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Analysis of multivariate time-series using the MARSS package

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Preface

The initial motivation for our work with MARSS models was a collaboration with Rich Hinrichsen. Rich developed a framework for analysis of multi-site population count data using MARSS models and bootstrap AICb (Hinrichsen and Holmes, 2009). Our work (EEH and EJW) extended Rich's framework, made it more general, and led to the development of a parametric bootstrap AICb for MARSS models, which allows one to do model-selection using datasets with missing values (Ward et al., 2009; Holmes and Ward, 2010). Later, we developed additional algorithms for simulation and confidence intervals. Discussions with Mark Scheuerell led to an extensive revision of the EM algorithm and to the development of a general EM algorithm for constrained MARSS models (Holmes, 2010). Discussions with Mark also led to a complete rewrite of the model specification so that the package could be used for MARSS models in general—rather than simply the form of MARSS model used in our (EEH and EJW) applications. Many collaborators have helped test the package; we thank especially Yasmin Lucero, Mark Scheuerell, Kevin See, and Brice Semmens. Development of the code into a R package would not have been possible without Kellie Wills, who wrote the much of the code outside of the algorithm functions. Finally, many users have contacted us regarding issues that were unclear in the manual, errors, or suggestions regarding new applications. Discussions with these users have helped us improve the manual and go in new directions.

The case studies were developed for workshops on analysis of multivariate time-series data given at the Ecological Society meetings since 2005 and taught by us (EEH and EJW) along with Yasmin Lucero, Stephanie Hampton, Brice Semmens, and Mark Scheuerell. The case study on extinction estimation and trend estimation was initially developed by Brice Semmens and later extended by us for this user guide. The case study on dynamic factor analysis was initially developed by Eli Holmes but later greatly revised and extended by Mark Scheuerell. The algorithm behind the TMU figure in Chapter 10 was developed during a collaboration with Steve Ellner (Ellner and Holmes, 2008).

EEH and EJW are research scientists at the Northwest Fisheries Science Center in the Mathematical Biology program. This work was conducted as part of our jobs at the Northwest Fisheries Science Center, a research center for NOAA Fisheries which is a US federal government agency. A CAMEO grant from NOAA Fisheries supported Kellie Wills. During the initial stages of this work, EJW was supported on a post-doctoral fellowship from the National Research Council.

You are welcome to use the code and adapt it with attribution. It may not be used in any commercial applications nor may it be copyrighted. Use of the EM algorithm should cite Holmes (2010). Links to more code and publications on MARSS applications can be found by following the links at EEH's website http://faculty.washington.edu/eeholmes. Links to our papers that use these methods can also be found at the same website.

Contents

1 The MARSS package 1
- 1.1 What does the MARSS package do? 2
- 1.2 How to get started (quickly) 4
- 1.3 Important notes about the algorithms 4
- 1.4 Troubleshooting 6
- 1.5 Other related packages 8

2 Overview of the package functions 11
- 2.1 The `MARSS()` function 11
- 2.2 Core functions for fitting a MARSS model 12
- 2.3 Functions for a fitted marssMLE object 12
- 2.4 Functions for marssm objects 13

3 The MARSS() function 15
- 3.1 $\mathbf{u}$, $\mathbf{a}$ and π model structures 16
- 3.2 $\mathbf{Q}$, $\mathbf{R}$, Λ model structures 18
- 3.3 $\mathbf{B}$ model structures 20
- 3.4 $\mathbf{Z}$ model 20
- 3.5 Default model structures 21

4 Model specification in the core functions 23
- 4.1 The fixed and free components of the model parameters 23
- 4.2 Limits on the model forms that can be fit 25

5 Algorithms used in the MARSS package 27
- 5.1 Kalman filter and smoother 27
- 5.2 The exact likelihood 28
- 5.3 Maximum-likelihood parameter estimation 29
- 5.4 Parametric and innovations bootstrapping 30
- 5.5 Simulation and forecasting 31
- 5.6 Model selection 31

6 Examples . . . 33
6.1 Fitting a general MARSS models . . . 33
6.2 Fitting different MARSS models to a harbor seal dataset . . . 34
6.3 Printing and summarizing models and model fits . . . 43
6.4 Confidence intervals on a fitted model . . . 44
6.5 Vectors of just the estimated parameters . . . 45
6.6 Degenerate variance estimates . . . 46
6.7 Bootstrap parameter estimates . . . 49
6.8 Random initial conditions . . . 49
6.9 Data simulation . . . 50
6.10 Bootstrap AIC . . . 50

7 Incorporating covariates into MARSS models . . . 53
7.1 Background . . . 53
7.2 Covariates with missing values or observation error . . . 53

8 Incorporating longer lags and autoregressive errors into MARSS models . . . 57
8.1 Background . . . 57
8.2 MAR(p) models . . . 57
8.3 MA(q) models . . . 59
8.4 Autoregressive process errors . . . 60
8.5 Univariate ARMA(p,q) . . . 60

9 Case study instructions . . . 61

10 Case Study 1: Count-based Population Viability Analysis using corrupted data . . . 63
10.1 The Problem . . . 63
10.2 Simulated data with process and observation error . . . 64
10.3 Maximum-likelihood parameter estimation . . . 67
10.4 Probability of hitting a threshold $\Pi(x_d, t_e)$ . . . 72
10.5 Certain and uncertain regions . . . 76
10.6 More risk metrics and some real data . . . 78
10.7 Confidence intervals . . . 80
10.8 Comments . . . 81

11 Case study 2: Combining multi-site and subpopulation data to estimate regional population dynamics . . . 83
11.1 The problem . . . 83
11.2 Analysis assuming a single total Puget Sound population . . . 85
11.3 Changing the assumption about the observation variances . . . 90
11.4 Analysis assuming north and south subpopulations . . . 93
11.5 Using `MARSS()` to fit other population structures . . . 97
11.6 Discussion . . . 99

12 Case Study 3: Using MARSS models to identify spatial population structure and covariance . . . 103
12.1 The problem . . . 103
12.2 How many distinct subpopulations? . . . 104
12.3 Is Hood Canal separate? . . . 107

13 Case Study 4: Dynamic Factor Analysis (DFA) with MARSS . . . 111
13.1 Dynamic Factor Analysis . . . 111
13.2 The data . . . 113
13.3 Setting up the model in MARSS . . . 114
13.4 Using model selection to determine the number of trends . . . 119
13.5 Using varimax rotation to determine the loadings and trends . . . 122
13.6 Examining model fits . . . 123
13.7 Adding covariates . . . 125
13.8 Other models and data . . . 126

14 Case Study 5: Using state-space models to analyze noisy animal tracking data . . . 127
14.1 A simple random walk model of animal movement . . . 127
14.2 The problem . . . 128
14.3 Estimate locations from bad tag data . . . 128
14.4 Comparing turtle tracks to proposed fishing areas . . . 132
14.5 Using specialized packages to analyze tag data . . . 133

15 Case Study 6: Detection of outliers and structural breaks using MARSS . . . 135
15.1 Detection of outliers and structural breaks . . . 135
15.2 Different models for the Nile flow levels . . . 135
15.3 Observation and state residuals . . . 140

16 Case Study 7: Estimation of species interaction strengths with and without covariates . . . 145
16.1 Background . . . 145
16.2 Two-species example using wolves and moose . . . 146
16.3 Analysis a four-species plankton community . . . 150

17 Case Study 8: Combining data from multiple time series . . . 163
17.1 Overview . . . 163
17.2 Analyzing time series of redd count data . . . 164
17.3 Analyzing time series of rockfish CPUE data . . . 166
17.4 Analyzing time series of American kestrel abundance indices . . . 170

A Textbooks and articles that use MARSS modeling for population modeling . . . 173

B Package MARSS: Warnings and errors 177

C Package MARSS: Object structures 183

D Package MARSS: The top-level MARSS functions and the base functions 187

References 189

Index 193

1

The MARSS package

MARSS stands for Multivariate Auto-Regressive(1) State-Space. The MARSS package is an *R* package for estimating the parameters of linear MARSS models with Gaussian errors. This class of model is extremely important in the study of linear stochastic dynamical systems, and these models are important in many different fields, including economics, engineering, genetics, physics and ecology (Appendix A). The model class has different names in other fields, for example in some fields they are termed dynamic linear models (DLMs) or vector autoregressive (VAR) state-space models.

The MARSS package allows you to easily fit constrained and unconstrained MARSS models to multivariate time-series data via maximum-likelihood using primarily an EM algorithm[1] A MARSS model, with Gaussian errors, takes the form:

$$\mathbf{x}_t = \mathbf{B}\mathbf{x}_{t-1} + \mathbf{u} + \mathbf{w}_t, \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}) \tag{1.1a}$$

$$\mathbf{y}_t = \mathbf{Z}\mathbf{x}_t + \mathbf{a} + \mathbf{v}_t, \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}) \tag{1.1b}$$

$$\mathbf{x}_1 \sim \text{MVN}(\pi, \Lambda) \text{ or } \mathbf{x}_0 \sim \text{MVN}(\pi, \Lambda) \tag{1.1c}$$

The **x** equation is termed the state process and the **y** is termed the observation process. Data traditionally enter the model as **y**'s; that is the **y** is treated as the data although there may be missing data.

The bolded terms are matrices with the following definitions:

$\mathbf{x}_t$ is a $m \times 1$ column vector of states at time t. It is a realization of the random variable $\mathbf{X}_t$.

$\mathbf{w}_t$ is a $m \times 1$ column vector of the process errors at time t. It is a realization from a multivariate normal random variable with mean 0 and covariance matrix $\mathbf{Q}$.

$\mathbf{y}_t$ is a $n \times 1$ column vector of the observations at time t. Some observations may be missing.

[1] Fitting via the BFGS algorithm is also provided using *R* 's optim function, but this is not the focus of the package.

$\mathbf{v}_t$ is a $n \times 1$ column vector of the non-process errors at time t. It is a realization from a multivariate normal random variable with mean 0 and covariance matrix $\mathbf{R}$.
$\mathbf{B}$ is a parameter and is a $m \times m$ matrix.
$\mathbf{u}$ is a parameter and is a $m \times 1$ column vector.
$\mathbf{Q}$ is a parameter and is a $m \times m$ variance-covariance matrix.
$\mathbf{Z}$ is a parameter and is a $n \times m$ matrix.
$\mathbf{a}$ is a parameter and is a $n \times 1$ column vector.
$\mathbf{R}$ is a parameter and is a $n \times n$ variance-covariance matrix.
π is either a parameter or a fixed prior. It is a $m \times 1$ matrix.
Λ is either a parameter or a fixed prior. It is a $m \times m$ variance-covariance matrix.

The meaning of the parameters in a MARSS model depends on the application. In some fields, the $\mathbf{u}$ and $\mathbf{a}$ terms are routinely set to 0 or the model is written in such a way that they are incorporated into $\mathbf{B}$ or $\mathbf{Z}$. However, in other fields, the $\mathbf{u}$ and $\mathbf{a}$ terms are the main objects of interest, and the model is written to explicitly show them. We include them throughout our discussion, but they can be set to zero if desired.

Although the MARSS model shown in Equation 1.1 appears to not include covariate information (termed exogenous variables in some fields), covariate information enters the model as data in the $\mathbf{y}$ equation with a corresponding covariate state process ($\mathbf{x}$); see chapter 7. The $\mathbf{R}$ or $\mathbf{Q}$ variances can be set to zero to specify partially deterministic systems. The model appears to be only AR(1) but AR(p) models can be written in the above form by properly defining the $\mathbf{x}$ vector; see chapter 8. Although the model appears to only include i.i.d. errors ($\mathbf{v}_t$ and $\mathbf{w}_t$), in practice, AR(p) errors can be included by moving the errors into the state model; see chapter 8. Similarly, the model appears to have independent process ($\mathbf{v}_t$) and observation ($\mathbf{w}_t$) errors, however, in practice, these can be modeled as identical or correlated by using one of the state processes to model the errors with the $\mathbf{B}$ matrix set appropriately for AR or white noise—although one may have to fix many of the parameters associated with the errors to have an identifiable model. Study the case studies in this User Guide and textbooks on MARSS models for examples of how a wide variety of autoregressive models can be written in MARSS form.

1.1 What does the MARSS package do?

Written in its most general and unconstrained form, a MARSS model can be written out as follows. Two state processes ($\mathbf{x}$) and three observation processes ($\mathbf{y}$) are used here for example's sake.

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_t = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{t-1} + \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}_t, \quad \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}_t \sim \text{MVN}\left(\begin{bmatrix} u_1 \\ u_2 \end{bmatrix}, \begin{bmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \end{bmatrix} \right)$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}_t = \begin{bmatrix} z_{11} & z_{12} \\ z_{21} & z_{22} \\ z_{31} & z_{32} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_t + \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}_t,$$
$$\begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}_t \sim \text{MVN}\left(\begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix}, \begin{bmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & r_{22} & r_{23} \\ r_{31} & r_{32} & r_{33} \end{bmatrix} \right)$$

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_0 \sim \text{MVN}\left(\begin{bmatrix} \pi_1 \\ \pi_2 \end{bmatrix}, \begin{bmatrix} \nu_{11} & \nu_{12} \\ \nu_{21} & \nu_{22} \end{bmatrix} \right) \quad \textit{or} \quad \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_1 \sim \text{MVN}\left(\begin{bmatrix} \pi_1 \\ \pi_2 \end{bmatrix}, \begin{bmatrix} \nu_{11} & \nu_{12} \\ \nu_{21} & \nu_{22} \end{bmatrix} \right)$$

However not all parameter elements can be estimated simultaneously. Constraints are required in order to specify a model with a unique solution. The MARSS package allows you to specify constraints by fixing elements in a parameter matrix or specifying that some, estimated, values in a matrix have the same value[2]. Here is an example of a MARSS model with fixed and shared parameter elements:

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_t = \begin{bmatrix} a & 0 \\ 0 & a \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{t-1} + \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}_t, \quad \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}_t \sim \text{MVN}\left(\begin{bmatrix} 0.1 \\ u \end{bmatrix}, \begin{bmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \end{bmatrix} \right)$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}_t = \begin{bmatrix} d & \\ c & d \\ e & e \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_t + \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}_t, \quad \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}_t \sim \text{MVN}\left(\begin{bmatrix} a_1 \\ a_2 \\ 0 \end{bmatrix}, \begin{bmatrix} r & 0 & 0 \\ 0 & r & 0 \\ 0 & 0 & r \end{bmatrix} \right)$$

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_0 \sim \text{MVN}\left(\begin{bmatrix} \pi \\ \pi \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right)$$

Specification of a properly constrained model with a unique solution is the responsibility of the user because MARSS has no way to tell if you have specified an insufficiently constrained model—with correspondingly an infinite number of solutions.

The MARSS package fits models via maximum likelihood. The MARSS package is unusual among packages for fitting MARSS models in that fitting is performed via an EM algorithm (Holmes, 2010), although fitting via the BFGS algorithm is also provided using *R* 's optim function. The EM algorithm gives robust estimation for datasets replete with missing values and for

[2] Actually the EM algorithm in the package allows much more general constraints. It will fit models with linear constraints of the form $\beta_i + \beta_{a,i}a + \beta_{b,i}b + \ldots$, but the current version of the package does not have a way for the user to specify those constraints.

high-dimensional models with various constraints. The EM algorithm is also often used to provide initial conditions for the BFGS algorithm (or an MCMC routine) in order to improve the performance of those algorithms. In addition, the MARSS package supplies functions for bootstrap and approximate confidence intervals, parametric and non-parametric bootstrapping, model selection (AIC and bootstrap AIC), simulation, and bootstrap bias correction.

1.2 How to get started (quickly)

If you already work with models in the form of Equation 1.1, you can immediately fit your model with the MARSS package. Install the MARSS package and then type `library(MARSS)` at the command line to load the package. Look at the Quick Start Guide and/or skim the first 2-4 pages of Chapter 3 then read through the first example in Chapter 6. Your data need to be a matrix (not dataframe) with time going across the columns and any non-data columns (like year) removed. The MARSS functions assume discrete time steps and you will need a column for each time step. Replace any missing time steps with a missing value holder (e.g. NA). Write your model down on paper and identify which parameters correspond to $\mathbf{B}$, $\mathbf{u}$, $\mathbf{Q}$, $\mathbf{Z}$, $\mathbf{a}$, and $\mathbf{R}$ in Equation 1.1. Call the `MARSS()` function (Chapter 3) using your data and using the `model` argument to specify the form of the parameters (Chapter 3 shows how to specify a MARSS model using a list of matrices).

1.3 Important notes about the algorithms

Specifying a properly constrained model with a unique solution is imperative. How do you know if the model is properly constrained? If you are using a MARSS model form that is widely used, then you can probably assume that it is properly constrained. If you go to papers where someone developed the model or method, the issue of constraints necessary to ensure "identifiability" will likely be addressed if it is an issue. Are you fitting novel MARSS models? Then you will need to do some study on identifiability in this class of models using textbooks (see the textbook list at end of this User Guide). Note, often textbooks do not address identifiability explicitly, rather it's addressed implicitly by only showing a model constructed in such a way that it is identifiable. In our work, if we suspect identification problems, we will often first do a Bayesian analysis with flat priors and look for oddities in the posteriors, such as ridges, plateaus or bimodality. This will often show the problem, though the solution can be a bit harder to determine.

All code in the MARSS package is in native *R* . Thus the model fitting is slow (relatively). In addition, the main Kalman filter/smoother algorithm used in MARSS is implemented exactly as you see it in Shumway and Stoffer (2006, p. 331-335), based on the original smoother presented in Rauch (1963).

Table 2 in Koopman (1993) indicates that this algorithm is 40-100 times slower than the algorithm given in Kohn and Ansley (1989), Koopman (1993), and Koopman et al. (1999). These faster filter and smoother algorithms are available in the KFAS package, but unfortunately the KFAS package is missing the lag-2 smoother needed by the EM algorithm and this limits its use in the MARSS package.

EM algorithms will quickly get in the vicinity of the maximum likelihood, but the final approach to the maximum is generally slow relative to quasi-Newton methods. On the flip side, EM algorithms are quite robust to initial conditions choices and can be extremely fast at getting close to the MLE values for high-dimensional models. The MARSS package also allows one to use the BFGS method to fit MARSS models, thus one can use an EM algorithm to "get close" and then the BFGS algorithm to polish off the estimate. Restricted maximum-likelihood algorithms are also available for AR(1) state-space models, both univariate (Staples et al., 2004) and multivariate (Hinrichsen, 2009). REML can give parameter estimates with lower variance than plain maximum-likelihood algorithms. However, the algorithms for REML when there are missing values are not currently available (although that will probably change in the near future). Another maximum-likelihood method is data-cloning which adapts MCMC algorithms used in Bayesian analysis for maximum-likelihood estimation (Lele et al., 2007).

Missing values are seamlessly accommodated with the MARSS package. Simply specify the way missing values are denoted in the data set (default is `miss.value=NA`). The likelihood computations are exact and will deal appropriately with missing values. However, no innovations[3] bootstrapping can be done if there are missing values. Instead parametric bootstrapping must be used.

You should be aware that maximum-likelihood estimates of variance in MARSS models are fundamentally biased, regardless of the algorithm used. This bias is more severe when one or the other of $\mathbf{R}$ or $\mathbf{Q}$ is very small, and the bias does not go to zero as sample size goes to infinity. The bias arises because variance is constrained to be positive. Thus if $\mathbf{R}$ or $\mathbf{Q}$ is essentially zero, the mean estimate will not be zero and thus the estimate will be biased high while the corresponding bias of the other variance will be biased low. You can generate unbiased variance estimates using a bootstrap estimate of the bias. The function `MARSSparamCIs()` will do this. However be aware that adding an *estimated* bias to a parameter estimate will lead to an increase in the variance of your parameter estimate. The amount of variance added will depend on sample size.

You should also be aware that mis-specification of the prior on the initial states (π and Λ) can have catastrophic effects on your parameter estimates if your prior conflicts with the distribution of the initial states implied by the MARSS model. These effects can be very difficult to detect because the

[3] referring to the non-parametric bootstrap developed by Stoffer and Wall (1991).

model will appear to be well-fitted. Unless you have a good idea of what the parameters should be, you might not realize that your prior conflicts.

The most common problems, we have found are the following. Problem 1) The correlation structure in Λ (whether the prior is diffuse or not) does not match the correlation structure in $\mathbf{x}_0$ implied by your model. For example, you specify a diagonal Λ (independent states), but the implied distribution has correlations. Problem 2) The correlation structure in Λ does not match the structure in $\mathbf{x}_0$ implied by constraints you placed on π. For example, you specify that all values in π are shared, yet you specify that Λ is diagonal (independent). Unfortunately, using a diffuse prior (using `method="BFGS"` and `model$diffuse=TRUE`) does not help with these two problems because the diffuse prior still has a correlation structure and can still conflict with the implied correlation in $\mathbf{x}_0$. One way to get around these problems is to set Λ=0 (a $m \times m$ matrix of zeros) and estimate $\pi \equiv \mathbf{x}_0$ only. Now π is a fixed but unknown (estimated) parameter, not the mean of a distribution. In this case, Λ does not exist in your model and there is no conflict with the model. Unfortunately estimating π as a parameter is not always robust. If you specify that Λ=0 and specify that π corresponds to $\mathbf{x}_0$, but your model "explodes" when run backwards, you cannot estimate π because you cannot get a good estimate of $\mathbf{x}_0$. Sometimes this can be avoided by specifying that π corresponds to $\mathbf{x}_1$ so that it can be constrained by the data $\mathbf{y}_1$. In summary, if the implied correlation structure of your initial states is independent (diagonal variance-covariance matrix), you should generally be ok with a diagonal and high variance prior or with treating the initial states as parameters (with $\Lambda = 0$). But if your initial states have an implied correlation structure that is not independent, then proceed with caution.

There is a large class of models in the statistical finance literature that have the form

$$\mathbf{x}_{t+1} = \mathbf{B}\mathbf{x}_t + \Gamma\eta_t$$
$$\mathbf{y}_t = \mathbf{Z}\mathbf{x}_t + \eta_t$$

For example, ARMA(p,q) models can be written in this form. The MARSS model framework in this package will not allow you to write models in that form. You can put the η_t into the $\mathbf{x}_t$ vector and set $\mathbf{R} = 0$ to make models of this form using the MARSS form, but the EM algorithm in the MARSS package won't let you estimate parameters because the parameters will drop out of the full likelihood being maximized in the algorithm. The EM algorithm could be written differently to avoid this constraint.

1.4 Troubleshooting

Numerical errors due to ill-conditioned matrices are not uncommon when fitting MARSS models. The Kalman and EM algorithms need inverses of matrices. If those matrices become ill-conditioned, for example all elements

are close to the same value, then the algorithm becomes unstable. Warning messages will be printed if the algorithms are becoming unstable and you can set `control$trace=1`, to see details of where the algorithm is becoming unstable. Whenever possible, you should avoid using shared π values in your model[4]. The way our algorithm deals with Λ tends to make this case unstable, especially if $\mathbf{R}$ is not diagonal. In general, estimation of a non-diagonal $\mathbf{R}$ is more difficult, more prone to ill-conditioning, and more data-hungry.

You may also see non-convergence warnings, especially if your MLE model turns out to be degenerate. This means that one of the elements on the diagonal of your $\mathbf{Q}$ or $\mathbf{R}$ matrix are going to zero (are degenerate). It will take the EM algorithm forever to get to zero. BFGS will have the same problem, although it will often get a bit closer to the degenerate solution. If you are using `method="kem"`, MARSS will warn you if it looks like the solution is degenerate. If you use `control=list(allow.degen=TRUE)`, the EM algorithm will attempt to set the degenerate variances to zero (instead of trying to get to zero using an infinite number of iterations). If you still get the non-convergence warnings, look at your data for anything obvious, like having only one data point in your time series or some really extreme outlier. Then try running the EM algorithm longer using `control=list(maxit=something big)`.

The algorithms in the MARSS package are designed for cases where the $\mathbf{Q}$ and $\mathbf{R}$ diagonals are all non-minuscule. For example, the EM update equation for $\mathbf{u}$ will grind to a halt (not update $\mathbf{u}$) if $\mathbf{Q}$ is tiny (like 1E-7). Conversely, the BFGS equations are likely to miss the maximum-likelihood when $\mathbf{R}$ is tiny because then the likelihood surface becomes hyper-sensitive to π. The solution is to use the degenerate likelihood function for the likelihood calculation and the EM update equations. MARSS will implement this automatically when $\mathbf{Q}$ or $\mathbf{R}$ diagonal elements are set to zero and will try setting $\mathbf{Q}$ and $\mathbf{R}$ terms to zero automatically if `control$allow.degen=TRUE`. One odd case can occur when $\mathbf{R}$ goes to zero (a matrix of zeros), but you are estimating π. If `model$tinitx=1`, then π must be $\mathbf{y}_1$ as $\mathbf{R}$ goes to zero, but as $\mathbf{R}$ goes to zero, the log-likelihood will go (correctly) to infinity. But if you set $\mathbf{R}=0$, the log-likelihood will be finite. The reason is that $\mathbf{R}\approx 0$ and $\mathbf{R}=0$ specify different likelihoods. In the first, the determinant $\mathbf{R}$ will appear, and this goes to positive infinity as $\mathbf{R}$ goes to zero. In the second case, $\mathbf{R}$ does not appear in the likelihood and so the determinant of $\mathbf{R}$ does not appear. If some elements of the diagonal of $\mathbf{R}$ are going to zero, you should be suspect of the parameter estimates. Sometimes the structure of your data, e.g. one data value followed by a long string of missing values, is causing an odd spike in the likelihood at $\mathbf{R}\approx 0$. Try manually setting $\mathbf{R}$ equal to zero to get the correct log-likelihood[5].

---

[4] An example of a π with shared values is $\pi = \left[\begin{smallmatrix} a \\ a \\ a \end{smallmatrix}\right]$.

[5] The likelihood returned when $\mathbf{R}\approx 0$ is not incorrect. It is just not the likelihood that you probably want. You want the likelihood where the $\mathbf{R}$ term is dropped because it is zero.

1.5 Other related packages

Packages that will do Kalman filtering and smoothing are many, but packages that estimate the parameters in a MARSS model, especially constrained MARSS models, are much less common. The following are those with which we are familiar, however there are certainly more packages for estimating MARSS models in engineering and economics of which we are unfamiliar. The MARSS package is unusual in that it uses an EM algorithm for maximizing the likelihood as opposed to a Newton-esque method (e.g. BFGS). The package is also unusual in that it allows you to specify the initial conditions at $t = 0$ or $t = 1$, allows degenerate models (with some of the diagonal elements of $\mathbf{R}$ or $\mathbf{Q}$ equal to zero). Lastly, model specification in the MARSS package has a one-to-one relationship between the model list in MARSS and the model as you would write it on paper. This makes the learning curve a bit less steep.

DLM DLM is an R package for fitting MARSS models. Our impression is that it is mainly Bayesian focused but it does allow MLE estimation via the `optim()` function. It has a book, Dynamic Linear Models with R by Petris et al., which has many examples of how to write MARSS models for different applications.

sspirs sspirs an R package for fitting ARSS (univariate) models with Gaussian, Poisson and binomial error distributions.

dse dse (Dynamic Systems Estimation) is a R package for multivariate Gaussian state space models with a focus on ARMA models.

SsfPack SsfPack is a package for Ox/Splus that fits constrained multivariate Gaussian state space models using mainly (it seems) the BFGS algorithm but the newer versions support other types of maximization. SsfPack is very flexible and written in C to be fast. It has been used extensively on statistical finance problems and is optimized for dealing with large (financial) data sets. It is used and documented in Time Series Analysis by State Space Methods by Durbin and Koopman, An Introduction to State Space Time Series Analysis by Commandeur and Koopman, and Statistical Algorithms for Models in State Space Form: SsfPack 3.0, by Koopman, Shephard, and Doornik.

Brodgar The Brodgar software was developed by Alain Zuur to do (among many other things) dynamic factor analysis, which involves a special type of MARSS model. The methods and many example analyses are given in Analyzing Ecological Data by Zuur, Ieno and Smith. This is the one package that we are aware of that also uses an EM algorithm for parameter estimation.

eViews eViews is a commercial economics software that will estimate at least some types of MARSS models.

KFAS The KFAS R package provides a fast Kalman filter and smoother. Examples in the package show how to estimate MARSS models using the KFAS functions and *R* 's optim() function. The MARSS package uses the

filter and smoother functions from the KFAS package when feasible; the KFAS package uses the initial condition set at $t = 1$ and cannot be used when the initial condition is set at $t = 0$.

S+FinMetrics An S-plus module for fitting MAR models, which are called vector autoregressive (VAR) models in the economics and finance literature. I has some support for state-space VAR models, though we haven't used it so are not sure which parameters it allows you to estimate. It was developed by Andrew Bruce, Doug Martin, Jiahui Wang, and Eric Zivot, and it has a book associated with it: Modeling Financial Time Series with S-plus by Eric Zivot and Jiahui Wang.

kftrack The kftrack R package provides a suite of functions specialized for fitting MARSS models to animal tracking data.

2

Overview of the package functions

The MARSS package is object-based. It has two main types of objects: a model object (class marssm) and a maximum-likelihood fitted model object (class marssMLE). A marssm object specifies the structure of the model to be fitted. It is an *R* code version of the MARSS equation (Equation 1.1). A marssMLE object specifies both the model and the information necessary for fitting (initial conditions, controls, method). If the model has been fitted, the marssMLE object will also have the parameter estimates and (optionally) confidence intervals and bias.

2.1 The `MARSS()` function

The function `MARSS()` is an interface to the core fitting functions in the MARSS package. It allows a user to fit a MARSS model using a list to describe the model structure. It returns marssm and marssMLE objects which the user can later use in other functions, e.g. simulating or computing bootstrap confidence intervals.

`MLEobj=MARSS(data, model=list(), ..., fit=TRUE)` This function will fit a MARSS model to the data using a model list which is a list describing the structure of the model parameter matrices. The default model has a one-to-one correspondence between the state processes and observation time series (**Z** is the identity matrix). The default has a diagonal observation error matrix (**R**) and process-error matrix (**Q**). The output is a marssMLE object where the estimated parameter matrices are in `MLEobj$par`. If `fit=FALSE`, it returns a minimal marssMLE object that is ready for passing to a fitting function (below) but with no `par` element.

2.2 Core functions for fitting a MARSS model

The following core functions are designed to work with 'unfitted' marssMLE objects, that is a marssMLE object without the `par` element. Users do not normally need to call the `MARSSkem` or `MARSSoptim` functions since `MARSS()` will call those. Below `MLEobj` means the argument is a marssMLE object. Note, these functions can be called with a marssMLE object with a `par` element, but these functions will overwrite that element.

`MLEobj=MARSSkem(MLEobj)` This will fit a MARSS model via the EM algorithm to the data using a properly specified marssMLE object, which has data, the marssm object and the necessary initial condition and control elements. See the appendix on the object structures in the MARSS package. `MARSSkem` does no error-checking. See `is.marssMLE()`. `MARSSkem` uses `MARSSkf` described below.

`MLEobj=MARSSoptim(MLEobj)` This will fit a MARSS model via the BFGS algorithm provided in `optim()`. This requires a properly specified marssMLE object, such as would be passed to `MARSSkem`.

`MLEobj=MARSSmcinit(MLEobj)` This will perform a Monte Carlo initial conditions search and update the marssMLE object with the best initial conditions from the search.

`is.marssMLE(MLEobj)` This will check that a marssMLE object is properly specified and ready for fitting. This should be called before `MARSSkem` or `MARSSoptim` is called. This function is not typically needed if using `MARSS()` since `MARSS()` builds the model object for the user and does error-checking on model structure.

2.3 Functions for a fitted marssMLE object

The following functions use a marssMLE object that has a populated `par` element, i.e. a marssMLE object returned from one of the fitting functions (`MARSS`, `MARSSkem`, `MARSSoptim`). Below `modelObj` means the argument is a marssm object and `MLEobj` means the argument is a marssMLE object. Type `?function.name` to see information on function usage and examples.

`kf=MARSSkf( MLEobj )` This will compute the expected values of the hidden states given data via the Kalman filter (to produce estimates conditioned on $1:t-1$) and the Kalman smoother (to produce estimates conditioned on $1:T$). The function also returns the exact likelihood of the data conditioned on `MLEobj$par`. A variety of other Kalman filter/smoother information is also output (`kf` is a list of output); see `?MARSSkf` for more details.

`MLEobj=MARSSaic(MLEobj)` This adds model selection criteria, AIC, AICc, and AICb, to a marssMLE object.

`boot=MARSSboot(MLEobj)` This returns a list containing bootstrapped parameters and data via parametric or innovations bootstrapping.

`MLEobj=MARSShessian(MLEobj)` This adds a numerically estimated Hessian matrix to a marssMLE object.

`MLEobj=MARSSparamCIs(MLEobj)` This adds standard errors, confidence intervals, and bootstrap estimated bias for the maximum-likelihood parameters using bootstrapping or the Hessian to the passed in marssMLE object.

`sim.data=MARSSsimulate(MLEobj)` This returns simulated data from a MARSS model specified via a list of parameter matrices in `MLEobj$parList` (this is a list with elements `Q`, `R`, `U`, etc).

`paramVec=MARSSvectorizeparam(MLEobj)` This returns the estimated (and only the estimated) parameters as a vector. This is useful for storing the results of simulations and for writing functions that fit MARSS models using R's `optim` function.

`new.MLEobj=MARSSvectorizeparam(MLEobj, paramVec)` This will return a marssMLE object in which the estimated parameters (which are in `MLEobj$par` along with the fixed values) are replaced with the values in `paramVec`.

2.4 Functions for marssm objects

`is.marssm(modelObj)` This will check that the free and fixed matrices in a marssm object are properly specified. This function is not typically needed if using `MARSS()` since `MARSS()` builds the marssm object for the user and does error-checking on model structure.

`summary(modelObj)` This will print the model parameter matrices showing the fixed values (in parentheses) and the location of the estimated elements. The estimated elements are shown as g1, g2, g3, ... which indicates which elements are shared (i.e., forced to have the same value). For example, an i.i.d. **R** matrix would appear as a diagonal matrix with just g1 on the diagonal.

3

The MARSS() function

From the user perspective, the main package function is `MARSS()`. This fits a MARSS model (Equation 1.1) to a matrix of data:

```
MARSS(data, model=list(Z=Z.model, B=B.model,
       U=U.model, Q=Q.model, A=A.model,
       R=R.model, x0=pi.model, V0=V.model) )
```

The data must be passed in as a $n \times T$ matrix, that is time goes across columns. A vector is not a matrix, nor is a dataframe. A data matrix of 3 inputs ($n = 3$) measured for 6 time steps might look like

$$\mathbf{y} = \begin{bmatrix} 1 & 2 & NA & NA & 3.2 & 8 \\ 2 & 5 & 3 & NA & 5.1 & 5 \\ 1 & NA & 2 & 2.2 & NA & 7 \end{bmatrix}$$

where NA denotes a missing value.

The argument `model` specifies the structure of the MARSS model (Equation 1.1). It is a list, where the list elements for each model parameter specifies the form of that parameter.

The most general way to specify model structure is to use a list matrix. The list matrix allows one to combine fixed and estimated elements in one's parameter specification. It allows a one-to-one correspondence between how you write the parameter matrix on paper and how you specify it in *R* . For example, let's say **Q** and **u** have the following forms in your model:

$$\mathbf{Q} = \begin{bmatrix} a & 0 & 0 \\ 0 & a & 0 \\ 0 & 0 & 1 \end{bmatrix} \text{ and } \mathbf{u} = \begin{bmatrix} 0.05 \\ b \\ c \end{bmatrix}$$

So **Q** is a diagonal matrix with the 3rd variance fixed at 1 and the 1st and 2nd estimated and equal. The 1st element of **u** is fixed, and the 2nd and 3rd are estimated and different. You can specify this using a list matrix:

```
Q.model=matrix(list("a",0,0,0,"a",0,0,0,1),3,3)
U.model=matrix(list(0.05,"b","c"),3,1)
```

If you print out `Q.model` and `U.model`, you will see they look exactly like **Q** and **u** written above. MARSS will keep the fixed values fixed and estimate a, b, and c.

List matrices allow the most flexible model structures, but MARSS also has text shortcuts for a number of common model structures. Below the possible ways to specify each model parameter are shown. The forms are shown using $m = 3$ (the number of hidden state processes) and $n = 3$ (number of observation time series).

3.1 u, a and π model structures

u, **a** and π are all row matrices and the options for specifying their structures are the same. The most general way to specify structure is to use a list matrix, but there are text shortcuts for the common structures. **a** has one special option, `"scaling"` described below. The allowable structures are shown using **u** as an example. Note that you should be careful about specifying shared structure in π because you need to make sure the structure in Λ matches. For example, if you require that all the π values are shared (equal) then Λ cannot be a diagonal matrix since that would be saying that the π values are independent, which they are clearly not if you force them to be equal.

`U.model=matrix(list(),m,1)`: This is the most general form and allows one to specify fixed and estimated elements in **u**. Each character string in **u** is the name of one of the **u** elements to be estimated. For example if `U.model=matrix(list(0.01,"u","u"),3,1)`, then **u** in the model has the following structure:

$$\begin{bmatrix} 0.01 \\ u \\ u \end{bmatrix}$$

`U.model=matrix(c(),m,1)`, where the values in `c()` all character strings: Each character string is the name of an element to be estimated. For example if `U.model=matrix(c("u1","u1","u2"),3,1)`, then **u** in the model has the following structure:

$$\begin{bmatrix} u_1 \\ u_1 \\ u_2 \end{bmatrix}$$

There are two values being estimated, u_1 and u_2. Note that `U.model=matrix(list("u1","u1","u2"),3,1)` also works.

`U.model="unequal"` or `U.model="unconstrained"`: Each element of **u** is estimated. If $m = 3$, then **u** would have the form:

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}$$

`U.model="equal"`: There is only one value in **u**:

$$\begin{bmatrix} u \\ u \\ u \end{bmatrix}$$

`U.model=matrix(c(),m,1)`, where the values in `c()` all numerical values: **u** is fixed and has no estimated values. For example if `U.model=matrix(c(0.01,1,-0.5),3,1)`, then **u** in the model has the following structure:

$$\begin{bmatrix} 0.01 \\ 1 \\ -0.5 \end{bmatrix}$$

Note that `U.model=matrix(list(0.01,1,-0.5),3,1)` works too.

You can also pass in a matrix with fixed values and NAs. For example, `matrix(c(0.1, NA, NA),3,1)`:

$$\begin{bmatrix} 0.1 \\ NA \\ NA \end{bmatrix}$$

The fixed values will be set to the fixed values and the elements specified by NAs will be estimated. The estimated elements are independent and not forced to be equal.

`U.model="zero"`: **u** is all zero:

$$\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

The **a** parameter has a special option, `"scaling"`, which is the default behavior. In this case, **a** is treated like a scaling parameter. If there is only one **y** row associated with an **x** row, then the corresponding **a** element is 0. If there are more than one **y** rows associated with an **x** row, then the first **a** element is set to 0 and the others are estimated. For example, say $m = 2$ and $n = 4$ and **Z** looks like the following:

$$\mathbf{Z} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Then the 1st-3rd rows of **y** are associated with the first row of **x**, and the 4th row of **y** is associated with the last row of **x**. Then if **a** is specified as `"scaling"`, **a** has the following structure:

$$\begin{bmatrix} 0 \\ a_1 \\ a_2 \\ 0 \end{bmatrix}$$

3.2 Q, R, Λ model structures

The possible **Q**, **R**, and Λ model structures are identical, except that **R** is $n \times n$ while **Q** and Λ are $m \times m$. The most general way to specify these variance-covariance matrices is using a list matrix. All types of structures can be specified using a list matrix, however there are also text shortcuts for specifying common structures. The structures are shown using **Q** as the example.

`Q.model=matrix(list(),m,m)`: This is the most general way to specify the parameters and allows there to be fixed and estimated elements. Each character string in the list matrix is the name of one of the **Q** elements to be estimated, and each numerical value is a fixed value. For example if `Q.model=matrix(list("s2a",0,0,0,"s2a",0,0,0,"s2b"),3,3)`, then **Q** has the following structure:

$$\begin{bmatrix} \sigma_a^2 & 0 & 0 \\ 0 & \sigma_a^2 & 0 \\ 0 & 0 & \sigma_b^2 \end{bmatrix}$$

Note that `diag(c("s2a","s2a","s2b"))` will not have the desired effect of producing a matrix with numeric 0s on the off-diagonals. It will have character 0s and MARSS will interpret "0" as the name of an element of **Q** to be estimated. Instead, the following two lines can be used:

```
Q.model=matrix(list(0),3,3)
diag(Q.model)=c("s2a","s2a","s2b")
```

`Q.model="diagonal and equal"`: There is only one process variance value in this case:

$$\begin{bmatrix} \sigma^2 & 0 & 0 \\ 0 & \sigma^2 & 0 \\ 0 & 0 & \sigma^2 \end{bmatrix}$$

`Q.model="diagonal and unequal"`: There are m process variance values in this case:

$$\begin{bmatrix} \sigma_1^2 & 0 & 0 \\ 0 & \sigma_2^2 & 0 \\ 0 & 0 & \sigma_3^2 \end{bmatrix}$$

`Q.model="unconstrained"`: There are values on the diagonal and the off-diagonals of **Q** and the variances and covariances are all different:

$$\begin{bmatrix} \sigma_1^2 & \sigma_{1,2} & \sigma_{1,3} \\ \sigma_{1,2} & \sigma_2^2 & \sigma_{2,3} \\ \sigma_{1,3} & \sigma_{2,3} & \sigma_3^2 \end{bmatrix}$$

There are m process variances and $(m^2 - m)/2$ covariances in this case, so $(m^2 + m)/2$ values to be estimated.

`Q.model="equalvarcov"`: There is one process variance and one covariance:

$$\begin{bmatrix} \sigma^2 & \beta & \beta \\ \beta & \sigma^2 & \beta \\ \beta & \beta & \sigma^2 \end{bmatrix}$$

`Q.model=matrix(c(), m, m)`, where all values in `c()` are character strings: Each element in **Q** is estimated and each character string is the name of a value to be estimated. Note if $m = 1$, you still need to wrap its value in `matrix()` so that its class is matrix.

`Q.model=matrix(c(), m, m)`, where all values in `c()` are numeric values: Each element in **Q** is fixed to the values in the matrix.

You can also pass in a diagonal matrix with fixed values and NAs:

$$\begin{bmatrix} NA & 0 & 0 \\ 0 & 0.1 & 0 \\ 0 & 0 & NA \end{bmatrix}$$

The fixed values will be set to the fixed values and the NAs will be estimated; the estimates are independent and not forced to be equal. The matrix must be diagonal (0s on the off-diagonals).

`Q.model="identity"`: The **Q** matrix is the identity matrix:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

`Q.model="zero"`: The **Q** matrix is all zeros:

$$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Be careful when setting Λ model structures. Mis-specifying the structure of Λ can have catastrophic, but difficult to discern, effects on your estimates. See the comments on priors in Chapter 1.

3.3 B model structures

Like the variance-covariance matrices ($\mathbf{Q}$,$\mathbf{R}$ and Λ), $\mathbf{B}$ can be specified with a list matrix to allow you to have both fixed and shared elements in the $\mathbf{B}$ matrix. Character matrices and matrices with fixed values and NAs operate the same way as for the variance-covariance matrices. In addition, the same text shortcuts are available: "identity", "diagonal and equal", "diagonal and unequal", "equalvarcov", and "zero". A fixed $\mathbf{B}$ can be specified with a numeric matrix, but all eigenvalues must fall within the unit circle; meaning `all(abs(eigen(B)$values)>=1)`..

3.4 Z model

Like $\mathbf{B}$ and the variance-covariance matrices, $\mathbf{Z}$ can be specified with a list matrix to allow you to have both fixed and estimated elements in $\mathbf{Z}$. If $\mathbf{Z}$ is a square matrix, many of the same text shortcuts are available: "diagonal and equal", "diagonal and equal", and "equalvarcov". If $\mathbf{Z}$ is a design matrix[1], then a special shortcut is available using `factor()` which allows you to specify which $\mathbf{y}$ rows are associated with which $\mathbf{x}$ rows. See Chapter 6 and the case studies chapters for more examples.

`Z.model=factor(c(1,1,1))`: All $\mathbf{y}$ time series are observing the same (and only) hidden state trajectory x ($n = 3$ and $m = 1$):

$$\mathbf{Z} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

`Z.model=factor(c(1,2,3))`: Each time series in $\mathbf{y}$ corresponds to a different hidden state trajectory. This is the default $\mathbf{Z}$ model and in this case $n = m$:

$$\mathbf{Z} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

`Z.model=factor(c(1,1,2))`: The first two time series in $\mathbf{y}$ corresponds to one hidden state trajectory and the third $\mathbf{y}$ time series corresponds to a different hidden state trajectory. Here $n = 3$ and $m = 2$:

$$\mathbf{Z} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}$$

The $\mathbf{Z}$ model can be specified using either numeric or character factor levels. `c(1,1,2)` is the same as `c("north","north","south")`

[1] a matrix with only 0s and 1s and where the row sums are all equal to 1

`Z.model="identity"`: This is the default behavior. This means $\mathbf{Z}$ is a $n \times n$ identity matrix and $m = n$. If $n = 3$, it is the same as `Z.model=factor(c(1,2,3))`.

`Z.model=matrix(..., n, m)`: Passing in a $n \times m$ character matrix, means that each character string is a value to be estimated. Be careful that you are specifying an identifiable model when using this option.

`Z.model=matrix(..., n, m)`: Passing in a $n \times m$ numeric matrix means that $\mathbf{Z}$ is fixed to the values in the matrix. The matrix must be numeric but it does not need to be a design matrix.

`Z.model=matrix(list(), n, m)`: Passing in a $n \times m$ list matrix allows you to combine fixed and estimated values in the $\mathbf{Z}$ matrix. Be careful that you are specifying an identifiable model when using this option.

3.5 Default model structures

The defaults are

`Z.model="identity"` each y in $\mathbf{y}$ corresponds to one x in $\mathbf{x}$
`B.model="identity"` no interactions between the x's in $\mathbf{x}$
`U.model="unequal"` the u's in $\mathbf{u}$ are all different
`Q.model="diagonal and unequal"` process errors are independent but have different variances
`R.model="diagonal and equal"` the observations are i.i.d.
`A.model="scaling"` $\mathbf{a}$ is a set of scaling factors
`pi.model="unequal"` all initial states are different
`V0.model="zero"` the initial condition on the states ($\mathbf{x}_0$ or $\mathbf{x}_1$) is fixed but unknown

4

Model specification in the core functions

Most users will not directly work with the core functions nor build marssm objects from scratch. Instead, they will usually interact with the core functions via the function `MARSS()` described in Chapter 3. With the `MARSS()` function, the user specifies the model structure with matrices or text strings ("diagonal", "unconstrained", etc.) and `MARSS()` builds the marssm object. However, a basic understanding of the structure of marssm objects is useful if one wants to interact directly with the core functions.

The first step of model specification is to write down (e.g. on paper) the model in matrix form (Equation 1.1) with notes on the dimensions (rows and columns) of each parameter and of $\mathbf{x}$ and $\mathbf{y}$. In the core functions, the parameters in the MARSS model must be passed as matrices of the correct dimension, and the parameters in the *R* functions correspond one-to-one to the mathematical equation. For example, $\mathbf{u}$ must be passed in as a matrix of dimension `c(m,1)`. The function will return an error if anything else is passed in (including a matrix with `dim=c(1,m)` or a vector of length m).

4.1 The fixed and free components of the model parameters

In a marssm object, each parameter must be specified by a pair of matrices: `free` which gives the location and sharing of the estimated elements in the parameter matrix and `fixed` which specifies the location and value of the fixed elements in the parameter matrix. For example, $\mathbf{Q}$ is specified by `free$Q` and `fixed$Q`.

4.1.1 The fixed matrices

The fixed matrix specifies the values (numeric) of the fixed (meaning not estimated) elements. In the fixed matrix, the free (meaning estimated or fitted)

elements are denoted with `NA`. The following shows some common examples of the fixed matrix using `fixed$Q` as the example. Each of the other fixed matrices for the other parameters uses the same pattern.

Q is unconstrained, so there are no fixed values

$$\texttt{fixed\$Q} = \begin{bmatrix} NA & NA & NA \\ NA & NA & NA \\ NA & NA & NA \end{bmatrix}$$

Q is a diagonal matrix, so the off-diagonals are fixed at 0. The diagonal elements will be estimated.

$$\texttt{fixed\$Q} = \begin{bmatrix} NA & 0 & 0 \\ 0 & NA & 0 \\ 0 & 0 & NA \end{bmatrix}$$

Q is fixed, i.e. will not be estimated rather all values in the **Q** matrix are fixed.

$$\texttt{fixed\$Q} = \begin{bmatrix} 0.1 & 0 & 0 \\ 0 & 0.1 & 0 \\ 0 & 0 & 0.1 \end{bmatrix}$$

4.1.2 The free matrices

The free matrix specifies which elements are estimated and specifies how (and whether) the free elements are shared. In the free matrix, the fixed elements are denoted `NA`. The following shows some common examples of `free` using `free$Q` as the example. `free` can be passed in as a character matrix or a numeric matrix, but if numeric, the numeric will be changed to character (thus 0 becomes "0" and is the name "0" not the number 0).

Q is a diagonal matrix in which there is only one, shared, value on the diagonal. Thus there is only one **Q** parameter.

$$\texttt{free\$Q} = \begin{bmatrix} 1 & NA & NA \\ NA & 1 & NA \\ NA & NA & 1 \end{bmatrix} \quad \texttt{or} \quad \begin{bmatrix} \text{“}a\text{”} & NA & NA \\ NA & \text{“}a\text{”} & NA \\ NA & NA & \text{“}a\text{”} \end{bmatrix}$$

Here "1" does not mean "number 1" but rather that the name of the shared parameter is "1". On the example at the right, the name of the shared parameter is "a".

Q is a diagonal matrix in which each of the diagonal elements are different.

$$\texttt{free\$Q} = \begin{bmatrix} 1 & NA & NA \\ NA & 2 & NA \\ NA & NA & 3 \end{bmatrix} \quad \texttt{or} \quad \begin{bmatrix} \text{“}north\text{”} & NA & NA \\ NA & \text{“}middle\text{”} & NA \\ NA & NA & \text{“}south\text{”} \end{bmatrix}$$

Q has one value on the diagonal and another one on the off-diagonals. There are no fixed values in **Q**.

$$\texttt{free\$Q} = \begin{bmatrix} 1 & 2 & 2 \\ 2 & 1 & 2 \\ 2 & 2 & 1 \end{bmatrix} \quad \texttt{or} \quad \begin{bmatrix} \text{“}a\text{”} & \text{“}b\text{”} & \text{“}b\text{”} \\ \text{“}b\text{”} & \text{“}a\text{”} & \text{“}b\text{”} \\ \text{“}b\text{”} & \text{“}b\text{”} & \text{“}a\text{”} \end{bmatrix}$$

Q is unconstrained. There are no fixed values in **Q** in this case. Note that since, **Q** is a variance-covariance matrix, it must be symmetric across the diagonal.

$$\texttt{free\$Q} = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 4 & 5 \\ 3 & 5 & 6 \end{bmatrix}$$

4.2 Limits on the model forms that can be fit

The main limitation is that one must specify a model that has only one solution. The core functions will allow you to attempt to fit an improper model (one with multiple solutions). If you do this accidentally, it may or may not be obvious that you have a problem. The estimation functions may chug along happily and return some solution. Careful thought about your model structure and the structure of the estimated parameter matrices will help you determine if your model is under-constrained and unsolvable.

5

Algorithms used in the MARSS package

5.1 Kalman filter and smoother

The MARSS model (Equation 1.1) is a linear dynamical system in discrete time. In 1960, Rudolf Kalman published the Kalman filter (Kalman, 1960), a recursive algorithm that solves for the expected value of the hidden state(s) at time t conditioned on the data up to time t: $\mathrm{E}(\mathbf{X}_t|\mathbf{y}_1^t)$. The Kalman filter gives the optimal (lowest mean square error) estimate of the unobserved $\mathbf{x}_t$ based on the observed data up to time t for this class of linear dynamical system. The Kalman smoother (Rauch et al., 1965) solves for the expected value of the hidden state(s) conditioned on all the data: $\mathrm{E}(\mathbf{X}_t|\mathbf{y}_1^T)$. If the errors in the stochastic process are Gaussian, then the estimators from the Kalman filter and smoother are also the maximum-likelihood estimates.

However, even if the the errors are not Gaussian, the estimators are optimal in the sense that they are estimators with the least variability possible. This robustness is one reason the Kalman filter is so powerful—it provides well-behaving estimates of the hidden states for all kinds of multivariate autoregressive processes, not just Gaussian processes. The Kalman filter and smoother are widely used in time-series analysis, and there are many textbooks covering it and its applications. In the interest of giving the reader a single point of reference, we use Shumway and Stoffer (2006) as our primary reference.

The `MARSSkf` function provides the Kalman filter and smoother in native *R* . The algorithm in `MARSSkf` is that shown in Shumway and Stoffer (2006). This algorithm is not computationally efficient; see Koopman et al. (1999, sec. 4.3) for a more efficient Kalman filter implementation. The Koopman et al. implementation is provided in the functions `MARSSkfas` using the KFAS *R* package. `MARSSkf` (and `MARSSkfas` with a few exceptions) has the following outputs:

`xtt1` The expected value of $\mathbf{X}_t$ conditioned on the data up to time $t-1$.
`xtt` The expected value of $\mathbf{X}_t$ conditioned on the data up to time t.

`xtT` The expected value of $\mathbf{X}_t$ conditioned on all the data from time 1 to T. This the smoothed state estimate.

`Vtt1` The variance of $\mathbf{X}_t$ conditioned on the data up to time $t-1$. Denoted P_t^{t-1} in section 6.2 in Shumway and Stoffer (2006).

`Vtt` The variance of $\mathbf{X}_t$ conditioned on the data up to time t. Denoted P_t^t in section 6.2 in Shumway and Stoffer (2006).

`VtT` The variance of $\mathbf{X}_t$ conditioned on all the data from time 1 to T.

`Vtt1T` The covariance of $\mathbf{X}_t$ and $\mathbf{X}_{t-1}$ conditioned on all the data, 1 to T. Not currently output by `MARSSkfas`.

`Kt` The Kalman gain. This is part of the update equations and relates to the amount `xtt1` is updated by the data at time t to produce `xtt`. Not currently output by `MARSSkfas`.

`J` This is similar to the Kalman gain but is part of the Kalman smoother. See Equation 6.49 in Shumway and Stoffer (2006). Not currently output by `MARSSkfas`.

`Innov` This has the innovations at time t, defined as $\varepsilon_t \equiv \mathbf{y}_t\text{-E}(\mathbf{Y}_t)$. These are the residuals, the difference between the data and their predicted values. See Equation 6.24 in Shumway and Stoffer (2006).

`Sigma` This has the Σ_t, the variance-covariance matrices for the innovations at time t. This is used for the calculation of confidence intervals, the s.e. on the state estimates and the likelihood. See Equation 6.25 in Shumway and Stoffer (2006) for the Σ_t calculation.

`logLik` The log-likelihood of the data conditioned on the model parameters.

5.2 The exact likelihood

The likelihood of the data given a set of MARSS parameters is part of the output of the `MARSSkf` and `MARSSkfas` functions. The likelihood computation is based on the innovations form of the likelihood (Schweppe, 1965) and uses the output from the Kalman filter:

$$\log \mathrm{L}(\Theta|data) = -\frac{N}{2\log(2\pi)} - \frac{1}{2}\left(\sum_{t=1}^{T}\log|\Sigma_t| + \sum_{t=1}^{T}(\varepsilon_t)^\top\Sigma_t^{-1}\varepsilon_t\right) \tag{5.1}$$

where N is the total number of data points, ε_t is the innovations at time t and $|\Sigma_t|$ is the determinant of the innovations variance-covariance matrix at time t. Reference Equation 6.62 in Shumway and Stoffer (2006). However there are a few differences between the log-likelihood output by `MARSSkf` and `MARSSkfas` and that described in Shumway and Stoffer (2006).

The standard likelihood calculation (Equation 6.62 in Shumway and Stoffer (2006)) is biased when there are missing values in the data, and the missing data modifications discussed in Section 6.4 in Shumway and Stoffer (2006) do not correct for this bias. Harvey (1989), Section 3.4.7, discusses at length that the standard missing values correction leads to an inexact likelihood when

there are missing values. The bias is minor if there are few missing values, but it becomes severe as the number of missing values increases. Many ecological datasets may have over 25% missing values and this level of missing values leads to a very biased likelihood if one uses the inexact formula. Harvey (1989) provides some non-trivial ways to compute the exact likelihood.

We use instead the exact likelihood correction for missing values that is presented in Section 12.3 in Brockwell and Davis (1991). This solution is straight-forward to implement. The correction involves the following changes to ε_t and Σ_t in the Equation 5.1. Suppose the value $y_{i,t}$ is missing. First, the corresponding i-th value of ε_t is set to 0. Second, the i-th diagonal value of Σ_t is set to 1 and the off-diagonal elements on the i-th column and i-th row are set to 0.

5.3 Maximum-likelihood parameter estimation

5.3.1 EM algorithm

The MARSS package provides a maximum-likelihood algorithm which uses an Expectation-Maximization (EM) algorithm (function `MARSSkem`) with output from the Kalman smoother. EM algorithms are widely used algorithms that extend maximum-likelihood estimation to cases where there are hidden random variables in a model (Dempster et al., 1977; Harvey, 1989; Harvey and Shephard, 1993; McLachlan and Krishnan, 2008).

The EM algorithm finds the maximum-likelihood estimates of the parameters in a MARSS model using an iterative process. Starting with an initial set of parameters[1], which we will denote $\hat{\Theta}_1$, an updated parameter set $\hat{\Theta}_2$ is obtaining by finding the $\hat{\Theta}_2$ that maximizes the expected value of the likelihood over the distribution of the states ($\mathbf{X}$) conditioned on $\hat{\Theta}_1$:

$$\hat{\Theta}_2 = \arg\max_{\Theta} \quad \mathrm{E}_{\mathbf{X}|\hat{\Theta}_1}[\log L(\Theta|\mathbf{Y}_1^T = \mathbf{y}_1^T, \mathbf{X})] \tag{5.2}$$

Then using $\hat{\Theta}_2$ in place of $\hat{\Theta}_1$ in Equation (5.2), an updated parameter set $\hat{\Theta}_3$ is calculated. This is repeated until the expected log-likelihood stops increasing (or increases less than some set tolerance level).

Implementing this algorithm is straight-forward, hence its popularity.

1. Set an initial set of parameters, $\hat{\Theta}_1$
2. E step: using the model for the hidden states ($\mathbf{X}$) and $\hat{\Theta}_1$, calculate the expected values of $\mathbf{X}$ conditioned on all the data $\mathbf{y}_1^T$; this is `xtT` output by `MARSSkf`. Also calculate expected values of any functions of $\mathbf{X}$, $g(\mathbf{X})$, that appear in your expected log-likelihood function.

[1] You can choose these however you wish, however choosing something not too far off from the correct values will make the algorithm go faster.

3. M step: put those $\mathrm{E}(\mathbf{X}|\mathbf{Y}_1^T = \mathbf{y}_1^T, \hat{\Theta}_1)$ and $\mathrm{E}(g(\mathbf{X})|\mathbf{Y}_1^T = \mathbf{y}_1^T, \hat{\Theta}_1)$ into your expected log-likelihood function in place of $\mathbf{X}$ (and $g(\mathbf{X})$) and maximize with respect to Θ. This gives you $\hat{\Theta}_2$.
4. Repeat the E and M steps until the log likelihood stops increasing.

The EM equations used in the MARSS package (function `MARSSkem`) are described in Holmes (2010) and are extensions of those in Shumway and Stoffer (1982) and Ghahramani and Hinton (1996). Our EM algorithm is an extended version because our algorithm is for cases where there are constraints within the parameter matrices (shared values, diagonal structure, block-diagonal structure, ...), where there are fixed values within the parameter matrices, and where there may be 0s on the diagonal of $\mathbf{Q}$, $\mathbf{R}$ and Λ.

The EM algorithm is a hill-climbing algorithm and like all hill-climbing algorithms can get stuck on local maxima. The MARSS package includes a Monte-Carlo initial conditions searcher (function `MARSSmcinit`) based on Biernacki et al. (2003) to minimize this problem. EM algorithms are also known to get close to the maximum very quickly but then creep toward the absolute maximum. Once in the vicinity of the maximum, quasi-Newton methods find the absolute maximum much faster, but they can be sensitive to initial conditions and in practice, we have found the EM algorithm to be much faster for large problems.

5.4 Parametric and innovations bootstrapping

Bootstrapping can be used to construct frequentist confidence intervals on the parameter estimates (Stoffer and Wall, 1991) and to compute the small-sample AIC corrector for MARSS models (Cavanaugh and Shumway, 1997); the functions `MARSSparamCIs` and `MARSSaic` do these computations.

The `MARSSboot` function provides both parametric and innovations bootstrapping of MARSS models. The innovations bootstrap algorithm by Stoffer and Wall (1991) bootstraps the model residuals (the innovations). This is a semi-parametric bootstrap since is uses, partially, the maximum-likelihood parameter estimates. This algorithm cannot be used if there are missing values in the data. Also for short time series, it gives biased bootstraps because one cannot resample the first few innovations.

`MARSSboot` also provides a fully parametric bootstrap. This uses the maximum-likelihood MARSS parameters to simulate data from which bootstrap parameter estimates are obtained. Our research (Holmes and Ward, 2010) indicates that this provides unbiased bootstrap parameter estimates, and it works with datasets with missing values. Lastly, `MARSSboot` can also output parameters sampled from a numerically estimated Hessian matrix.

5.5 Simulation and forecasting

The `MARSSsimulate` function simulates from a MARSS model using a list of parameter matrices. It use the `mvrnorm` function to produce draws of the process and observation errors from multivariate normal distributions for each time step.

5.6 Model selection

The package provides a `MARSSaic` function for computing AIC, AICc and AICb. The latter is a small-sample corrector for autoregressive state-space models. The bias problem with AIC and AICc for short time-series data has been shown in Cavanaugh and Shumway (1997) and Holmes and Ward (2010). AIC and AICc tend to select overly complex MARSS models when the time-series data are short. AICb corrects this bias. The algorithm for a non-parametric AICb is given in Cavanaugh and Shumway (1997). Their algorithm uses the innovations bootstrap (Stoffer and Wall, 1991), which means it cannot be used when there are missing data. We added a parametric AICb (Holmes and Ward, 2010), which uses a parametric bootstrap. This algorithm allows one to compute AICb when there are missing data and it provides unbiased AIC even for short time series. See Holmes and Ward (2010) for discussion and testing of parametric AICb for MARSS models.

AICb is comprised of the familiar AIC fit term, $-2\log L$, plus a penalty term that is the mean difference between the log likelihood the data under the bootstrapped maximum-likelihood parameter estimates and the log likelihood of the data under the original maximum-likelihood parameter estimate:

$$AICb = -2\log \mathrm{L}(\hat{\Theta}|\mathbf{y}) + 2\left(\frac{1}{N_b}\sum_{i=1}^{N_b} -\log\frac{\mathrm{L}(\hat{\Theta}^*(i)|\mathbf{y})}{\mathrm{L}(\hat{\Theta}|\mathbf{y})}\right) \tag{5.3}$$

where $\hat{\Theta}$ is the maximum-likelihood parameter set under the original data $\mathbf{y}$, $\hat{\Theta}^*(i)$ is a maximum-likelihood parameter set estimated from the i-th bootstrapped data set $\mathbf{y}^*(i)$, and N_b is the number of bootstrap data sets. It is important to notice that the likelihood in the AICb equation is $\mathrm{L}(\hat{\Theta}^*|\mathbf{y})$ not $\mathrm{L}(\hat{\Theta}^*|\mathbf{y}^*)$. In other words, we are taking the average of the likelihood of the original data given the bootstrapped parameter sets.

6

Examples

In this chapter, we show how to fit the most general MARSS, and then work through a series of short examples using the MARSS package functions. This chapter is oriented towards those who are already somewhat familiar with MARSS models and want to get started quickly. We provide no explanatory text. Those unfamiliar with MARSS models would do better to start with the case studies.

6.1 Fitting a general MARSS models

The short examples below show models which you can fit using some model specification shortcuts. But we will start by showing the most general form, so you will know how to fit (most) any MARSS model you can write on paper. In the most general form a MARSS model can look like so (m=2 and n=3). The numeric values are arbitrary and just show that in the MARSS model specification you can mix estimated, fixed, and shared values. In addition, you can have 0s on the diagonals of your variance-covariance matrices, which allows you to mix deterministic processes, zero measurement error processes, and white noise into your models.

$$\begin{bmatrix} x_{1,t} \\ x_{2,t} \end{bmatrix} = \begin{bmatrix} b_1 & 0.1 \\ b_2 & 2 \end{bmatrix} \begin{bmatrix} x_{1,t-1} \\ x_{2,t-1} \end{bmatrix} + \begin{bmatrix} u \\ u \end{bmatrix} + \begin{bmatrix} w_{1,t} \\ w_{2,t} \end{bmatrix}, \ \mathbf{w}_t \sim \text{MVN}\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} q_1 & q_3 \\ q_3 & q_2 \end{bmatrix} \right)$$

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \end{bmatrix} = \begin{bmatrix} z_1 & z_2 & 0 \\ 0 & z_2 & 3 \end{bmatrix} \begin{bmatrix} x_{1,t} \\ x_{2,t} \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \end{bmatrix}, \ \mathbf{v}_t \sim \text{MVN}\left(\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} r & 0 & 0 \\ 0 & r & 0 \\ 0 & 0 & 1 \end{bmatrix} \right)$$

$$\mathbf{x}_0 \sim \text{MVN}\left(\begin{bmatrix} \pi_1 \\ \pi_2 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right)$$

Notice how we have mixed fixed values, estimated values and shared values. The MARSS model specification is a list with the names, Z,A,R,B,U,Q. Each

element is matrix (class matrix) with the same dimensions as your model on paper. MARSS distinguishes between the estimated and fixed values by using list matrices in which you can have numeric and character elements. Numeric elements are fixed; character elements are names of things to be estimated.

```
Z=matrix(list("z1","z2",0,0,"z2",3),3,2)
A=matrix(0,3,1)
R=matrix(list(0),3,3); diag(R)=c("r","r",1)
B=matrix(list("b1",0.1,"b2",2),2,2)
U=matrix(c("u","u"),2,1)
Q=matrix(c("q1","q3","q3","q2"),2,2)
x0=matrix(c("pi1","pi2"),2,1)
V0=diag(1,2)
model.gen=list(Z=Z,A=A,R=R,B=B,U=U,Q=Q,x0=x0,V0=V0)
```

Notice that there is a one-to-one correspondence between the model list in *R* and the model on paper. Fitting the model is then just a matter of passing the data and model list to the MARSS function:

```
kemfit = MARSS(dat, model=model.gen)
```

If you work often with MARSS models then you will probably know whether prior sensitivity is a problem for your types of MARSS applications. If so, note that the MARSS package is unusual in that it allows you to set $\Lambda = 0$ and treat $\mathbf{x}_0$ as an unknown estimated parameter. This eliminates the prior and thus the prior sensitivity problems—at the cost of adding m parameters. Depending on your application, you may need to set the initial conditions at $t = 1$ instead of the default of $t = 0$. If you are unsure, look in the index and read all the sections that talk about troubleshooting priors.

6.2 Fitting different MARSS models to a harbor seal dataset

Here we show a series of short examples using a dataset on Washington harbor seals (`?harborSealWA`), which has five observation time series. The dataset is a little unusual in that it has four missing years from year 2 to 5. This causes some interesting issues with prior specification. Before starting the harbor seal examples, we set up the data, making time go across the columns and removing the year column:

```
dat = t(harborSealWA)
dat = dat[2:nrow(dat),] #remove the year row
```

6.2.1 One hidden state process for each observation time series

This is the default model for the `MARSS()` function. In this case, $n = m$, the observation errors are i.i.d. and the process errors are independent and have

different variances. The elements in **u** are all different (meaning, they are not forced to be the same). Mathematically, the MARSS model being fit is:

$$\begin{bmatrix} x_{1,t} \\ x_{2,t} \\ x_{3,t} \\ x_{4,t} \\ x_{5,t} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_{1,t-1} \\ x_{2,t-1} \\ x_{3,t-1} \\ x_{4,t-1} \\ x_{5,t-1} \end{bmatrix} + \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} + \begin{bmatrix} w_{1,t} \\ w_{2,t} \\ w_{3,t} \\ w_{4,t} \\ w_{5,t} \end{bmatrix}, \ \mathbf{w}_t \sim \text{MVN}\left(\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} q_1 & 0 & 0 & 0 & 0 \\ 0 & q_2 & 0 & 0 & 0 \\ 0 & 0 & q_3 & 0 & 0 \\ 0 & 0 & 0 & q_4 & 0 \\ 0 & 0 & 0 & 0 & q_5 \end{bmatrix} \right)$$

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_{1,t} \\ x_{2,t} \\ x_{3,t} \\ x_{4,t} \\ x_{5,t} \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \end{bmatrix}, \ \mathbf{v}_t \sim \text{MVN}\left(\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} r & 0 & 0 & 0 & 0 \\ 0 & r & 0 & 0 & 0 \\ 0 & 0 & r & 0 & 0 \\ 0 & 0 & 0 & r & 0 \\ 0 & 0 & 0 & 0 & r \end{bmatrix} \right)$$

This is the default model, so you can fit it by simply passing `dat` to `MARSS()`.

```
kemfit = MARSS(dat)
```

```
Success! Parameters converged at 30 iterations.
Alert: conv.test.slope.tol is 0.5.
Test with smaller values (<0.1) to ensure convergence.

MARSS fit is
Estimation method: kem
Estimation converged in 30 iterations.
Log-likelihood: 19.11755
AIC: -6.235105   AICc: 3.838969

          Estimate
R.R(diag)  0.00927
U.U1       0.06840
U.U2       0.07170
U.U3       0.04171
U.U4       0.05230
U.U5      -0.00286
Q.Q(1,1)   0.03068
Q.Q(2,2)   0.01078
Q.Q(3,3)   0.00694
Q.Q(4,4)   0.00434
Q.Q(5,5)   0.05308
x0.x01     5.98840
x0.x02     6.72740
x0.x03     6.66616
```

```
x0.x04     5.83845
x0.x05     6.60533

Standard errors have not been calculated.
Use MARSSparamCIs to compute CIs and bias estimates.
```

Notice that the output warns you that the convergence tolerance is high. You can set it lower by passing in `control=list(conv.test.slope.tol=0.1)`. `MARSS()` is automatically creating parameter names since you did not tell it the names. To see exactly where each parameter element (e.g. `Q.2`) appears in its parameter matrix, type `summary(kemfit$model)`.

Though it is not necessary to specify the model for this example since it is the default, here is how you would do so using matrices:

```
B=Z=diag(1,5)
U=matrix(c("u1","u2","u3","u4","u5"),5,1)
x0=A=matrix(0,5,1)
R=Q=matrix(list(0),5,5)
diag(R)="r"
diag(Q)=c("q1","q2","q3","q4","q5")
```

Notice that there is a one-to-one relationship between the model on paper and the model specification for MARSS. Notice also that when a matrix has both fixed and estimated elements (like **R** and **Q**), a list matrix is used to allow you to specify the fixed elements as numeric and to give the estimated elements character names.

The default MLE method is the EM algorithm (`method="kem"`). You can also use a quasi-Newton method (BFGS) by setting `method="BFGS"`.

```
kemfit.bfgs = MARSS(dat, method="BFGS")
```

```
Success! Converged in 99 iterations.
Function MARSSkf used for likelihood calculation.

MARSS fit is
Estimation method: BFGS
Estimation converged in 99 iterations.
Log-likelihood: 19.13936
AIC: -6.278712   AICc: 3.795362

          Estimate
R.R(diag)  0.00849
U.U1       0.06838
U.U2       0.07152
U.U3       0.04188
U.U4       0.05233
U.U5      -0.00271
```

```
Q.Q(1,1)   0.03368
Q.Q(2,2)   0.01124
Q.Q(3,3)   0.00722
Q.Q(4,4)   0.00437
Q.Q(5,5)   0.05600
x0.x01     5.98437
x0.x02     6.72169
x0.x03     6.65689
x0.x04     5.83527
x0.x05     6.60425

Standard errors have not been calculated.
Use MARSSparamCIs to compute CIs and bias estimates.
```

Using the default EM convergence criteria, the EM algorithm stops at a log-likelihood a little lower than the BFGS algorithm does, but the EM algorithm was considerable faster, 19.848 times faster in this case. If you wanted to use the EM fit as the initial conditions, pass in the `inits` argument.

```
kemfit.bfgs2 = MARSS(dat, method="BFGS", inits=kemfit$par)
```

The BFGS algorithm now converges in 85 iterations. Output not shown.

We mentioned that the missing years from year 2 to 4 creates an interesting issue with the prior specification. The default behavior of MARSS is to treat the initial state as at $t = 0$ instead of $t = 1$. Usually this doesn't make a difference, but for this dataset, if we set the prior at $t = 1$, the MLE estimate of $\mathbf{R}$ becomes 0. If we estimate $\mathbf{x}_1$ as a parameter and let $\mathbf{R}$ go to 0, the likelihood will go to infinity (slowly but surely). This is neither an error nor a pathology, but is probably not what you would like to have happen. Note that the "BFGS" algorithm will not find the maximum in this case; it will stop before $\mathbf{R}$ gets small and the likelihood gets very large. However, the EM algorithm will climb up the peak. You can try it by running the following code. It will report warnings which you can read about in Appendix B.

```
kemfit.strange = MARSS(dat, model=list(tinitx=1))
```

6.2.2 Five correlated hidden state processes

This is the same model except that the hidden states have temporally correlated process errors. Mathematically, this is the model:

$$\begin{bmatrix} x_{1,t} \\ x_{2,t} \\ x_{3,t} \\ x_{4,t} \\ x_{5,t} \end{bmatrix} = \begin{bmatrix} x_{1,t-1} \\ x_{2,t-1} \\ x_{3,t-1} \\ x_{4,t-1} \\ x_{5,t-1} \end{bmatrix} + \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} + \begin{bmatrix} w_{1,t} \\ w_{2,t} \\ w_{3,t} \\ w_{4,t} \\ w_{5,t} \end{bmatrix}, \ \mathbf{w}_t \sim \text{MVN}\left(0, \begin{bmatrix} q_1 & c_{1,2} & c_{1,3} & c_{1,4} & c_{1,5} \\ c_{1,2} & q_2 & c_{2,3} & c_{2,4} & c_{2,5} \\ c_{1,3} & c_{2,3} & q_3 & c_{3,4} & c_{3,5} \\ c_{1,4} & c_{2,4} & c_{3,4} & q_4 & c_{4,5} \\ c_{1,5} & c_{2,5} & c_{3,5} & c_{4,5} & q_5 \end{bmatrix}\right)$$

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_{1,t} \\ x_{2,t} \\ x_{3,t} \\ x_{4,t} \\ x_{5,t} \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \end{bmatrix}, \ \mathbf{v}_t \sim \text{MVN}\left(0, \begin{bmatrix} r & 0 & 0 & 0 & 0 \\ 0 & r & 0 & 0 & 0 \\ 0 & 0 & r & 0 & 0 \\ 0 & 0 & 0 & r & 0 \\ 0 & 0 & 0 & 0 & r \end{bmatrix}\right)$$

B is not shown in the top equation; it is a $m \times m$ identity matrix. To fit, use `MARSS()` with the `model` argument set. The output is not shown but it will appear if you type this on the *R* command line.

```
kemfit = MARSS(dat, model=list(Q="unconstrained"))
```

This shows one of the text shortcuts, `"unconstrained"`, which means estimate all elements in the matrix. This shortcut can be used for all parameters.

6.2.3 Five equally correlated hidden state processes

This is the same model except that now there is only one process error variance and one process error covariance. Mathematically, the model is:

$$\begin{bmatrix} x_{1,t} \\ x_{2,t} \\ x_{3,t} \\ x_{4,t} \\ x_{5,t} \end{bmatrix} = \begin{bmatrix} x_{1,t-1} \\ x_{2,t-1} \\ x_{3,t-1} \\ x_{4,t-1} \\ x_{5,t-1} \end{bmatrix} + \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} + \begin{bmatrix} w_{1,t} \\ w_{2,t} \\ w_{3,t} \\ w_{4,t} \\ w_{5,t} \end{bmatrix}, \ \mathbf{w}_t \sim \text{MVN}\left(0, \begin{bmatrix} q & c & c & c & c \\ c & q & c & c & c \\ c & c & q & c & c \\ c & c & c & q & c \\ c & c & c & c & q \end{bmatrix}\right)$$

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_{1,t} \\ x_{2,t} \\ x_{3,t} \\ x_{4,t} \\ x_{5,t} \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \end{bmatrix}, \ \mathbf{v}_t \sim \text{MVN}\left(0, \begin{bmatrix} r & 0 & 0 & 0 & 0 \\ 0 & r & 0 & 0 & 0 \\ 0 & 0 & r & 0 & 0 \\ 0 & 0 & 0 & r & 0 \\ 0 & 0 & 0 & 0 & r \end{bmatrix}\right)$$

Again **B** is not shown in the top equation; it is a $m \times m$ identity matrix. To fit, use the following code (output not shown):

```
kemfit = MARSS(dat, model=list(Q="equalvarcov"))
```

The shortcut '`"equalvarcov"` means one value on the diagonal and one on the off-diagonal. It can be used for all square matrices (**B**,**Q**,**R**, and Λ).

6.2.4 Five hidden state processes with a "north" and a "south" u and Q elements

Here we fit a model with five independent hidden states where each observation time series is an independent observation of a different hidden trajectory but the hidden trajectories 1-3 share their **u** and **Q** elements, while hidden trajectories 4-5 share theirs. This is the model:

$$\begin{bmatrix} x_{1,t} \\ x_{2,t} \\ x_{3,t} \\ x_{4,t} \\ x_{5,t} \end{bmatrix} = \begin{bmatrix} x_{1,t-1} \\ x_{2,t-1} \\ x_{3,t-1} \\ x_{4,t-1} \\ x_{5,t-1} \end{bmatrix} + \begin{bmatrix} u_n \\ u_n \\ u_n \\ u_s \\ u_s \end{bmatrix} + \begin{bmatrix} w_{1,t} \\ w_{2,t} \\ w_{3,t} \\ w_{4,t} \\ w_{5,t} \end{bmatrix}, \ \mathbf{w}_t \sim \text{MVN}\left(0, \begin{bmatrix} q_n & 0 & 0 & 0 & 0 \\ 0 & q_n & 0 & 0 & 0 \\ 0 & 0 & q_n & 0 & 0 \\ 0 & 0 & 0 & q_s & 0 \\ 0 & 0 & 0 & 0 & q_s \end{bmatrix}\right)$$

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_{1,t} \\ x_{2,t} \\ x_{3,t} \\ x_{4,t} \\ x_{5,t} \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \end{bmatrix}, \ \mathbf{v}_t \sim \text{MVN}\left(0, \begin{bmatrix} r & 0 & 0 & 0 & 0 \\ 0 & r & 0 & 0 & 0 \\ 0 & 0 & r & 0 & 0 \\ 0 & 0 & 0 & r & 0 \\ 0 & 0 & 0 & 0 & r \end{bmatrix}\right)$$

To fit use the following code, we specify the `model` argument for **u** and **Q** using list matrices. List matrices allow us to combine numeric and character values in a matrix. MARSS will interpret the numeric values as fixed, and the character values as parameters to be estimated. Parameters with the same name are constrained to be identical.

```
regions=list("N","N","N","S","S")
U.model=matrix(regions,5,1)
Q.model=matrix(list(0),5,5); diag(Q.model)=regions
kemfit = MARSS(dat, model=list(U=U.model, Q=Q.model))
```

Only **u** and **Q** need to be specified since the other parameters are at their default values.

6.2.5 Fixed observation error variance

Here we fit the same model but with a known observation error variance. This is the model:

$$\begin{bmatrix} x_{1,t} \\ x_{2,t} \\ x_{3,t} \\ x_{4,t} \\ x_{5,t} \end{bmatrix} = \begin{bmatrix} x_{1,t-1} \\ x_{2,t-1} \\ x_{3,t-1} \\ x_{4,t-1} \\ x_{5,t-1} \end{bmatrix} + \begin{bmatrix} u_n \\ u_n \\ u_n \\ u_s \\ u_s \end{bmatrix} + \begin{bmatrix} w_{1,t} \\ w_{2,t} \\ w_{3,t} \\ w_{4,t} \\ w_{5,t} \end{bmatrix}, \ \mathbf{w}_t \sim \text{MVN}\left(0, \begin{bmatrix} q_n & 0 & 0 & 0 & 0 \\ 0 & q_n & 0 & 0 & 0 \\ 0 & 0 & q_n & 0 & 0 \\ 0 & 0 & 0 & q_s & 0 \\ 0 & 0 & 0 & 0 & q_s \end{bmatrix}\right)$$

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_{1,t} \\ x_{2,t} \\ x_{3,t} \\ x_{4,t} \\ x_{5,t} \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \end{bmatrix},$$

$$\mathbf{v}_t \sim \text{MVN}\left(0, \begin{bmatrix} 0.01 & 0 & 0 & 0 & 0 \\ 0 & 0.01 & 0 & 0 & 0 \\ 0 & 0 & 0.01 & 0 & 0 \\ 0 & 0 & 0 & 0.01 & 0 \\ 0 & 0 & 0 & 0 & 0.01 \end{bmatrix}\right)$$

To fit this model, use the following code (output not shown):

```
regions=list("N","N","N","S","S")
U.model=matrix(regions,5,1)
Q.model=matrix(list(0),5,5); diag(Q.model)=regions
kemfit = MARSS(dat, model=list(U=U.model, Q=Q.model,
          R=diag(0.01,5)))
```

6.2.6 One hidden state and five i.i.d. observation time series

Instead of five hidden state trajectories, we specify that there is only one and all the observations are of that one trajectory. Mathematically, the model is:

$$x_t = x_{t-1} + u + w_t, \ w_t \sim \text{N}(0, q)$$

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} x_t + \begin{bmatrix} 0 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \end{bmatrix}, \ \mathbf{v}_t \sim \text{MVN}\left(0, \begin{bmatrix} r & 0 & 0 & 0 & 0 \\ 0 & r & 0 & 0 & 0 \\ 0 & 0 & r & 0 & 0 \\ 0 & 0 & 0 & r & 0 \\ 0 & 0 & 0 & 0 & r \end{bmatrix}\right)$$

Note the default model for **R** is `"diagonal and equal"`' so we can leave this off when specifying the `model` argument. To fit, use this code (output not shown):

```
kemfit =
   MARSS(dat, model=list(Z=factor(c(1,1,1,1,1))))
```

```
Success! Parameters converged at 21 iterations.
Alert: conv.test.slope.tol is 0.5.
Test with smaller values (<0.1) to ensure convergence.

MARSS fit is
Estimation method: kem
Estimation converged in 21 iterations.
Log-likelihood: 3.57983
AIC: 8.840339   AICc: 11.16292

          Estimate
A.2        0.80533
A.3        0.28632
A.4       -0.54281
A.5       -0.62036
R.R(diag)  0.04514
U.U        0.04762
Q.Q        0.00452
x0.x0      6.38367

Standard errors have not been calculated.
Use MARSSparamCIs to compute CIs and bias estimates.
```

You can also pass in **Z** exactly as it is in the equation: `Z=matrix(1,5,1)`.

6.2.7 One hidden state and five independent observation time series with different variances

Mathematically, this model is:

$$x_t = x_{t-1} + u + w_t,\ w_t \sim \mathrm{N}(0, q)$$

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} x_t + \begin{bmatrix} 0 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \end{bmatrix},\ \mathbf{v}_t \sim \mathrm{MVN}\left(0, \begin{bmatrix} r_1 & 0 & 0 & 0 & 0 \\ 0 & r_2 & 0 & 0 & 0 \\ 0 & 0 & r_3 & 0 & 0 \\ 0 & 0 & 0 & r_4 & 0 \\ 0 & 0 & 0 & 0 & r_5 \end{bmatrix}\right)$$

To fit this model:

```
kemfit =
   MARSS(dat, model=list(Z=factor(c(1,1,1,1,1)),
   R="diagonal and unequal"))
```

```
Success! Parameters converged at 21 iterations.
Alert: conv.test.slope.tol is 0.5.
Test with smaller values (<0.1) to ensure convergence.

MARSS fit is
Estimation method: kem
Estimation converged in 21 iterations.
Log-likelihood: 16.65845
AIC: -9.316899   AICc: -3.937589

         Estimate
A.2       0.79446
A.3       0.27429
A.4      -0.53850
A.5      -0.61041
R.R(1,1)  0.03216
R.R(2,2)  0.03505
R.R(3,3)  0.01362
R.R(4,4)  0.01095
R.R(5,5)  0.19665
U.U       0.05276
Q.Q       0.00607
x0.x0     6.26665

Standard errors have not been calculated.
Use MARSSparamCIs to compute CIs and bias estimates.
```

6.2.8 Two hidden state processes

Here we fit a model with two hidden states (north and south) where observation time series 1-3 are for the north and 4-5 are for the south. We make the hidden state processes independent (meaning a diagonal **Q** matrix) but with the same process variance. We make the observation errors i.i.d. (the default) and the **u** elements equal. Mathematically, this is the model:

$$\begin{bmatrix} x_{n,t} \\ x_{s,t} \end{bmatrix} = \begin{bmatrix} x_{n,t-1} \\ x_{s,t-1} \end{bmatrix} + \begin{bmatrix} u \\ u \end{bmatrix} + \begin{bmatrix} w_{n,t} \\ w_{s,t} \end{bmatrix}, \ \mathbf{w}_t \sim \text{MVN}\left(0, \begin{bmatrix} q & 0 \\ 0 & q \end{bmatrix}\right)$$

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_{n,t} \\ x_{s,t} \end{bmatrix} + \begin{bmatrix} 0 \\ a_2 \\ a_3 \\ 0 \\ a_5 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \end{bmatrix}, \ \mathbf{v}_t \sim \text{MVN}\left(0, \begin{bmatrix} r & 0 & 0 & 0 & 0 \\ 0 & r & 0 & 0 & 0 \\ 0 & 0 & r & 0 & 0 \\ 0 & 0 & 0 & r & 0 \\ 0 & 0 & 0 & 0 & r \end{bmatrix}\right)$$

To fit the model, use the following code (output not shown):

```
kemfit =
   MARSS(dat, model=list(Z=factor(c("N","N","N","S","S")),
   Q="diagonal and equal",U="equal"))
```

You can also pass in **Z** exactly as it is in the equation as a numeric matrix; the `factor` notation is a shortcut for making a design matrix (as **Z** is in these examples). `"equal"` is a shortcut meaning all elements in a matrix are constrained to be equal. It can be used for all column matrices (**a**, **u** and π). `"diagonal and equal"` can be used as a shortcut for all square matrices (**B**,**Q**,**R**, and Λ).

6.2.9 Time-varying parameters

Pass an array of matrices (list, numeric or character) for each time-varying parameters. The 3rd dimension of the array is time and must be the same value as the 2nd (time) dimension of the data matrix. No text shortcuts are allowed for time-varying parameters; you need to use the matrix form. Here is an example with a different **U** for the first half versus second half of the harbor seal time series:

```
U1=matrix("t1",5,1); U2=matrix("t2",5,1)
Ut=array(U2,dim=c(dim(U1),dim(dat)[2]))
Ut[,,1:11]=U1
kemfit.tv=MARSS(dat,model=list(U=Ut,Q="diagonal and equal"))
```

You can have some elements in a parameter matrix be time-constant and some be time-varying:

```
U1=matrix(c(rep("t1",4),"hc"),5,1); U2=matrix(c(rep("t2",4),"hc"),5,1)
Ut=array(U2,dim=c(dim(U1),dim(dat)[2]))
Ut[,,1:11]=U1
kemfit.tv=MARSS(dat,model=list(U=Ut,Q="diagonal and equal"))
```

Note that how the time-varying model is specified for MARSS is the same as you would write the time-varying model on paper in matrix math form.

6.3 Printing and summarizing models and model fits

The package includes print functions for marssm objects (model objects) and marssMLE objects (fitted models).

```
print(kemfit)
print(kemfit$model)
```

This will print the basic information on model structure and model fit that you have seen in the previous examples.

The package also includes a summary function for models.

```
summary(kemfit$model)
```

Output is not shown because it is verbose, but it prints each matrix with the fixed elements denoted with their values and the free elements denoted by their names. This is very helpful for confirming exactly what model structure you are fitting to the data.

6.4 Confidence intervals on a fitted model

The function `MARSSparamCIs()` is used to compute confidence intervals. The function can compute approximate confidence intervals using a numerically estimated Hessian matrix (`method="hessian"`) or via parametric (`method="parametric"`) or non-parametric (`method="innovations"`) bootstrapping.

6.4.1 Approximate confidence intervals from a Hessian matrix

```
#default uses an est Hessian matrix
kem.with.hess.CIs = MARSSparamCIs(kemfit)
```

Use `print` or just type the marssMLE object name to see the confidence intervals:

```
print(kem.with.hess.CIs)
```

```
MARSS fit is
Estimation method: kem
Estimation converged in 18 iterations.
Log-likelihood: 7.941363
AIC: 0.1172745   AICc: 2.439855

            ML.Est Std.Err    low.CI  up.CI
A.2        0.79556 0.06146  0.675107 0.9160
A.3        0.27502 0.06247  0.152570 0.3975
A.5       -0.06913 0.08880 -0.243174 0.1049
R.R(diag)  0.03399 0.00645  0.021351 0.0466
U.U        0.04315 0.01459  0.014550 0.0717
Q.Q(diag)  0.00793 0.00434 -0.000577 0.0164
x0.x01     6.17149 0.14643  5.884501 6.4585
x0.x02     6.20544 0.15802  5.895717 6.5152

CIs calculated at alpha = 0.05 via method=hessian
```

The Hessian matrix is an estimate of the variance-covariance matrix of the parameter estimates. For the variances, **Q** and **R**, the normality assumption is not so good because they are constrained to be positive. Thus you may see lower confidence intervals on variances that are negative using the Hessian approximation.

6.4.2 Confidence intervals from a parametric bootstrap

Use `method="parametric"` to use a parametric bootstrap to compute confidence intervals and bias using a parametric bootstrap.

```
kem.w.boot.CIs=MARSSparamCIs(kemfit,method="parametric",nboot=10)
#nboot should be more like 1000, but set low for example's sake
print(kem.w.boot.CIs)
```

```
MARSS fit is
Estimation method: kem
Estimation converged in 18 iterations.
Log-likelihood: 7.941363
AIC: 0.1172745   AICc: 2.439855

            ML.Est Std.Err  low.CI   up.CI  Est.Bias
A.2        0.79556 0.07968  0.6460 0.88696  0.002577
A.3        0.27502 0.04763  0.1933 0.33533  0.018971
A.5       -0.06913 0.09438 -0.2064 0.07730 -0.013383
R.R(diag)  0.03399 0.00564  0.0248 0.04072  0.000571
U.U        0.04315 0.01712  0.0152 0.06375  0.004937
Q.Q(diag)  0.00793 0.00257  0.0000 0.00709  0.004852
x0.x01     6.17149 0.21584  6.0296 6.64700 -0.122539
x0.x02     6.20544 0.35796  5.4418 6.58250  0.109144
          Unbias.Est
A.2           0.7981
A.3           0.2940
A.5          -0.0825
R.R(diag)     0.0346
U.U           0.0481
Q.Q(diag)     0.0128
x0.x01        6.0490
x0.x02        6.3146

CIs calculated at alpha = 0.05 via method=parametric
Bias calculated via parametric bootstrapping with 10 bootstraps.
```

6.5 Vectors of just the estimated parameters

Often it is useful to have a vector of the estimated parameters. For example, if you are writing a call to `optim`, you will need a vector of just the estimated parameters.

```
parvec=MARSSvectorizeparam(kemfit)
parvec
```

```
         A.2          A.3          A.5    R.R(diag)
 0.795564837  0.275016071 -0.069133139  0.033992394
         U.U    Q.Q(diag)       x0.x01       x0.x02
 0.043148375  0.007929747  6.171492396  6.205435799
```

If you want to replace the estimated parameter values with different values, you can use the same function:

```
parvec.new=parvec
parvec.new[6]=parvec.new[6]+0.02
kem.new=MARSSvectorizeparam(kemfit, parvec.new)
```

Then you might want to find out the likelihood of the data using those new parameter values. You compute that with the Kalman filter function `MARSSkf()`, sending it the MLE object, kem.new.

```
kf=MARSSkf( kem.new )
kf$logLik
```

```
[1] 4.479739
```

6.6 Degenerate variance estimates

If your data are short relative to the number of parameters you are estimating, then you are liable to find that some of the variance elements are degenerate (equal to zero). Try the following:

```
dat.short = dat[1:4,1:10]
kem.degen = MARSS(dat.short,control=list(allow.degen=FALSE))
```

```
Warning! Reached maxit before parameters converged. Maxit was 500.

MARSS fit is
Estimation method: kem
WARNING: maxit reached, 500 iter, before convergence.
 The likelihood and params are not at the ML values.
 Try setting control$maxit higher.
Log-likelihood: 11.67854
AIC: 2.642914   AICc: 63.30958

          Estimate
R.R(diag) 1.22e-02
U.U1      9.79e-02
U.U2      1.09e-01
U.U3      9.28e-02
U.U4      1.11e-01
Q.Q(1,1)  1.89e-02
```

```
Q.Q(2,2)  1.03e-05
Q.Q(3,3)  8.24e-06
Q.Q(4,4)  3.05e-05
x0.x01    5.96e+00
x0.x02    6.73e+00
x0.x03    6.60e+00
x0.x04    5.71e+00

Standard errors have not been calculated.
Use MARSSparamCIs to compute CIs and bias estimates.

Convergence warnings
 Warning: the  Q.Q(2,2)  parameter value has not converged.
 Warning: the  Q.Q(3,3)  parameter value has not converged.
 Warning: the  Q.Q(4,4)  parameter value has not converged.
```

This will print a warning that the maximum number of iterations was reached before convergence of some of the **Q** parameters. It might be that if you just ran a few more iterations the variances will converge. So first try setting `control$maxit` higher.

```
kem.degen2 = MARSS(dat.short, control=list(maxit=1000,
      allow.degen=FALSE), silent=2)
```

Output not shown, but if you run the code, you will see that some of the **Q** terms are still not converging. MARSS can detect if a variance is going to zero and it will try zero to see if that has a higher likelihood. Try removing the `allow.degen=FALSE` which was turning off this feature.

```
kem.short = MARSS(dat.short)
```

```
Warning! Reached maxit before parameters converged. Maxit was 500.

MARSS fit is
Estimation method: kem
WARNING: maxit reached, 500 iter, before convergence.
 The likelihood and params are not at the ML values.
 Try setting control$maxit higher.
Log-likelihood: 11.6907
AIC: 2.6186   AICc: 63.28527

          Estimate
R.R(diag) 1.22e-02
U.U1      9.79e-02
U.U2      1.09e-01
U.U3      9.24e-02
U.U4      1.11e-01
```

```
Q.Q(1,1)  1.89e-02
Q.Q(2,2)  1.03e-05
Q.Q(3,3)  0.00e+00
Q.Q(4,4)  3.04e-05
x0.x01    5.96e+00
x0.x02    6.73e+00
x0.x03    6.60e+00
x0.x04    5.71e+00

Standard errors have not been calculated.
Use MARSSparamCIs to compute CIs and bias estimates.

Convergence warnings
 Warning: the  Q.Q(2,2)  parameter value has not converged.
 Warning: the  Q.Q(4,4)  parameter value has not converged.
```

So three of the four **Q** elements are going to zero. This often happens when you do not have enough data to estimate both observation and process variance.

Perhaps we are trying to estimate too many variances. We can try using only one variance value in **Q** and one u value in **u**:

```
kem.small=MARSS(dat.short,model=list(Q="diagonal and equal",
   U="equal"))
```

```
Success! Parameters converged at 155 iterations.
Alert: conv.test.slope.tol is 0.5.
Test with smaller values (<0.1) to ensure convergence.

MARSS fit is
Estimation method: kem
Estimation converged in 155 iterations.
Log-likelihood: 11.18769
AIC: -8.375378   AICc: 0.9579553

          Estimate
R.R(diag)   0.0194
U.U         0.1030
Q.Q(diag)   0.0000
x0.x01      6.0585
x0.x02      6.7671
x0.x03      6.5293
x0.x04      5.7435

Standard errors have not been calculated.
Use MARSSparamCIs to compute CIs and bias estimates.
```

No, there are simply not enough data to estimate both process and observation variances.

6.7 Bootstrap parameter estimates

You can easily produce bootstrap parameter estimates from a fitted model using `MARSSboot()`:

```
boot.params = MARSSboot(kemfit,
     nboot=20, output="parameters", sim="parametric")$boot.params
```

```
          |2%      |20%      |40%      |60%      |80%      |100%
Progress: ||||||||||||||||||||||||||||||||||||||||||||||||||||||||
```

Use `silent=TRUE` to stop the progress bar from printing. The function will also produce parameter sets generated using a Hessian matrix (`sim="hessian"`) or a non-parametric bootstrap (`sim="innovations"`).

6.8 Random initial conditions

You can use random initial conditions by passing in `MCInit=TRUE`:

```
Z.model = factor(c(1,1,2,2,2))
U.model = "equal"
Q.model =  "diagonal and unequal"
R.model = "diagonal and equal"
model.list=list(Z=Z.model, R=R.model, U=U.model, Q=Q.model)
#Set the numInits very low so the example runs quickly
cntl.list=list(MCInit=TRUE,numInits=10)
kem.mcinit = MARSS(dat, model=model.list, control=cntl.list)
```

```
> Starting Monte Carlo Initializations
          |2%      |20%      |40%      |60%      |80%      |100%
Progress: ||||||||||||||||||||||||||||||||||||||||||||||||||||||||
Success! Parameters converged at 16 iterations.
Alert: conv.test.slope.tol is 0.5.
Test with smaller values (<0.1) to ensure convergence.

MARSS fit is
Estimation method: kem
Monte Carlo initialization with random starts.
Estimation converged in 16 iterations.
Log-likelihood: 11.98254
AIC: -5.965073   AICc: -3.014253
```

```
          Estimate
A.2        0.79888
A.4       -0.77733
A.5       -0.84387
R.R(diag)  0.02881
U.U        0.04335
Q.Q(1,1)   0.01139
Q.Q(2,2)   0.00516
x0.x01     6.04849
x0.x02     6.87387

Standard errors have not been calculated.
Use MARSSparamCIs to compute CIs and bias estimates.
```

6.9 Data simulation

6.9.1 Simulated data from a fitted MARSS model

You can easily simulate data from a fitted model using `MARSSsimulate()`.

```
sim.data=MARSSsimulate(kemfit, nsim=2, tSteps=100)$sim.data
```

Then you might want to estimate parameters from that simulated data. Above we created two simulated datasets (`nsim=2`). We will fit to the first one. Here the default settings for `MARSS()` are used.

```
kem.sim.1 = MARSS(sim.data[,,1])
```

Then we might like to see the likelihood of the second set of simulated data under the model fit to the first set of data. We do that with the Kalman filter function. This function takes a MLE object (as output by say the MARSS function), and we have to replace the data in kem.sim.1 with the second set of simulated data.

```
kem.sim.2 = kem.sim.1
kem.sim.2$model$data = sim.data[,,2]
MARSSkf( kem.sim.2 )$logLik
```

```
[1] -23.23208
```

6.10 Bootstrap AIC

The function `MARSSaic()` computes a bootstrap AIC for model selection purposes. Use `output="AICbp"` to produce a parameter bootstrap. Use `output="AICbb"` to produce a non-parameter bootstrap AIC.

```
kemfit.with.AICb = MARSSaic(kemfit, output = "AICbp",
   Options = list(nboot = 10, silent=TRUE))
#nboot should be more like 1000, but set low here for example sake

print(kemfit.with.AICb)
```

```
MARSS fit is
Estimation method: kem
Estimation converged in 18 iterations.
Log-likelihood: 7.941363
AIC: 0.1172745   AICc: 2.439855   AICbp(param): 183.0742

          Estimate
A.2        0.79556
A.3        0.27502
A.5       -0.06913
R.R(diag)  0.03399
U.U        0.04315
Q.Q(diag)  0.00793
x0.x01     6.17149
x0.x02     6.20544

Standard errors have not been calculated.
Use MARSSparamCIs to compute CIs and bias estimates.
```

We used only 10 bootstraps so the AICb estimate will be terrible, but this shows you how to comput AICb with the MARSS package.

7

Incorporating covariates into MARSS models

7.1 Background

A MARSS model with covariate effects in both the process and observation components is often written as:

$$\begin{aligned} \mathbf{x}_t &= \mathbf{B}\mathbf{x}_{t-1} + \mathbf{U}\mathbf{u}_t + \mathbf{w}_t, \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}) \\ \mathbf{y}_t &= \mathbf{Z}\mathbf{x}_t + \mathbf{A}\mathbf{a}_t + \mathbf{v}_t, \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}) \end{aligned} \tag{7.1}$$

where $\mathbf{u}_t$ is the $p \times 1$ vector of covariates (e.g., temperature, rainfall) which affects the states and $\mathbf{a}_t$ is a vector of covariates (potentially the same at $\mathbf{u}_t$) which affect the observations[1]. Also a regression model with autoregressive errors (Harvey and Phillips, 1979) is of this form slso. $\mathbf{U}$ is an $m \times p$ matrix of coefficients relating the effects of $\mathbf{u}_t$ to the $m \times 1$ state vector $\mathbf{x}_t$, and $\mathbf{A}$ is an $n \times q$ matrix of coefficients relating the effects of $\mathbf{a}_t$ to the $n \times 1$ observation vector $\mathbf{y}_t$. An example is Eqns 6.3, 6.4 in Shumway and Stoffer (2006), where $\mathbf{f}_t \equiv \mathbf{u}_t$ in their equation and $\mathbf{u}$ and $\mathbf{a}$ do not appear.

In MARSS using `form=''marxss''` (the default), one can fit this model by simply passing in `model$u` and/or `model$a` in the MARSS() call as a $m \times T$ or $n \times T$ matrix, respectively. As usual, the $\mathbf{U}$, $\mathbf{u}$, $\mathbf{A}$, and $\mathbf{a}$ are passed in via the model argument using a one-to-one relationship between the specification in math matrix form and the form in *R* .

7.2 Covariates with missing values or observation error

The specific formulation of Equation 16.3 creates restrictions on the assumptions regarding the covariate data. You have to assume that your covariate data has no error, which is probably not true. You cannot have missing values in your covariate data, again unlikely. You cannot combine instrument time

[1] One must be careful here that the model is identifiable.

series; for example, if you have two temperature recorders with different error rates and biases. Also, what if you have one noisy temperature recorder in the first part of your time series and then you switch to a much better recorder in the second half of your time series? All these problems require pre-analysis massaging of the covariate data, leaving out noisy and gappy covariate data, and making what can feel like arbitrary choices about which covariate time series to include.

To circumvent these potential problems and allow more flexibility in how we incorporate covariate data, one can instead treat the covariates as components of an auto-regressive process by including them in both the process and observation models. Beginning with the process equation, we can write

$$\begin{bmatrix}\mathbf{x}^{(v)}\\ \mathbf{x}^{(c)}\end{bmatrix}_t = \begin{bmatrix}\mathbf{B}^{(v)} & \mathbf{C}\\ 0 & \mathbf{B}^{(c)}\end{bmatrix}\begin{bmatrix}\mathbf{x}^{(v)}\\ \mathbf{x}^{(c)}\end{bmatrix}_{t-1} + \begin{bmatrix}\mathbf{u}^{(v)}\\ \mathbf{u}^{(c)}\end{bmatrix} + \mathbf{w}_t,\ \mathbf{w}_t \sim \mathrm{MVN}\left(0, \begin{bmatrix}\mathbf{Q}^{(v)} & 0\\ 0 & \mathbf{Q}^{(c)}\end{bmatrix}\right) \tag{7.2}$$

The elements with superscript (v) are for the k variate states and those with superscript (c) are for the q covariate states. The dimension of $\mathbf{x}^{(c)}$ is $q \times 1$ and q is not necessarily equal to p, the number of covariate observation time series in your dataset. Imagine, for example, that you have two temperature sensors and you are combining these data. Then you have two covariate observation time series ($p = 2$) but only one underlying covariate state time series ($q = 1$). The matrix $\mathbf{C}$ is dimension $k \times q$, and $\mathbf{B}^{(c)}$ and $\mathbf{Q}^{(c)}$ are dimension $q \times q$. The dimension[2] of $\mathbf{x}^{(v)}$ is $k \times 1$, and $\mathbf{B}^{(v)}$ and $\mathbf{Q}^{(v)}$ are dimension $k \times k$.

Next, we can write the observation equation in an analogous manner, such that

$$\begin{bmatrix}\mathbf{y}^{(v)}\\ \mathbf{y}^{(c)}\end{bmatrix}_t = \begin{bmatrix}\mathbf{Z}^{(v)} & \mathbf{D}\\ 0 & \mathbf{Z}^{(c)}\end{bmatrix}\begin{bmatrix}\mathbf{x}^{(v)}\\ \mathbf{x}^{(c)}\end{bmatrix}_t + \begin{bmatrix}\mathbf{a}^{(v)}\\ \mathbf{a}^{(c)}\end{bmatrix} + \mathbf{v}_t,\ \mathbf{v}_t \sim \mathrm{MVN}\left(0, \begin{bmatrix}\mathbf{R}^{(v)} & 0\\ 0 & \mathbf{R}^{(c)}\end{bmatrix}\right) \tag{7.3}$$

The dimension of $\mathbf{y}^{(c)}$ is $p \times 1$, where p is the number of covariate observation time series in your dataset. The dimension of $\mathbf{y}^{(v)}$ is $l \times 1$, where l is the number of variate observation time series in your dataset. The total dimension of $\mathbf{y}$ is $l + p$. The matrix $\mathbf{D}$ is dimension $l \times q$, $\mathbf{Z}^{(c)}$ is dimension $p \times q$, and $\mathbf{R}^{(c)}$ are dimension $p \times p$. The dimension of $\mathbf{Z}^{(v)}$ is dimension $l \times k$, and $\mathbf{R}^{(v)}$ are dimension $l \times l$.

The $\mathbf{D}$ matrix would presumably have a number of all zero rows in it, as would the $\mathbf{C}$ matrix. The covariates that affect the states would often be different than the covariates that affect the observations. For example, mean annual temperature would affect population growth rates for many species while having little or no affect on observability, and turbidity might strongly affect observability in many types of aquatic, say, surveys but have little affect on population growth rate.

[2] The dimension of $\mathbf{x}$ is always denoted m. If your process model includes only variates, then $k = m$, but now your process model includes k variates and q covariate states so $m = k + q$.

Our MARSS model with covariates now looks on the surface like a regular MARSS model:

$$\begin{aligned} \mathbf{x}_t &= \mathbf{B}\mathbf{x}_{t-1} + \mathbf{U} + \mathbf{w}_t, \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}) \\ \mathbf{y}_t &= \mathbf{Z}\mathbf{x}_t + \mathbf{A} + \mathbf{v}_t, \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}) \end{aligned} \tag{7.4}$$

with the $\mathbf{x}_t$, $\mathbf{y}_t$ and parameter matrices redefined as in Equations 7.2 and 7.3:

$$\begin{aligned} \mathbf{x} &= \begin{bmatrix} \mathbf{x}^{(v)} \\ \mathbf{x}^{(c)} \end{bmatrix} \quad \mathbf{B} = \begin{bmatrix} \mathbf{B}^{(v)} & \mathbf{C} \\ 0 & \mathbf{B}^{(c)} \end{bmatrix} \quad \mathbf{U} = \begin{bmatrix} \mathbf{U}^{(v)} \\ \mathbf{U}^{(c)} \end{bmatrix} \quad \mathbf{Q} = \begin{bmatrix} \mathbf{Q}^{(v)} & 0 \\ 0 & \mathbf{Q}^{(c)} \end{bmatrix} \\ \mathbf{y} &= \begin{bmatrix} \mathbf{y}^{(v)} \\ \mathbf{y}^{(c)} \end{bmatrix} \quad \mathbf{Z} = \begin{bmatrix} \mathbf{Z}^{(v)} & \mathbf{D} \\ 0 & \mathbf{Z}^{(c)} \end{bmatrix} \quad \mathbf{A} = \begin{bmatrix} \mathbf{A}^{(v)} \\ \mathbf{A}^{(c)} \end{bmatrix} \quad \mathbf{R} = \begin{bmatrix} \mathbf{R}^{(v)} & 0 \\ 0 & \mathbf{R}^{(c)} \end{bmatrix} \end{aligned} \tag{7.5}$$

Note $\mathbf{Q}$ and $\mathbf{R}$ are written as diagonal matrices, but you could allow covariances if that made sense. $\mathbf{U}$ and $\mathbf{A}$ are column vectors here. We can fit the model (Equation 7.4) as usual using the `MARSS()` function. Note that the likelihood returned from MARSS will include the likelihood of the covariates under their assumed or estimated state model.

The log-likelihood that is returned by MARSS will include the log-likelihood of the covariates under the covariate state model. If you want only the the log-likelihood of the non-covariate data, you will need to substract off the log-likelihood of the covariate model:

$$\begin{aligned} \mathbf{x}_t^{(c)} &= \mathbf{B}^{(c)}\mathbf{x}_{t-1}^{(c)} + \mathbf{U}^{(c)} + \mathbf{w}_t, \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}^{(c)}) \\ \mathbf{y}_t^{(c)} &= \mathbf{Z}^{(c)}\mathbf{x}_t^{(c)} + \mathbf{A}^{(c)} + \mathbf{v}_t, \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}^{(c)}) \end{aligned} \tag{7.6}$$

So if your augmented model (Equation 7.4 with terms defined as in Equation 7.5), and easy way to get the log-likelihood for the covariate data only is to pass in missing values for the non-covariate data.

```
y.aug=rbind(data,covariates)
fit.aug=MARSS(y.aug, model=model.aug)
#fit.aug is now the MLE object that can be passed to MARSSkf
#you need to make a version with the non-covariate data filled with NAs
fit.cov=fit.aug; fit.cov$model$data[1:dim(data)[1],]=NA
extra.LL=MARSSkf(fit.cov)$logLik
```

Also when you fit the augmented model, the estimates of $\mathbf{C}$ and $\mathbf{B}^{(c)}$ are affected by the non-covariate data since the model for both the non-covariate and covariate data are estimated simultaneously and are not independent (since the covariate states affect the non-covariates states). If you want the covariate model to be unaffected by the non-covariate data, you can fit the covariate model separately and use the estimates for $\mathbf{B}^{(c)}$ and $\mathbf{Q}^{(c)}$ as fixed values in your augmented model.

8

Incorporating longer lags and autoregressive errors into MARSS models

8.1 Background

Many types of time-series models, for example AR(p), ARMA(p,q), and ARMAX(p,q), can be written in state-space form specifically MARSS(1) (see section 11.3.2 in (Tsay, 2010)). Writing these models in state-space form allows one to take advantage of the fitting algorithms for MARSS(1) models[1]. When written in state-space form, it does not necessarily mean that the process is observed with error, i.e. the ARMA(p,q) is not overlaid with an observation model. Rather the original model, with no observation process, is rewritten in the state-space form to facilitate statistical analysis.

8.2 MAR(p) models

The MARSS model (equation 1.1) is written such that $\mathbf{x}_t$ is only affected by $\mathbf{x}_{t-1}$. This is called a lag-1 model. A model in which lags up to time p are included allows that $\mathbf{x}_t$ may be affected by $\mathbf{x}_{t-p}$. These are called lag-p models. A MARSS model with p lags in the process model can be equivalently rewritten as a MARSS(1) model by redefining the $\mathbf{x}$ state vector.

Let's start with a lag-2 model:

$$\mathbf{x}'_t = \mathbf{B}_1\mathbf{x}'_{t-1} + \mathbf{B}_2\mathbf{x}'_{t-2} + \mathbf{u} + \mathbf{w}_t, \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}) \tag{8.1}$$

We rewrite this as lag-1 by defining $\mathbf{x}_t = \begin{bmatrix} \mathbf{x}'_t \\ \mathbf{x}'_{t-1} \end{bmatrix}$:

[1] There are many packages for fitting AR-p and ARMA(p,q) models. If you are only interested in univariate models then I suggest looking into packages that specialize in fitting ARMA models to univariate data. The forecast package in *R* is a good place to start but others can be found on the *R* time-series review. This chapter is focused on fitting such models by converting to a MARSS.

$$\begin{bmatrix} \mathbf{x}_t' \\ \mathbf{x}_{t-1}' \end{bmatrix} = \begin{bmatrix} \mathbf{B}_1 & \mathbf{B}_2 \\ \mathbf{I}_m & 0 \end{bmatrix} \begin{bmatrix} \mathbf{x}_{t-1}' \\ \mathbf{x}_{t-2}' \end{bmatrix}_{t-1} + \begin{bmatrix} \mathbf{u} \\ 0 \end{bmatrix} + \mathbf{w}_t,\ \mathbf{w}_t \sim \mathrm{MVN}\left(0, \begin{bmatrix} \mathbf{Q} & 0 \\ 0 & 0 \end{bmatrix}\right)$$
$$\begin{bmatrix} \mathbf{x}_0' \\ \mathbf{x}_{-1}' \end{bmatrix} \sim \mathrm{MVN}(\pi, \Lambda) \tag{8.2}$$

Here is an example of fitting a AR lag-2 model to AR lag-2 data. First, let's generate some simulated AR lag-2 data:

```
temp=arima.sim(n=50,list(ar=c(-1.5,-.75)),sd=1)
sim.ar2=matrix(temp,nrow=1)
```

Next, we write the AR lag-2 model (Equation 8.2) as a MARSS model in R :

```
Z=matrix(c(1,0),1,2)
B=matrix(list("b.1",1,"b.2",0),2,2)
U=matrix(0,2,1)
Q=matrix(list("q.1",0,0,0),2,2)
A=matrix(0,1,1)
R=matrix(0,1,1)
pi=matrix(list(sim.ar2[1],"x0"),2,1)
V=matrix(0,2,2)
model.list=list(Z=Z,B=B,U=U,Q=Q,A=A,R=R,x0=pi,V0=V,tinitx=1)
```

Notice that we do not need to estimate π for x_1 since we are setting $\pi = \begin{bmatrix} x_1 \\ x_0 \end{bmatrix}$ by using `kf.x0="x10"` and $\mathbf{R} = 0$. Thus x_1, and by extension the first element of π, is known from y_1.

Then we can fit the AR-2 model to this simulated data. We pass in good initial conditions so it does not take quite so long to run.

```
init.list=list(x0=matrix(sim.ar2[1],1,1),Q=matrix(1,1,1),B=matrix(1,2,1))
ar2=MARSS(sim.ar2,model=model.list,inits=init.list)
```

```
Success! algorithm run for 15 iterations and parameters converged.
Alert: conv.test.slope.tol is 0.5.
Test with smaller values (<0.1) to ensure convergence.

MARSS fit is
Estimation method: kem
Algorithm ran 15 (=minit) iterations and convergence was reached.
Log-likelihood: -71.68132
AIC: 151.3626   AICc: 152.2515

      Estimate
B.b.1   -1.465
B.b.2   -0.755
Q.q.1    1.052
x0.x0   -2.270
```

```
Standard errors have not been calculated.
Use MARSSparamCIs to compute CIs and bias estimates.
```

A lag-p model would be:

$$\mathbf{x}_t' = \mathbf{B}_1\mathbf{x}_{t-1}' + \mathbf{B}_2\mathbf{x}_{t-2}' + \cdots + \mathbf{B}_p\mathbf{x}_{t-p}' + \mathbf{u}' + \mathbf{w}_t', \text{ where } \mathbf{w}_t' \sim \text{MVN}(0, \mathbf{Q}')$$

and the lag-1 version is

$$\mathbf{x}_t = \mathbf{B}\mathbf{x}_{t-1} + \mathbf{u} + \mathbf{w}_t, \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q})$$

where

$$\mathbf{x}_t = \begin{bmatrix} \mathbf{x}_t' \\ \mathbf{x}_{t-1}' \\ \vdots \\ \mathbf{x}_{t-p}' \end{bmatrix}, \mathbf{B} = \begin{bmatrix} \mathbf{B}_1 & \mathbf{B}_2 & \dots & \mathbf{B}_p \\ \mathbf{I}_m & 0 & \dots & 0 \\ 0 & \mathbf{I}_m & \dots & 0 \\ 0 & 0 & \ddots & \vdots \\ 0 & 0 & \dots & 0 \end{bmatrix}, \mathbf{u} = \begin{bmatrix} \mathbf{u}' \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \mathbf{Q} = \begin{bmatrix} \mathbf{Q}' & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ 0 & 0 & \ddots & \vdots \\ 0 & 0 & \dots & 0 \end{bmatrix} \tag{8.3}$$

This would be fairly straight-forward except one must define π and Λ. The joint distribution of $\mathbf{x}_{1:p}'$ is a function of our model, and the $\mathbf{x}_{1:p}'$ are definitely not independent of each other. Since we are trying to estimate the model, we do not know the distribution of $\mathbf{x}_{1:p}'$ even if we assume stationarity. One possibility is to treat $\mathbf{x}_0 \equiv \mathbf{x}_{1:p}'$ as an estimated parameter. This means estimating $m \times p$ initial state parameters. This might not be very robust. You might try fixing π, using knowledge of its expected value, and estimating Λ (as suggested in Harvey and Phillips (1979)). Or try researching in the finance literature on state-space VAR(p) model (the name for a MARSS(p) model in that literature). However, be aware that finance data is often so long that the effects of a mis-specified prior can be overcome by the information in the data. Ecological data are shorter and more susceptible to problems from a mis-specified initial state distribution.

8.3 MA(q) models

In a moving-average model (MA), the process error term is a sum of i.i.d. errors. Let's start with a MA(2) model:

$$\mathbf{x}_t' = \mathbf{w}_t' + {}_1\mathbf{w}_{t-1}' + {}_2\mathbf{w}_{t-2}', \text{ where } \mathbf{w}_t' \sim \text{MVN}(0, \mathbf{Q}') \tag{8.4}$$

We rewrite this as MARSS(1) by defining $\mathbf{x}_t = \begin{bmatrix} \mathbf{x}_{t-2}' \\ \mathbf{x}_{t-1}' \\ \mathbf{x}_t' \end{bmatrix}$:

$$\begin{bmatrix} \mathbf{x}'_{t-2} \\ \mathbf{x}'_{t-1} \\ \mathbf{x}'_t \end{bmatrix} = \begin{bmatrix} 0 & \mathbf{I}_m & 0 \\ 0 & 0 & \mathbf{I}_m \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \mathbf{x}'_{t-3} \\ \mathbf{x}'_{t-2} \\ \mathbf{x}'_{t-1} \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ \mathbf{w}'_t \end{bmatrix}, \ \mathbf{w}_t \sim \text{MVN}\left(0, \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \mathbf{Q}' \end{bmatrix}\right) \tag{8.5}$$

$$\mathbf{y}_t = \begin{bmatrix} 2 & 1 & 1 \end{bmatrix} \mathbf{x}_t$$

8.4 Autoregressive process errors

$$\mathbf{x}'_t = \mathbf{B}\mathbf{x}'_{t-1} + \mathbf{u}' + \eta_t$$

where η_t is a AR-1 (or p) process.

We can model this process using the MARSS form by moving the $m \times 1$ AR process error term into the state vector.

$$\mathbf{x}_t = \mathbf{B}\mathbf{x}_{t-1} + \mathbf{u} + \mathbf{w}_t, \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q})$$

where the terms are redefined as follows:

$$\begin{bmatrix} \mathbf{x}' \\ \eta \end{bmatrix}_t = \begin{bmatrix} \mathbf{B}_x & \mathbf{I}_m \\ 0 & \mathbf{B}_\eta \end{bmatrix} \begin{bmatrix} \mathbf{x}' \\ \eta \end{bmatrix}_{t-1} + \begin{bmatrix} \mathbf{u}' \\ 0 \end{bmatrix} + \mathbf{w}_t, \ \mathbf{w}_t \sim \text{MVN}\left(0, \begin{bmatrix} 0 & 0 \\ 0 & \mathbf{Q}_\eta \end{bmatrix}\right)$$

8.5 Univariate ARMA(p,q)

There are a few different ways to write a univariate ARMA(p,q), $p \geq q$, model in state-space form (see section 11.3.2 in (Tsay, 2010)). They all (at least in (Tsay, 2010)) put the ARMA(p,q) model in the following state-space form:

$$\begin{aligned} \mathbf{x}_{t+1} &= \mathbf{B}\mathbf{x}_t + \Gamma a_t \\ \mathbf{y}_t &= \mathbf{Z}\mathbf{x}_t \end{aligned}$$

or

$$\begin{aligned} \mathbf{x}_{t+1} &= \mathbf{B}\mathbf{x}_t + \Gamma a_t \\ \mathbf{y}_t &= \mathbf{Z}\mathbf{x}_t + a_t \end{aligned}$$

Unfortunately, the EM algorithm in MARSS 3.0 is not able to estimate the parameters. This will have to wait for a rewrite of the EM algorithm to allow the form $\Gamma\eta_t$ for the process errors.

9

Case study instructions

The case studies walk you through some analyses of multivariate population count data using MARSS models and the `MARSS()` function. This will take you through both the conceptual steps (with pencil and paper) and a *R* step which translates the conceptual model into code.

Set-up

- If you haven't already, install the MARSS package. See directions on the CRAN webpage (http://cran.r-project.org/) for instructions on installing packages. You will need write permissions for your *R* program directories to install packages. See the help pages on CRAN for workarounds if you don't have write permission.
- Type in `library(MARSS)` at the *R* command line to load the package after you install it.
- To open up a copy of the case study script with the code you need to do the exercises, type `RShowDoc("Case_study_X.R",package="MARSS")` (with X replaced by the case study number).

Tips

- `summary(foo$model)`, where `foo` is a fitted model object, will print detailed information on the structure of the MARSS model that was fit in the call `foo = MARSS(logdata)`. This allows you to double check the model you fit. `print(foo)` will print a 'English' version of the model structure along with the parameter estimates.
- When you run `MARSS()`, it will output the number of iterations used. If you reached the maximum, re-run with `control=list(maxit=...)` set higher than the default.

- If you mis-specify the model, `MARSS()` will post an error that should give you an idea of the problem (make sure `silent=FALSE` to see full error reports). Remember, the number of rows in your data is n, time is across the columns, and the length of the vector or factors passed in for `model$Z` must be m, the number of x hidden state trajectories in your model.
- The default missing value indicator is NA. You can change that by passing in `miss.value=...`.
- Running `MARSS(data)`, with no arguments except your data, will fit a MARSS model with $m = n$, a diagonal $\mathbf{Q}$ matrix with m variances, and i.i.d. observation errors.

10

Case Study 1: Count-based Population Viability Analysis using corrupted data

10.1 The Problem

Estimates of extinction and quasi-extinction risk are an important risk metric used in the management and conservation of endangered and threatened species. By necessity, these estimates are based on data that contain both variability due to real year-to-year changes in the population growth rate (process errors) and variability in the relationship between the true population size and the actual count (observation errors). Classic approaches to extinction risk assume the data have only process error, i.e. no observation error. In reality, observation error is ubiquitous both because of the sampling variability and also because of year-to-year (and day-to-day) variability in sightability.

In this case study, we use the Kalman filter to fit a univariate (meaning one time series) state-space model to count data for a population. We will compute the extinction risk metrics given in Dennis et al. (1991), however instead of using a process-error only model (as is done in the original paper), we use a model with both process and observation error. The risk metrics and their interpretations are the same as in Dennis et al. (1991). The only real difference is how we compute $\boldsymbol{\sigma}^2$, the process error variance. However this difference has a large effect on our risk estimates, as you will see.

In this case study, we use a density-independent model, a stochastic exponential growth model in log space. This equivalent to a MARSS model with $\mathbf{B} = 1$. Density-independence is often a reasonable assumption when doing a population viability analysis because we do such calculations for at-risk populations that are either declining or that are well below historical levels (and presumably carrying capacity). In an actual population viability analysis, it is necessary to justify this assumption and if there is reason to doubt the assumption, one tests for density-dependence (Taper and Dennis, 1994) and does sensitivity analyses using state-space models with density-dependence (Dennis et al., 2006).

The univariate model is written:

$$x_t = x_{t-1} + u + w_t \qquad \text{where } w_t \sim \mathrm{N}(0, \sigma^2) \tag{10.1}$$

$$y_t = x_t + v_t \qquad \text{where } v_t \sim \mathrm{N}(0, \eta^2) \tag{10.2}$$

where y_t is the logarithm of the observed population size at time t, x_t is the unobserved state at time t, u is the growth rate, and σ^2 and η^2 are the process and observation error variances, respectively. In the *R* code to follow, σ^2 is denoted `Q` and η^2 is denoted `R` because the functions we are using are also for multivariate state-space models and those models use **Q** and **R** for the respective variance-covariance matrices.

10.2 Simulated data with process and observation error

We will start by using simulated data to see the difference between data and estimates from a model with process error only versus a model that also includes observation error. For our simulated data, we used a decline of 5% per year, process variability of 0.02 (typical for small to medium-sized vertebrates), and a observation variability of 0.05 (which is a bit on the high end). We'll randomly set 10% of the values as missing. Here is the code:

First, set things up:

```
sim.u = -0.05          # growth rate
sim.Q = 0.02           # process error variance
sim.R = 0.05           # non-process error variance
nYr= 50                # number of years of data to generate
fracmissing = 0.1      # fraction of years that are missing
init = 7               # log of initial pop abundance
years = seq(1:nYr)     # sequence 1 to nYr
x = rep(NA,nYr)        # replicate NA nYr times
y = rep(NA,nYr)
```

Then generate the population sizes using Equation 10.1:

```
x[1]=init
for(t in 2:nYr){
   x[t] = x[t-1]+ sim.u + rnorm(1,mean=0,sd=sqrt(sim.Q)) }
```

Lastly, add observation error using Equation 10.2 and then add missing values:

```
for(t in 1:nYr){
  y[t]= x[t] + rnorm(1,mean=0,sd=sqrt(sim.R))
}
missYears = sample(years[2:(nYr-1)],floor(fracmissing*nYr),
   replace = FALSE)
y[missYears]=NA
```

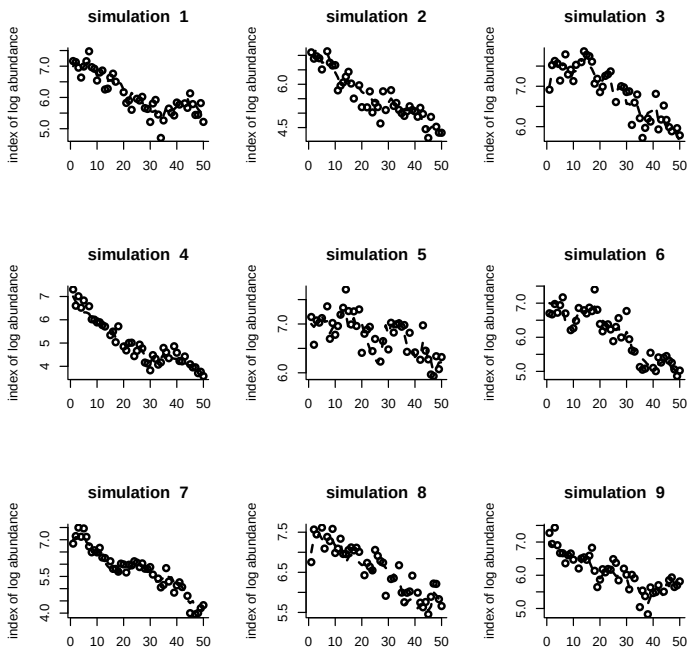

Fig. 10.1. Plot of nine simulated population time series with process and observation error. Circles are observation and the dashed line is the true population size.

Stochastic population trajectories show much variation, so it is best to look at a few simulated data sets at once. In Figure 10.1, nine simulations from the identical parameters are shown.

Example 10.1 (The effect of parameter values on parameter estimates)

A good way to get a feel for reasonable σ^2 *values is to generate simulated data and look at the time series. As a biologist, you probably have a pretty good idea of what kind of year-to-year population changes are reasonable for your species. For example for many large mammalian species, the maximum population yearly increase would be around 50% (the population could go from 1000 to 1500 in one year), but some of fish species could easily double or even triple in a really good year. Your observed data may bounce around a lot for many different reasons having to do with sightability, sampling error, age-structure, etc., but the underlying population trajectory is constrained by the*

kinds of year-to-year changes in population size that are biologically possible for your species. σ^2 *describes those true population changes.*

Run the exercise code several times using different parameter values to get a feel for how different the time series can look based on identical parameter values. You can cut and paste from the pdf into the R command line. Typical vertebrate σ^2 *values are 0.002 to 0.02, and typical* η^2 *values are 0.005 to 0.1. A* u *of -0.01 translates to an average 1% per year decline and a* u *of -0.1 translates to an average 10% per year decline (approximately).*

Example 10.1 code

Type `RShowDoc("Case_study_1.R",package="MARSS")` *to open a file with all the example code.*

```
par(mfrow=c(3,3))
sim.u = -0.05
sim.Q = 0.02
sim.R = 0.05
nYr= 50
fracmiss = 0.1
init = 7
years = seq(1:nYr)
for(i in 1:9){
  x = rep(NA,nYr) # vector for ts w/o measurement error
  y = rep(NA,nYr) # vector for ts w/ measurement error
  x[1]=init
  for(t in 2:nYr){
    x[t] = x[t-1]+ sim.u + rnorm(1, mean=0, sd=sqrt(sim.Q)) }
  for(t in 1:nYr){
    y[t]= x[t] + rnorm(1,mean=0,sd=sqrt(sim.R)) }
  missYears =
    sample(years[2:(nYr-1)],floor(fracmiss*nYr),replace = FALSE)
  y[missYears]=NA
  plot(years, y,
    xlab="",ylab="log abundance",lwd=2,bty="l")
  lines(years,x,type="l",lwd=2,lty=2)
  title(paste("simulation ",i) )
}
legend("topright", c("Observed","True"),
  lty = c(-1, 2), pch = c(1, -1))
```

10.3 Maximum-likelihood parameter estimation

10.3.1 Model with process and observation error

Using the simulated data, we estimate the parameters, u, σ^2, and η^2, and the hidden population sizes. These are the estimates using a model with process and observation variability. The function call is `kem = MARSS(data)`, where `data` is a vector of logged (base e) counts with missing values denoted by NA. After this call, the maximum-likelihood parameter estimates are `kem$par$U`, `kem$par$Q` and `kem$par$R`. There are numerous other outputs from the `MARSS()` function. To get a list of the outputs type in `names(kem)`. Note that `kem` is just a name; the output could have been called `foo`. Here's code to fit to the simulated time series:

```
kem = MARSS(y)
```

Let's look at the parameter estimates for the nine simulated time series in Figure 10.1 to get a feel for the variation. The `MARSS()` function was used on each time series to produce parameter estimate for each simulation. The estimates are followed by the mean (over the nine simulations) and the true values:

```
               kem.U       kem.Q      kem.R
sim 1    -0.03483592 0.021970029 0.04881205
sim 2    -0.05447465 0.005501265 0.08235375
sim 3    -0.02880985 0.022911155 0.05726041
sim 4    -0.06997490 0.018438108 0.04722468
sim 5    -0.01665368 0.010979111 0.05894114
sim 6    -0.03601471 0.036771464 0.03511144
sim 7    -0.05717600 0.028139051 0.02696387
sim 8    -0.03697083 0.000000000 0.07277042
sim 9    -0.02938939 0.021319142 0.04594110
mean sim -0.04047777 0.018447703 0.05281987
true     -0.05000000 0.020000000 0.05000000
```

As expected, the estimated parameters do not exactly match the true parameters, but the average should be fairly close (although nine simulations is a small sample size). Also note that although we do not get u quite right, our estimates are usually negative. Thus our estimates usually indicate declining dynamics. Some of the `kem.Q` estimates may be 0. This means that the maximum-likelihood estimate that the data are generated by is a process with no environment variation and only observation error.

The MARSS model fit also gives an estimate of the true population size with observation error removed. This is in `kem$states`. Figure 10.2 shows the estimated true states of the population over time as a solid line. Note that the solid line is considerably closer to the actual true states (dashed line) than the observations. On the other hand with certain datasets, the estimates can be quite wrong as well!

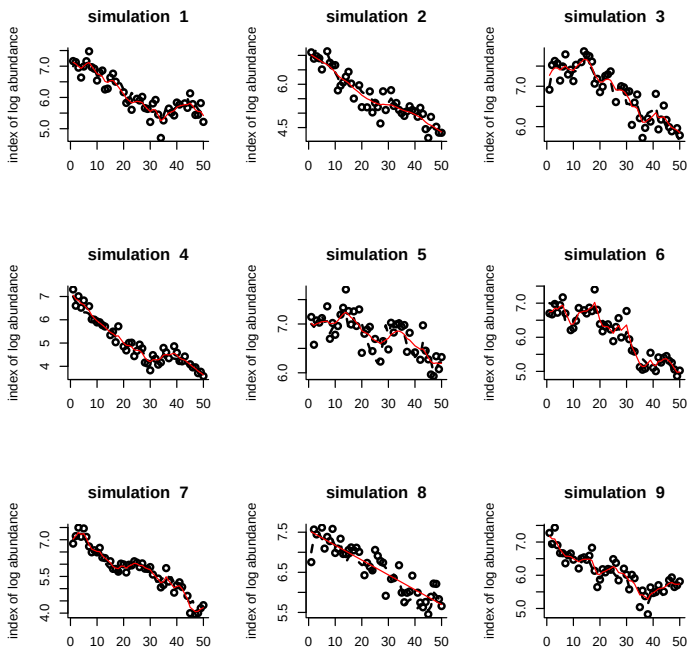

Fig. 10.2. The circles are the observed population sizes with error. The dashed lines are the true population sizes. The solid thin lines are the estimates of the true population size from the MARSS model. When the process error variance is 0, these lines are straight.

10.3.2 Model with no observation error

We used the MARSS model to estimate the mean population rate u and process variability σ^2 under the assumption that the count data have observation error. However, the classic approach to this problem, referred to as the "Dennis model" (Dennis et al., 1991), uses a model that assumes the data have no observation error (a MAR model); all the variability in the data is assumed to result from process error. This approach works well if the observation error in the data is low, but not so well if the observation error is high. We will next fit the data using the classic approach so that we can compare and contrast parameter estimates from the different methods.

Using the estimation method in Dennis et al. (1991), our data need to be re-specified as the observed population changes (`delta.pop`) between censuses along with the time between censuses (`tau`). We re-specify the data as follows:

```
den.years = years[!is.na(y)] # the non missing years
den.y = y[!is.na(y)] # the non missing counts
```

```
den.n.y = length(den.years)
delta.pop = rep(NA, den.n.y-1 ) # population transitions
tau = rep(NA, den.n.y-1 ) # step sizes
for (i in 2:den.n.y ){
  delta.pop[i-1] = den.y[i] - den.y[i-1]
  tau[i-1] =  den.years[i] - den.years[i-1]
} # end i loop
```

Next, we regress the changes in population size between censuses (`delta.pop`) on the time between censuses (`tau`) while setting the regression intercept to 0. The slope of the resulting regression line is an estimate of u, while the variance of the residuals around the line is an estimate of σ^2. The regression is shown in Figure 10.3. Here is the code to do that regression:

```
den91 <- lm(delta.pop ~ -1 + tau)
# note: the "-1" specifies no intercept
den91.u = den91$coefficients
den91.Q = var(resid(den91))
#type ?lm to learn about the linear regression function in R
#form is lm(dependent.var ~ response.var1 + response.var2 + ...)
#type summary(den91) to see other info about our regression fit
```

Here are the parameter values for the data in Figure 10.2 using the process-error only model:

```
             den91.U    den91.Q
sim 1    -0.03028947 0.11433055
sim 2    -0.02296138 0.18350968
sim 3    -0.01129879 0.13970451
sim 4    -0.08521759 0.12513762
sim 5    -0.02995212 0.13647436
sim 6    -0.02452939 0.11608571
sim 7    -0.06217300 0.07977847
sim 8    -0.02022198 0.11736175
sim 9    -0.03544077 0.12108485
mean sim -0.03578716 0.12594083
true     -0.05000000 0.02000000
```

Notice that the u estimates are similar to those from MARSS model, but the σ^2 estimate (`Q`) is much larger. That is because this approach treats all the variance as process variance, so any observation variance in the data is lumped into process variance (in fact it appears as an additional variance of twice the observation variance).

Example 10.2 (The variability in parameter estimates)

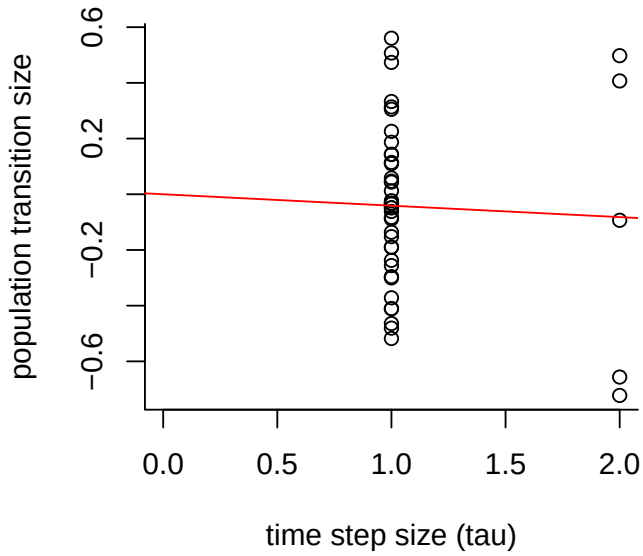

Fig. 10.3. The regression of $log(N_{t+\tau}) - log(N_t)$ against τ. The slope is the estimate of u and the variance of the residuals is the estimate of σ^2.

In this example, you will look at how variable the parameter estimates are by generating multiple simulated data sets and then estimating parameter values for each. You'll compare the MARSS estimates to the estimates using a process error only model (i.e. ignoring the observation error).

Example 10.2 code

Type `RShowDoc("Case_study_1.R",package="MARSS")` *to open a file with all the example code. You will not be able to edit this file. To edit, copy and paste into a new script file.*

```
sim.u = -0.05   # growth rate
sim.Q = 0.02    # process error variance
sim.R = 0.05    # non-process error variance
nYr= 50         # number of years of data to generate
fracmiss = 0.1  # fraction of years that are missing
init = 7        # log of initial pop abundance (~1100 individuals)
nsim = 9
years = seq(1:nYr)  # col of years
params = matrix(NA, nrow=(nsim+2), ncol=5,
  dimnames=list(c(paste("sim",1:nsim),"mean sim","true"),
c("kem.U","den91.U","kem.Q","kem.R", "den91.Q")))
x.ts = matrix(NA,nrow=nsim,ncol=nYr)  # ts w/o measurement error
y.ts = matrix(NA,nrow=nsim,ncol=nYr)  # ts w/ measurement error
for(i in 1:nsim){
  x.ts[i,1]=init
  for(t in 2:nYr){
    x.ts[i,t] = x.ts[i,t-1]+sim.u+rnorm(1,mean=0,sd=sqrt(sim.Q))}
  for(t in 1:nYr){
    y.ts[i,t] = x.ts[i,t]+rnorm(1,mean=0,sd=sqrt(sim.R))}
  missYears = sample(years[2:(nYr-1)], floor(fracmiss*nYr),
    replace = FALSE)
  y.ts[i,missYears]=NA

  #MARSS estimates
  kem = MARSS(y.ts[i,], silent=TRUE)
  params[i,c(1,3,4)] = c(kem$par$U,kem$par$Q,kem$par$R)

  #Dennis et al 1991 estimates
  den.years = years[!is.na(y.ts[i,])]  # the non missing years
  den.yts = y.ts[i,!is.na(y.ts[i,])]   # the non missing counts
  den.n.yts = length(den.years)
  delta.pop = rep(NA, den.n.yts-1 ) # transitions
  tau = rep(NA, den.n.yts-1 )       # time step lengths
  for (t in 2:den.n.yts ){
    delta.pop[t-1] = den.yts[t] - den.yts[t-1] # transitions
    tau[t-1] =  den.years[t]-den.years[t-1]    # time step length
  } # end i loop
  den91 <- lm(delta.pop ~ -1 + tau) # -1 specifies no intercept
  params[i,c(2,5)] = c(den91$coefficients, var(resid(den91)))
}
params[nsim+1,]=apply(params[1:nsim,],2,mean)
params[nsim+2,]=c(sim.u,sim.u,sim.Q,sim.R,sim.Q)
```

Here is an example of the output from the code:

```
print(params,digits=3)
```

```
           kem.U den91.U   kem.Q  kem.R den91.Q
sim 1    -0.0586 -0.0240 0.02433 0.0545   0.145
sim 2    -0.0452 -0.0615 0.00000 0.0517   0.105
sim 3    -0.0417 -0.0286 0.02134 0.0377   0.103
sim 4    -0.0762 -0.0758 0.01385 0.0726   0.173
sim 5    -0.0433 -0.0495 0.02281 0.0567   0.136
sim 6    -0.0494 -0.0512 0.01977 0.0540   0.130
sim 7    -0.0744 -0.0509 0.02904 0.0469   0.122
sim 8    -0.0589 -0.0555 0.00442 0.0635   0.158
sim 9    -0.0326 -0.0369 0.01767 0.0421   0.110
mean sim -0.0534 -0.0482 0.01703 0.0533   0.131
true     -0.0500 -0.0500 0.02000 0.0500   0.020
```

1. *Re-run the code a few times to see the performance of the estimates using a state-space model (*`kem`*) versus the model with no observation error (*`den91`*). You can copy and paste the code from the pdf file into* R *.*

2. *Alter the observation variance,* `sim.R`*, in the data generation step in order to get a feel for performance as observations are further corrupted. What happens as observation error is increased?*

3. *Decrease the number of years of data,* `nYr`*, and re-run the parameter estimation. What changes?*

If you find that the exercise code takes too long to run, reduce the number of simulations (by reducing `nsim` *in the code).*

10.4 Probability of hitting a threshold $\Pi(x_d, t_e)$

A common extinction risk metric is 'the probability that a population will hit a certain threshold x_d within a certain time frame t_e – *if the observed trends continue*'. In practice, the threshold used is not $N_e = 1$, which would be true extinction. Often a 'functional' extinction threshold will be used ($N_e >> 1$). Other times a threshold representing some fraction of current levels is used. The latter is used because we often have imprecise information about the relationship between the true population size and what we measure in the field; that is, many population counts are index counts. In these cases, one

must use 'fractional declines' as the threshold. Also, extinction estimates that use an absolute threshold (like 100 individuals) are quite sensitive to error in the estimate of true population size. Here, we are going to use fractional declines as the threshold, specifically $p_d = 0.1$ which means a 90% decline.

The probability of hitting a threshold, denoted $\Pi(x_d, t_e)$, is typically presented as a curve showing the probabilities of hitting the threshold (y-axis) over different time horizons (t_e) on the x-axis. Extinction probabilities can be computed through Monte Carlo simulations or analytically using Equation 16 in Dennis et al. (1991) (note there is a typo in Equation 16; the last + is supposed to be a −). We will use the latter method:

$$\Pi(x_d, t_e) = \pi(u) \times \Phi\left(\frac{-x_d + |u|t_e}{\sqrt{\sigma^2 t_e}}\right) + \exp(2x_d|u|/\sigma^2)\Phi\left(\frac{-x_d - |u|t_e}{\sqrt{\sigma^2 t_e}}\right) \quad (10.3)$$

where x_e is the threshold and is defined as $x_e = \log(N_0/N_e)$. N_0 is the current population estimate and N_e is the threshold. If we are using fractional declines then $x_e = \log(N_0/(p_d \times N_0)) = -\log(p_d)$. $\pi(u)$ is the probability that the threshold is eventually hit (by $t_e = \infty$). $\pi(u) = 1$ if $u <= 0$ and $\pi(u) = \exp(-2ux_d/\sigma^2)$ if $u > 0$. $\Phi()$ is the cumulative probability distribution of the standard normal (mean = 0, sd = 1).

Here is the R code for that computation:

```
pd = 0.1 #means a 90 percent decline
tyrs = 1:100
xd = -log(pd)
p.ever = ifelse(u<=0,1,exp(-2*u*xd/Q)) #Q=sigma2
for (i in 1:100){
 Pi[i] = p.ever * pnorm((-xd+abs(u)*tyrs[i])/sqrt(Q*tyrs[i]))+
   exp(2*xd*abs(u)/Q)*pnorm((-xd-abs(u)*tyrs[i])/sqrt(Q*tyrs[i]))
}
```

Figure 10.4 shows the estimated probabilities of hitting the 90% decline for the nine 30-year times series simulated with $u = -0.05$, $\sigma^2 = 0.01$ and $\eta^2 = 0.05$. The dashed line shows the estimates using the MARSS parameter estimates and the solid line shows the estimates using a process-error only model (the `den91` estimates). The circles are the true probabilities. The difference between the estimates and the true probalities is due to errors in $\hat{u}$. Those errors are due largely to process error—not observation error. As we saw earlier, by chance population trajectories with a $u < 0$ will increase, even over a 50-year period. In this case, $\hat{u}$ will be positive when in fact $u < 0$.

Looking at the figure, it is obvious that the probability estimates are highly variable. However, look at the first panel. This is the average estimate (over nine simulations). Note that on average (over nine simulations), the estimates are good. If we had averaged over 1000 simulations instead of nine, you would see that the MARSS line falls on the true line. It is an unbiased predictor. While that may seem a small consolation if estimates for individual simulations

are all over the map, it is important for correctly specifying our uncertainty about our estimates. Second, rather than focusing on how the estimates and true lines match up, see if there are any types of forecasts that seem better than others. For example, are 20-year predictions better than 50-year and are 100-year forecasts better or worse. In Exercise 3, you will remake this figure with different u. You'll discover from that forecasts are more certain for populations that are declining faster.

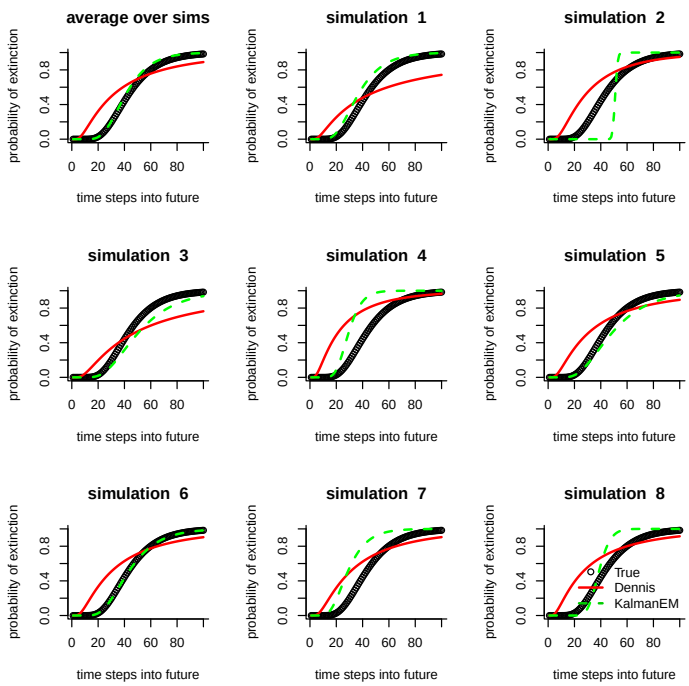

Fig. 10.4. Plot of the true and estimated probability of declining 90% in different time horizons for nine simulated population time series with observation error. The plot may look like a step-function if the σ^2 estimate is very small (<1e-4 or so).

Example 10.3 (The effect of parameter values on risk estimates)

In this example, you will recreate Figure 10.4 using different parameter values. This will give you a feel for how variability in the data and population process affect the risk estimates. You'll need to run the Example 10.2 code before running the Example 10.3 code.

Example 10.3 code

Type `RShowDoc("Case_study_1.R",package="MARSS")` *to open a file with all the example code.*

```
#Needs Exercise 2 to be run first
par(mfrow=c(3,3))
pd = 0.1; xd = -log(pd)   # decline threshold
te = 100; tyrs = 1:te   # extinction time horizon
for(j in c(10,1:8)){
  real.ex = denn.ex = kal.ex = matrix(nrow=te)

  #MARSS parameter estimates
  u=params[j,1];   Q=params[j,3]
  if(Q==0) Q=1e-4  #just so the extinction calc doesn't choke
  p.ever = ifelse(u<=0,1,exp(-2*u*xd/Q))
  for (i in 1:100){
    if(is.finite(exp(2*xd*abs(u)/Q))){
          sec.part = exp(2*xd*abs(u)/Q)*pnorm((-xd-abs(u)* tyrs[i])/sqrt(Q*tyrs[i]))
    }else sec.part=0
    kal.ex[i]=p.ever*pnorm((-xd+abs(u)*tyrs[i])/sqrt(Q*tyrs[i]))+sec.part
  } # end i loop

  #Dennis et al 1991 parameter estimates
  u=params[j,2];   Q=params[j,5]
  p.ever = ifelse(u<=0,1,exp(-2*u*xd/Q))
  for (i in 1:100){
    denn.ex[i]=p.ever*pnorm((-xd+abs(u)*tyrs[i])/sqrt(Q*tyrs[i]))+
      exp(2*xd*abs(u)/Q)*pnorm((-xd-abs(u)*tyrs[i])/sqrt(Q*tyrs[i]))
  } # end i loop

  #True parameter values
  u=sim.u;   Q=sim.Q
  p.ever = ifelse(u<=0,1,exp(-2*u*xd/Q))
  for (i in 1:100){
    real.ex[i]=p.ever*pnorm((-xd+abs(u)*tyrs[i])/sqrt(Q*tyrs[i]))+
      exp(2*xd*abs(u)/Q)*pnorm((-xd-abs(u)*tyrs[i])/sqrt(Q*tyrs[i]))
  } # end i loop

  #plot it
  plot(tyrs, real.ex, xlab="time steps into future",
    ylab="probability of extinction", ylim=c(0,1), bty="l")
  if(j<=8) title(paste("simulation ",j) )
  if(j==10) title("average over sims")
  lines(tyrs,denn.ex,type="l",col="red",lwd=2,lty=1)
  lines(tyrs,kal.ex,type="l",col="green",lwd=2,lty=2)
}
legend("bottomright",c("True","Dennis","KalmanEM"),pch=c(1,-1,-1),
  col=c(1,2,3),lty=c(-1,1,2),lwd=c(-1,2,2),bty="n")
```

1. *Change* `sim.R` *and rerun the Example 10.2 code. Then run the Example 10.3 code. When are the estimates using the process-error only model (*`den91`*) worse and in what way are they worse?*

2. *You might imagine that you should always use a model that includes observation error, since in practice observations are never perfect. However, there is a cost to estimating that extra variance parameter and the cost is a more variable* σ^2 *(*`Q`*) estimate. Play with shortening the time series and decreasing the* `sim.R` *values. Are there situations when the 'cost' of the extra parameter is greater than the 'cost' of ignoring observation error?*

3. *How does changing the extinction threshold (*`pd`*) change the extinction probability curves? (Do not remake the data, i.e. don't rerun the Example 10.2 code.)*

4. *How does changing the rate of decline (*`sim.u`*) change the estimates of risk? Rerun the Example 10.2 code using a lower* `u`*; this will create a new matrix of parameter estimates. Then run the Example 10.3 code. Do the estimates seem better of worse for rapidly declining populations?*

5. *Rerun the Example 10.2 code using fewer number of years (*`nYr` *smaller) and increase* `fracmiss`*. Then run the Example 10.3 code. The graphs will start to look peculiar. Why do you think it is doing that? Hint: look at the estimated parameters.*

10.5 Certain and uncertain regions

From Example 10.3, you have observed one of the problems with estimates of the probability of hitting thresholds. Looking over the nine simulations, your risk estimates will be on the true line sometimes and other times they are way off. So your estimates are variable and one should not present only the point estimates of the probability of 90% decline. At the minimum, confidence intervals need to be added (next section), but even with confidence intervals, the probability of hitting declines often does not capture our certainty and uncertainty about extinction risk estimates.

From Example 10.3, you might have also noticed that there are some time horizons (10, 20 years) for which the estimate are highly certain (the threshold is never hit), while for other time horizons (30, 50 years) the estimates are all over the map. Put another way, you may be able to say with high confidence that a 90% decline will not occur between years 1 to 20 and that by year 100 it most surely will have occurred. However, between the years 20 and 100, you are very uncertain about the risk. The point is that you can be certain about some forecasts while at the same time being uncertain about other forecasts.

One way to show this is to plot the uncertainty as a function of the forecast, where the forecast is defined in terms of the forecast length (number of years) and forecasted decline (percentage). Uncertainty is defined as how much of the 0-1 range your 95% confidence interval covers. Ellner and Holmes (2008) show such a figure (their Figure 1). Figure 10.5 shows a version of this figure that you can produce with the function `CSEGtmufigure(u= val, N= val, s2p= val)`. For the figure, the values $u = -0.05$ which is a 5% per year decline, $N = 25$ so 25 years between the first and last census, and $s_p^2 = 0.01$ are used. The process variability for big mammals is typically in the range of 0.002 to 0.02.

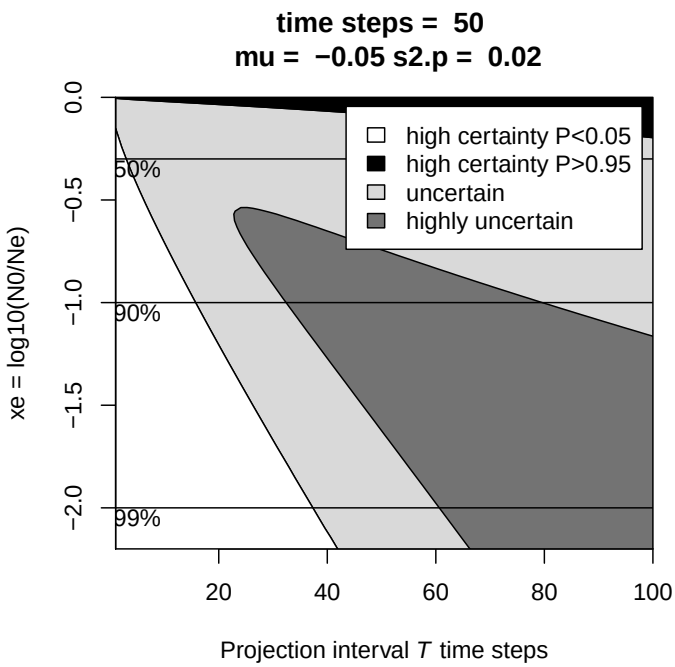

Fig. 10.5. This figure shows your region of high uncertainty (dark grey). In this region, the minimum 95% confidence intervals (meaning if you had no observation error) span 80% of the 0 to 1 probability. That is, you are uncertain if the probability of a specified decline is close to 0 or close to 1. The white area shows where your upper 95% CIs does not exceed P=0.05. So you are quite sure the probability of a specified decline is less than 0.05. The black area shows where your lower 95% confidence interval is above P=.95. So you are quite sure the probability is greater than P=0.95. The light grey is between these two certain/uncertain extremes.

Example 10.4 (Uncertain and certain regions)

Use the Example 10.4 code to re-create Figure 10.5 and get a feel for when risk estimates are more certain and when they are less certain. `N` *are the number of years of data,* `u` *is the mean population growth rate, and* `s2p` *is the process variance.*

Exercise 10.4 code

Type `RShowDoc("Case_study_1.R",package="MARSS")` *to open a file with all the example code.*

```
par(mfrow = c(1, 1))
CSEGtmufigure(N = 50, u = -0.05, s2p = 0.02)
```

10.6 More risk metrics and some real data

The previous sections have focused on the probability of hitting thresholds because this is an important and common risk metric used in population viability analysis and it appears in IUCN Red List criteria. However, as you have seen, there is high uncertainty associated with such estimates. Part of the problem is that probability is constrained to be 0 to 1, and it is easy to get estimates with confidence intervals that span 0 to 1. Other metrics of risk, $\hat{u}$ and the distribution of the time to hit a threshold (Dennis et al., 1991), do not have this problem and may be more informative. Figure 10.6 shows different risk metrics from Dennis et al. (1991) on a single plot. This figure is generated by a call to the function `CSEGriskfigure()`:

```
dat=read.table(datafile, skip=1)
dat=as.matrix(dat)
CSEGriskfigure(dat)
```

The `datafile` is the name of the data file, with years in column 1 and population count (logged) in column 2. `CSEGriskfigure()` has a number of arguments that can be passed in to change the default behavior. The variable `te` is the forecast length (default is 100 years), `threshold` is the extinction threshold either as an absolute number, if `absolutethresh=TRUE`, or as a fraction of current population count, if `absolutethresh=FALSE`. The default is `absolutethresh=FALSE` and `threshold=0.1`. `datalogged=TRUE` means the data are already logged; this is the default.

Example 10.5 (Risk figures for different species)

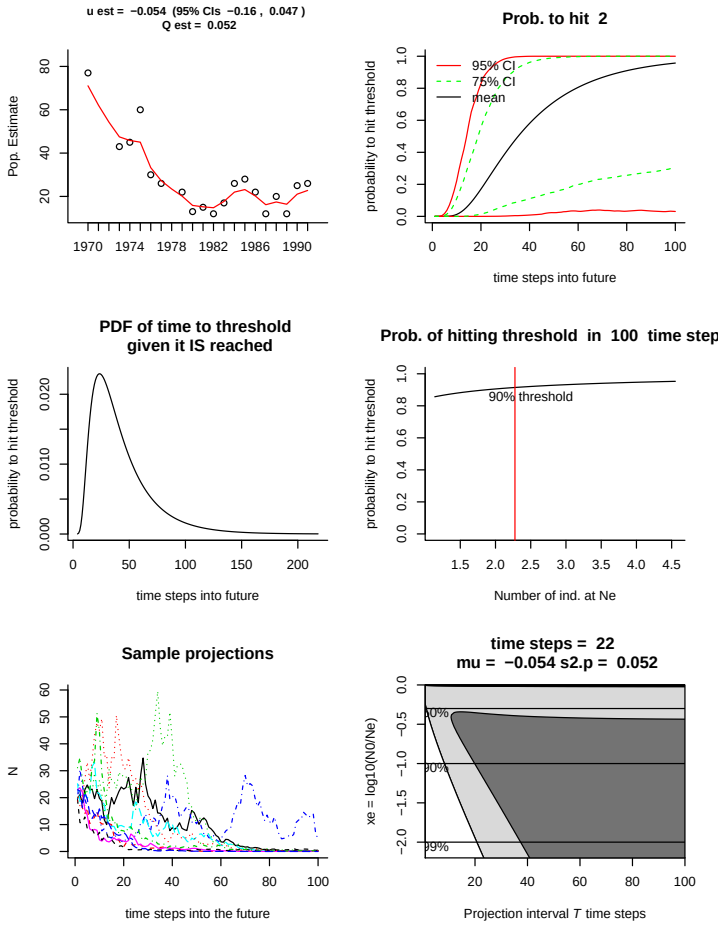

Fig. 10.6. Risk figure using data for the critically endangered African Wild Dog (data from Ginsberg et al. 1995). This population went extinct after 1992.

Use the Example 10.5 code to re-create Figure 10.6. The package includes other data for you to run: `prairiechicken` *from the endangered Attwater Prairie Chicken,* `graywhales` *from Gerber et al. (1999), and* `grouse` *from the Sharptailed Grouse (a species of U.S. federal concern) in Washington State. Note for some of these other datasets, the Hessian matrix cannot be inverted and you will need to use* `CI.method="parametric"`*. If you have other text files of data, you can run those too. The commented lines show how to read in data from a tab-delimited text file with a header line.*

Exercise 5 code
Type `RShowDoc("Case_study_1.R",package="MARSS")` *to open a file with the example code.*

```
#If you have your data in a tab delimited file with a header
#This is how you would read it in using file.choose()
#to call up a directory browser.
#However, the package has the datasets for the exercises
#dat=read.table(file.choose(), skip=1)
#dat=as.matrix(dat)
dat = wilddogs
CSEGriskfigure(dat, CI.method="hessian", silent=TRUE)
```

10.7 Confidence intervals

The figures produced by `CSEGriskfigure()` have confidence intervals (95% and 75%) on the probabilities in the top right panel. A standard way to produce these intervals is via parametric bootstrapping. Here are the steps in a parametric bootstrap:

- You estimate u, σ^2 and η^2
- Then you simulate time series using those estimates and Equations 10.1 and 10.2
- Then you re-estimate your parameters from the simulated data (using say `MARSS(simdata)`
- Repeat for 1000s of time series simulated using your estimated parameters. This gives you a large set of bootstrapped parameter estimates
- For each bootstrapped parameter set, compute a set of extinction estimates (you use Equation 10.3 and code from Example 10.3)
- The α% ranges on those bootstrapped extinction estimates gives you your α confidence intervals on your probabilities of hitting thresholds

The MARSS package provides the function `MARSSparamCIs()` to add bootstrapped confidence intervals to fitted models (type `?MARSSparamCIs` to learn about the function).

In the function `CSEGriskfigure()`, you can set `CI.method = c("hessian", "parametric", "innovations", "none")` to tell it how to compute the confidence intervals. The methods 'parametric' and 'innovations' specify parametric and non-parametric bootstrapping respectively. Producing parameter estimates by bootstrapping is quite slow. Approximate confidence intervals on the parameters can be generated rapidly using the inverse of a numerically estimated Hessian matrix (method 'hessian'). This uses an estimate of the

variance-covariance matrix of the parameters (the inverse of the Hessian matrix). Using an estimated Hessian matrix to compute confidence intervals is a handy trick that can be used for all sorts of maximum-likelihood parameter estimates.

10.8 Comments

Data with cycles, from age-structure or predator-prey interactions, are difficult to analyze and the EM algorithm used in the MARSS package will give poor estimates for this type of data. The slope method (Holmes, 2001) is more robust to those problems. Holmes et al. (2007) used the slope method in a large study of data from endangered and threatened species, and Ellner and Holmes (2008) showed that the slope estimates are close to the theoretical minimum uncertainty. Especially, when doing a population viability analysis using a time series with fewer than 25 years of data, the slope method is often less biased and (much) less variable because that method is less data-hungry (Holmes, 2004). However the slope method is not a true maximum-likelihood method and thus constrains the types of further analyses you can do (such as model selection).

11

Case study 2: Combining multi-site and subpopulation data to estimate regional population dynamics

11.1 The problem

In this case study, we will use multivariate state-space models to combine surveys from multiple regions (or sites) into one estimate of the average long-term population growth rate and the year-to-year variability in that growth rate. Note this is not quite the same as estimating the 'trend'; 'trend' often means what population change happened, whereas the long-term population growth rate refers to the underlying population dynamics. We will use as our example a dataset from harbor seals in Puget Sound, Washington, USA.

We have five regions (or sites) where harbor seals were censused from 1978-1999 while hauled out of land[1]. During the period of this dataset, harbor seals were recovering steadily after having been reduced to low levels by hunting prior to protection. The methodologies were consistent throughout the 20 years of the data but we do not know what fraction of the population that each region represents nor do we know the observation-error variance for each region. Given differences between behaviors of animals in different regions and the numbers of haul-outs in each region, the observation errors may be quite different. The regions have had different levels of sampling; the best sampled region has only 4 years missing while the worst has over half the years missing.

Figure 11.1 shows the data. The numbers on each line denote the different regions:

```
1 SJF
2 SJI
3 EBays
4 PSnd
5 HC
```

[1] Jeffries et al. 2003. Trends and status of harbor seals in Washington State: 1978-1999. Journal of Wildlife Management 67(1):208–219

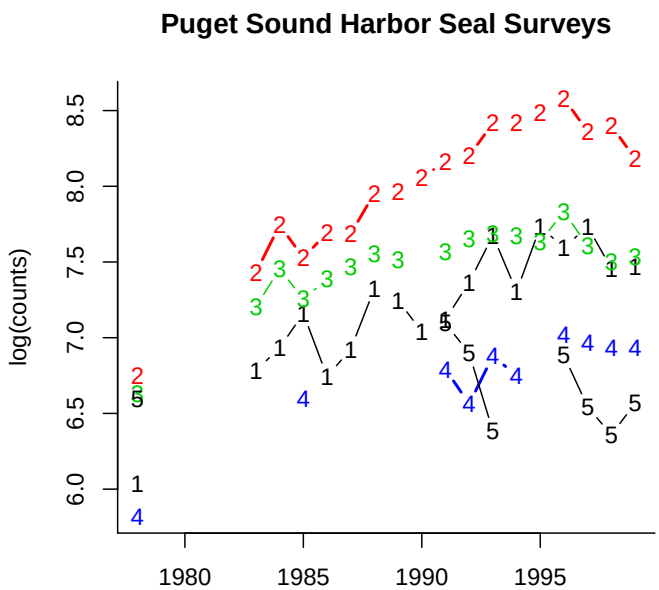

Fig. 11.1. Plot of the of the count data from the five harbor seal regions (Jeffries et al. 2003). Each region is an index of the total harbor seal population, but the bias (the difference between the index and the true population size) for each region is unknown.

For this case study, we will assume that the underlying population process is a stochastic exponential growth process with rates of increase that were not changing through 1978-1999. However, we are not sure if all five regions sample a single "total Puget Sound" population or if there are independent subpopulations. You are going to estimate the long-term population growth rate using different assumptions about the population structures (one big population versus multiple smaller ones) and observation error structures to see how your assumptions change your estimates.

The data for this case study are in the MARSS package. The data have time running down the rows and years in the first column. We need time across the columns for the `MARSS()` function, so we will transpose the data:

```
dat=t(harborSealWA) #Transpose
years = dat[1,] #[1,] means row 1
n = nrow(dat)-1
dat = dat[2:nrow(dat),] #no years
```

If you needed to read data in from a comma-delimited or tab-delimited file, these are the commands to do that:

```
dat = read.csv("datafile.csv",header=TRUE)
dat = read.table("datafile.csv",header=TRUE)
```

The years are in column 1 of `dat` and the logged data are in the rest of the columns. The number of observation time series (`n`) is the number of rows in `dat` minus 1 (for years row). Let's look at the first few years of data:

```
print(harborSealWA[1:8,], digits=3)
```

```
     Year  SJF  SJI EBays PSnd  HC
[1,] 1978 6.03 6.75  6.63 5.82 6.6
[2,] 1979   NA   NA    NA   NA  NA
[3,] 1980   NA   NA    NA   NA  NA
[4,] 1981   NA   NA    NA   NA  NA
[5,] 1982   NA   NA    NA   NA  NA
[6,] 1983 6.78 7.43  7.21   NA  NA
[7,] 1984 6.93 7.74  7.45   NA  NA
[8,] 1985 7.16 7.53  7.26 6.60  NA
```

The `NA`'s in the data are missing values. The algorithm will ignore those values.

11.2 Analysis assuming a single total Puget Sound population

The first step in a state-space modeling analysis is to specify the population structure and how the regions relate to that structure. The general state-space model is

$$\begin{aligned}\mathbf{x}_t &= \mathbf{B}\mathbf{x}_{t-1} + \mathbf{u} + \mathbf{w}_t, \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}) \\ \mathbf{y}_t &= \mathbf{Z}\mathbf{x}_t + \mathbf{a} + \mathbf{v}_t, \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R})\end{aligned}$$

where all the bolded symbols are matrices. To specify the structure of the population and observations, we will specify what those matrices look like.

11.2.1 A single population process, x

When we are looking at data over a large geographic region, we might make the assumption that the different census regions are measuring a single population if we think animals are moving sufficiently such that the whole area (multiple regions together) is "well-mixed". We write a model of the total population abundance as:

$$n_t = \exp(u + w_t) n_{t-1}, \tag{11.1}$$

where n_t is the total count in year t, u is the mean population growth rate, and w_t is the deviation from that average in year t. We then take the log of both sides and write the model in log space:

$$x_t = x_{t-1} + u + w_t, \text{ where } w_t \sim \mathrm{N}(0,q) \tag{11.2}$$

$x_t = \log n_t$. When there is one effective population, there is one x, therefore $\mathbf{x}_t$ is a 1×1 matrix. There is one population growth rate (u) and there is one process variance (q). Thus $\mathbf{u}$ and $\mathbf{Q}$ are 1×1 matrices.

11.2.2 The observation process, y

For this first analysis, we assume that all five regional time series are observing this one population trajectory but they are scaled up or down relative to that trajectory. In effect, we think that animals are moving around a lot and our regional samples are some fraction of the population. There is year-to-year variation in the fraction in each region, just by chance. Notice that under this analysis, we do not think the regions represent independent subpopulations but rather independent observations of one population. Our model for the data, $\mathbf{y}_t = \mathbf{Z}\mathbf{x}_t + \mathbf{a} + \mathbf{v}_t$, is written as:

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} x_t + \begin{bmatrix} 0 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \end{bmatrix} \tag{11.3}$$

Each y_i is the time series for a different region. The a's are the bias between the regional sample and the total population. The a's are scaling (or intercept-like) parameters[2]. We allow that each region could have a unique observation variance and that the observation errors are independent between regions. Lastly, we assume that the observations errors on log(counts) are normal and thus the errors on (counts) are log-normal.[3]

We specify independent observation errors with unique variances by specifying that the v's come from a multivariate normal distribution with variance-covariance matrix $\mathbf{R}$ ($\mathbf{v} \sim \mathrm{MVN}(0,\mathbf{R})$), where

[2] To get rid of the a's, we scale multiple observation time series against each other; thus one a will be fixed at 0. Estimating the bias between regional indices and the total population is important for getting an estimate of the total population size. The type of time-series analysis that we are doing here (trend analysis) is not useful for estimating a's. Instead to get a's one would need some type of mark-recapture data. However, for trend estimation, the a's are not important. The regional observation variance captures increased variance due to a regional estimate being a smaller sample of the total population.

[3] The assumption of normality is not unreasonable since these regional counts are the sum of counts across multiple haul-outs.

$$\mathbf{R} = \begin{bmatrix} r_1 & 0 & 0 & 0 & 0 \\ 0 & r_2 & 0 & 0 & 0 \\ 0 & 0 & r_3 & 0 & 0 \\ 0 & 0 & 0 & r_4 & 0 \\ 0 & 0 & 0 & 0 & r_5 \end{bmatrix} \tag{11.4}$$

$\mathbf{Z}$ specifies which observation time series, $y_{i,1:T}$, is associated with which population trajectory, $x_{j,1:T}$. $\mathbf{Z}$ is like a look up table with 1 row for each of the n observation time series and 1 column for each of the m population trajectories. A 1 in row i column j means that observation time series i is measuring state process j. Otherwise the value in $\mathbf{Z}_{ij} = 0$. Since we have only 1 population trajectory, all the regions must be measuring that one population trajectory. Thus $\mathbf{Z}$ is $n \times 1$:

$$\mathbf{Z} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \tag{11.5}$$

11.2.3 Set the model structure for `MARSS`

Now that we have specified our state-space model, we set the arguments that will tell the function `MARSS()` the structure of our model. We do this by passing in the argument `model` to `MARSS()`. The argument `model` is a list which specifies the model structure for $\mathbf{Z}$, $\mathbf{u}$, $\mathbf{Q}$, etc. The function call will now look like:

```
kem1 = MARSS(dat, model=list(Z=Z.model, U=U.model,
      Q=Q.model, R=R.model) )
```

First we set the $\mathbf{Z}$ model. We need to tell the `MARSS` function that $\mathbf{Z}$ is a 5×1 matrix of 1s (as in Equation 11.3). We can do this two ways. We can pass in `Z.model` as a matrix of ones, `matrix(1,5,1)`, just like in Equation (11.3) or we can pass in a vector of five factors, `factor(c(1,1,1,1,1))`. The i-th factor specifies which population trajectory the i-th observation time series belongs to. Since there is only one population trajectory in this first analysis, we will have a vector of five 1's: every observation time series is measuring the first, and only, population trajectory.

```
Z.model = factor(c(1,1,1,1,1))
```

Note, the vector (the `c()` bit) must be wrapped in `factor()` so that `MARSS` recognizes what it is. You can use either numeric or character vectors: `c(1,1,1,1,1)` is the same as `c("PS","PS","PS","PS","PS")`.

Next we specify that the $\mathbf{R}$ variance-covariance matrix only has terms on the diagonal (the variances) with the off-diagonal terms (the covariances) equal to zero:

```
R.model = "diagonal and unequal"
```

The 'and unequal' part specifies that the variances are allowed to be unique on the diagonal. If we wanted to force the observation variances to be equal at all regions, we would use `"diagonal and equal"`.

For the first analysis, we only need to set the model structure for **Z** and **R**. Since there is only one population, there is only one **u** and **Q** (they are scalars), so there are no constraints to set on them.

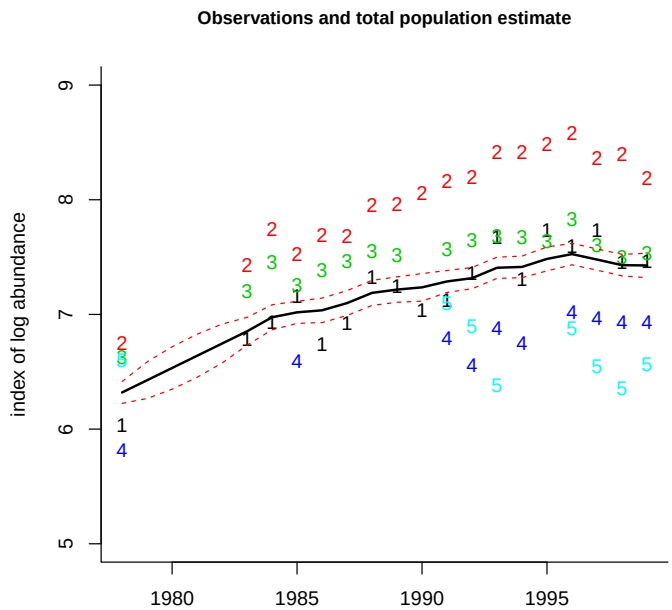

Fig. 11.2. Plot of the estimate of "log total harbor seals in Puget Sound" (minus the unknown bias for time series 1) against the data. The estimate of the total seal count has been scaled relative to the first time series. The 95% confidence intervals on the population estimates are the dashed lines. These are not the confidence intervals on the observations, and the observations (the numbers) will not fall between the confidence interval lines.

11.2.4 The `MARSS()` output

The output from `MARSS()`, here assigned the name `kem`, is a list of objects. To see all the objects in it, type:

```
names(kem1)
```

The maximum-likelihood estimates of "total harbor seal population" scaled to the first observation data series (Figure 11.2) are in `kem1$states`, and `kem1$states.se` are the standard errors on those estimates. To get 95% confidence intervals, use `kem1$states +/- 1.96*kem1$states.se`. Figure 11.2 shows a plot of `kem1$states` with its 95% confidence intervals over the data. Because `kem1$states` has been scaled relative to the first time series, it is on top of that time series. One of the biases, the as, cannot be estimated and arbitrarily our algorithm choses $a_1 = 0$, so the population estimate is scaled to the first observation time series.

The estimated parameters are a list: `kem1$par`. To get the element `U` of that list, which is the estimated long-term population growth rate, type in `kem1$par$U`. Multiply by 100 to get the percent increase per year. The estimated process variance is given by `kem1$par$Q`.

The log-likelihood of the fitted model is in `kem1$logLik`. We estimated one initial x ($t = 1$), one process variance, one u, four a's, and five observation variances's. So $K = 12$ parameters. The AIC of this model is $-2 \times$ log-like $+ 2K$, which we can show by typing `kem1$AIC`.

Example 11.1 (Fit the single population model)

Analyze the harbor seal data using the single population model (Equations 11.2 and 11.3). The code for Example 11.1 shows you how to input data and send it to the function `MARSS()`*. As you run the examples, add the estimates to the table at the end of the chapter so you can compare estimates across the examples.*

Example 11.1 code

Type `RShowDoc("Case_study_2.R",package="MARSS")` *to open a file with all the example code.*

```
#Read in data
dat=t(harborSealWA) #Transpose since MARSS needs time ACROSS columns
years = dat[1,]
n = nrow(dat)-1
dat = dat[2:nrow(dat),]
legendnames = (unlist(dimnames(dat)[1]))
#estimate parameters
Z.model = factor(c(1,1,1,1,1))
R.model = "diagonal and unequal"
kem1 = MARSS(dat, model=
  list(Z=Z.model, R=R.model))
#make figure
matplot(years, t(dat),xlab="",ylab="index of log abundance",
  pch=c("1","2","3","4","5"),ylim=c(5,9),bty="L")
lines(years,kem1$states-1.96*kem1$states.se,type="l",
  lwd=1,lty=2,col="red")
lines(years,kem1$states+1.96*kem1$states.se,type="l",
  lwd=1,lty=2,col="red")
lines(years,kem1$states,type="l",lwd=2)
title("Observations and total population estimate",cex.main=.9)
#show just the estimated parameter elements
kem1$par
#show the parameters matrices with fixed and estimated elements
parmat(kem1)
#show the log-likelihood and AIC
kem1$logLik
kem1$AIC
```

11.3 Changing the assumption about the observation variances

The variable `kem1$par$R` contains the estimates of the observation error variances. It is a matrix. Here is **R** from Example 11.1. Notice that the function `parmat` is used. The list element `kem1$par` is just the estimated values in a matrix. The function `parmat()` is used to construct the full parameter matrix that includes the fixed and estimated elements.

```
print(parmat(kem1,"R"), digits=3)
```

```
$R
       [,1]   [,2]   [,3]  [,4]  [,5]
[1,] 0.0322 0.0000 0.0000 0.000 0.000
[2,] 0.0000 0.0351 0.0000 0.000 0.000
[3,] 0.0000 0.0000 0.0136 0.000 0.000
[4,] 0.0000 0.0000 0.0000 0.011 0.000
[5,] 0.0000 0.0000 0.0000 0.000 0.197
```

Notice that the variances along the diagonal are all different—we estimated five unique observation variances. We might be able to improve the fit (relative to the number of estimated parameters) by assuming that the observation variance is equal across regions but the errors are independent. This means we estimate one observation variance instead of five. This is a fairly standard assumption for data that come from the uniform survey methodology[4].

To impose this model, we set the **R** model to

```
R.model="diagonal and equal"
```

This tells `MARSS` that all the r's along the diagonal in **R** are the same. To fit this model to the data, call `MARSS()` as:

```
Z.model = factor(c(1,1,1,1,1))
R.model = "diagonal and equal"
kem2 = MARSS(dat, model=
       list(Z=Z.model, R=R.model))
```

We estimated one initial x, one process variance, one u, four a's, and one observation variance. So $K = 8$ parameters. The AIC for this new model compared to the old model with five observation variances is:

```
c(kem1$AIC,kem2$AIC)
```

```
[1] -9.316899  8.840339
```

A smaller AIC means a better model. The difference between the one observation variance versus the unique observation variances is >10, suggesting that the unique observation variances model is better.

One of the key diagnostics when you are comparing fits from multiple models, it to examine whether the model is flexible enough to fit the data. You do this by looking for temporal trends in the the residuals between the estimated population states (e.g. `kem2$states`) and the data. In Figure 11.3, the residuals for the second analysis are shown. Ideally, these residuals should not have a temporal trend. They should look cloud-like. The fact that the

[4] By the way, this is not a good assumption for these data since the number haul-outs in each region varies and the regional counts are the sums across all haul-outs in a region. We will see that this is a poor assumption when we look at the AIC values.

residuals have a strong temporal trend is an indication that our one population model is too restrictive for the data[5].

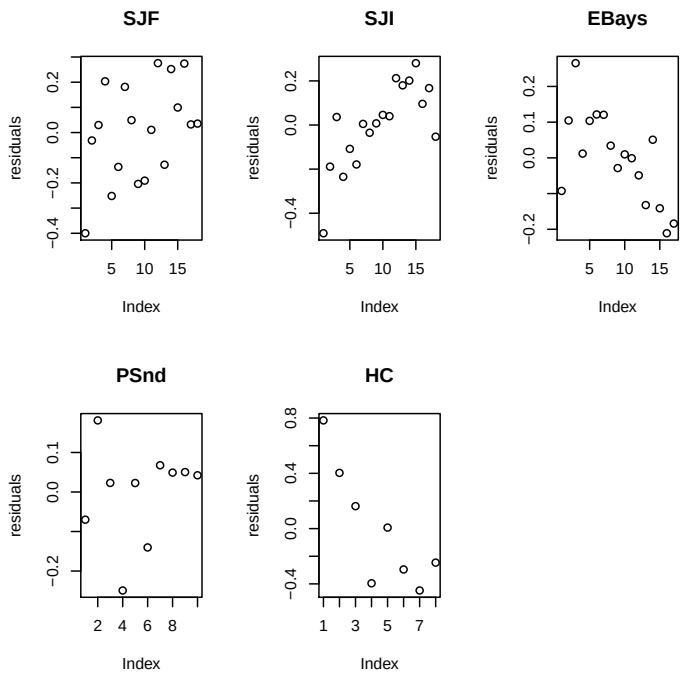

Fig. 11.3. Residuals for the model with a single population. The plots of the residuals should not have trends with time, but they do... This is an indication that the single population model is inconsistent with the data. The code to make this plot is given in the script file for this case study.

Example 11.2 (Fit a model with shared observation variances)

Analyze the data using the same population model as in Example 11.1, but constrain the **R** *matrix so that all five census regions have the same observation variance. The Example 11.2 code shows you how to do this. It also shows you how to make the diagnostics figure (Figure 11.3).*

[5] When comparing models via AIC, it is important that you only compare models that are flexible enough to fit the data. Fortunately if you neglect to do this, the inadequate models will usually have very high AICs and fall out of the mix anyhow.

Example 11.2 code

Type `RShowDoc("Case_study_2.R",package="MARSS")` *to open a file with all the example code.*

```
#fit model
Z.model = factor(c(1,1,1,1,1))
R.model = "diagonal and equal"
kem2 = MARSS(dat, model=
  list(Z=Z.model, R=R.model))
#show the estimated parameter elements
kem2$par$U       #population growth rate
kem2$par$Q       #process variance
kem2$par$R  #observation variance
kem2$logLik #log likelihood
c(kem1$AIC,kem2$AIC)
#plot residuals
plotdat = t(dat)
matrix.of.biases = matrix(parmat(kem2)$A,
  nrow=nrow(plotdat),ncol=ncol(plotdat),byrow=T)
xs = matrix(kem2$states,
  nrow=dim(plotdat)[1],ncol=dim(plotdat)[2],byrow=F)
resids = plotdat-matrix.of.biases-xs
par(mfrow=c(2,3))
for(i in 1:n){
  plot(resids[!is.na(resids[,i]),i],ylab="residuals")
  title(legendnames[i])
}
par(mfrow=c(1,1))
```

11.4 Analysis assuming north and south subpopulations

For the third analysis, we will change our assumption about the structure of the population. We will assume that there are two subpopulations, north and south, and that regions 1 and 2 (Strait of Juan de Fuca and San Juan Islands) fall in the north subpopulation and regions 3, 4 and 5 fall in the south subpopulation. For this analysis, we will assume that these two subpopulations share their growth parameter, u, and process variance, q, since they share a similar environment and prey base. However we postulate that because of fidelity to natal rookeries for breeding, animals do not move much year-to-year between the north and south and the two subpopulations are independent.

We need to write down the state-space model to reflect this population structure. There are two subpopulations, x_n and x_s, and they have the same growth rate u:

$$\begin{bmatrix} x_{n,t} \\ x_{s,t} \end{bmatrix} = \begin{bmatrix} x_{n,t-1} \\ x_{s,t-1} \end{bmatrix} + \begin{bmatrix} u \\ u \end{bmatrix} + \begin{bmatrix} w_{n,t} \\ w_{s,t} \end{bmatrix} \tag{11.6}$$

We specify that they are independent by specifying that their year-to-year population fluctuations (their process errors) come from a multivariate normal with no covariance:

$$\begin{bmatrix} w_{n,t} \\ w_{s,t} \end{bmatrix} \sim MVN\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} q & 0 \\ 0 & q \end{bmatrix} \right) \tag{11.7}$$

For the observation process, we use the **Z** matrix to associate the regions with their respective x_n and x_s values:

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_{n,t} \\ x_{s,t} \end{bmatrix} + \begin{bmatrix} 0 \\ a_2 \\ 0 \\ a_4 \\ a_5 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \end{bmatrix} \tag{11.8}$$

11.4.1 Specifying the `MARSS()` arguments

We need to change the **Z** model to specify that there are two subpopulations (north and south), and that regions 1 and 2 are in the north subpopulation and regions 3,4 and 5 are in the south subpopulation. There are a few ways, we can specify this **Z** matrix for `MARSS()`:

```
Z.model = matrix(c(1,1,0,0,0,0,0,1,1,1),5,2)
Z.model = factor(c(1,1,2,2,2))
Z.model = factor(c("N","N","S","S","S"))
```

Which you choose is a matter of preference as they all specify the same form for **Z**.

We also want to specify that the u's are the same for each subpopulation and that **Q** is diagonal with equal q's. To do this, we set

```
U.model = "equal"
Q.model = "diagonal and equal"
```

This says that there is one u and one q parameter and both subpopulations share it (if we wanted the u's to be different, we would use `U.model="unequal"` or leave off the **u** model since the default behavior is `U.model="unequal"`).

Now we specify the new model structures and fit this model to the data:

```
Z.model = factor(c(1,1,2,2,2))
U.model = "equal"
Q.model = "diagonal and equal"
```

```
R.model = "diagonal and equal"
kem3 = MARSS(dat, model=list(Z=Z.model,
   R=R.model, U=U.model, Q=Q.model))
```

```
Success! Parameters converged at 20 iterations.
Alert: conv.test.slope.tol is 0.5.
Test with smaller values (<0.1) to ensure convergence.

MARSS fit is
Estimation method: kem
Estimation converged in 20 iterations.
Log-likelihood: 11.52392
AIC: -7.047848   AICc: -4.725268

          Estimate
A.2        0.79876
A.4       -0.75537
A.5       -0.81630
R.R(diag)  0.02929
U.U        0.05036
Q.Q(diag)  0.00812
x0.x01     6.06229
x0.x02     6.83345

Standard errors have not been calculated.
Use MARSSparamCIs to compute CIs and bias estimates.
```

Figure 11.4 shows the residuals for the two subpopulations case. The residuals look better (more cloud-like) but the Hood Canal residuals are still temporally correlated.

Example 11.3 (Fit a model with north and south subpopulations)

Analyze the data using a model with two subpopulations, northern and southern. Assume that the subpopulation are independent (diagonal $\mathbf{Q}$*), however let each subpopulation share the same population parameters,* $\boldsymbol{u}$ *and* q*. The Example 11.3 code shows how to set the* `MARSS()` *arguments for this case.*

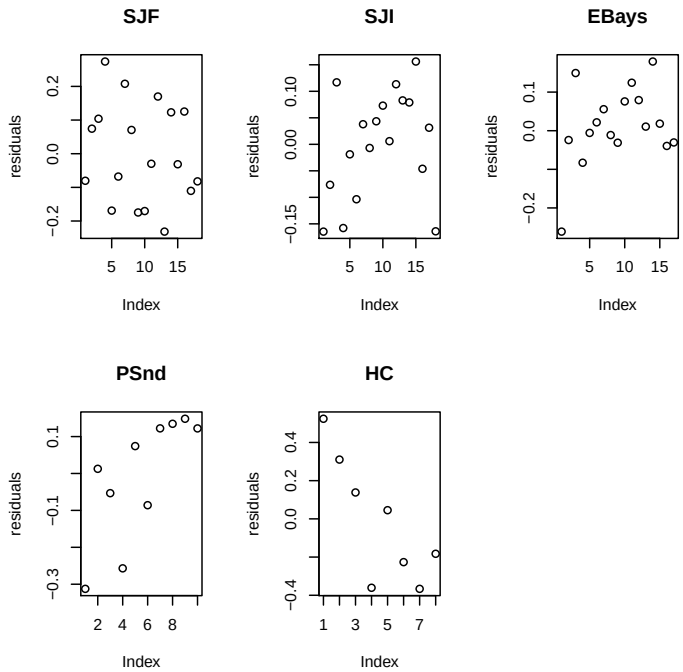

Fig. 11.4. The residuals for the analysis with a north and south subpopulation. The plots of the residuals should not have trends with time. Compare with the residuals for the analysis with one subpopulation.

Example 11.3 code

Type `RShowDoc("Case_study_2.R",package="MARSS")` *to open a file with all the example code.*

```
#fit model
Z.model = factor(c(1,1,2,2,2))
U.model = "equal"
Q.model = "diagonal and equal"
R.model = "diagonal and equal"
kem3 = MARSS(dat, model=list(Z=Z.model,
  R=R.model, U=U.model, Q=Q.model))
#plot residuals
plotdat = t(dat)
matrix.of.biases = matrix(parmat(kem3)$A,
  nrow=nrow(plotdat),ncol=ncol(plotdat),byrow=T)
par(mfrow=c(2,3))
for(i in 1:n){
  j=c(1,1,2,2,2)
  xs = kem3$states[j[i],]
  resids = plotdat[,i]-matrix.of.biases[,i]-xs
  plot(resids[!is.na(resids)],ylab="residuals")
  title(legendnames[i])
}
par(mfrow=c(1,1))
```

11.5 Using MARSS() to fit other population structures

Now work through a number of different structures and fill out the table at the back of this case study. At the end you will see how your estimation of the mean population growth rate varies under different assumptions about the population and the data.

Example 11.4 (Five subpopulations)

Analyze the data using a model with five subpopulations, where each of the five census regions is sampling one of the subpopulations. Assume that the subpopulation are independent (diagonal $\mathbf{Q}$*), however let each subpopulation share the same population parameters,* u *and* q*. The Example 11.4 code shows how to set the* `MARSS()` *arguments for this case. You can use* `R.model="diagonal and equal"` *to make all the observation variances equal.*

Example 11.4 code

Type `RShowDoc("Case_study_2.R",package="MARSS")` *to open a file with all the example code.*

```
Z.model=factor(c(1,2,3,4,5))
U.model="equal"
Q.model="diagonal and equal"
R.model="diagonal and unequal"
kem=MARSS(dat, model=list(Z=Z.model,
  U=U.model, Q=Q.model, R=R.model) )
```

Example 11.5 (Two subpopulations with different population parameters)

Analyze the data using a model that assumes that the Strait of Juan de Fuca and San Juan Islands census regions represent a northern Puget Sound subpopulation, while the other three regions represent a southern Puget Sound subpopulation. This time assume that each population trajectory (north and south) has different u *and* q *parameters:* u_n,u_s *and* q_n,q_s*. Also assume that each of the five census regions has a different observation variance. Try to write your own code. If you get stuck (or want to check your work, you can open a script file with all the Case Study 2 examples by typing* `RShowDoc("Case_study_2.R",package="MARSS")` *at the R command line.*

In math form, this model is:

$$\begin{bmatrix} x_{n,t} \\ x_{s,t} \end{bmatrix} = \begin{bmatrix} x_{n,t-1} \\ x_{s,t-1} \end{bmatrix} + \begin{bmatrix} u_n \\ u_s \end{bmatrix} + \begin{bmatrix} w_{n,t} \\ w_{s,t} \end{bmatrix}, \begin{bmatrix} w_{n,t} \\ w_{s,t} \end{bmatrix} \sim \text{MVN}\left(0, \begin{bmatrix} q_n & 0 \\ 0 & q_s \end{bmatrix}\right) \tag{11.9}$$

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_{n,t} \\ x_{s,t} \end{bmatrix} + \begin{bmatrix} 0 \\ a_2 \\ 0 \\ a_4 \\ a_5 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \end{bmatrix} \tag{11.10}$$

Example 11.6 (Hood Canal covaries with the other regions)

Analyze the data using a model with two subpopulations with the divisions being Hood Canal versus everywhere else. In math form, this model is:

$$\begin{bmatrix} x_{p,t} \\ x_{h,t} \end{bmatrix} = \begin{bmatrix} x_{p,t-1} \\ x_{h,t-1} \end{bmatrix} + \begin{bmatrix} u_p \\ u_h \end{bmatrix} + \begin{bmatrix} w_{p,t} \\ w_{h,t} \end{bmatrix}, \begin{bmatrix} w_{p,t} \\ w_{h,t} \end{bmatrix} \sim \text{MVN}\left(0, \begin{bmatrix} q & c \\ c & q \end{bmatrix}\right) \tag{11.11}$$

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_{p,t} \\ x_{h,t} \end{bmatrix} + \begin{bmatrix} 0 \\ a_2 \\ a_3 \\ a_4 \\ 0 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \end{bmatrix} \tag{11.12}$$

To specify that **Q** *has one value on the diagonal (one variance) and one value on the off-diagonal (covariance) you can specify* `Q.model` *two ways:*

```
Q.model = "equalvarcov"
Q.model = matrix(c("q","c","c","q"),2,2)
```

Example 11.7 (Three subpopulations with shared parameter values)

Analyze the data using a model with three subpopulations as follows: north (regions 1 and 2), south (regions 3 and 4), Hood Canal (region 5). You can specify that some subpopulations share parameters while others do not. First, let's specify that each population is affected by independent environmental variability, but that the variance of that variability is the same for the two interior populations:

```
Q.model=matrix(list(0),3,3)
diag(Q.model)=c("coastal","interior","interior")
print(Q.model)
```

Notice that **Q** *is a diagonal matrix (independent year-to-year environmental variability) but the variance of two of the populations is the same. Notice too that the off-diagonal terms are numeric; they do not have quotes. We specified* **Q** *using a matrix of class list, so that we could have numeric values (fixed) and character values (estimated parameters).*

In a similar way, we specify that the observation errors are independent but that estimates from a plane do not have the same variance as those from a boat:

```
R.model=matrix(list(0),5,5)
diag(R.model)=c("boat","boat","plane","plane","plane")
```

For the long-term trends, we specify that x_1 *and* x_2 *share a long-term trend ("puget sound") while* x_3 *is allowed to have a separate trend ("hood canal").*

```
U.model=matrix(c("puget sound","puget sound","hood canal"),3,1)
```

11.6 Discussion

There are a number of corners that we cut in order to have case study code that runs quickly:

- We ran the code starting from one initial condition. For a real analysis, you should start from a large number of random initial conditions and use the one that gives the highest likelihood. Since the EM algorithm is a "hill-climbing" algorithm, this ensures that it does not get stuck on a local maxima. `MARSS()` will do this for you if you pass it the argument `control=list(MCInit=TRUE)`. This will use a Monte Carlo routine to try many different initial conditions. See the help file on `MARSS()` for more information (by typing `?MARSS` at the *R* prompt).
- We assume independent observation and process errors. Depending on your system, observation errors may be driven by large-scale environmental factors (temperature, tides, prey locations) that would cause your observation errors to covary across regions. If your observation errors strongly covary between regions and you treat them as independent, this could be bad for your analysis. Unfortunately, separating covariance across observation

versus process errors will require much data (to have any power). In practice, the first step is to think hard about what drives sightability for your species and what are the relative levels of process and observation variance. You may be able to subsample your data in a way that will make the observation errors more independent.

- The `MARSS()` argument `control` specifies the options for the EM algorithm. We left the default tolerance for the convergence test. You would want to set this lower for a real analysis. You will need to up the `maxit` argument correspondingly.
- We used the large-sample approximation for AIC instead of a bootstrap AIC that is designed to correct for small sample size in state-space models. The bootstrap metric, AICb, takes a long time to run. Use the call `MARSSaic(kem, output=c("AICbp"))` to compute AICb. We could have shown AICc, which is the small-sample size corrector for non-state-space models. Type `kem$AICc` to get that.

Finally, in a real (maximum-likelihood) analysis, one needs to be careful not to dredge the data. The temptation is to look at the data and pick a population structure that will fit that data. This can lead to including models in your analysis that have no biological basis. In practice, we spend a lot of time discussing the population structure with biologists working on the species and review all the biological data that might tell us what are reasonable structures. From that, a set of model structures to use are selected. Other times, a particular model structure needs to be used because the population structure is not in question rather it is a matter of using that pre-specified structure and using all the data to get parameter estimates for forecasting.

Results table

Ex.		pop. growth rate `kem$par$U`	process variance `kem$par$Q`	K `kem$num. params`	log-like `kem$ logLik`	AIC `kem$AIC`
1	one population different obs. vars uncorrelated					
2	one population identical obs vars uncorrelated					
3	N+S subpops identical obs vars uncorrelated;					
4	5 subpops unique obs vars u's + q's identical					
5	N+S subpops unique obs vars u's + q's identical					
6	PS + HC subpops unique obs vars u's + q's unique					
7	N + S + HC subpops unique obs vars u's + q's unique					

For AIC, lower is better and only the relative differences matter. A difference of 10 between two AICs means substantially more support for the model with lower AIC. A difference of 30 or 40 between two AICs is very large.

Questions

1. Do different assumptions about whether the observation error variances are all identical versus different affect your estimate of the long-term population growth rate (u)? You may want to rerun examples 3-7 with the `R.model` changed. `R.model="diagonal and unequal"` means measurement variances all different versus `"diagonal and equal"`.
2. Do assumptions about the underlying structure of the population affect your estimates of u? Structure here means number of subpopulations and which areas are in which subpopulation.

3. The confidence intervals for the first two analyses are very tight because the estimate process variance was very small, `kem1$par$Q`. Why do you think process variance (q) was forced to be so small? [Hint: We are forcing there to be one and only one true population trajectory and all the observation time series have to fit that one time series. Look at the AICs too.]

12

Case Study 3: Using MARSS models to identify spatial population structure and covariance

12.1 The problem

In this case study, we use time series of observations from nine sites along the west coast to examine large-scale spatial structure in harbor seals (Jeffries et al., 2003). Harbor seals are distributed along the west coast of the U.S. from California to Washington. The populations in Oregon and Washington have been surveyed for over 25 years at a number of haul-out sites (Figure 12.1). In general, these populations have been increasing steadily since the 1972 Marine Mammal Protection Act. It remains unknown whether they are at carrying capacity.

For management purposes, two stocks are recognized; the coastal stock consists of four sites (Northern/Southern Oregon, Coastal Estuaries, Olympic Peninsula), and the inland WA stock consists of the remaining five sites (Figure 12.1). Subtle differences exist in the demographics across sites (e.g. pupping dates), however mtDNA analyses and tagging studies have suggested that these sites may be structured on a much larger scale. Harbor seals are known for strong site fidelity, but at the same time travel large distances to forage.

Our goal for this case study is to address the following questions about spatial structure: 1) Does population abundance data support the existing management boundaries, or are there alternative groupings that receive more support? and 2) Does the Hood Canal site represent a distinct subpopulation? To address these questions, we will mathematically formulate different hypotheses about population structure via different MARSS models; each model represents a different population structure. We will then compare the data support for different models using model selection criteria, specifically AIC.

Type `RShowDoc("Case_study_3.R",package="MARSS")` to open a file with the *R* code to get you started on the analyses in this chapter.

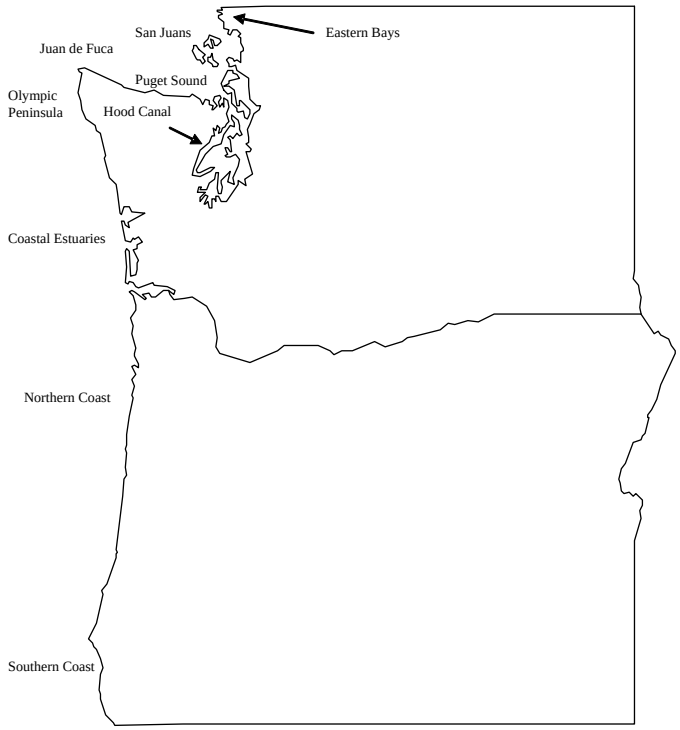

Fig. 12.1. Map of spatial distribution of 9 harbor seal sites in Washington and Oregon.

12.2 How many distinct subpopulations?

We will analyze the support for five hypotheses about the population structure. These do not represent all possible structures but instead represent those that are considered most biologically plausible given the geography and the behavior of harbor seals.

Hypothesis 1 Sites are grouped by stock ($m = 2$), unique process variances
Hypothesis 2 Sites are grouped by stock ($m = 2$), same process variance
Hypothesis 3 Sites are grouped by state ($m = 2$), unique process variances
Hypothesis 4 Sites are grouped by state ($m = 2$), same process variance
Hypothesis 5 All sites are part of the same panmictic population ($m = 1$)

Aerial survey methodology has been relatively constant across time and space, and we will assume that all sites have identical and independent observation error variance.

12.2.1 Specify the design, Z, matrices

Write down the **Z** matrices for the hypotheses. Hint: Hypothesis 1 and 2 have the same **Z** matrix, Hypothesis 3 and 4 have the same **Z** matrix and Hypothesis 5 is a column of 1s.

	H 1 and 2 **Z** subpop 1	H 1 and 2 **Z** subpop 2	H 3 and 4 **Z** subpop 1	H 3 and 4 **Z** subpop 2	H 5 **Z** subpop 1
`Coastal Estuaries`					
`Olympic Peninsula`					
`Str. Juan de Fuca`					
`San Juan Islands`					
`Eastern Bays`					
`Puget Sound`					
`Hood Canal`					
`OR North Coast`					
`OR South Coast`					

Next you need to specify the `model` argument so that `MARSS` knows the structure of your **Z**'s. The **Z** model will be a vector of factors, i.e. it will have the form `factor(c(....))`.

- Hypothesis 1 and 2: `Z.model=`
- Hypothesis 3 and 4: `Z.model=`
- Hypothesis 5: `Z.model=`

12.2.2 Specify the grouping arguments

For this case study, we will assume that subpopulations share the same growth rate. What should `U.model` be for each hypothesis? To specify shared u parameters, `U.model` is set as a character vector where shared elements in **u** have the same character name. Written in *R* it takes the form `matrix(c(#,#,...),m,1)`

- Hypothesis 1-4: `U.model=`
- Hypothesis 5: `U.model=`

What about `Q.model`? To specify a diagonal **Q** matrix with shared values along the diagonal, we will need to have a matrix with numeric values (0) on the off-diagonals and character values (names of parameters to estimate) on the diagonal. We do this with a matrix of class list.

```
Q.model=matrix(list(0),m,1)
diag(Q.model)=c("q1","q1","q2","q2","...")
```

Notice that first, we set up `Q.model` as a list matrix with numeric 0s everywhere and then set the diagonals to a vector of character strings. Character strings that are the same are shared (identical) values.

Look at each hypothesis (above) and write down *R* code for the corresponding `Q.model`.

- Hypothesis 1: `Q.model=`
- Hypothesis 2: `Q.model=`
- Hypothesis 3: `Q.model=`
- Hypothesis 4: `Q.model=`
- Hypothesis 5: `Q.model=`

Lastly, specify `R.model`. As we mentioned above, we will assume that the observation errors are independent and the observation variance is the same across sites. You can specify this model with the text string `"equal"`.

- Hypothesis 1-5: `R.model=`

12.2.3 Fit models and summarize results

Fit each model for each hypothesis to the seal data (look at the script `Case_Study_3.R` for the code to load the data). Each call to `MARSS()` will look like

```
kem = MARSS(sealData, model=list(Z = Z.model,
  Q = Q.model, R = R.model, U = U.model))
```

Fill in the following table, by fitting the five state-space models—for the five hypotheses—to the harbor seal data (using `MARSS()`). Use the `Case_Study_3.R` script so you do not have to type in all the commands.

12.2.4 Interpret results for question 1

What do these results indicate about the process error grouping and spatial grouping? A lower AIC means a more parsimonious model (highest likelihood given the number of parameters). A difference of 10 between AICs is large, and means the model with the higher AIC is unsupported relative to the model with lower AIC.

Extra analysis (if you have time): Do your results change if you assume that observation errors are independent but have unique variances? The nine sites have different numbers of haul-outs and so the observation variances

Table 12.1. Table to fill out for the five hypotheses from the first analysis (Section 12.2). The code of the form `$foo$bar` shows you what to type at the command line to output each parameter or metric. Remember to add the name of the model fit, e.g. `kem$foo$bar` where `kem` is the name you gave to the model fit.

H	pop. growth rate `$par$U`	proc. variance `$par$Q`	obs. variance `$par$R`	K `$num. params`	log-like `$logLik`	AIC `$AIC`	AICc `$AICc`
1							
2							
3							
4							
5							

might be different. Repeat the analysis with unique observation variances for each site (this means changing `R.model`). You can also try the analysis with temporally co-varying subpopulations (good and bad years correlated) by setting `Q.model="unconstrained"` or `Q.model="equalvarcov"`.

12.3 Is Hood Canal separate?

The Hood Canal site may represent a distinct population, and has recently been subjected to a number of catastrophic events (hypoxic events, possibly leading to reduced prey availability, and several killer whale predation events, removing up to 50% of animals per occurrence). Build four models, assuming that each site (other than Hood Canal) is assigned to its current management stock, but Hood Canal is a different subpopulation ($m = 3$). Again, assume that observation error variance is identical and independent across sites.

Hypothesis 1 Subpopulations have the same process variance and growth rate

Hypothesis 2 Each subpopulation has a unique process variance and growth rate

Hypothesis 3 Hood Canal has the same process variance but different growth rate

Hypothesis 4 Hood Canal has unique process variance and unique growth rate

12.3.1 Specify the Z matrix and `Z.model`

The **Z** matrix for each hypothesis is the same. The coastal subpopulation consists of 4 sites (Northern/Southern Oregon, Coastal Estuaries, Olympic Peninsula), the Hood Canal subpopulation is the Hood Canal site, and the inland WA subpopulation consists of the remaining 4 sites. Thus $m = 3$ and **Z** is a 9×3 matrix:

$$
\begin{array}{r}
\\ \\ \\ \\ \\ \\ \\ \\ \\
\end{array}
\begin{array}{c}
\begin{array}{ccc} \text{subpop} & \text{subpop} & \text{subpop} \\ 1 & 2 & 3 \end{array} \\
\begin{bmatrix} \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{bmatrix}
\end{array}
\begin{array}{r}
\texttt{Coastal Estuaries} \\
\texttt{Olympic Peninsula} \\
\texttt{Str. Juan de Fuca} \\
\texttt{San Juan Islands} \\
\texttt{Eastern Bays} \\
\texttt{Puget Sound} \\
\texttt{Hood Canal} \\
\texttt{OR North Coast} \\
\texttt{OR South Coast}
\end{array}
$$

Then write down `Z.model` for this **Z**: `factor(c(...))`

12.3.2 Specify which parameters are shared across which subpopulations

`U.groups` specifies which u are shared across subpopulations. Look at the hypothesis descriptions above which will specify whether subpopulations share their population growth rate or have unique population growth rates.

- Hypothesis 1: `U.model=`
- Hypothesis 2: `U.model=`
- Hypothesis 3: `U.model=`
- Hypothesis 4: `U.model=`

`U.model` will be a $m \times 1$ matrix of character strings; `matrix(c("c1","c2","....."),m,1)` Once you have more than two subpopulations, it can get hard to keep straight which `U.model` goes to which subpopulation. It is best to sketch your **Z** matrix (which tells you which site in the rows corresponds to which subpopulation in the columns). Then remember that the elements of `U.model` correspond one-to-one with the columns of **Z**:

`U.model=matrix(c(col 1 Z, col 2 Z, col 3 Z, ..),m,1)`.

Specify `Q.groups` showing which subpopulations share their process variance parameter.

- Hypothesis 1: `Q.model=`
- Hypothesis 2: `Q.model=`
- Hypothesis 3: `Q.model=`
- Hypothesis 4: `Q.model=`

`Q.model` will be specified using the matrix of class list again. For example,

```
Q.model=matrix(list(0),3,3)
diag(Q.model)=c("q1","q2","q3")
```

`R.model` is set so that the observation variances are the same for each site.

12.3.3 Fit the models and summarize results

Fit each model for each hypothesis to the seal data. Each call to `MARSS()` will look like

```
kem = MARSS(sealData, model=list(Z = Z.model,
  Q = Q.model, R = R.model, U = U.model))
```

Table 12.2. Table to fill out for the four hypotheses from the second analysis (Section 12.3). The code of the form `$foo$bar` shows you what to type at the command line to output each parameter or metric. Remember to add the name of the model fit, e.g. `kem$foo$bar` where `kem` is the name you gave to the model fit.

H	pop. growth rate `$par$U`	proc. variance `$par$Q`	obs. variance `$par$R`	K `$num. params`	log-like `$logLik`	AIC `$AIC`	AICc `$AICc`
1							
2							
3							
4							

12.3.4 Interpret results for question 2

How do the residuals for the Hood Canal site compare from these models relative to the best model from question 1? Hint: If you have the vector of estimated population states (`Xpred = t(kem$states)`) and the data (`Xobs = sealData`), the residuals for site i can be plotted in R as:

```
Xpred = t(kem$states)
Xobs = sealData
plot(Xpred[, Z.model[i]] - Xobs[,i],
      ylab="Predicted-Observed Data")
```

In R , if you have a matrix `Y[1:numYrs, 1:n]`, you can extract column j by writing `Yj = Y[,j]`.

Relative to the previous models from question 1, do these scenarios have better or worse AIC scores (smaller AIC is better)? If you were to provide advice to managers, would you recommend that the Hood Canal population is a source or sink? What implications does this have for population persistence?

Code for Case Study 3
Type `RShowDoc("Case_study_3.R",package="MARSS")` to open a file in R with all the example code.

13

Case Study 4: Dynamic Factor Analysis (DFA) with MARSS

13.1 Dynamic Factor Analysis

In this case study, we use MARSS to do Dynamic Factor Analysis (DFA), which allows us to look for a set of common underlying trends among a relatively large set of time series (Harvey, 1989, sec. 8.5). This is conceptually different than what we have been doing in the previous case studies. Here we are trying to explain temporal variation in a set of n time series using linear combinations of a set of m hidden random walks, where $m << n$. Zuur et al. (2003) show a number of examples of DFA applied to fisheries catch data and densitites of zoobenthos.

A DFA model is a type of MARSS model with the following structure:

$$\begin{aligned} \mathbf{x}_t &= \mathbf{x}_{t-1} + \mathbf{w}_t \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}) \\ \mathbf{y}_t &= \mathbf{Z}\mathbf{x}_t + \mathbf{a} + \mathbf{v}_t \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}) \\ \mathbf{x}_0 &\sim \text{MVN}(\boldsymbol{\pi}, \boldsymbol{\Lambda}) \end{aligned} \tag{13.1}$$

The general idea is that the observations ($\mathbf{y}$) are modeled as a linear combination of hidden trends ($\mathbf{x}$) and factor loadings ($\mathbf{Z}$) plus some offsets ($\mathbf{a}$). The DFA model in Equation 13.11 and the standard MARSS model in Equation 1.1 are equivalent–we have simply set the matrix $\mathbf{B} = \mathbf{I}_m$[1] and the vector $\mathbf{u} = \mathbf{0}$.

13.1.1 Writing out the model

Imagine a case where we had a data set with six observed time series ($n = 6$) and we want to fit a model with three hidden trends ($m = 3$). If we write out our DFA model in MARSS matrix form (ignoring the error structures and initial conditions for now), it would look like this:

[1] $\mathbf{I}_m$ is an $m \times m$ identity matrix (i.e., a diagonal matrix with 1's on the diagonal and 0's elsewhere).

$$\begin{bmatrix} x_{1,t} \\ x_{2,t} \\ x_{3,t} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_{1,t-1} \\ x_{2,t-1} \\ x_{3,t-1} \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} w_{1,t} \\ w_{2,t} \\ w_{3,t} \end{bmatrix}$$

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \\ y_{6,t} \end{bmatrix} = \begin{bmatrix} z_{11} & z_{12} & z_{13} \\ z_{21} & z_{22} & z_{23} \\ z_{31} & z_{32} & z_{33} \\ z_{41} & z_{42} & z_{43} \\ z_{51} & z_{52} & z_{53} \\ z_{61} & z_{62} & z_{63} \end{bmatrix} \begin{bmatrix} x_{1,t} \\ x_{2,t} \\ x_{3,t} \end{bmatrix} + \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \\ v_{6,t} \end{bmatrix}. \tag{13.2}$$

The process errors of the hidden trends would be

$$\begin{bmatrix} w_{1,t} \\ w_{2,t} \\ w_{3,t} \end{bmatrix} \sim \text{MVN}\left(\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \end{bmatrix} \right), \tag{13.3}$$

and the observation errors would be

$$\begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \\ v_{6,t} \end{bmatrix} \sim \text{MVN}\left(\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} r_{11} & r_{12} & r_{13} & r_{14} & r_{15} & r_{16} \\ r_{21} & r_{22} & r_{23} & r_{24} & r_{25} & r_{26} \\ r_{31} & r_{32} & r_{33} & r_{34} & r_{35} & r_{36} \\ r_{41} & r_{42} & r_{43} & r_{44} & r_{45} & r_{46} \\ r_{51} & r_{52} & r_{53} & r_{54} & r_{55} & r_{56} \\ r_{61} & r_{62} & r_{63} & r_{64} & r_{65} & r_{66} \end{bmatrix} \right). \tag{13.4}$$

13.1.2 Constraints to ensure identifiability

If $\mathbf{Z}$, $\mathbf{a}$, and $\mathbf{Q}$ in Equation 13.11 are not constrained, then the DFA model above is unidentifiable (Harvey, 1989, sec 4.4). Harvey (1989, sec. 8.5.1), suggests the following parameter constraints to make the model identifiable:

- in the first $m-1$ rows of $\mathbf{Z}$, the z-value in the j-th column and i-th row is set to zero if $j > i$;
- $\mathbf{a}$ is constrained so that the first m values are set to zero; and
- $\mathbf{Q}$ is set equal to the identity matrix ($\mathbf{I}_m$).

Zuur et al. (2003), however, note that with Harvey's second constraint, the EM-algorithm is not particularly robust, and it takes a long time to converge. Zuur et al. show that the EM estimates are much better behaved if you instead constrain each of the time-series in $\mathbf{x}$ to have a mean of zero across $t = 1$ to T. To do so, replace the estimates of the hidden states, $\mathbf{x}_t^T$, coming out of the Kalman smoother with $\mathbf{x}_t^T - \bar{\mathbf{x}}$ for $t = 1$ to T (*NOTE*: $\bar{\mathbf{x}}$ is the mean of $\mathbf{x}_t$ across t, not m). With this approach, you estimate all of the $\mathbf{a}$ elements, which represent the average level of $\mathbf{y}_t$ relative to $\mathbf{Z}(\mathbf{x}_t - \bar{\mathbf{x}})$ (However, we will

demean our data and thus will set **a** to zero). Forcing the hidden states to have a mean of zero is easily implemented in the `MARSS()` function by setting the control value `demean.states=TRUE`.

Using these constraints, the DFA model in Equation 13.2 becomes

$$\begin{bmatrix} x_{1,t} \\ x_{2,t} \\ x_{3,t} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_{1,t-1} \\ x_{2,t-1} \\ x_{3,t-1} \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} w_{1,t} \\ w_{2,t} \\ w_{3,t} \end{bmatrix}$$

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \\ y_{6,t} \end{bmatrix} = \begin{bmatrix} z_{11} & 0 & 0 \\ z_{21} & z_{22} & 0 \\ z_{31} & z_{32} & z_{33} \\ z_{41} & z_{42} & z_{43} \\ z_{51} & z_{52} & z_{53} \\ z_{61} & z_{62} & z_{63} \end{bmatrix} \begin{bmatrix} x_{1,t} \\ x_{2,t} \\ x_{3,t} \end{bmatrix} + \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \\ v_{6,t} \end{bmatrix}. \tag{13.5}$$

The process errors of the hidden trends in Equation 13.3 would then become

$$\begin{bmatrix} w_{1,t} \\ w_{2,t} \\ w_{3,t} \end{bmatrix} \sim \text{MVN}\left(\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \right), \tag{13.6}$$

but the observation errors in Equation 13.4 would stay the same, such that

$$\begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \\ v_{6,t} \end{bmatrix} \sim \text{MVN}\left(\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} r_{11} & r_{12} & r_{13} & r_{14} & r_{15} & r_{16} \\ r_{21} & r_{22} & r_{23} & r_{24} & r_{25} & r_{26} \\ r_{31} & r_{32} & r_{33} & r_{34} & r_{35} & r_{36} \\ r_{41} & r_{42} & r_{43} & r_{44} & r_{45} & r_{46} \\ r_{51} & r_{52} & r_{53} & r_{54} & r_{55} & r_{56} \\ r_{61} & r_{62} & r_{63} & r_{64} & r_{65} & r_{66} \end{bmatrix} \right). \tag{13.7}$$

To complete our model, we still need the final form for the initial conditions of the state. Following Zuur et al. (2003), we set the initial state vector ($\mathbf{x}_0$) to have zero mean and a diagonal variance-covariance matrix with large variances, such that

$$\mathbf{x}_0 \sim \text{MVN}\left(\begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 5 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 5 \end{bmatrix} \right). \tag{13.8}$$

13.2 The data

For this case study, we will analyze some of the Lake Washington plankton data included in the MARSS package. This dataset includes 33 years of

monthly counts for 13 plankton species along with data on water temperature, total phosphorous (TP), and pH. First, we load the data and then extract a subset of columns corresponding to the phytoplankton species only.

```
# load the data
data(lakeWAplankton)
# use only the data from 1977 onward
dat.spp.1977 = lakeWAplankton[lakeWAplankton[,"Year"]>=1977,]
# create vector of phytoplankton group names
phytoplankton = c("Cryptomonas", "Diatoms", "Greens",
                  "Bluegreens", "Unicells", "Other.algae")
# get only the phytoplankton
dat.spp.1977 = dat.spp.1977[,phytoplankton]
```

Next, we transpose the data and calculate the number of time series and their length.

```
# transpose data so time goes across columns
dat.spp.1977 = t(dat.spp.1977)
# get number of time series
N.ts = dim(dat.spp.1977)[1]
# get length of time series
TT = dim(dat.spp.1977)[2]
```

It is normal in this type of analysis to standardize each time series by first substracting its mean and then dividing by its standard deviation (i.e., create a z-score $\mathbf{y}_t^*$ with mean = 0 and SD = 1), such that

$$\mathbf{y}_t^* = \blacksquare^{-1}(\mathbf{y}_t - \bar{\mathbf{y}}),$$

$\blacksquare$ is a diagonal matrix with the standard deviations of each time series along the diagonal, and $\bar{\mathbf{y}}$ is a vector of the means. In R, this can be done as follows

```
Sigma = sqrt(apply(dat.spp.1977, 1, var, na.rm=TRUE))
y.bar = apply(dat.spp.1977, 1, mean, na.rm=TRUE)
dat.z = (dat.spp.1977 - y.bar) * (1/Sigma)
rownames(dat.z) = rownames(dat.spp.1977)
```

Figure 13.1 shows time series of Lake Washington phytoplankton data following z-score transformation.

13.3 Setting up the model in MARSS

As we have seen in other cases, setting up the model structure for MARSS requires that the parameter matrices have a one-to-one correspondence to the model as you would write it on paper (i.e., Equations 13.5 through 13.8). If a parameter matrix has a combination of fixed and estimated values, then you

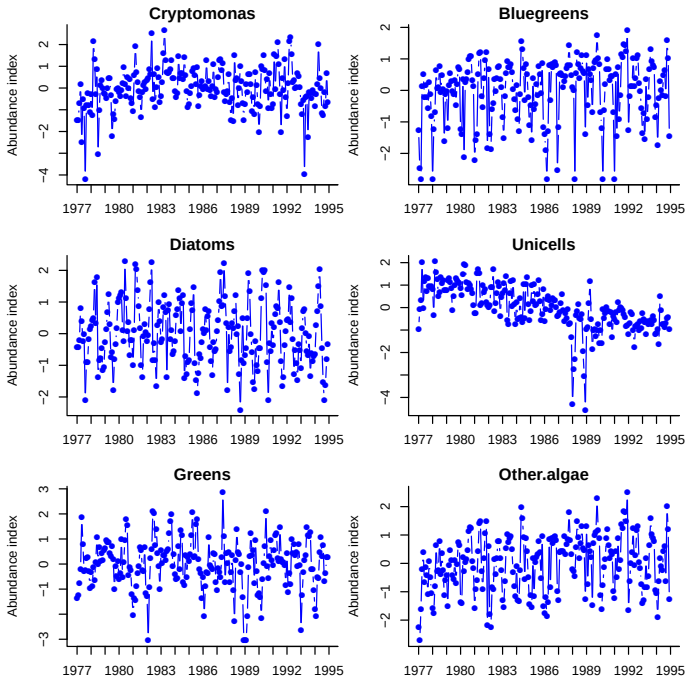

Fig. 13.1. Time series of Lake Washington phytoplankton data following z-score transformation.

specify that using `matrix(list(), nrow, ncol)`. This is a matrix of class list and allows you to combine numeric and character values in a single matrix. MARSS recognizes the numeric values as fixed values and the character values as estimated values.

This is how we set up **Z** for MARSS:

```
Z.vals = list(
"z11",  0  ,  0  ,
"z21","z22",  0  ,
"z31","z32","z33",
"z41","z42","z43",
"z51","z52","z53",
"z61","z62","z63")
Z = matrix(Z.vals, nrow=N.ts, ncol=3, byrow=TRUE)
```

When specifying the list values, spacing and carriage returns were added to help show the correspondence with the **Z** matrix in Equation 13.3. If you print **Z** (at the `R` command line), you will see that it is a matrix with character values (the estimated elements) and numeric values (the fixed 0's).

```
print(Z)
```

```
     [,1]  [,2]  [,3]
[1,] "z11" 0     0
[2,] "z21" "z22" 0
[3,] "z31" "z32" "z33"
[4,] "z41" "z42" "z43"
[5,] "z51" "z52" "z53"
[6,] "z61" "z62" "z63"
```

Notice that the `0`'s do not have quotes around them. If they did, it would mean the `"0"` is a character value and would be interpreted as the name of a parameter to be estimated rather than a fixed numeric value.
The parameter vector **a** is set up similarly.

```
A.vals = list("a1","a2","a3","a4","a5","a6")
A = matrix(A.vals, nrow=N.ts, ncol=1)
```

However, there are no missing values in the Lake Washington plankton dataset and we have demeaned the data. Therefore we can set $\mathbf{a} = 0$.
The **Q** and **B** matrices are both set equal to the identity matrix using `diag()`.

```
Q = B = diag(1,3)
```

For our first analysis, we will assume that each time series of phytoplankton has a different observation variance, but that there is no covariance among time series. Thus, **R** should be a diagonal matrix that looks like:

$$\begin{bmatrix} r_{11} & 0 & 0 & 0 & 0 & 0 \\ 0 & r_{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & r_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & r_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & r_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & r_{66} \end{bmatrix},$$

and each of the r_{ii} values is a different parameter to be estimated. We can also specify this **R** structure using a list matrix as follows:

```
R.vals = list(
"r11",0,0,0,0,0,
0,"r22",0,0,0,0,
0,0,"r33",0,0,0,
0,0,0,"r44",0,0,
0,0,0,0,"r55",0,
0,0,0,0,0,"r66")
R = matrix(R.vals, nrow=N.ts, ncol=N.ts, byrow=TRUE)
```

You can print **R** at the `R` command line to see what it looks like:

```
print(R)
```

```
     [,1]  [,2]  [,3]  [,4]  [,5]  [,6]
[1,] "r11" 0     0     0     0     0
[2,] 0     "r22" 0     0     0     0
[3,] 0     0     "r33" 0     0     0
[4,] 0     0     0     "r44" 0     0
[5,] 0     0     0     0     "r55" 0
[6,] 0     0     0     0     0     "r66"
```

It turns out that this form of variance-covariance matrix is commonly used, and therefore MARSS has a built-in shorthand for this structure. Alternatively, we could simply type:

```
R = "diagonal and unequal"
```

As mentioned in earlier chapters, there are other shorthand notations for many of the common parameter structures. Type ?MARSS at the `R` command line to see a list of the shorthand options for each parameter vector/matrix.

The parameter vectors π (termed `x0` in MARSS) and $\mathbf{u}$ are each set to be a column vector of zeros. Either of the following can be used:

```
x0 = U = matrix(0, nrow=3, ncol=1)
x0 = U = "zero"
```

The Λ matrix (termed `V0` in MARSS) is a diagonal matrix with 5's along the diagonal:

```
V0 = diag(5,3)
```

Finally, we make a list of the model parameters to pass to the `MARSS()` function and set the control list:

```
dfa.model = list(Z=Z, A="zero", R=R, B=B, U=U, Q=Q, x0=x0, V0=V0)
cntl.list = list(demean.states=TRUE, maxit=50)
```

For example purposes so that the code runs quicker, we set the maximum iterations to 50. The parameter estimates will not have converged to the maximum likelihood values. That would take closer to 1000 iterations, but that takes a long time so we set the maximum iterations lower so you can see results quicker.

13.3.1 Fitting the model

We can now pass the DFA model list to `MARSS()` to estimate the $\mathbf{Z}$ matrix and underlying hidden states ($\mathbf{x}$). The output is not shown because it is voluminous.

```
kemz.3 = MARSS(dat.z, model=dfa.model, control=cntl.list)
```

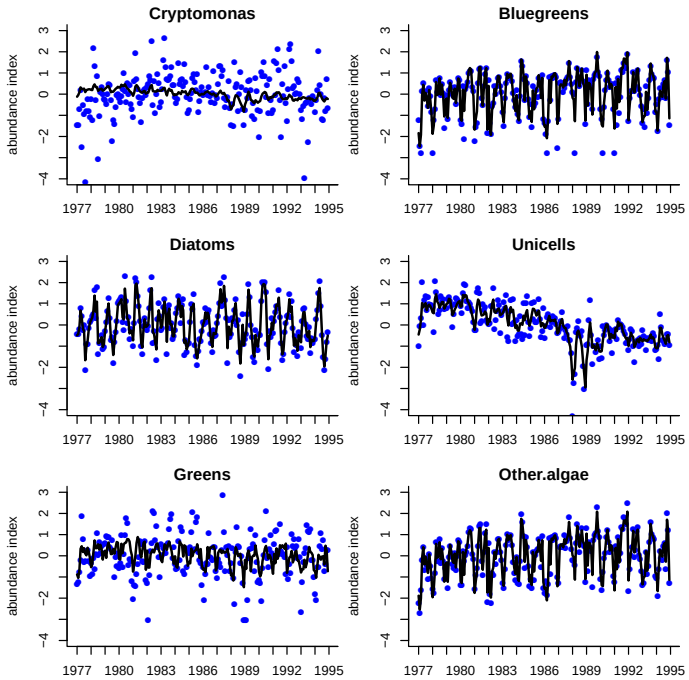

Fig. 13.2. Plots of Lake Washington phytoplankton data with model fits (dark lines) from a model with 3 trends and a diagonal and unequal variance-covariance matrix for the observation errors.

13.4 Using model selection to determine the number of trends

Following Zuur et al. (2003), we use model selection criteria (specifically AICc) to determine the number of underlying trends that have the highest data support. Our first model had three underlying trends ($m = 3$). Let's compare this to a model with two underlying trends. The forms for parameter matrix **R** and vector **a** will stay the same but we need to change the other parameter vectors and matrices because m is different.

After showing you the matrix math behind a DFA model, we will now use the `form` argument for a MARSS call to specify that we want to fit a DFA model. This will set up the **Z** matrix and the other parameters for you. Specify how many trends you want by passing in `model=list(m=x)`. You can also pass in different forms for the **R** matrix in the usual way.

Bere is how to fit two trends using `form="dfa"`:

```
model.list=list(m=2,R="diagonal and unequal")
kemz.2 = MARSS(dat.spp.1977, model=model.list,
    z.score=TRUE, form="dfa", control=cntl.list)
```

```
Success! Parameters converged at 28 iterations.
Alert: conv.test.slope.tol is 0.5.
Test with smaller values (<0.1) to ensure convergence.

MARSS fit is
Estimation method: kem
Estimation converged in 28 iterations.
Log-likelihood: -1597.725
AIC: 3229.451   AICc: 3229.929

         Estimate
Z.11       0.4866
Z.21       0.4832
Z.31       0.3020
Z.41       0.4679
Z.51       0.2703
Z.61       0.5117
Z.22      -0.2968
Z.32       0.2739
Z.42       0.8390
Z.52      -0.1205
Z.62       0.8468
R.R(1,1)   0.6483
R.R(2,2)   0.4131
R.R(3,3)   0.8393
R.R(4,4)   0.1236
R.R(5,5)   0.8408
R.R(6,6)   0.0801

Standard errors have not been calculated.
Use MARSSparamCIs to compute CIs and bias estimates.
```

and compare its AICc value to that from the 3-trend model.

```
print(c(kemz.3$AICc, kemz.2$AICc))
```

```
[1] 3135.878 3229.929
```

It looks like a model with 3 trends has a lot more support from the data because its AICc value is about 90 units less than that for the 2-trend model.

13.4.1 Comparing many model structures

Now let's examine a larger suite of possible models. We will test from one to five underlying trends ($m = 1$ to 5) and three different structures for the **R** matrix:

1. diagonal and equal,
2. diagonal and unequal, and
3. unconstrained.

The following code builds our model matrices; you could also write out each matrix as we did in the first example, but this allows us to build and run all of the models together.

```
# set up forms of R matrices
levels.R = c("diagonal and equal",
             "diagonal and unequal",
             "unconstrained")
model.data = data.frame()
# fit lots of models & store results
for(R in levels.R) {
    for(m in 1:(N.ts-1)) {
        dfa.model = list(A="zero", R=R, m=m)
        kemz = MARSS(dat.spp.1977, model=dfa.model, control=cntl.list,
            form="dfa", z.score=TRUE)
        model.data = rbind(model.data,
                           data.frame(R=R,
                                      m=m,
                                      logLik=kemz$logLik,
                                      K=kemz$num.params,
                                      AICc=kemz$AICc,
                                      stringsAsFactors=FALSE))
        assign(paste("kemz", m, R, sep="."), kemz)
        } # end m loop
    } # end R loop
```

Model selection results are shown in Table 13.1. The model with lowest AICc has 4 trends and an unconstrained **R** matrix. It also appears that, in general, models with an unconstrained **R** matrix fit the data much better than those models with less complex structures for the observation errors (i.e., models with unconstrained forms for **R** had all of the AICc weight).

Table 13.1. Model selection results.

R	m	logLik	AICc	delta.AICc	Ak.wt	Ak.wt.cum
unconstrained	3	-1471.5	3017	0.0	1.00	1.00
unconstrained	4	-1478.1	3037	19.6	0.00	1.00
unconstrained	5	-1481.9	3049	31.4	0.00	1.00
unconstrained	2	-1493.4	3052	35.3	0.00	1.00
diagonal and unequal	5	-1520.2	3094	76.5	0.00	1.00
diagonal and unequal	4	-1529.1	3107	90.0	0.00	1.00
diagonal and equal	5	-1544.9	3132	115.4	0.00	1.00
diagonal and unequal	3	-1546.6	3136	118.8	0.00	1.00
diagonal and equal	4	-1586.5	3212	194.5	0.00	1.00
diagonal and unequal	2	-1597.7	3230	212.8	0.00	1.00
diagonal and equal	3	-1607.5	3247	230.2	0.00	1.00
unconstrained	1	-1604.3	3264	246.7	0.00	1.00
diagonal and unequal	1	-1644.7	3314	296.5	0.00	1.00
diagonal and equal	2	-1688.5	3401	384.1	0.00	1.00
diagonal and equal	1	-1770.4	3555	537.9	0.00	1.00

13.5 Using varimax rotation to determine the loadings and trends

As Harvey (1989, p. 450) discusses in section 8.5.1, there are multiple equivalent solutions to the dynamic factor loadings. We arbitrarily constrained $\mathbf{Z}$ in such a way to choose only one of these solutions, but fortunately the different solutions are equivalent, and they can be related to each other by a rotation matrix $\mathbf{H}$. Let $\mathbf{H}$ be any $m \times m$ non-singular matrix. The following are then equivalent solutions:

$$\begin{aligned} \mathbf{y}_t &= \mathbf{Z}\mathbf{x}_t + \mathbf{a} + \mathbf{v}_t \\ \mathbf{x}_t &= \mathbf{x}_{t-1} + \mathbf{w}_t \end{aligned} \tag{13.9}$$

and

$$\begin{aligned} \mathbf{y}_t &= \mathbf{Z}\mathbf{H}^{-1}\mathbf{H}\mathbf{x}_t + \mathbf{a} + \mathbf{v}_t \\ \mathbf{H}\mathbf{x}_t &= \mathbf{H}\mathbf{x}_{t-1} + \mathbf{H}\mathbf{w}_t \end{aligned} \tag{13.10}$$

There are many ways of doing factor rotations, but a common approach is the varimax rotation which seeks a rotation matrix $\mathbf{H}$ that creates the largest difference beween loadings. For example, let's say there are three trends in our model. In our estimated $\mathbf{Z}$ matrix, let's say row 3 is $(0.2, 0.2, 0.2)$. That would mean that data series 3 is equally described by trends 1, 2, and 3. If instead row 3 was $(0.8, 0.1, 0.1)$, this would make interpretation easier because we could say that data time series 3 was mostly described by trend 1. The varimax rotation finds the $\mathbf{H}$ matrix that makes the $\mathbf{Z}$ rows more like $(0.8, 0.1, 0.1)$ and less like $(0.2, 0.2, 0.2)$.

The varimax rotation is easy to compute because R has a built in function for this. To do so, we first get the model fits from the highest ranked model.

```
# get the "best" model
best.model = model.tbl[1,]
fitname = paste("kemz",best.model$m,best.model$R,sep=".")
best.fit = get(fitname)
```

Next, we retrieve the matrix used for varimax rotation.

```
# get the inverse of the rotation matrix
H.inv = varimax(parmat(best.fit)$Z)$rotmat
```

Finally, we use $\mathbf{H}^{-1}$ to rotate the factor loadings and $\mathbf{H}$ to rotate the trends as in Equation 13.10.

```
# rotate factor loadings
Z.rot = parmat(best.fit)$Z %*% H.inv
# rotate trends
trends.rot = solve(H.inv) %*% best.fit$states
```

Rotated factor loadings for the best model are shown in Figure 13.3. Oddly, some taxa appear to have no loadings on some trends (e.g., bluegreens on trend 2). The reason is that, merely for display puroposes, we chose to plot only those loadings that are greater than 0.05, and it turns out that after varimax rotation, several loadings are close to 0. This is interesting given the pronounced shape of trend 4 (Figure 13.4). If we compare the loadings on trends 1-3 to those from a model with $m = 3$ (instead of $m = 4$), we would see that they are quite similar. This suggests that we might choose the model with $m = 3$ (2nd row in table) instead of $m = 4$.

Recall that we set $\mathrm{Var}(\mathbf{w}_t) = \mathbf{Q} = \mathbf{I}_m$ in order to make our DFA model identifiable. Does the variance in the process errors also change following varimax rotation? Interestingly, no. Because $\mathbf{H}$ is a non-singular, orthogonal matrix, $\mathrm{Var}(\mathbf{H}\mathbf{w}_t) = \mathbf{H}\mathrm{Var}(\mathbf{w}_t)\mathbf{H}^\top = \mathbf{H}\mathbf{I}_m\mathbf{H}^\top = \mathbf{I}_m$.

13.6 Examining model fits

Now that we have found a "best" model and done the appropriate factor and trends rotations, we should examine some plots of model fits (see Figure 13.5). First, it looks like the model did an adequate job of capturing some of the high frequency variation (i.e., seasonality) in the time series. Second, some of the time series had much better overall fits than others (e.g., compare Diatoms versus Cryptomonas). Given the obvious seasonal patterns in the phytoplankton data, it might be worthwhile to first "detrend" the data and then repeat the model fitting exercise to see (1) how many trends would be favored, and (2) the shape of those trends.

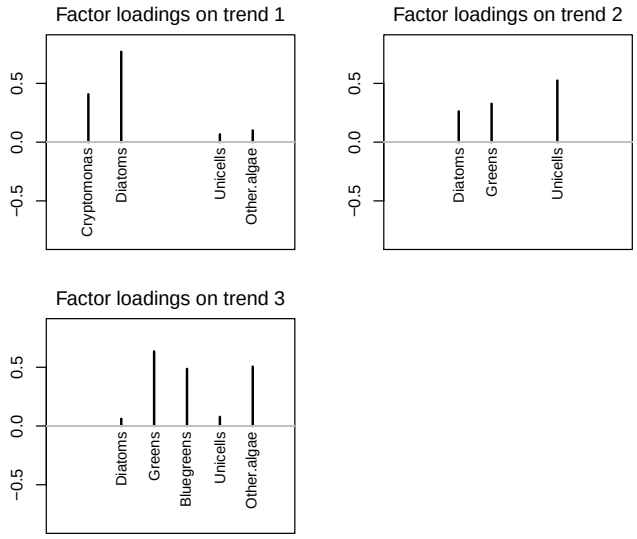

Fig. 13.3. Plot of the factor loadings (following varimax rotation) from the best model fit to the phytoplankton data.

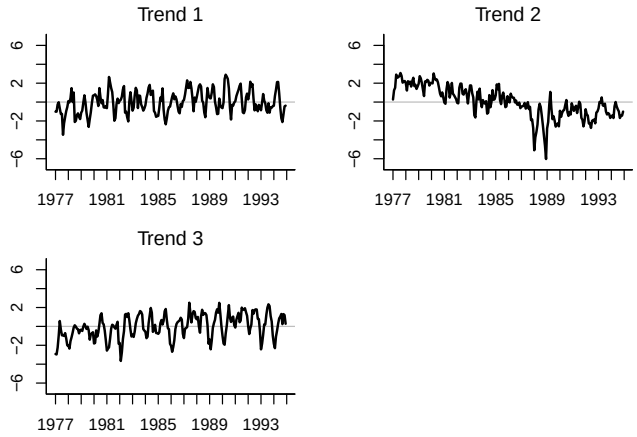

Fig. 13.4. Plot of the unobserved trends (following varimax rotation) from the best model fit to the phytoplankton data.

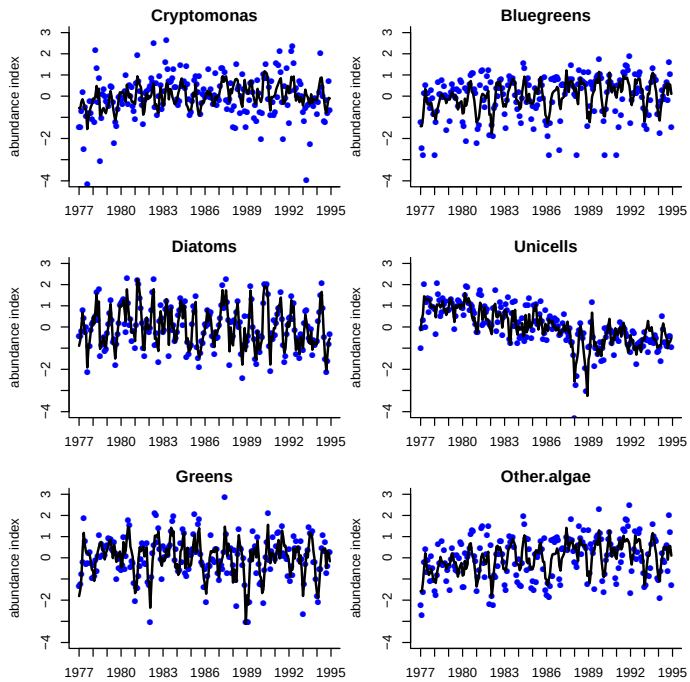

Fig. 13.5. Plot of the "best" model fits to the phytoplankton data.

13.7 Adding covariates

It is standard to add covariates to the analysis so that one removes known important drivers. The DFA with covariates is written:

$$\begin{aligned} \mathbf{x}_t &= \mathbf{x}_{t-1} + \mathbf{w}_t \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}) \\ \mathbf{y}_t &= \mathbf{Z}\mathbf{x}_t + \mathbf{a} + \mathbf{D}\mathbf{d}_t + \mathbf{v}_t \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}) \\ \mathbf{x}_0 &\sim \text{MVN}(\pi, \Lambda) \end{aligned} \tag{13.11}$$

where the $\mathbf{d}_t$ are the covariates at time t. This way of including covariates means that the covariates are input, not data, and there can be no missing values in the covariates.

Using `form="dfa"`, we can easily add covariates to our DFA. The Lake Washington dataset has two environmental covariates, temperature and total phosphorous.

```
temp = t(lakeWAplankton[lakeWAplankton[,"Year"]>=1977,"Temp"])
TP = t(lakeWAplankton[lakeWAplankton[,"Year"]>=1977,"TP"])
```

We need the covariate inputs to have the same number of time steps as the variate data, thus we limit the covariate data to years afer 1977 also.

We

```
model.list=list(m=3,R="unconstrained")
kemz.temp = MARSS(dat.spp.1977, model=model.list,z.score=TRUE,form="dfa",
   control=cntl.list, covariates=temp)
kemz.TP = MARSS(dat.spp.1977, model=model.list,z.score=TRUE,form="dfa",
   control=cntl.list, covariates=TP)
kemz.both = MARSS(dat.spp.1977, model=model.list,z.score=TRUE,form="dfa",
   control=cntl.list, covariates=rbind(temp,TP))
```

We can then compare whether the addition of the covariates improves the model fit.

```
print(c(kemz.temp$AICc,kemz.TP$AICc,kemz.both$AICc))
```

```
[1] 2931.711 3089.863 3011.685
```

This suggests that using temperature as a covariate is warranted but total phosphorous does not add information. However, keep in mind that these results are using a low maximum number of iterations (`maxit=20`) and the fits have not converged yet.

When you fit the models, the output looks a bit odd as you will see terms like `A.D1` listed. MARSS works by recasting different models into MARSS(1) form, and in this case the **D** matrix appears in the **A** term of the equivalent MARSS(1) model. You can ignore the `A.` part and just focus on the `D` part which gives the name of the DFA parameter. When you write your own models, it is often useful to specify your own names for parameters. For example, we could use

```
D=matrix(c("D(Crypto,Temp)","D(Diatoms,Temp)",
  "D(Grn,Temp)","D(BG,Temp)","D(Uni,Temp)",
  "D(Other,Temp)"), 6,1)
```

That way the model output will remind us exactly what each **D** term means, e.g. the effect of temperature on Cryptomonas (z-scored) abundance.

13.8 Other models and data

We analyzed the phytoplankton data alone. You can try analyzing the zooplankton data (type `head(lakeWAplankton)`) to see the names. You can also try analyzing the phytoplankton and zooplankton together. You can also try different assumptions concerning the structure of **R**; we just tried unconstrained, diagonal and unequal, and diagonal and equal. To see all the `R` code behind the figures, type `RShowDoc("Case_study_4.R",package="MARSS")`. This opens a file with all the code. Copy and paste the code into a new file, and then you can edit that code. These models can take a long time to converge. In a real DFA, you will want to make sure to try different inits values and force the algorithm to run a long time by using `control=list(minit=x, maxit=(x+c))`, where `x` and `c` are something like 200 and 800, respectively.

14

Case Study 5: Using state-space models to analyze noisy animal tracking data

14.1 A simple random walk model of animal movement

A simple random walk model of movement with drift (directional movement) but no correlation is

$$x_{1,t} = x_{1,t-1} + u_1 + w_{1,t}, \;\; w_{1,t} \sim \mathrm{N}(0, \sigma_1^2) \tag{14.1}$$

$$x_{2,t} = x_{2,t-1} + u_2 + w_{2,t}, \;\; w_{2,t} \sim \mathrm{N}(0, \sigma_2^2) \tag{14.2}$$

where $x_{1,t}$ is the location at time t along one axis (here, longitude) and $x_{2,t}$ is for another, generally orthogonal, axis (in here, latitude). The parameter u_1 is the rate of longitudinal movement and u_2 is the rate of latitudinal movement. We add errors to our observations of location:

$$y_{1,t} = x_{1,t} + v_{1,t}, \;\; v_{1,t} \sim \mathrm{N}(0, \eta_1^2) \tag{14.3}$$

$$y_{2,t} = x_{2,t} + v_{2,t}, \;\; v_{2,t} \sim \mathrm{N}(0, \eta_2^2), \tag{14.4}$$

This model is actually comprised of two separate univariate state-space models. Note that y_1 depends only on x_1 and y_2 depends only on x_2. There are no actual interactions between these two univariate models. However, we can write the model down in the form of a multivariate model using diagonal variance-covariance matrices and a diagonal design ($\mathbf{Z}$) matrix. Because the variance-covariance matrices and $\mathbf{Z}$ are diagonal, the x_1:y_1 and x_2:y_2 processes will be independent as intended. Here are Equations 14.2 and 14.4 written as a MARSS model (in matrix form):

$$\begin{bmatrix} x_{1,t} \\ x_{2,t} \end{bmatrix} = \begin{bmatrix} x_{1,t-1} \\ x_{2,t-1} \end{bmatrix} + \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} + \begin{bmatrix} w_{1,t} \\ w_{2,t} \end{bmatrix}, \;\; \mathbf{w}_t \sim \mathrm{MVN}\left(0, \begin{bmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{bmatrix}\right) \tag{14.5}$$

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_{1,t} \\ x_{2,t} \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \end{bmatrix}, \;\; \mathbf{v}_t \sim \mathrm{MVN}\left(0, \begin{bmatrix} \eta_1^2 & 0 \\ 0 & \eta_2^2 \end{bmatrix}\right) \tag{14.6}$$

The variance-covariance matrix for $\mathbf{w}_t$ is a diagonal matrix with unequal variances, σ_1^2 and σ_2^2. The variance-covariance matrix for $\mathbf{v}_t$ is a diagonal matrix with unequal variances, η_1^2 and η_2^2. We can write this succinctly as

$$\mathbf{x}_t = \mathbf{x}_{t-1} + \mathbf{u} + \mathbf{w}_t, \;\; \mathbf{w}_t \sim \mathrm{MVN}(0, \mathbf{Q}) \tag{14.7}$$

$$\mathbf{y}_t = \mathbf{Z}\mathbf{x}_t + \mathbf{v}_t, \;\; \mathbf{v}_t \sim \mathrm{MVN}(0, \mathbf{R}). \tag{14.8}$$

The $\mathbf{Z}$ matrix is a 2×2 identity matrix.

14.2 The problem

Loggerhead sea turtles (*Caretta caretta*) are listed as threatened under the United States Endangered Species Act of 1973. Over the last ten years, a number of state and local agencies have been deploying ARGOS tags on loggerhead turtles on the east coast of the United States. We have data on eight individuals over that period. In this case study, we use some turtle data from the WhaleNet Archive of STOP Data, however we have corrupted this data severely by adding random errors in order to create a "Bad Tag" problem. We corrupted latitude and longitude data by errors (Figure 14.1) and it would appear that our sea turtles are becoming land turtles (at least part of the time).

For this case study, we will use the `MARSS()` function to estimate true positions and speeds from the corrupted data. We will use a mapping package to plot the results: the `maps` package. If you have not already, install this package by selecting the 'Packages' menu and then 'Install packages' and then select `maps`. If you are on a Mac, remember to select "binaries" for the package type. Type `RShowDoc("Case_study_5.R",package="MARSS")` to open a file in *R* with all *R* code to get you started on the analyses in this chapter.

14.3 Estimate locations from bad tag data

14.3.1 Read in the data and load `maps` package

Our noisy data are in `loggerheadNoisy`. They consist of daily readings of location (longitude/latitude). The data are recorded daily and `MARSS()` requires a data entry for each day. If data are missing for a day, then the entries for latitude and longitude for that day should be NA. However, to make this case study run quickly, we have interpolated all missing values in the original, uncorrupted, dataset (`loggerhead`). The corrupted data are a dataframe and the first six lines look like so

```
loggerheadNoisy[1:6,]
```

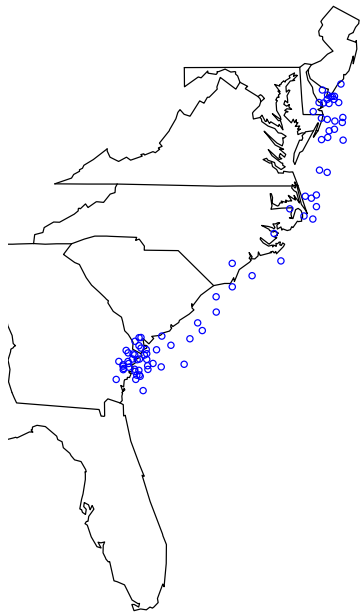

Fig. 14.1. Plot of the tag data from the turtle Big Mama. Errors in the location data make it seem that Big Mama has been moving overland.

```
   turtle month day year       lon      lat
1 BigMama     5  28 2001 -81.45989 31.70337
2 BigMama     5  29 2001 -80.88292 32.18865
3 BigMama     5  30 2001 -81.27393 31.67568
4 BigMama     5  31 2001 -81.59317 31.83092
5 BigMama     6   1 2001 -81.35969 32.12685
6 BigMama     6   2 2001 -81.15644 31.89568
```

The file has data for eight turtles:

```
levels(loggerheadNoisy$turtle)
```

```
[1] "BigMama"  "Bruiser"  "Humpty"   "Isabelle" "Johanna"
[6] "MaryLee"  "TBA"      "Yoto"
```

We will first analyze the position data for "Big Mama". We put the data for "Big Mama" into variable `dat`. `dat` is transposed because we need time across the columns.

```
turtlename="BigMama"
dat = loggerheadNoisy[which(loggerheadNoisy$turtle==turtlename),5:6]
dat = t(dat) #transpose
```

We will begin by specifying the structure of the MARSS model and then use `MARSS()` to fit that model to the data. There are two state processes (one for latitude and the other for longitude), and there is one observation time series for each state process. As we saw in Equation 14.6, $\mathbf{Z}$ is the an identity matrix (a diagonal matrix with 1s on the diagonal). We could specify this structure as `Z.model="identity"` or `Z.model=factor(c(1,2))`. Although technically, this is unnecessary as this is the default contraint for $\mathbf{Z}$.

We will assume that the errors are independent and that there are different drift rates (u), process variances (σ^2) and observation variances for latitude and longitude (η^2).

```
Z.model=factor(c(1,2))
U.model="unequal"
Q.model="diagonal and unequal"
R.model="diagonal and unequal"
```

Fit the model to the data:

```
kem = MARSS(dat, model=list(Z = Z.model,
      Q = Q.model, R = R.model, U = U.model))
```

14.3.2 Compare state estimates to the real positions

The real locations (from which `loggerheadNoisy` was produced by adding noise) are in `loggerhead`. In Figure 14.2, we compare the tracks estimated from the noisy data with the original, good, data (see `Case_Study_5.R` for the code to make this plot. There are only a few data points for the real data because in the real tag data, there are many missing days.

14.3.3 Estimate speeds for each turtle

Turtle biologists designated one of these loggerheads "Big Mama," presumably for her size and speed. For each of the eight turtles, estimate the average miles traveled per day. To calculate the distance traveled by a turtle each day, you use the estimate (from `MARSS()`) of the lat/lon location of turtle at day t and at day $t-1$. To calculate distance traveled in miles from lat/lon start and finish locations, we will use the function `GCDF` defined at the beginning of the *R* script, `Case_Study_5.R`):

```
distance[i-1]=GCDF(pred.lon[i-1],pred.lon[i],
                   pred.lat[i-1],pred.lat[i])
```

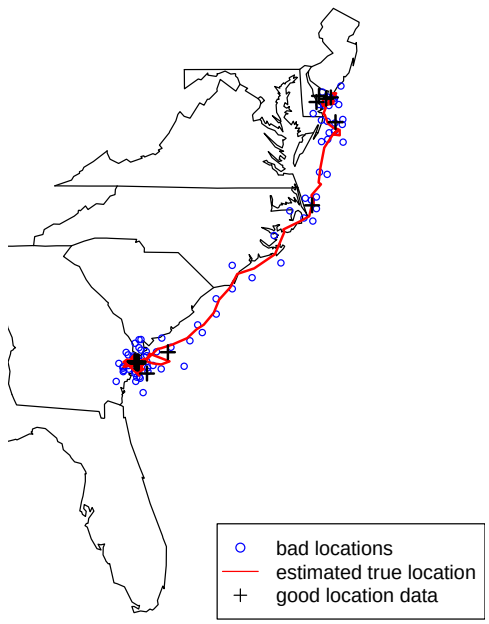

Fig. 14.2. Plot of the estimated track of the turtle Big Mama versus the good location data (before we corrupted it with noise).

`pred.lon` and `pred.lat` are the predicted longitudes and latitudes from `MARSS()`: rows one and two in `kem$states`. To calculate the distances for all days, we put this through a `for` loop:

```
distance = array(NA, dim=c(dim(dat)[2]-1,1))
for(i in 2:dim(dat)[2])
   distance[i-1]=GCDF(pred.lon[i-1],pred.lon[i],
      pred.lat[i-1],pred.lat[i])
```

The command `mean(distance)` gives us the average distance per day. We can also make a histogram of the distances traveled per day (Figure 14.3). Repeat the analysis done for "Big Mama" for each of the other turtles and fill out the speed table (Table 14.1).

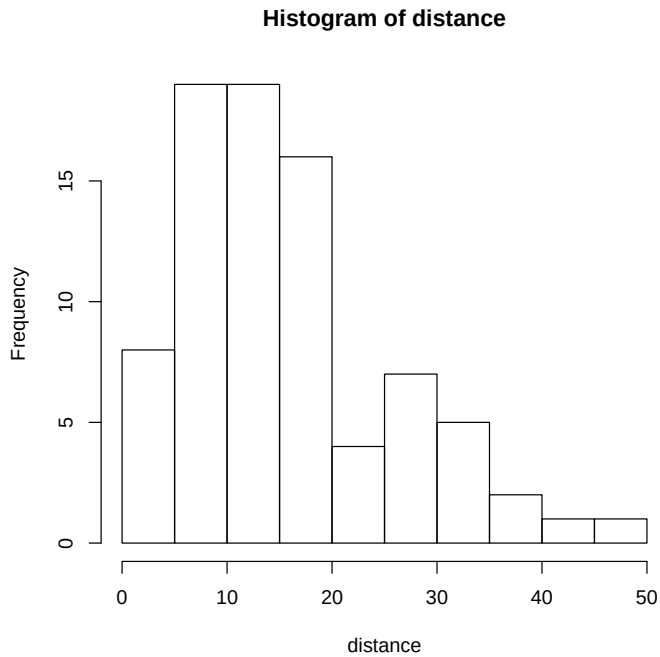

Fig. 14.3. Histogram of the miles traveled per day for Big Mama. Compare this to the estimate of miles traveled per day if you had not accounted for measurement errors. See the script file, `Case_Study_5.R`, for the code to do this.

14.4 Comparing turtle tracks to proposed fishing areas

One of the greatest threats to the long term viability of loggerhead turtles is incidental take by net/pot fisheries. Add two proposed fishing areas to your turtle plots:

```
# the proposed fishery areas
lines(c(-77,-78,-78,-77,-77),
      c(33.5,33.5,32.5,32.5,33.5),col="red",lwd=2)
lines(c(-75,-76,-76,-75,-75),
      c(38,38,37,37,38),col="red",lwd=2)
```

Given that only one area can be chosen as a future fishery, what do your predicted movement trajectories for our eight turtles tell you?

Table 14.1. Estimated speeds with location errors included in model versus speeds when we assume that the data have no location error.

Turtle	Location error included in model	Data assumed to be error free
Big Mama		
Bruiser		
Humpty		
Isabelle		
Johanna		
Mary Lee		
TBA		
Yoto		

14.5 Using specialized packages to analyze tag data

If you have real tag data to analyze, you should use a state-space modeling package that is customized for fitting MARSS models to tracking data. The MARSS package does not have all the bells and whistles that you would want for analyzing tracking data, particularly tracking data in the marine environment. These are a couple *R* packages that we have come across for this purpose:

UKFSST http://www.soest.hawaii.edu/tag-data/tracking/ukfsst/
KFTRACK http://www.soest.hawaii.edu/tag-data/tracking/kftrack/

`kftrack` is a full-featured toolbox for analyzing tag data with extended Kalman filtering. It incorporates a number of extensions that are important for analyzing track data: barriers to movement such as coastlines and non-Gaussian movement distributions. With `kftrack`, you can use the real tag data which has big gaps, i.e. days with no location. `MARSS()` will struggle with these data because it will estimate states for all the unseen days; `kftrack` only fits to the seen days.

To use `kftrack` to fit the turtle data, type

```
library(kftrack) # must be installed from a local zip file
loggerhead = loggerhead
# Run kftrack with the first turtle (BigMama)
```

```
turtlename = "BigMama"
dat = loggerhead[which(loggerhead$turtle == turtlename),2:6]
model = kftrack(dat, fix.first=F, fix.last=F,
       var.struct="uniform")
```

15

Case Study 6: Detection of outliers and structural breaks using MARSS

15.1 Detection of outliers and structural breaks

This case study is based on a short example shown on page 147-148 in Koopman et al. (1999) using a 100-year record of river flow on the Nile River. The methods are based on Harvey et al. (1998) which is in turn based on techniques in Harvey and Koopman (1992) and Koopman (1993). The Nile dataset is included in *R* . Figure 15.1 shows the data. To see all the *R* code behind the figures in the chapter, type `RShowDoc("Case_study_6.R",package="MARSS")`.

15.2 Different models for the Nile flow levels

We begin by fitting different flow models to the data and compare these models with AIC. After that, we will use the model residuals to look for outliers and structural breaks.

15.2.1 Flat level model

We will start by modeling these data as a simple average river flow with variability around this level.

$$y_t = a + v_t \text{ where } v_t \sim \mathrm{N}(0, r) \tag{15.1}$$

where y_t is the river flow volume at year t and x is some constant average flow level (notice it has no t subscript).

To fit this model with MARSS, we will explicitly show all the MARSS parameters.

$$\begin{aligned} x_t &= 1 \times x_{t-1} + 0 + w_t \text{ where } w_t \sim \mathrm{N}(0,0) \\ y_t &= 0 \times x_t + a + v_t \text{ where } v_t \sim \mathrm{N}(0,r) \\ x_0 &= 0 \end{aligned} \tag{15.2}$$

```
#load the datasets package
library(datasets)
data(Nile)   #load the data
plot(Nile,ylab="Flow volume",xlab="Year")
```

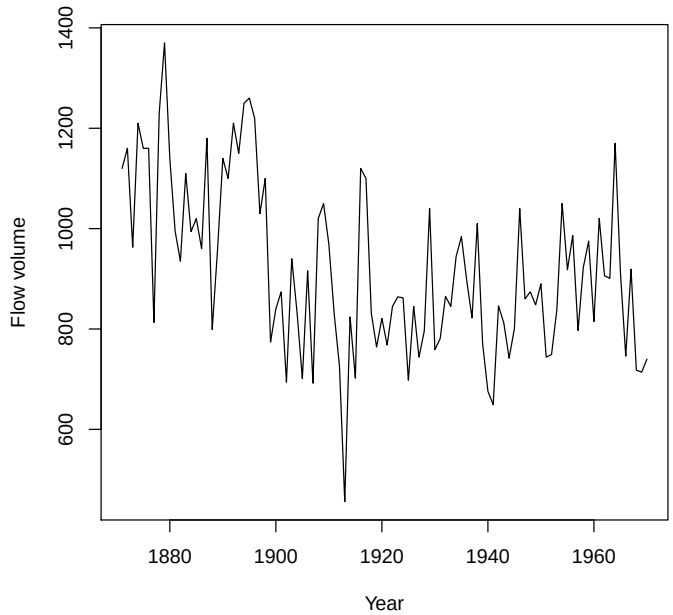

Fig. 15.1. The Nile River flow volume 1871 to 1970 (included dataset in *R*).

MARSS includes the state process x_t but we are setting $\mathbf{Z}$ to zero so that does not appear in our observation model. We need to fix all the state parameters to zero so that the algorithm doesn't "chase its tail" trying to fit x_t to the data.

An equivalent way to write this model is to use x_t as the average flow level and make it be a constant level by setting $q = 0$. The average flow appears as the x_0 parameter. In MARSS form, the model is then:

$$\begin{aligned} x_t &= 1 \times x_{t-1} + 0 + w_t \text{ where } w_t \sim \mathrm{N}(0,0) \\ y_t &= 1 \times x_t + 0 + v_t \text{ where } v_t \sim \mathrm{N}(0,r) \\ x_0 &= a \end{aligned} \tag{15.3}$$

We will use this latter format since we will be building on this form. The model is specified as a list as follows and we denote this model "0":

```
mod.nile.0 = list(
Z=matrix(1), A=matrix(0), R=matrix("r"),
B=matrix(1), U=matrix(0), Q=matrix(0),
x0=matrix("a")
)
```

We then fit the model with `MARSS()`:

```
#The data is in a ts format,
#and we need a matrix with time across columns
dat = t(as.matrix(Nile))
#Now we fit the model
kem.0 = MARSS(dat, model=mod.nile.0)
```

```
Success! algorithm run for 15 iterations and parameters converged.
Alert: conv.test.slope.tol is 0.5.
Test with smaller values (<0.1) to ensure convergence.

MARSS fit is
Estimation method: kem
Algorithm ran 15 (=minit) iterations and convergence was reached.
Log-likelihood: -654.5157
AIC: 1313.031   AICc: 1313.155

     Estimate
R.r     28352
x0.a      919

Standard errors have not been calculated.
Use MARSSparamCIs to compute CIs and bias estimates.
```

15.2.2 Linear trend in flow model

Figure 15.2 shows the fit for the flat average river flow model. Looking at the data, we might expect that a declining average river flow would be better. In MARSS form, that model would be:

$$\begin{aligned} x_t &= 1 \times x_{t-1} + u + w_t \text{ where } w_t \sim \mathrm{N}(0,0) \\ y_t &= 1 \times x_t + 0 + v_t \text{ where } v_t \sim \mathrm{N}(0,r) \\ x_0 &= a \end{aligned} \tag{15.4}$$

where u is now the average per-year decline in river flow volume. The model is specified as a list as follows and we denote this model "1":

```
mod.nile.1 = list(
Z=matrix(1), A=matrix(0), R=matrix("r"),
B=matrix(1), U=matrix("u"), Q=matrix(0),
```

```
x0=matrix("a")
)
```

We then fit the model with `MARSS()`:

```
kem.1 = MARSS(dat, model=mod.nile.1)
```

```
Success! algorithm run for 15 iterations and parameters converged.
Alert: conv.test.slope.tol is 0.5.
Test with smaller values (<0.1) to ensure convergence.

MARSS fit is
Estimation method: kem
Algorithm ran 15 (=minit) iterations and convergence was reached.
Log-likelihood: -642.3214
AIC: 1290.643   AICc: 1290.893

     Estimate
R.r  22217.87
U.u     -2.66
x0.a  1052.95

Standard errors have not been calculated.
Use MARSSparamCIs to compute CIs and bias estimates.
```

Figure 15.2 shows the fits for the two models with deterministic models (flat and declining) for mean river flow along with their AICc values (smaller AICc is better). The AICc for the model with a declining river flow is lower by over 20 (which is a lot).

15.2.3 Stochastic level model

Looking at the flow levels, we might suspect first that a model that allows the average flow to change would model the data better and we might suspect that there have been sudden, and anomalous, changes in the river flow level. We will now model the average river flow at year t as a random walk, specifically an autoregressive process which means that average river flow is year t is a function of average river flow in year $t-1$.

$$\begin{aligned} x_t &= x_{t-1} + w_t \text{ where } w_t \sim \mathrm{N}(0,q) \\ y_t &= x_t + v_t \text{ where } v_t \sim \mathrm{N}(0,r) \\ x_0 &= \pi \end{aligned} \tag{15.5}$$

As before, y_t is the river flow volume at year t. With all the MARSS parameters shown, the model is:

$$
\begin{aligned}
x_t &= 1 \times x_{t-1} + 0 + w_t \text{ where } w_t \sim \mathrm{N}(0,q) \\
y_t &= 1 \times x_t + 0 + v_t \text{ where } v_t \sim \mathrm{N}(0,r) \\
x_0 &= \pi
\end{aligned}
\tag{15.6}
$$

Thus, $\mathbf{Z} = 1$, $\mathbf{a} = 0$, $\mathbf{R} = r$, $\mathbf{B} = 1$, $\mathbf{u} = 0$, $\mathbf{Q} = q$, and $\mathbf{x}_0 = \pi$. The model is then specified as:

```
mod.nile.2 = list(
Z=matrix(1), A=matrix(0), R=matrix("r"),
B=matrix(1), U=matrix(0), Q=matrix("q"),
x0=matrix("pi")
)
```

We could also use the text shortcuts to specify the model. Because **R** and **Q** are 1×1 matrices, "unconstrained", "diagonal and unequal", "diagonal and equal" and "equalvarcov" will all lead to a 1×1 matrix with one estimated element. For **a** and **u**, the following shortcut could be used:

```
A=U="zero"
```

Because $\mathbf{x}_0$ is 1×1, it could be specified as "unequal", "equal" or "unconstrained".

We fit the model with the `MARSS()` function. We are using the "BFGS" algorithm to polish off the estimates, since it will get the maximum faster than the default EM algorithm as long as we start it close to the maximum.

```
kem.2em = MARSS(dat, model=mod.nile.2, silent=TRUE)
kem.2 = MARSS(dat, model=mod.nile.2,
  inits=kem.2em$par, method="BFGS")
```

```
Success! Converged in 13 iterations.
Function MARSSkf used for likelihood calculation.

MARSS fit is
Estimation method: BFGS
Estimation converged in 13 iterations.
Log-likelihood: -637.7462
AIC: 1281.492   AICc: 1281.742

      Estimate
R.r      15356
Q.q       1237
x0.pi     1114

Standard errors have not been calculated.
Use MARSSparamCIs to compute CIs and bias estimates.
```

This is the same model fit in Koopman et al. (1999, p. 148) except that we estimate x_1 as parameter rather than specifying x_1 via a diffuse prior. As

a result, the log-likelihood value and **R** and **Q** are a little different than in Koopman et al. (1999). To fit the model as Koopman et al. did, use the following specifications:

```
mod.nile.3 = list(
Z=matrix(1), A=matrix(0), R=matrix("r"),
B=matrix(1), U=matrix(0), Q=matrix("q"),
x0=matrix("pi"), tinitx=1, diffuse=TRUE
)
kem.3.koop=MARSS(dat, model=mod.nile.3,
  inits=kem.2em$par, method="BFGS")
```

```
Success! Converged in 12 iterations.
Function MARSSkf used for likelihood calculation.

MARSS fit is
Estimation method: BFGS
Estimation converged in 12 iterations.
Log-likelihood: -637.6043
AIC: 1281.209   AICc: 1281.459

      Estimate
R.r      15305
Q.q       1273
x0.pi     1114

Standard errors have not been calculated.
Use MARSSparamCIs to compute CIs and bias estimates.
```

Initial conditions are set using the results from the EM algorithm, otherwise the BFGS algorithm takes a long time. The `model$diffuse=TRUE` specification means to use a true diffuse prior (variance is infinite). When using a diffuse prior make sure that Λ in the model has a correlation structure that matches that of $\text{var}(\mathbf{x}_0)$ implied by the model. In our case, $\text{var}(\mathbf{x}_0)$ is scalar (1×1) so Λ has no structure. If you are unsure of the structure of the initial conditions, fit your model and look at `MLEobj$kf$VtT[,,1]`, which is the variance-covariance matrix for $(\mathbf{x}_1|\mathbf{y}_0)$ that is implied by your model. You want to be particularly alert for cases where Λ is specified as a diagonal variance-covariance matrix but `MLEobj$kf$VtT[,,1]` is not diagonal. You may need to set `control$trace=1` to add the `kf` list to your MLE object.

15.3 Observation and state residuals

Figure 15.2 shows the MARSS fits to the data. From these model fits, auxiliary residuals can be computed which contain information about whether the

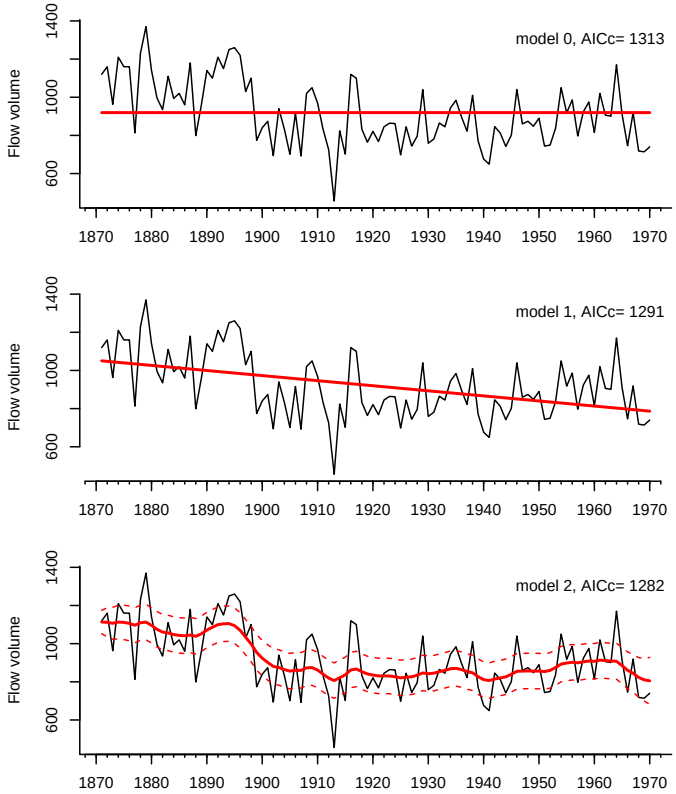

Fig. 15.2. The Nile River flow volume with the model estimated flow rates (solid lines). The bottom model is a stochastic level model, and the 2 standard deviations for the level are also shown. The other two models are deterministic level models so the state is not stochastic and does not have a standard deviation.

data and models fits at time t differ more than you would expect given the model and the model fits at time $t-1$. In this section, we follow the example shown on page 147-148 in Koopman et al. (1999) and use these residuals to look for outliers and sudden flow level changes. Using auxiliary residuals this way follows mainly from Harvey and Koopman (1992), but see slso Koopman (1993, sec. 3), de Jong and Penzer (1998) and Penzer (2001) for discussions of using auxiliary residuals for detection of outliers and structural breaks.

The MARSS function will output the expected values of x_t conditioned on the maximum-likelihood values of q, r, and x_1 and on the data (y). In time series literature, these are called the smoothed state estimates and they are output by the Kalman filter-smoother. We will call these smoothed estimates

$\hat{x}_t$ and from them, we can compute the model predicted value of y_t or $\hat{y}_t$:

$$\begin{aligned}\hat{x}_t &= \mathrm{E}(x_t|\hat{\theta}, y_1^T) \\ \hat{y}_t &= \mathrm{E}(y_t|\hat{\theta}, y_1^T) \\ &= \mathrm{E}(x_t|\hat{\theta}, y_1^T) + \mathrm{E}(w_t|\hat{\theta}, y_1^T) = \hat{x}_t\end{aligned} \tag{15.7}$$

where $\hat{\theta}$ are the maximum-likelihood estimates of the parameters. The $\hat{y}_t$ equation comes directly from equation (15.5).

15.3.1 Using observation residuals to detect outliers

The standardized smoothed observation residuals[1] are the difference between the data at time t and the model fit at time t conditioned on all the data standardized by the observation variance:

$$\begin{aligned}\hat{v}_t &= y_t - \hat{y}_t \\ e_t &= \frac{1}{\sqrt{\mathrm{var}(\hat{v}_t)}}\hat{v}_t\end{aligned} \tag{15.8}$$

These residuals should have (asymptotically) a t-distribution (Kohn and Ansley, 1989, sec. 3) and by looking at the residuals, we can identify potential outlier data points–or more accurately, we can identify data points that do not fit the model (Equation 15.5). The function `MARSSresids()` will compute these residuals. It returns the standardized residuals (also called auxiliary residuals) as a $n+m \times T$ matrix. The first n rows are the estimated $\mathbf{v}_t$ standardized observation residuals and the next m rows are the estimated $\mathbf{w}_t$ standardized state residuals (discussed below).

```
resids.0=MARSSresids(kem.0)$std.et
resids.1=MARSSresids(kem.1)$std.et
resids.2=MARSSresids(kem.2)$std.et
```

Figure 15.3 shows the observation residuals for the three models developed above. We immediately see that model 0 (flat level) and model 1 (linear declining level) have problems because the residuals are all positive for the first part of the time series and then all negative. The residuals should not be temporally correlated like that. Model 2 with a stochastic level shows well-behaving residuals with low temporal correlation between t and $t-1$. Looking at the residuals for model 2, we see that there are a number of years with flow levels that appear to be outliers (are beyond the dashed level lines).

[1] also called smoothations in the literature to distinguish them from innovations, which are $\mathbf{y}_t - \mathrm{E}(\mathbf{y}_t|\mathbf{y}_1^{t-1})$. Notice that for innovations the expectation is conditioned on the data up to time $t-1$ while for smoothations, we condition on all the data.

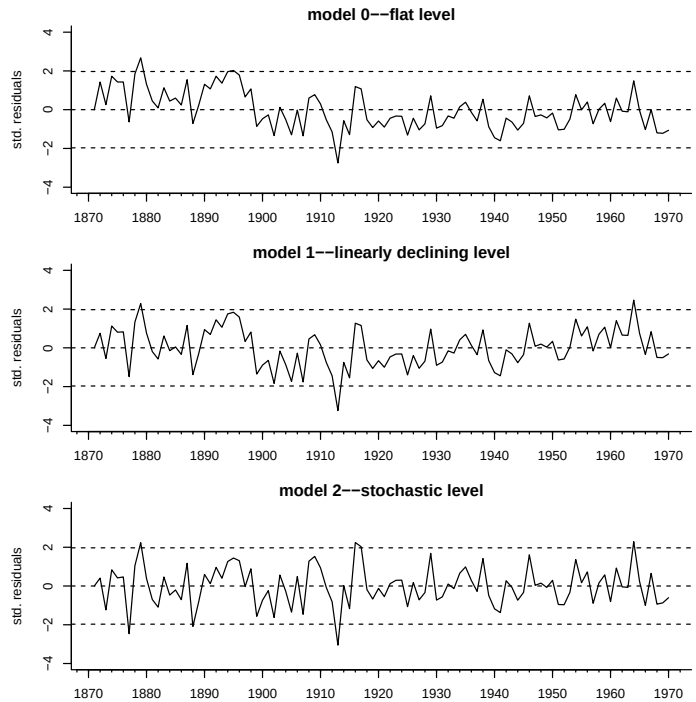

Fig. 15.3. The standardized observation residuals from models 0, 1, and 2. These residuals are the standardized $\hat{v}_t$. The dashed lines are the 95% CIs for a t-distribution.

15.3.2 Detecting sudden level changes

The standardized smoothed state residuals (f_t below) are the difference between the estimated state at time t and the estimated state at time $t-1$ conditioned on all the data standardized by the standard deviation:

$$\begin{aligned} \hat{w}_t &= \hat{x}_t - \hat{x}_{t-1} \\ f_t &= \frac{1}{\sqrt{\mathrm{var}(\hat{w}_t)}}\hat{w}_t \end{aligned} \tag{15.9}$$

These state residuals do not show simple changes in the average level; x_t is clearly changing in Figure 15.2, bottom panel. Instead we are looking for "breaks" or sudden changes in the level. The bottom panel of Figure 15.4 shows the standardized state residuals (f_t). This shows, as we can see by eye, the average flow level in the Nile appears to have suddenly changed around the turn of the century when the first Aswan dam was built. The top panel shows the standardized observaton residuals for comparison.

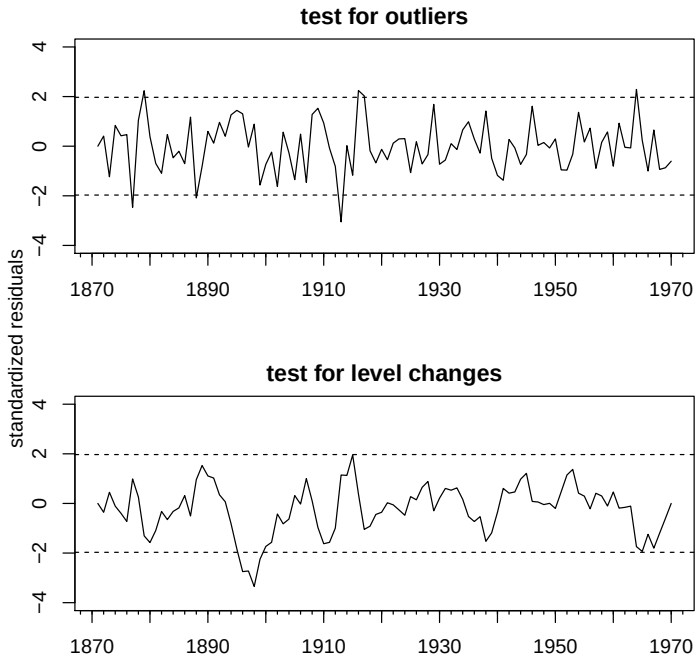

Fig. 15.4. Top panel, the standardized observation residuals. Bottom panel, the standardized state residuals. This replicates Figure 12 in Koopman et al. (1999).

16

Case Study 7: Estimation of species interaction strengths with and without covariates

16.1 Background

Multivariate autoregressive models (commonly termed MAR models) have been developed as a tool for analyzing community dynamics from time series data (Ives, 1995; Ives et al., 1999, 2003). This approach has been used estimate species interaction strengths, stability metrics, and environmental drivers for a variety of freshwater plankton systems (Ives, 1995; Ives et al., 1999, 2003; Hampton et al., 2008, 2006; Hampton and Schindler, 2006; Klug and Cottingham, 2001). These models are based on a process model for log abundances ($\mathbf{x}$) of the form

$$\mathbf{x}_t = \mathbf{B}\mathbf{x}_{t-1} + \mathbf{U} + \mathbf{w}_t \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}) \tag{16.1}$$

$\mathbf{B}$ is the interaction matrix; self interaction strengths (density-dependence) is on the diagonal and inter-specific interaction strengths are on the off-diagonals such that $\mathbf{B}_{i,j}$ is the 'effect' of species j on species i. This model has a stochastic equilibrium—it fluctuates around mean, $(\mathbf{I}-\mathbf{B})^{-1}\mathbf{U}$. The term $\mathbf{U}$ determines the mean level but once the system is at equalibrium, it does not affect the fluctuations relative to the mean. To see this, compare two models with $b = 0.5$ and $u = 1$ versus $u = 0$. The mean for the first is $1/(1-0.5) = 2$ and for the second is 0. If we start both 1 above the mean, the next x is the same distance from the mean: $x_2 = 0.5(2+1)+1 = 2.5$ and $x_2 = 0.5(0+1)+0 = 0.5$. So both end up at 0.5 above the mean. So once the system is at equalibrium, it is 'scale invariant', where $\mathbf{U}$ is the scaling term. The way that Ives et al. (2003) write their process model (their Equation 10) is $\mathbf{X}_t = \mathbf{A} + \mathbf{B}\mathbf{X}_{t-1} + \mathbf{E}_t$, using their terminology. The $\mathbf{A}$ in Ives's equation is the $\mathbf{U}$ appearing in Equation 16.1 and the $\mathbf{E}_t$ is a scaling term.

Often the models include environmental covariates, but we will leave that off for the moment and address that at the end of this case study. If we add

a measurement process[1], we have a MARSS model:

$$\mathbf{y}_t = \mathbf{Z}\mathbf{x}_t + \mathbf{A} + \mathbf{v}_t \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}) \tag{16.2}$$

Typically, we have one time series per species and thus we assume that $m = n$ and $\mathbf{Z}$ is an $m \times m$ identity matrix (when $m = n$, $\mathbf{A}$ is set to 0). However, it is certainly possible to have multiple time series per species (for example data taken at multiple sites).

In this case study, we will use the MARSS package to estimate the $\mathbf{B}$ matrix of species interactions for a simple wolf-moose system and for a four-species freshwater plankton system.

16.2 Two-species example using wolves and moose

Population dynamics of wolves and moose on Isle Royale make an interesting case study of a two-species predator-prey interactions. These populations have been studied intensively since 1958, making the time-series length relatively unique. Unlike other populations of grey wolves, the Isle Royale population has a diet dominated by one prey item (ca. 90% moose). The only predator of moose on Isle Royale is the grey wolf, as this population is not hunted.

We will use the wolf and moose census data from Isle Royale to learn how to fit community dynamics models to time-series data. The data we are using are the raw aerial survey data, rather than the reconstructed numbers that one normally sees presented for the Isle Royale moose. This is to remove the smoothing that the reconstruction introduces.

16.2.1 Load in and plot the data

```
royale.dat = log(t(isleRoyal[,2:3]))
```

16.2.2 Fit the model to the wolf-moose data

The naive way to fit the model is to use Equations 16.2 and 16.1 "as is":

```
royale.model.0=list(B="unconstrained",Q="diagonal and unequal",
      R="diagonal and unequal",U="unequal")
kem.0=MARSS(royale.dat,model=royale.model.0)
```

If you try this, you will notice that it does not converge but stops when it reaches `maxit` and prints a number of warnings about non-convergence. The problem is that when you try to estimate $\mathbf{B}$ and $\mathbf{u}$, they are often confounded.

[1] You can fit a MAR model with no observation error by setting $\mathbf{R} = 0$, but a conditional least-squares algorithm is vastly faster than EM or BFGS for the $\mathbf{R} = 0$ case (assuming no missing data).

```
matplot(isleRoyal[,1],log(isleRoyal[,2:3]),
    ylab="log count",xlab="Year",type="l",
    lwd=3,bty="L",col="black")
legend("topright",c("Wolf","Moose"), lty=c(1,2), bty="n")
```

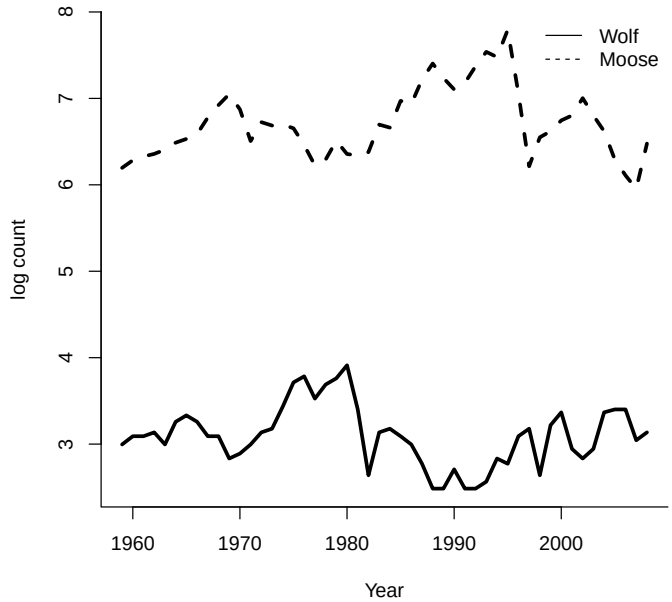

Fig. 16.1. Plot of the Isle Royale wolf and moose data.

This a well-known problem, and you will need to find a way to fix **u** at some value. If you are willing to assume that the process is at equilibrium (i.e. not recovering to equilibrium from a big perturbation), then you can simply demean the data and set **u** to 0. It is also standard to standardize the variance by dividing by the square root of the variance of the data. This is called z-scoring the data.

```
#if missing values are in the data, they should be NAs
z.royale.dat=(royale.dat-apply(royale.dat,1,mean,na.rm=TRUE))/
     sqrt(apply(royale.dat,1,var,na.rm=TRUE))
```

We also need to change a couple settings before fitting the model. In the default MARSS model, the initial value of **x** is treated as being at $t = 0$. If we are estimating the **B** matrix, we need to set this to be at $t = 1$ so that the initial

x is constrained by the data at $t = 1$[2]. The reason is that we need to estimate the initial **x**. Even if we use a prior on the initial **x**, we are still estimating its value[3]. A model with a non-diagonal **B** matrix, does not "run backwards" well and the estimation of the initial **x** will run in circles. If we constrain it by data (at $t = 1$), we avoid this problem. So we will set `model$tinitx=1`.

The other setting we want to change is `allow.degen`. This sets the diagonals of **Q** or **R** to zero if they are heading towards zero. When the initial **x** is at $t = 1$, this can have non-intuitive (not wrong but puzzling; see Appendix B) consequences if **R** is going to zero. So, we will set `control$allow.degen=FALSE` and manually set **R** to 0 if needed.

```
royale.model.1=list(Z="identity", B="unconstrained",
      Q="diagonal and unequal", R="diagonal and unequal", U="zero", tinitx=1)
cntl.list=list(allow.degen=FALSE,maxit=200)
kem.1=MARSS(z.royale.dat, model=royale.model.1, control=cntl.list)
```

```
Warning! Reached maxit before parameters converged. Maxit was 200.

MARSS fit is
Estimation method: kem
WARNING: maxit reached, 200 iter, before convergence.
 The likelihood and params are not at the ML values.
 Try setting control$maxit higher.
Log-likelihood: -83.28397
AIC: 186.5679   AICc: 189.0398

         Estimate
R.R(1,1)  0.00172
R.R(2,2)  0.00036
B.B(1,1)  0.69461
B.B(2,1) -0.27502
B.B(1,2) -0.06822
B.B(2,2)  0.63271
Q.Q(1,1)  0.45211
Q.Q(2,2)  0.27980
x0.x01   -0.28324
x0.x02   -1.26168

Standard errors have not been calculated.
```

[2] If there are many missing values at $t = 1$, we might still have problems and have to adjust accordingly.

[3] Also putting a prior on the initial **x**'s requires specifying their variance-covariance structure, which depends on the unknown **B**, and specifying some variance-covariance structure that conflicts with **B** will change your **B** estimates. So, in general, using a prior on the initial **x**'s when estimating **B** is a bad idea.

```
Use MARSSparamCIs to compute CIs and bias estimates.

Convergence warnings
 Warning: the  R.R(1,1)  parameter value has not converged.
 Warning: the  R.R(2,2)  parameter value has not converged.
```

It looks like **R** is going to zero, meaning that the maximum-likelihood model is a process error only model. That is not too surprising given that the data look more like a random walk than white noise. We will set **R** manually to zero:

```
royale.model.2=list(Z="identity", B="unconstrained",
    Q="diagonal and unequal", R="zero", U="zero")
kem.2=MARSS(z.royale.dat, model=royale.model.2, control=cntl.list)
```

16.2.3 Look at the estimated interactions

The estimated **B** matrix is `kem.2$par$B`.

```
wolf.B=parmat(kem.2)$B
rownames(wolf.B)=colnames(wolf.B)=rownames(royale.dat)
print(wolf.B, digits=2)
```

```
       Wolf  Moose
Wolf   0.69 -0.069
Moose -0.27  0.633
```

Does the **B** matrix make sense ecologically? Element row=i, col=j in **B** is the effect of species j on species i, so $\mathbf{B}[2,1]$ is the effect of wolves on moose and $\mathbf{B}[1,2]$ is the effect of moose on wolves. The diagonals are interpreted differently than the off-diagonals since the diagonals are $(b_{i,i}-1)$ so subtract off 1 from the diagonals to get the effect of species i on itself. If the species are density-independent, then $b_{i,i}$ would equal 1. Smaller $b_{i,i}$ means more density dependence.

The **B** matrix suggests that wolves have a negative effect on moose (as you might expect), but that moose also have a slightly negative effect on wolves. The negative effect of moose on wolf is not what we would expect. We have modeled the effect of moose numbers last year on wolf numbers this year. It may be that the effects are delayed or that it is moose numbers in winter (say) that are most important to wolf population increase. Or perhaps the negative effect (actually correlation) between moose numbers last year and wolf numbers this year is not surprising if actual numbers are less important than the condition of the moose. Low moose numbers may be correlated with 'weak moose' which provides an abundant wolf food supply

This analysis was for teaching purposes and one should not make too much of the **B** estimates because we have not included any environmental covariates. It is well-known that other factors have large effects on moose numbers. Moose

numbers are strongly affected by winter temperatures and snow depth. If we had data on winter temperature and snow depth, we might find that the effect of wolves on moose is considerably different than that estimated with just wolf and moose data.

16.2.4 Change the model and data

You can explore the sensitivity of the **B** estimates when the measurement error is increased by adding white noise to the data:

```
bad.data=z.royale.dat+matrix(rnorm(100,0,sqrt(.2)),2,50)
kem.bad=MARSS(bad.data, model=model, control=cntl.list)
```

You can change the model by changing the constraints on **R** and **Q**.

16.3 Analysis a four-species plankton community

Ives et al. (2003) presented weekly data on the biomass of two species of phytoplankton and two species of zooplankton in two lakes, one with low planktivory and one with high planktivory. They used these data to estimate the interaction terms for the four species. Here we will reanalyze data and compare our results.

Ives et al. (2003) explain the data as: "The data consist of weekly samples of zooplankton and phytoplankton, which for the analyses were divided into two zooplankton groups (Daphnia and non-Daphnia) and two phytoplankton groups (large and small phytoplankton). Daphnia are large, effective herbivores, and small phytoplankton are particularly vulnerable to herbivory, so we anticipate strong interactions between Daphnia and small phytoplankton groups." Figure 16.2 shows the data. What you can see from the figure is that the data are only collected in the summer.

16.3.1 Load in the plankton data

```
# only use the plankton, daphnia, & non-daphnia
plank.dat = ivesDataByWeek[,c("Large Phyto","Small Phyto","Daphnia","Non-daphnia")]
#The data are not logged
plank.dat = log(plank.dat)
#Transpose to get time going across the columns
plank.dat = t(plank.dat)
#make a demeaned version
d.plank.dat = (plank.dat-apply(plank.dat,1,mean,na.rm=TRUE))
```

As before, we will demean the data so we can set **u** to 0. We do not standardize by the variance, however because we are going to fix the **R** variance later as Ives et al. did.

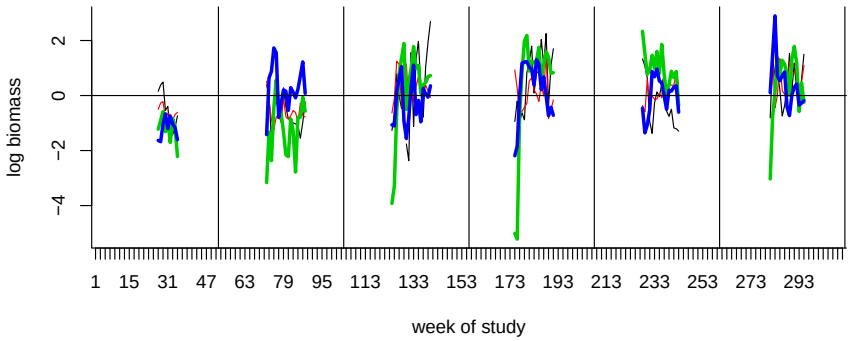

Fig. 16.2. Plot of the plankton data. Zooplankton are the thicker lines. Phytoplankton are the thinner lines.

16.3.2 Specify a MARSS model for the plankton data

We will start by fitting a model with the following assumptions:

- All phytoplankton share the same process variance.
- All zooplankton share the same process variance.
- Phytoplankton and zooplankton have different measurement variances
- Measurement errors are independent.
- Process errors are independent.

```
Z="identity"
U="zero"
B="unconstrained"
Q=matrix(list(0),4,4); diag(Q)=c("Phyto","Phyto","Zoo","Zoo")
R=matrix(list(0),4,4); diag(R)=c("Phyto","Phyto","Zoo","Zoo")
plank.model.0=list(Z=Z, U=U, Q=Q, R=R, B=B)
```

Why did we set `U="zero"`? Equation 16.1 is a stationary model; it fluctuates about a mean. The **u** in Equation 16.1 is a scaling term that just affects the mean level—once the system is at equilibrium. If we assume that the mean of **y** (the mean of our data) is a good estimate of the mean of the system (the **x**), then we can set **U** equal to zero.

16.3.3 Fit the plankton model and look at the estimated B matrix

The call to fit the model is standard with the addition of setting `model$tinitx` so that the initial states (**x**) are set at $t = 1$ instead of $t = 0$.

```
plank.model.0$tinitx=1
kem.plank.0 = MARSS(d.plank.dat, model=plank.model.0 )
```

Now we can print the **B** matrix, with a little cleaning up so it looks prettier.

```
#Cleaning up the B matrix for printing
B.0 = parmat(kem.plank.0)$B[1:4,1:4]
rownames(B.0) = colnames(B.0) = c("LP","SP","D","ND")
B.0[B.0==0]=NA
print(B.0,digits=2,na.print="--")
```

```
       LP   SP       D     ND
LP  0.834 0.10 -0.0025  0.076
SP  0.016 0.77  0.0139 -0.030
D   0.122 0.39  0.6036  0.470
ND -0.011 0.43 -0.1773  0.954
```

LP stands for large phytoplankton, SP for small phytoplankton, D for Daphnia and ND for non-Daphnia.

We can compare this to the Ives et al. estimates (in their Table 2, bottom right) and see a few differences:

```
     LP    SP     D    ND
LP 0.48 -0.39    --    --
SP   --  0.25 -0.17 -0.11
D    --    --  0.74  0.00
ND   --  0.10  0.00  0.60
```

First, thing you will notice is that the Ives et al. matrix is missing values. The matrix they show is after a model selection step to determine which interactions had little data support and thus could be set to zero. Also, they fixed apriori the interactions between Daphnia and non-Daphnia at zero because they do not prey on each other. The second thing you will notice is that the estimates are not particularly similar. Next we will try some other ways of fitting the data that are closer to the way that Ives et al. fitted the data.

By the way, if you are curious what would happen if we removed all those NAs, you can run the following code.

```
test.dat=d.plank.dat[,!is.na(d.plank.dat[1,])]
test = MARSS(test.dat, model=plank.model.0 )
```

Removing all the NAs would mean that the end of summer 1 is connected to the beginning of summer 2. This adds some steep steps in the Daphnia time series where Daphnia ended the summer high and started the next summer low.

16.3.4 Look at different ways to fit the model

We will try a series of changes to get closer and closer to the way Ives et al. fit the data, and you will see how different assumptions change (or do not change) our species interaction estimates.

First, we change **Q** to be unconstrained. Making **Q** diagonal in model 0 meant that we were assuming that whatever environmental factor is driving variation in phytoplankton numbers is uncorrelated with the environmental factor driving zooplankton variation. That is probably not true since they are all in the same lake. This case takes awhile to run.

```
plank.model.1=plank.model.0
plank.model.1$Q="unconstrained"
kem.plank.1 = MARSS(d.plank.dat, model=plank.model.1)
```

Notice that the **Q** specification changed to "unconstrained". Everything else stays the same as in model 0. The code now runs longer, and the **B** estimates are not particulaly closer to Ives et al.

```
       LP    SP      D     ND
LP  0.536 0.012  0.082 0.1196
SP -0.157 0.845  0.065 0.0043
D   0.139 0.350  0.654 0.3754
ND  0.045 0.303 -0.153 0.8886
```

Next, we will set some of the interactions to zero as in Table 2 in Ives et al. (2003). In that table, certain interactions were fixed at 0 (denoted with 0s), and some were made 0 after fitting (the blanks). We will fix all to zero. To do this, we need to write out the **B** matrix as a list matrix so that we can have estimated and fixed values (the 0s) in the **B** specification.

```
B.2=matrix(list(0),4,4) #set up the list matrix
diag(B.2)=c("B11","B22","B33","B44") #give names to diagonals
#and names to the estimated non-diagonals
B.2[1,2]="B12"; B.2[2,3]="B23"; B.2[2,4]="B24"; B.2[4,2]="B42"
print(B.2)
```

```
     [,1]  [,2]  [,3]  [,4]
[1,] "B11" "B12" 0     0
[2,] 0     "B22" "B23" "B24"
[3,] 0     0     "B33" 0
[4,] 0     "B42" 0     "B44"
```

As you can see, the **B** matrix now has elements that will be estimated (the names in quotes) and fixed values (the numbers with no quotes). When preparing your list matrix, make sure your fixed values do not have have quotes around them. If they do, they are strings (class character) not numbers (class numeric), and MARSS will interpret a string as the name of something to be

estimated. If you use the same name for an element, then MARSS will force those elements to be shared (have the same value). This one will take a while to run also.

```
#model 2
plank.model.2=plank.model.1
plank.model.2$B = B.2
kem.plank.2= MARSS(d.plank.dat, model=plank.model.2)
```

Now we are getting closer to the Ives et al. estimates:

```
     LP     SP      D    ND
LP 0.75 -0.304     --    --
SP   --  0.747 -0.015 0.032
D    --     --  0.884    --
ND   --  0.059     -- 0.664
```

Ives et al. did not estimate **R**. Instead they used a fixed observation variance of 0.04 for phytoplankton and 0.16 for zooplankton. Interestingly, these values are opposite to what you get if you estimate these variances (look at `kem.plank.2$par$R`). You can fit the model with their fixed **R** as follows:

```
#model 3
plank.model.3=plank.model.2
plank.model.3$R=diag(c(.04,.04,.16,.16))
kem.plank.3= MARSS(d.plank.dat, model=plank.model.3)
```

As you can see from Table 16.1, we are getting closer to Ives et al. estimates, but we are still a bit off. Now we need to add the environmental covariates: phosphorous and fish biomass.

16.3.5 Adding covariates

A standard way that you will see covariate data added to a MARSS model is the following:

$$\begin{aligned} \mathbf{x}_t &= \mathbf{B}\mathbf{x}_{t-1} + \mathbf{U} + \mathbf{C}\mathbf{c}_t + \mathbf{w}_t, \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}) \\ \mathbf{y}_t &= \mathbf{Z}\mathbf{x}_t + \mathbf{A} + \mathbf{D}\mathbf{d}_t + \mathbf{v}_t, \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}) \end{aligned} \tag{16.3}$$

$\mathbf{c}_t$ and $\mathbf{d}_t$ are covariate data, like temperature. At time t and $\mathbf{C}$ is a matrix with the (linear) effects of $\mathbf{c}_t$ on $\mathbf{x}_t$, and $\mathbf{D}$ is a matrix with the (linear) effects of $\mathbf{d}_t$ on $\mathbf{y}_t$.

Ives et al. (2003) only include covariates in their process model, and their process model (their Equation 27) is written $\mathbf{X}_t = \mathbf{A} + \mathbf{B}\mathbf{X}_{t-1} + \mathbf{C}\mathbf{U}_t + \mathbf{E}_t$. In our Equation 16.3, $\mathbf{U}_t = \mathbf{c}_t$, and $\mathbf{C}$ is a $m \times p$ matrix, where p is the number of covariates in $\mathbf{c}_t$. For this case study, we set $\mathbf{A} = 0$ by demeaning the $\mathbf{y}$ and implicitly assuming that the mean of the $\mathbf{y}$ is a good estimate of the mean of the $\mathbf{x}$'s. If we assume that the process is stochastically stable, meaning it

is fluctuating about a mean, we can also set $\mathbf{U} = 0$ after demeaning the data. Thus the model where covariates only affect the underlying process is

$$\begin{aligned} \mathbf{x}_t &= \mathbf{B}\mathbf{x}_{t-1} + \mathbf{C}\mathbf{c}_t + \mathbf{w}_t, \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}) \\ \mathbf{y}_t &= \mathbf{x}_t + \mathbf{v}_t, \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}) \end{aligned} \tag{16.4}$$

We can fit this model as follows in MARSS. First we need to prepare the covariate data. We will just use the phosphorous data.

```
#transpose to make time go across columns
#drop=FALSE so that R doesn't change our matrix to a vector
phos = t(log(ivesDataByWeek[,"Phosph",drop=FALSE]))
d.phos = (phos-apply(phos,1,mean,na.rm=TRUE))
```

Why log the covariate data? It is what Ives et al. did, so we follow their method. However, in general, you want to think about what relationshipyou want to assume between the covariates and their effects. For example, log (or square-root) transformations mean that extremes have less impact relative to their untransformed value and that a small absolute change, say from 0.01 to 0.0001 in the untransformed value, can mean large difference in the effects since $\log(0.0001) \blacksquare \log(0.01)$.

Phosporous is assumed to only affect phytoplankton so the other terms in $\mathbf{C}$, corresponding to the zooplankton and fish biomass, are set to 0. The $\mathbf{C}$ matrix is defined as follows:

$$\mathbf{C} = \begin{bmatrix} C_{LP,phos} \\ C_{SP,phos} \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{16.5}$$

To add $\mathbf{C}$ and $\mathbf{c}$ to our latest model, we just add $\mathbf{C}$ and $\mathbf{c}$ to the model list:

```
plank.model.4=plank.model.3
plank.model.4$C=matrix(list("C11","C21",0,0),4,1)
plank.model.4$c=d.phos
```

Then we fit the model as usual:

```
kem.plank.4= MARSS(d.plank.dat, model=plank.model.4)
```

```
Success! Parameters converged at 20 iterations.
Alert: conv.test.slope.tol is 0.5.
Test with smaller values (<0.1) to ensure convergence.

MARSS fit is
Estimation method: kem
Estimation converged in 20 iterations.
Log-likelihood: -393.8637
```

```
AIC: 835.7274   AICc: 839.2777

         Estimate
B.B11      0.6302
B.B12     -0.4805
B.B22      0.3640
B.B42      0.0400
B.B23     -0.0302
B.B33      0.9017
B.B24     -0.0239
B.B44      0.7020
U.C11      0.1407
U.C21      0.1506
Q.Q(1,1)   0.7300
Q.Q(2,1)   0.2202
Q.Q(3,1)   0.0761
Q.Q(4,1)   0.0261
Q.Q(2,2)   0.2639
Q.Q(3,2)  -0.1343
Q.Q(4,2)  -0.0943
Q.Q(3,3)   0.8635
Q.Q(4,3)   0.4499
Q.Q(4,4)   0.3389
x0.x01     0.1603
x0.x02    -0.5248
x0.x03    -1.1112
x0.x04    -1.8190

Standard errors have not been calculated.
Use MARSSparamCIs to compute CIs and bias estimates.
```

16.3.6 Including a covariate observation model

The difficulty with the standard approach to including covariates (Equation 16.3) is that it limits what kind of covariate data you can use and how you model that covariate data. You have to assume that your covariate data has no error, which is probably not true. Assuming that your covariate has no error reduces the reported uncertainty in your covariate effect because you did not include uncertainty in those values. The standard approach also does not allow missing values in your covariate data, which is why we did not include the fish covariate data in the last model. Also you cannot combine instrument time series; for example, if you have two temperature recorders with different error rates and biases. Also, what if you have one noisy temperature recorder in the first part of your time series and then you switch to a much better recorder in the second half of your time series? All these problems require pre-analysis

massaging of the covariate data, leaving out noisy and gappy covariate data, and making what can feel like arbitrary choices about which covariate time series to include which is especially worrisome when the covariates are then incorporated in the model as known without error.

Instead one can include an observation and process model for the covariates just like for the non-covariate data. Now the covariates are included in $\mathbf{y}_t$ and are modeled with their own state process(es) in $\mathbf{x}_t$. A MARSS model with a covariate observation and process model is shown below. The elements with superscript (v) are for the variates and those with superscript (c) are for the covariates. The superscripts just help us keep straight which of the state processes and parameters corresponding to the parts that correspond abundances and which correspond to the environmental covariates.

$$\begin{bmatrix}\mathbf{x}^{(v)}\\ \mathbf{x}^{(c)}\end{bmatrix}_t = \begin{bmatrix}\mathbf{B}^{(v)} & \mathbf{C}\\ 0 & \mathbf{B}^{(c)}\end{bmatrix}\begin{bmatrix}\mathbf{x}^{(v)}\\ \mathbf{x}^{(c)}\end{bmatrix}_{t-1} + \begin{bmatrix}\mathbf{u}^{(v)}\\ \mathbf{u}^{(c)}\end{bmatrix} + \mathbf{w}_t,\ \mathbf{w}_t \sim \text{MVN}\left(0, \begin{bmatrix}\mathbf{Q}^{(v)} & 0\\ 0 & \mathbf{Q}^{(c)}\end{bmatrix}\right)$$

$$\begin{bmatrix}\mathbf{y}^{(v)}\\ \mathbf{y}^{(c)}\end{bmatrix}_t = \begin{bmatrix}\mathbf{Z}^{(v)} & 0\\ 0 & \mathbf{Z}^{(c)}\end{bmatrix}\begin{bmatrix}\mathbf{x}^{(v)}\\ \mathbf{x}^{(c)}\end{bmatrix}_t + \begin{bmatrix}\mathbf{a}^{(v)}\\ \mathbf{a}^{(c)}\end{bmatrix} + \mathbf{v}_t,\ \mathbf{v}_t \sim \text{MVN}\left(0, \begin{bmatrix}\mathbf{R}^{(v)} & 0\\ 0 & \mathbf{R}^{(c)}\end{bmatrix}\right) \tag{16.6}$$

Note that when you fit your covariate and non-covariate data jointly as in Equation 16.6, your non-covariate data affect the estimates of the covariate models. When you maximize the likelihood, you do so conditioned on all the data. The likelihood that is output is the likelihood of the non-covariate and covariate data. Depending on your system, you might not want the covariate model affected by the non-covariate data. In this case, you can fit the covariate model separately:

$$\begin{aligned}\mathbf{x}_t^{(c)} &= \mathbf{B}^{(c)}\mathbf{x}_{t-1}^{(c)} + \mathbf{u}^{(c)} + \mathbf{w}_t,\ \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}^{(c)})\\ \mathbf{y}_t^{(c)} &= \mathbf{Z}^{(c)}\mathbf{x}_t^{(c)} + \mathbf{a}^{(c)},\ \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}^{(c)})\end{aligned} \tag{16.7}$$

At this point, you have another choice. Do you want the estimated covariates states, the $\mathbf{x}^{(c)}$, to be affected by the non-covariate data? For example, you have temperature data. You can estimates true temperature for the temperture only from the temperature data or you can decide that the non-covariate data has information about the true temperature, because the non-covariate states are affected by the true temperature. If you want the covariate states to only be affected by the covariate data, then use Equation 16.3 with $\mathbf{u}_t$ set from your estimates of $\mathbf{x}^{(c)}$ from Equation 16.7. Or if you want the non-covariate data to affect the estimates of the covariate states, use Equation 16.6 with the parameters estimated from equation 16.7.

16.3.7 The MARSS model with covariates following Ives et al.

Ives et al. used Equation 16.3 for phosporous and Equation 16.6 for fish biomass. Phosporous was treated as observed with no error since it was ex-

perimentally manipulated and there were no missing values. Fish biomass was treated as having observation error and was modeled as a autoregressive process with unknown parameters as in Equation 16.6.

Their MARSS model takes the form:

$$\begin{aligned} \mathbf{x}_t &= \mathbf{B}\mathbf{x}_{t-1} + \mathbf{C}\mathbf{c}_t + \mathbf{w}_t, \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}) \\ \mathbf{y}_t &= \mathbf{x}_t + \mathbf{v}_t, \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}) \end{aligned} \tag{16.8}$$

where $\mathbf{x}$ and $\mathbf{y}$ are redefined as

$$\begin{bmatrix} \text{large phyto} \\ \text{small phyto} \\ \text{Daphnia} \\ \text{Non-Daphnia zooplank} \\ \text{fish biomass} \end{bmatrix} \tag{16.9}$$

The covariate fish biomass appears in $\mathbf{x}$ because it will be modeled, and its interaction terms (Ives et al.'s $\mathbf{C}$ terms) appear in $\mathbf{B}$. pH appears in the $\mathbf{c}_t$ terms because it is treated as a known additive term and its interaction terms appear in $\mathbf{C}$. Recall that we set $\mathbf{U}$ to 0 by demeaning the plankton data, so it does not appear above. The $\mathbf{Z}$ matrix does not appear in front of the $\mathbf{x}_t$ since there is a one-to-one correspondence the $\mathbf{x}$'s and $\mathbf{y}$'s, and thus $\mathbf{Z}$ is the identity matrix.

The $\mathbf{B}$ matrix is

$$\mathbf{B} = \begin{bmatrix} \mathbf{B}^{(v)} & \mathbf{C} \\ 0 & \mathbf{B}^{(c)} \end{bmatrix} = \begin{bmatrix} b_{LP} & b_{LP,SP} & 0 & 0 & 0 \\ 0 & b_{SP} & b_{SP,D} & b_{SP,ND} & 0 \\ 0 & 0 & b_D & 0 & C_{D,fish} \\ 0 & b_{ND,SP} & 0 & b_{ND,ND} & C_{ND,fish} \\ 0 & 0 & 0 & 0 & b_{fish} \end{bmatrix} \tag{16.10}$$

The $\mathbf{B}$ elements have some interactions fixed at 0 as in our last model fit. The c's are the interactions between the fish and the species. We will estimate a b term for fish since Ives et al. did, but this is an odd thing to do for the fish data since these data were interpolated from two samples per season.

The $\mathbf{Q}$ matrix is the same as that in our last model fit, with the addition of an element for the variance for the fish biomass:

$$\mathbf{Q} = \begin{bmatrix} \mathbf{Q}^{(v)} & 0 \\ 0 & \mathbf{Q}^{(c)} \end{bmatrix} = \begin{bmatrix} q_{LP} & q_{LP,SP} & q_{LP,D} & q_{LP,ND} & 0 \\ q_{LP,SP} & q_{SP} & q_{SP,D} & q_{SP,ND} & 0 \\ q_{LP,D} & q_{SP,D} & q_D & q_{D,ND} & 0 \\ q_{LP,ND} & q_{SP,ND} & q_{D,ND} & q_{ND} & 0 \\ 0 & 0 & 0 & 0 & 0 \; q_{fish} \end{bmatrix} \tag{16.11}$$

Again it is odd to estimate a variance term for data interpolated from two points, but we follow Ives et al. here.

Ives et al. set the observation variance for the logged fish biomass data to 0.36 (page 320 in Ives et al. (2003)). The observation variances for the species data was set as in our previous model.

$$\mathbf{R} = \begin{bmatrix} 0.04 & 0 & 0 & 0 & 0 \\ 0 & 0.04 & 0 & 0 & 0 \\ 0 & 0 & 0.16 & 0 & 0 \\ 0 & 0 & 0 & 0.16 & 0 \\ 0 & 0 & 0 & 0 & 0.36 \end{bmatrix} \tag{16.12}$$

16.3.8 Setting the model structure for the model with fish covariate data

First we need to add the logged fish biomass to our data matrix since we are treating it as data with error and thus it needs to appear in **y**.

```
#transpose to make time go across columns
#drop=FALSE so that R doesn't change our matrix to a vector
fish = t(log(ivesDataByWeek[,"Fish biomass",drop=FALSE]))
d.fish = (fish-apply(fish,1,mean,na.rm=TRUE))
#plank.dat.w.fish = rbind(plank.dat,fish)
d.plank.dat.w.fish = rbind(d.plank.dat,d.fish)
```

Next make the **B** matrix. Some elements are estimated and others are fixed at 0.

```
B=matrix(list(0),5,5)
diag(B)=list("B11","B22","B33","B44","Bfish")
B[1,2]="B12";B[2,3]="B23"; B[2,4]="B24"
B[4,2]="B42";
B[1:4,5]=list(0,0,"C32","C42")
print(B)
```

```
     [,1]  [,2]  [,3]  [,4]  [,5]
[1,] "B11" "B12" 0     0     0
[2,] 0     "B22" "B23" "B24" 0
[3,] 0     0     "B33" 0     "C32"
[4,] 0     "B42" 0     "B44" "C42"
[5,] 0     0     0     0     "Bfish"
```

Now we have a **B** matrix that looks like that in Equation 16.10.

We need to add an extra row to **C** for the fish biomass row in **x**:

```
C=matrix(list("C11","C21",0,0,0),5,1)
```

Then we set up the **R** matrix.

```
R=matrix(list(0),5,5)
diag(R)=list(0.04,0.04,0.16,0.16,0.36)
```

Last, we need to set up the **Q** matrix:

```
Q=matrix(list(0),5,5);
Q[1:4,1:4]=paste(rep(1:4,times=4),rep(1:4,each=4),sep="")
Q[5,5]="fish"
Q[lower.tri(Q)]=t(Q)[lower.tri(Q)]
print(Q)
```

```
     [,1] [,2] [,3] [,4] [,5]
[1,] "11" "12" "13" "14" 0
[2,] "12" "22" "23" "24" 0
[3,] "13" "23" "33" "34" 0
[4,] "14" "24" "34" "44" 0
[5,] 0    0    0    0    "fish"
```

16.3.9 Fit the model with covariates

The model is the same as the previous model with updated process parameters and updated **R**. We will pass in the updated data matrix with the fish biomass added:

```
plank.model.5=plank.model.4
plank.model.5$B=B
plank.model.5$C=C
plank.model.5$Q=Q
plank.model.5$R=R
kem.plank.5=MARSS(d.plank.dat.w.fish, model=plank.model.5)
```

This is the new **B** matrix using covariates.

```
     LP     SP      D     ND
LP 0.63 -0.484     --     --
SP   --  0.365 -0.032 -0.023
D    --     --  0.911     --
ND   --  0.036     --  0.716
```

Now we are getting are getting close to Ives et al.'s estimates. Compare model 5 in Table 16.1 to the first column.

NOTE! When you include your covariates in your state model (the **x** part), the reported log-likelihood is for the variate plus the covariate data. If you want just the log-likelihood for the variates, then your replace the covariate data with NAs and run the Kalman filter with your estimated model:

```
tmp=kem.plank.5
tmp$model$data[5,]=NA
LL.variates=MARSSkf(tmp)$logLik
```

`MARSSkf` is the Kalman filter function and it needs a fitted model as output by a `MARSS` call. We set up a temporary fitted model, `tmp`, equal to our fitted model and then set the covariate data in that to NAs. We then pass that temporary fitted model to `MARSSkf` to get the log-likelihood of just the variates.

Table 16.1. The parameter estimates under the different plankton models. Models 0 to 3 do not include covariates, so the C elements are blank. Bij is the effect of species i on species j. 1=large phytoplankton, 2=small phytoplankton, 3=Daphnia, 4=non-Daphnia zooplankton. The Ives et al. (2003) estimates are from their table 2 for the low planktivory lake with the observation model.

	Ives et al.	Model 0	Model 1	Model 2	Model 3	Model 4	Model 5
B11	0.48	0.83	0.54	0.75	0.64	0.63	0.63
B22	0.25	0.77	0.84	0.75	0.53	0.36	0.37
B33	0.74	0.60	0.65	0.88	0.90	0.90	0.91
B44	0.60	0.95	0.89	0.66	0.71	0.70	0.72
B12	-0.39	0.10	0.01	-0.30	-0.33	-0.48	-0.48
B23	-0.17	0.01	0.06	-0.02	-0.03	-0.03	-0.03
B24	-0.11	-0.03	0.00	0.03	0.03	-0.02	-0.02
B42	0.10	0.43	0.30	0.06	0.07	0.04	0.04
C11	0.25					0.14	0.14
C21	0.25					0.15	0.15
C32	-0.14						-0.04
C42	-0.04						-0.00

16.3.10 Discussion

The estimates for model 4 are fairly close to the Ives et al. estimates, but still a bit different. There are two big difference between model 4 and the Ives et al. analysis. Ives et al. had data from three lakes and the estimate of $\mathbf{Q}$ used the data from all lakes.

Combining data, whether it be from different areas or years, can be done in a MARSS model as follows. Let $\mathbf{y}_1$ be the first data set (say from site 1) and $\mathbf{y}_2$ be the second data set (say from site 2). Then a MARSS model with shared parameters values across datasets would be

$$\begin{aligned} \mathbf{x}_t^+ &= \mathbf{B}^+\mathbf{x}_{t-1}^+ + \mathbf{u}^+\mathbf{w}_t, \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}^+) \\ \mathbf{y}_t^+ &= \mathbf{Z}^+\mathbf{x}_t^+ + \mathbf{a}^+ + \mathbf{v}_t, \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}^+) \end{aligned} \tag{16.13}$$

where the + matrices are stacked matrices from the different sites (1 and 2):

$$\begin{aligned} \begin{bmatrix} \mathbf{x}_{1,t} \\ \mathbf{x}_{2,t} \end{bmatrix} &= \begin{bmatrix} \mathbf{B} & 0 \\ 0 & \mathbf{B} \end{bmatrix} \begin{bmatrix} \mathbf{x}_{1,t-1} \\ \mathbf{x}_{2,t-1} \end{bmatrix} + \begin{bmatrix} \mathbf{u} \\ \mathbf{u} \end{bmatrix} + \mathbf{w}_t, \ \mathbf{w}_t \sim \text{MVN}\left(0, \begin{bmatrix} \mathbf{Q} & \mathbf{q} \\ \mathbf{q} & \mathbf{Q} \end{bmatrix}\right) \\ \begin{bmatrix} \mathbf{y}_{1,t} \\ \mathbf{y}_{2,t} \end{bmatrix} &= \begin{bmatrix} \mathbf{Z} & 0 \\ 0 & \mathbf{Z} \end{bmatrix} \begin{bmatrix} \mathbf{x}_{1,t} \\ \mathbf{x}_{2,t} \end{bmatrix} + \begin{bmatrix} \mathbf{a} \\ \mathbf{a} \end{bmatrix} + \mathbf{v}_t, \ \mathbf{v}_t \sim \text{MVN}\left(0, \begin{bmatrix} \mathbf{R} & 0 \\ 0 & \mathbf{R} \end{bmatrix}\right) \end{aligned} \tag{16.14}$$

The $\mathbf{q}$ in the process variance allows that the environmental variabililty might might be correlated between datasets, i.e. if they are replicate plots that are nearby, say. If you did not want all the parameters shared, then you replace the $\mathbf{B}$ in $\mathbf{B}^+$ with $\mathbf{B}_1$ and $\mathbf{B}_2$, say.

The second big difference is that Ives et al. did not demean their data, but estimated **u**. We could have done that too, but with all the NAs in the data (during winter), estimating **u** is not robust and takes a long time. You can try the analysis on the data that has not been demeaned and set `U="unequal"`. The results are not particularly different, but it takes a long, long,...long time to converge.

You can also try using the actual fish data instead of the interpolated data. Fish biomass was estimated at the end and start of the season, so only the values at the start and finish of strings of fish numbers are the real data. The others are interpolated. You can fill in those interpolated values with NAs (missing values) and rerun model 4. The results are not appreciably different, but the effect of fish drops a bit as you might expect when you have less fish information. You don't see it here, but your estimated confidence in the fish effects would also drop since this estimate is based on less fish data.

17

Case Study 8: Combining data from multiple time series

17.1 Overview

In this section, we will consider the case where multiple time series exist and we want to use all the datasets to estimate a common underlying state-process or common underlying parameters. In ecological applications, these time series may take on two common forms: 1) They are time series of observations from the same species as the original time series (e.g. aerial and land based surveys of Marbled Murrelets). or 2) They are time series collected in the same survey, but represent observations of other species (e.g. we might be using a time series from a survey that counts multiple species in a marine fish community).

Why should we consider using other time series? In the first scenario, where methodology differs between time series of the same species, observation error may be survey-specific. These time series may represent observations of multiple populations (with separate state / process vectors), or these may represent multiple observations of the same population. In the second scenario, each species should be treated as a separate process (given its own state vector), but because the survey methodology is the same across species, it might be reasonable to assume a shared observation error variance. If these species have a similar response to environmental stochasticity, it might be possible to also assume a shared process variance.

In both of the above examples, MARSS models offer a way to linking multiple time series. If parameters are allowed to be shared among state / process vectors (trend parameters, process variances) or observed time series (observation variances), parameter estimates will be more precise than if we treated each time series as independent. By improving estimates of variance parameters, we will also be better able to discriminate between process and observation error variances.

The multivariate first-order autoregressive process can be described as:

$$\mathbf{x}_t = \mathbf{B}\mathbf{x}_{t-1} + \mathbf{u} + \mathbf{w}_t \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}) \tag{17.1}$$

The true states at time t are represented by the vector $\mathbf{x}_t$, whose dimensions are equal to the number of processes (m). The $m \times m$ matrix $\mathbf{B}$ allows interaction between processes (density dependence and competition, for instance), $\mathbf{u}$ is a vector describing the mean trend, and the correlation of the process deviations is determined by the structure of the matrix $\mathbf{Q}$.

The multivariate observation error model is expressed as,

$$\mathbf{y}_t = \mathbf{Z}\mathbf{x}_t + \mathbf{a} + \mathbf{v}_t \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}) \tag{17.2}$$

where $\mathbf{y}_t$ is a vector of observations at time t, $\mathbf{Z}$ is a design matrix of 0s and 1s, $\mathbf{a}$ is a vector of bias adjustments, and the correlation structure of observation matrices is specified with the matrix $\mathbf{R}$. Including $\mathbf{Z}$ and $\mathbf{a}$ will not be required for every model, but is useful when some processes are observed multiple times.

17.2 Analyzing time series of redd count data

In our first application combining multiple time series, we will analyze a dataset on Chinook salmon (*Oncorhynchus tshawytscha*). This data comes from the Okanagan River in Washington state, a major tributary of the Columbia River (headwaters in British Columbia). As an index of adult / spawning population abundance, biologists have conducted redd surveys during summer months (redds are nests or collection of rocks on stream bottoms where females deposit eggs). Aerial surveys of redds on the Okanagan have been conducted 1956-2008. Alternative ground surveys of were initiated in 1990, and have been conducted annually.

17.2.1 Read in and plot the raw data

```
head(okanaganRedds)
```

```
     Year aerial ground
[1,] 1956     37     NA
[2,] 1957     53     NA
[3,] 1958     94     NA
[4,] 1959     50     NA
[5,] 1960     29     NA
[6,] 1961     NA     NA
```

```
logRedds = log(t(okanaganRedds)[2:3,])
```

Year is in the first column, and the counts (in normal space) are in columns 2:3. Missing observations are represented by NAs.

```
# Code for plotting raw Okanagan redd counts
plot(okanaganRedds[,1], okanaganRedds[,2],
    xlab = "Year", ylab="Redd counts",main="", col="red")
points(okanaganRedds[,1], okanaganRedds[,3], col="blue")
legend('topleft', inset=0.1, legend=c("Aerial survey","Ground survey"),
 col=c("red","blue"), pch=21)
```

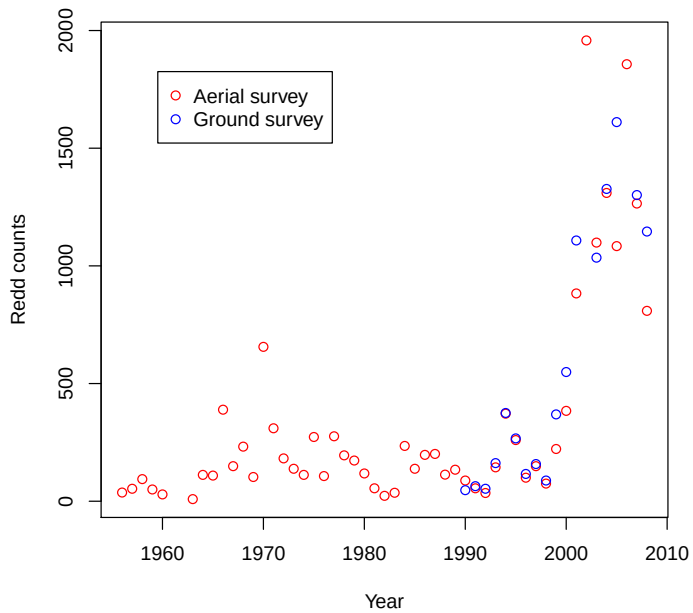

Fig. 17.1. The two time series look to be pretty close to one another in the years there is overlap.

17.2.2 Test hypotheses about whether the data can be combined

Do these surveys represent observations of the same underlying process? We can evaluate data support for this question by testing a few relatively simple models. First, we need to make sure the data are logged:

Using the logged data, we will start with a simple model that assumes the underlying process is univariate. This assumes that the time series are observations of the same population, and there are 2 process parameters (1 trend, 1 process variance).

```
Q.model="diagonal and equal"
R.model="diagonal and equal"
U.model="equal"
```

```
Z.model=factor(c(1,1)) #1 observation time series
# Fit the single state model, where the time series are assumed
# to be from thesame population.
kem1 = MARSS(logRedds, model=list(Z = Z.model, Q = Q.model,
   R = R.model, U = U.model))
```

We can print the AIC value for this model by typing `kem$AIC` and `kem$AICc`.

How would we modify the above model to let the observation error variances to be unique? We can do this in our second model:

```
R.model="diagonal and unequal"
kem2 = MARSS(logRedds, model=list(Z = Z.model, Q = Q.model,
   R = R.model, U = U.model))
```

It is possible that these models are measuring different processes, so we will fit a model with two state vectors. For simplicity (and because of the AIC values from our first two models), we will keep the trend and variance parameters the same.

```
Q.constraint="diagonal and equal"
R.constraint="diagonal and equal"
U.constraint="equal"
Z.constraint=factor(c(1,2))
model3=list(Z = Z.model, Q = Q.model, R = R.model, U = U.model)
kem3 = MARSS(logRedds, model=model3)
```

Which of the above models receives the most support from the data? It looks like the best model is also the simplest one, with one state vector. This suggests that the two different surveys are not only measuring the same thing, but have the same observation error variance. Finally,we will make a plot of the model-predicted states (with +/- 2 s.e.s) and the log-transformed data (Figure 17.2).

17.3 Analyzing time series of rockfish CPUE data

We want to estimate the average long-term trend in total rockfish abundance in the Puget Sound, Washington. There are over a dozen species of rockfish within the Puget Sound, the most prevalent in commercial and recreational catches have been Copper, Quillback, Canary, and Yelloweye rockfish. “Total rockfish” thus represents the sum of multiple population trajectories and, like the individual population trajectories, is also a random walk.

We will assume that the underlying process is a univariate stochastic exponential growth process with rates of decline that are not changing through time. The stochastic exponential is often a decent approximation for many different types of density-independent population processes, and total rockfish catches have been declining over the last 30 years. Because we are interested

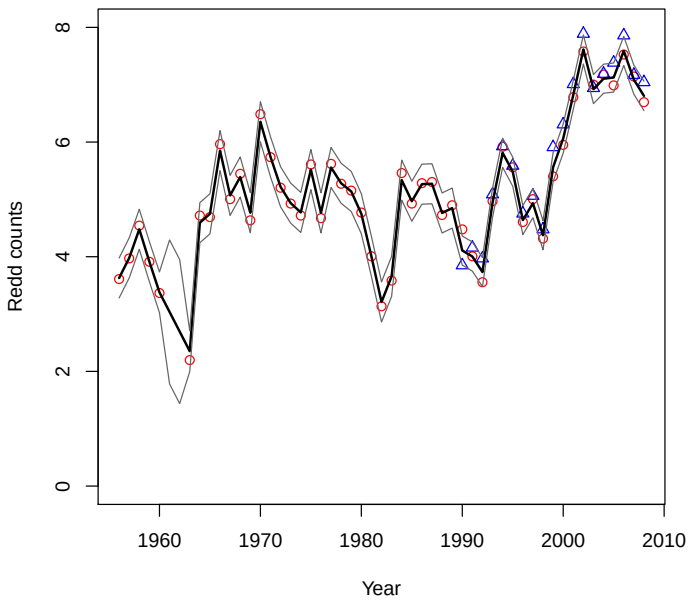

Fig. 17.2. The data support the hypothesis that the two time series are from the same population. The points are the data and the thick black line is the estimated underlying state.

in the total trend, there is only one state vector to be estimated. Our uncertainty lies in how observation errors may be differing among different types of data.

17.3.1 Read in and plot the data

```
1 Bottom.trawl
2 Bottom.trawl.1
3 Rec..targeting.bottomfish
4 Rec..targeting.bottomfish.1
5 Rec..targeting.bottomfish.2
6 Rec..targeting.bottomfish.3
7 Rec..targeting.bottomfish.4
8 SCUBA.survey
9 WDFW.ind..survey
```

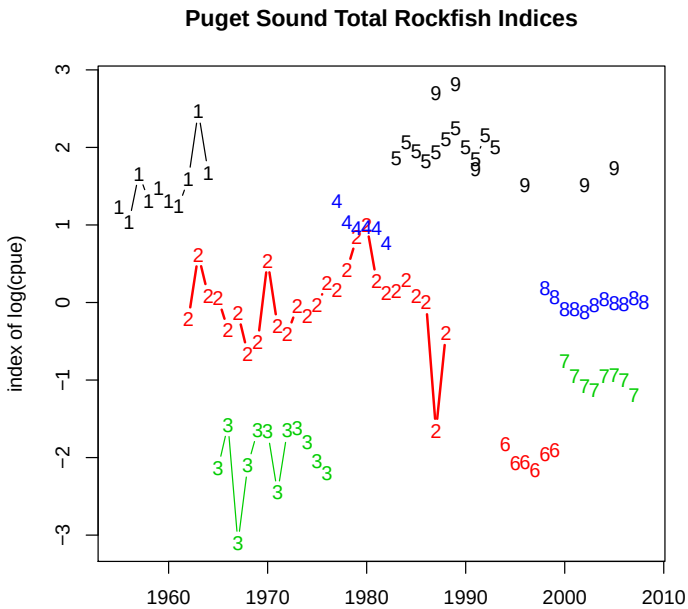

Fig. 17.3. Plot of the catch per unit effort data for Puget Sound total rockfish. Each time series has been given an arbitrary bias (up or down) to purposefully mask any trend in the data that you might pick out by eye – for teaching purposes not for analysis purposes.

17.3.2 Construct models with different configurations of observation error

First, let's fit a model that allows unique variances for each time series.

```
fishdat = t(rockfish[,2:dim(rockfish)[2]])
Q.model="diagonal and equal"
R.model="diagonal and unequal"
U.model="equal"
Z.model=factor(rep(1,dim(fishdat)[1]))
model1 = list(Z = Z.model, Q = Q.model, R = R.model, U = U.model)
kem1 = MARSS(fishdat, model=model1)
```

At the other end of the spectrum, we can build a model that assumes each of the time series has the same observation error.

```
R.model="diagonal and equal"
model2 = list(Z = Z.model, Q = Q.model, R = R.model, U = U.model)
kem2 = MARSS(fishdat, model=model2)
```

Neither of these models fits particularly well. We can improve the partitioning of the variances by constraining some of the measurement variances. We know that the recreational CPUE data from 1977 on represents a consistent measure of catch effort. It is the average fish per angler trip over 8 standardized regions in the Puget Sound. The error between this metric and "total rockfish" equals (sampling error variance + variance due to real year-to-year changes in catchability). The sampling error variance is something we control by our sampling design and sample size. The year-to-year changes in catchability have to do with things we cannot control – weather, how hunger fish are, where the fish are, sizes of the fish, etc. etc. For the recreational data, our sample size is very large: ca 100,000 to 300,000 angler trips. So we can probably safely say that the measurement error variance is driven by year-to-year changes in catchability rather than changes in sample size. Thus we will assume that that the measurement errors for time series 4,5,6, and 7 have an identical variance (so there are six observation variances, rather than nine).

```
R.model=matrix(list(0),9,9)
diag(R.model)=list("1","2","3","4","4","4","4","5","6")
model3 = list(Z = Z.model, Q = Q.model, R = R.model, U = U.model)
kem3 = MARSS(fishdat, model=model3)
```

17.3.3 Last analysis: Only fit model to 1980-2008 data

It is apparent that there is a conflict between and the model for pre-1980 and post-1980. Thus the pre-1980 "total rockfish" estimates produced by this model (with u=constant) are unsupported by the data. The reasons for this could be that the population was stable pre-1980 and then decline post-1980. In this case, our assumption that u is constant over the whole time series is poor, and we should have fit a model using $u_{\text{pre-1980}}$ and $u_{\text{post-1980}}$. As a last example, we will drop the data before 1980 (and the time series that do not have data after this year).

Pull out data years 1980 on and drop the columns (observation time series) with no data after 1980:

```
years = rockfish[,1]
dat = rockfish[,-1]
dat4 = dat[years>=1980,]
years4=years[years>=1980]
isdata = apply(is.na(dat4),2,sum)!=length(years4)
dat4 = dat4[,isdata]
```

Redo the **Z** matrix since we now have fewer time series and change the `R.model` argument to reflect the missing time series:

```
n4 = ncol(dat4)
Z4 = as.factor(rep(1,n4))
R.model4=matrix(list(0),n4,n4)
diag(R.model4)=list("1","2","2","2","2","3","4")
```

Rerun the analysis:

```
model4 =  list(Z = Z4, Q = Q.model, R = R.model4, U = U.model)
kem4 = MARSS(t(dat4), model=model4)
```

17.4 Analyzing time series of American kestrel abundance indices

In previous applications, we were interested in whether time series were from the same population (or not) and we explored alternative groupings of observation errors. In this application, we evaluate uncertainty in the structure of process variability (environmental stochasticity) using some bird survey data. Breeding Bird Surveys have been conducted in the U.S. and Canada for 50+ years. In this analysis, we focus on 3 time series of American kestrel (*Falco sparverius*) abundance from adjacent Canadian provinces along a longitudinal gradient (British Columbia, Alberta, Saskatchewan). Data have been collected annually, and corrected for changes in observer coverage and detectability.

17.4.1 Read in and look at the data

Figure 17.4 shows the data.

```
birddat = t(kestrel[,2:4])
head(kestrel)
```

```
     Year British.Columbia Alberta Saskatchewan
[1,] 1969            0.754   0.460        0.000
[2,] 1970            0.673   0.899        0.192
[3,] 1971            0.734   1.133        0.280
[4,] 1972            0.589   0.528        0.386
[5,] 1973            1.405   0.789        0.451
[6,] 1974            0.624   0.528        0.234
```

We know that the surveys use the same design, so we will force observation error to be shared. Our uncertainty lies in whether these time series are sampling the same population, and how environmental stochasiticity varies by subpopulation. Our first model has 1 state vector, and equal observation variances:

```
Q.model="diagonal and equal"
R.model="diagonal and equal"
```

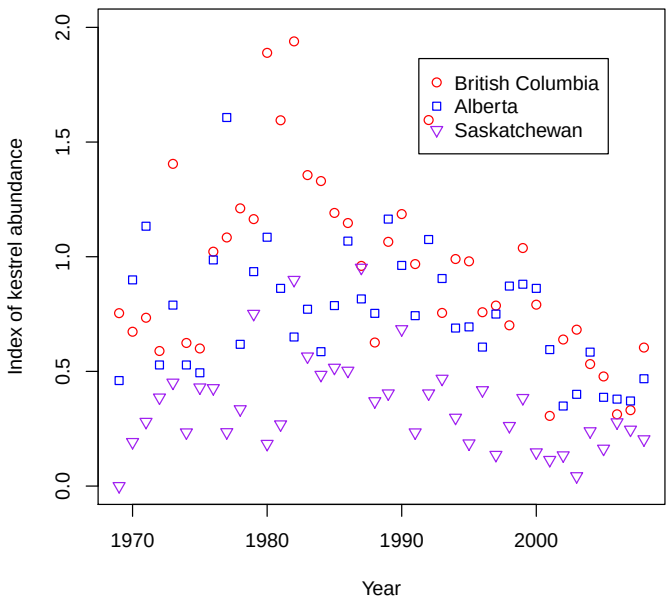

Fig. 17.4. The kestrel data.

```
U.model="equal"
Z.model=factor(c(1,1,1))
model1=list(Z = Z.model, Q = Q.model, R = R.model, U = U.model)
kem1 = MARSS(birddat, model=model1, control=list(minit=100) )
```

```
kem1$AICc
```

```
[1] 20.9067
```

Let's compare this to a model with separate state vectors:

```
Z.model=factor(c(1,2,3))
model2=list(Z = Z.model, Q = Q.model, R = R.model, U = U.model)
kem2 = MARSS(birddat, model=model2)
```

```
kem2$AICc
```

```
[1] 23.13879
```

Because these populations are surveyed over a relatively large geographic area, it is reasonable to expect that environmental variation may differ between populations. Third, we will fit a model with separate processes and unequal process variance parameters.

```
Q.model="diagonal and unequal"
model3=list(Z = Z.model, Q = Q.model, R = R.model, U = U.model)
kem3 = MARSS(birddat, model=model3)
```

```
kem3$AICc
```

```
[1] 19.34103
```

Finally for a fourth model, we will consider lumping Alberta/Saskatchewan, because the time series indicate similar trends.

```
Z.model=factor(c(1,2,2)) #1 observation time series for each x time series
model4=list(Z = Z.model, Q = Q.model, R = R.model, U = U.model)
kem4 = MARSS(birddat, model=model4)
```

```
kem4$AICc
```

```
[1] 12.50061
```

This last model was superior to the others, improving the AICc value compared to model 1 by 8 units. Figure 17.5 shows the fits for this model.

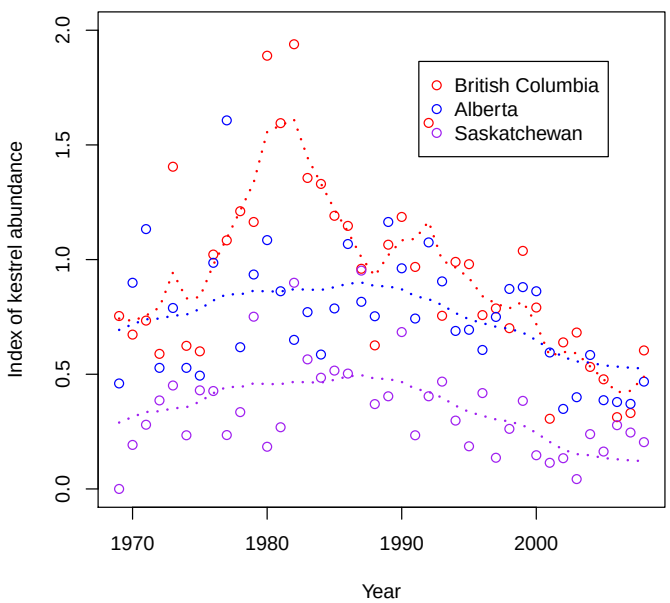

Fig. 17.5. Plot model 4 fits to the kestrel data.

A

Textbooks and articles that use MARSS modeling for population modeling

Textbooks Describing the Estimation of Process and Non-process Variance

There are many textbooks on Kalman filtering and estimation of state-space models. The following are a sample of books on state-space modeling that we have found especially helpful.

Shumway, R. H., and D. S. Stoffer. 2006. Time series analysis and its applications. Springer-Verlag.

Harvey, A. C. 1989. Forecasting, structural time series models and the Kalman filter. Cambridge University Press.

Durbin, J., and S. J. Koopman. 2001. Time series analysis by state space methods. Oxford University Press.

Kim, C. J. and Nelson, C. R. 1999. State space models with regime switching. MIT Press.

King, R., G. Olivier, B. Morgan, and S. Brooks. 2009. Bayesian analysis for population ecology. CRC Press.

Giovanni, P., S. Petrone, and P. Campagnoli. 2009. Dynamic linear models in R. Springer-Verlag.

Pole, A., M. West, and J. Harrison. 1994. Applied Bayesian forecasting and time series analysis. Chapman and Hall.

Bolker, B. 2008. Ecological models and data in R. Princeton University Press.

West, M. and Harrison, J. 1997. Bayesian forecasting and dynamic models. Springer-Verlag.

Tsay, R. S. 2010. Analysis of financial time series. Wiley.

Maximum-likelihood papers

This is just a sample of the papers from the population modeling literature.

de Valpine, P. 2002. Review of methods for fitting time-series models with process and observation error and likelihood calculations for nonlinear, non-Gaussian state-space models. Bulletin of Marine Science 70:455-471.

de Valpine, P. and A. Hastings. 2002. Fitting population models incorporating process noise and observation error. Ecological Monographs 72:57-76.

de Valpine, P. 2003. Better inferences from population-dynamics experiments using Monte Carlo state-space likelihood methods. Ecology 84:3064-3077.

de Valpine, P. and R. Hilborn. 2005. State-space likelihoods for nonlinear fisheries time series. Canadian Journal of Fisheries and Aquatic Sciences 62:1937-1952.

Dennis, B., J.M. Ponciano, S.R. Lele, M.L. Taper, and D.F. Staples. 2006. Estimating density dependence, process noise, and observation error. Ecological Monographs 76:323-341.

Ellner, S.P. and E.E. Holmes. 2008. Resolving the debate on when extinction risk is predictable. Ecology Letters 11:E1-E5.

Erzini, K. 2005. Trends in NE Atlantic landings (southern Portugal): identifying the relative importance of fisheries and environmental variables. Fisheries Oceanography 14:195-209.

Erzini, K., Inejih, C. A. O., and K. A. Stobberup. 2005. An application of two techniques for the analysis of short, multivariate non-stationary time-series of Mauritanian trawl survey data ICES Journal of Marine Science 62:353-359.

Hinrichsen, R.A. and E.E. Holmes. 2009. Using multivariate state-space models to study spatial structure and dynamics. In Spatial Ecology (editors Robert Stephen Cantrell, Chris Cosner, Shigui Ruan). CRC/Chapman Hall.

Hinrichsen, R.A. 2009. Population viability analysis for several populations using multivariate state-space models. Ecological Modelling 220:1197-1202.

Holmes, E.E. 2001. Estimating risks in declining populations with poor data. Proceedings of the National Academy of Sciences of the United States of America 98:5072-5077.

Holmes, E.E. and W.F. Fagan. 2002. Validating population viability analysis for corrupted data sets. Ecology 83:2379-2386.

Holmes, E.E. 2004. Beyond theory to application and evaluation: diffusion approximations for population viability analysis. Ecological Applications 14:1272-1293.

Holmes, E.E., W.F. Fagan, J.J. Rango, A. Folarin, S.J.A., J.E. Lippe, and N.E. McIntyre. 2005. Cross validation of quasi-extinction risks from real time series: An examination of diffusion approximation methods. U.S. Department of Commerce, NOAA Tech. Memo. NMFS-NWFSC-67, Washington, DC.

Holmes, E.E., J.L. Sabo, S.V. Viscido, and W.F. Fagan. 2007. A statistical approach to quasi-extinction forecasting. Ecology Letters 10:1182-1198.

Kalman, R.E. 1960. A new approach to linear filtering and prediction problems. Journal of Basic Engineering 82:35-45.

Lele, S.R. 2006. Sampling variability and estimates of density dependence: a composite likelihood approach. Ecology 87:189-202.

Lele, S.R., B. Dennis, and F. Lutscher. 2007. Data cloning: easy maximum likelihood estimation for complex ecological models using Bayesian Markov chain Monte Carlo methods. Ecology Letters 10:551-563.

Lindley, S.T. 2003. Estimation of population growth and extinction parameters from noisy data. Ecological Applications 13:806-813.

Ponciano, J.M., M.L. Taper, B. Dennis, S.R. Lele. 2009. Hierarchical models in ecology: confidence intervals, hypothesis testing, and model selection using data cloning. Ecology 90:356-362.

Staples, D.F., M.L. Taper, and B. Dennis. 2004. Estimating population trend and process variation for PVA in the presence of sampling error. Ecology 85:923-929.

Zuur, A. F., and G. J. Pierce. 2004. Common trends in Northeast Atlantic squid time series. Journal of Sea Research 52:57-72.

Zuur, A. F., I. D. Tuck, and N. Bailey. 2003. Dynamic factor analysis to estimate common trends in fisheries time series. Canadian Journal of Fisheries and Aquatic Sciences 60:542-552.

Zuur, A. F., R. J. Fryer, I. T. Jolliffe, R. Dekker, and J. J. Beukema. 2003. Estimating common trends in multivariate time series using dynamic factor analysis. Environmetrics 14:665-685.

Bayesian papers

This is a sample of the papers from the population modeling and animal tracking literature.

Buckland, S.T., K.B. Newman, L. Thomas and N.B. Koestersa. 2004. State-space models for the dynamics of wild animal populations. Ecological modeling 171:157-175.

Calder, C., M. Lavine, P. Müller, J.S. Clark. 2003. Incorporating multiple sources of stochasticity into dynamic population models. Ecology 84:1395-1402.

Chaloupka, M. and G. Balazs. 2007. Using Bayesian state-space modelling to assess the recovery and harvest potential of the Hawaiian green sea turtle stock. Ecological Modelling 205:93-109.

Clark, J.S. and O.N. Bjørnstad. 2004. Population time series: process variability, observation errors, missing values, lags, and hidden states. Ecology 85:3140-3150.

Jonsen, I.D., R.A. Myers, and J.M. Flemming. 2003. Meta-analysis of animal movement using state space models. Ecology 84:3055-3063.

Jonsen, I.D, J.M. Flemming, and R.A. Myers. 2005. Robust state-space modeling of animal movement data. Ecology 86:2874-2880.

Meyer, R. and R.B. Millar. 1999. BUGS in Bayesian stock assessments. Can. J. Fish. Aquat. Sci. 56:1078-1087.

Meyer, R. and R.B. Millar. 1999. Bayesian stock assessment using a state-space implementation of the delay difference model. Can. J. Fish. Aquat. Sci. 56:37-52.

Meyer, R. and R.B. Millar. 2000. Bayesian state-space modeling of age-structured data: fitting a model is just the beginning. Can. J. Fish. Aquat. Sci. 57:43-50.

Newman, K.B., S.T. Buckland, S.T. Lindley, L. Thomas, and C. Fernández. 2006. Hidden process models for animal population dynamics. Ecological Applications 16:74-86.

Newman, K.B., C. Fernández, L. Thomas, and S.T. Buckland. 2009. Monte Carlo inference for state-space models of wild animal populations. Biometrics 65:572-583

Rivot, E., E. Prévost, E. Parent, and J.L. Baglinière. 2004. A Bayesian state-space modelling framework for fitting a salmon stage-structured population dynamic model to multiple time series of field data. Ecological Modeling 179:463-485.

Schnute, J.T. 1994. A general framework for developing sequential fisheries models. Canadian J. Fisheries and Aquatic Sciences 51:1676-1688.

Swain, D.P., I.D. Jonsen, J.E. Simon, and R.A. Myers. 2009. Assessing threats to species at risk using stage-structured state-space models: mortality trends in skate populations. Ecological Applications 19:1347-1364.

Thogmartin, W.E., J.R. Sauer, and M.G. Knutson. 2004. A hierarchical spatial model of avian abundance with application to cerulean warblers. Ecological Applications 14:1766-1779.

Trenkel, V.M., D.A. Elston, and S.T. Buckland. 2000. Fitting population dynamics models to count and cull data using sequential importance sampling. J. Am. Stat. Assoc. 95:363-374.

Viljugrein, H., N.C. Stenseth, G.W. Smith, and G.H. Steinbakk. 2005. Density dependence in North American ducks. Ecology 86:245-254.

Ward, E.J., R. Hilborn, R.G. Towell, and L. Gerber. 2007. A state-space mixture approach for estimating catastrophic events in time series data. Can. J. Fish. Aquat. Sci., Can. J. Fish. Aquat. Sci. 644:899-910.

Wikle, C.K., L.M. Berliner, and N. Cressie. 1998. Hierarchical Bayesian space-time models. Journal of Environmental and Ecological Statistics 5:117-154

Wikle, C.K. 2003. Hierarchical Bayesian models for predicting the spread of ecological processes. Ecology 84:1382-1394.

B

Package MARSS: Warnings and errors

The following is brief descriptions of the warning and error message you may see and what they mean (or might mean).

B update is outside the unit circle

If you are estimating $\mathbf{B}$, then if the absolute value of all the eigenvalues of $\mathbf{B}$ are less than 1, the system is stationary (meaning the $\mathbf{X}$'s have some multivariate distribution that does not change over time). In this case, we say that $\mathbf{B}$ is within the unit circle. A pure univariate random walk for example would have $\mathbf{B}$=1 and it is not stationary. The distribution of $\mathbf{X}$ has a variance that increases with time. If on the other hand $|\mathbf{B}| < 1$, you have an Ornstein-Uhlenbeck process and is stationary, with a stationary variance of $\mathbf{Q}/(1-\mathbf{B}^2)$ (note $\mathbf{B}$ is a scalar here because in this example $\mathbf{X}$ is univariate). If any of the eigenvalues (real part) are greater than 1, then the system with "explode"—it rapidly diverges.

In the EM algorithm, there is nothing to force $\mathbf{B}$ to be on or within the unit circle (real part of the eigenvalues less than or equal to 1). It is possible at an update that $\mathbf{B}$ will be outside the unit circle. The problem is that if you get too far outside the unit circle, the algorithm becomes numerically unstable since small errors are magnified by the "explosive" $\mathbf{B}$ term. If you see the 'B outside the unit circle' warning, it is fine as long as it is temporary and the log-likelihood does not start decreasing (you will see a separate warning if that happens).

If you do see $\mathbf{B}$ outside the unit circle and the log-likelihood decreases, then it probably means that you have poorly specified the model somehow. An easy way to do this is to poorly specify the initial conditions, π and Λ. If, say, you try to specify a vague prior on $\mathbf{x}_0$ (or $\mathbf{x}_1$) with π equal to zero and Λ equal to a diagonal matrix with a large variance on the diagonal, you will likely run into trouble if $\mathbf{B}$ has off-diagonal terms. The reason is that by specifying that Λ is diagonal, you specified that the individual X's in $\mathbf{X}_0$ are

independent, yet if $\mathbf{B}$ has off-diagonal terms, the stationary distribution of $\mathbf{X}_1$ is NOT independent. If you force the diagonal terms on Λ to be big enough, you can force the maximum-likelihood estimate of $\mathbf{B}$ to be outside the unit circle since this is the only way to account for $\mathbf{X}_0$ independent and $\mathbf{X}_1$ highly correlated.

The problem is that you will not know the stationary distribution of the $\mathbf{X}$'s (from which $\mathbf{X}_0$ was presumably drawn) without knowing the parameters you are trying to estimate. One approach is the estimate both π and Λ by setting `x0="unconstrained"` and `V0="unconstrained"` in the model specification. Estimating both π and Λ cannot be done robustly for all MARSS models, and in general, one probably wants to specify the model in such a way as to fix one or both of these. Another, more robust approach, is to treat $\mathbf{x}_1$ as fixed but unknown (instead of $\mathbf{x}_0$). You do this by setting `model$tinitx=1`, so that π refers to $t = 1$ not $t = 0$. Then estimate π and fix $\Lambda = 0$. This eliminates Λ from the model and often eliminates the problems with prior specification—as the expense of m more parameters. Note, when you set $\Lambda = 0$, Λ is truly eliminated from the model by MARSS; the likelihood function is different, so do not expect $\Lambda = 0$ and $\Lambda \sim 0$ to have the same likelihood under all conditions.

Warning! Reached maxit before parameters converged

The maximum number of EM iterations is set by `control$maxit`. If you get this warning, it means that one of the parameters or log-likelihood had not yet reached the convergence stopping criteria before `maxit` was reached. There are many situations where you might want to set `control$maxit` lower than the value needed to reach convergence. For example, if you are using the EM algorithm to produce initial values for a different algorithm (like a Bayesian MCMC algorithm or a Newton method) then you can set `maxit` low, say 20 or 50.

Stopped at iter=xx in MARSSkem() because numerical errors were generated in MARSSkf

This means the Kalman filter/smoother algorithm became unstable and most likely one of the variances became ill-conditioned. When that happens the inverses of those matrices are poor, and you will start to get negative values on the diagonals of your var-covariance matrices. Once that happens, the inverse of that var-covariance matrix produces an error. If you get this error, turn on tracing with `control$trace=1`. This will store the error messages so you can see what is going on. It may be that you have specified the model in such a way that some of the variances are being forced very close to 0, which makes the var-covariance matrix ill-conditioned. The output from the MARSS call will be the parameter values just before

Warning: the xyz parameter value has not converged

The algorithm checks whether the log-likelihood and each individual parameter has converged. If a parameter has not converged, you can try upping `control$maxit` and see if it converges. If you set, `maxit` high, but the parameter is still not converging, then it suggests that one of the variance parameters is so small that the EM update steps for that parameter are tiny. For example, as $\mathbf{Q}$ goes to zero, the update steps for $\mathbf{u}$ go to zero. As Λ goes to zero, the update steps for π go to zero. The first thing to do is to reflect on whether you are inadvertently specifying the model in such a way that one of the variances is forced to zero. For example, if the total variance in $\mathbf{X}$ is 0.1 and you fix $\mathbf{R} = 0.2$ then $\mathbf{Q}$ must go to zero. The second thing to do is to try using a Newton algorithm, using your last EM values as the initial conditions for the Newton algorithm. The initial values are set using the `inits` argument for the `MARSS()` function.

Errors were caught in checkPopWrap

You will get this error if your model is internally inconsistent or your model is inconsistent with your data. For example, $\mathbf{B}$ and $\mathbf{Q}$ must have the same dimensions. If you set them to have different dimensions, you will get the `checkPopWrap` error. Often just running `dim(data)` and then looking at your model matrices, will reveal the problem. Other times you will get this error, because say you passed in a character value for something that must be numeric. The errors listed under this message will tell you what is wrong.

MARSSkem: The soln became unstable and logLik DROPPED

This is a more serious error as in the EM algorithm, the log-likelihood should never drop. The first thing to do is check if you have specified a bizarre model or data, inadvertently. Plot the data you are trying to fit. Often, this error arises when a user has inadvertently scrambled their data order during a demeaning or variance-standardization step. Second, check the model you are trying to fit. Use `test=MARSS(data, model=xyz, fit=FALSE)` and then `summary(test$model)`. This shows you what MARSS() thinks your model is, with fixed values in parentheses and estimated values without. You may be trying to fit an illogical model.

If those checks looks good, then pass `trace=1` into the `MARSS()` call. This will report a fuller set of warnings. Look if the error "B is outside the unit circle" appears. If so, you are probably specifying a strange $\mathbf{B}$ matrix. Are you forcing the $\mathbf{B}$ matrix to be outside the unit circle (eigenvalues > 1)? If so, you need to rethink your $\mathbf{B}$ matrix contraints. If you do not see that error, look at

`test$iter.record$logLik`. If the log-likelihood is steadily dropping (at each iteration) or drops by large amounts (much larger than the machine precision), that is bad and means that the EM algorithm did not work. If however the log-likelihood is just fluctuating by small amounts about some steady value, that is ok as it means that the values converged but the parameters are such that there are slight numerical fluctuations. Try passing `safe=TRUE` in via the `control` argument for `MARSS()`. This can sometimes help as it inserts a call to the Kalman filter after each individual parameter update.

Stopped at iter=xx in MARSSkem: solution became unstable. R (or Q) update is not positive definite

First check if you have specified an illegally constrained variance-covariance matrix. For example, if the variances (diagonal) are constrained to be equal, you cannot specify the covariances (off-diagonals) as unequal. Or if you specify that some of the covariances are equal, you cannot specify the variances as all unequal. These are illegal constraints on a variance-covariance matrix from a statistical perspective (nothing to do with MARSS specifically).

This could also be due to numerical instability as **B** leaves the unit circle or one of the variance matrix becomes ill-conditioned. Try turning on tracing with `control$trace=1` and turn on safe with `control$safe=TRUE`. This will print out the error warnings at each parameter update step. Then consider whether you have inadvertently specified the model in such a way as to force this behavior in the **B** parameter.

You might also get this error if you inadvertantly specified an improper structure for **R** or **Q**. For example, if you used `R=diag(c(1,1,"r"))` with the intent of specifying a diagonal matrix with fixed variance 1 at $\mathbf{R}[1,1]$ and $\mathbf{R}[2,2]$ and an estimated $\mathbf{R}[3,3]$, you would have actually specified a character matrix with `"0"` on the off-diagonals and `c("1","1","r")` on the diagonal. MARSS() interprets all elements in quotes as names of parameters to be estimated. Thus it will estimate one off-diagonal covariance and two diagonal variances. That happens to put illegal constraints on estimation of a variance-covariance matrix having nothing to do with MARSS() but with estimation of variance-covariance matrices in general.

iter=xx MARSSkf: logLik computation is becoming unstable. Condition num. of Sigma[t=1] = Inf and of R = Inf.

This means, generally, that V0 is very small, say 0, and R is very small and very close to zero.

Warning: setting diagonal to 0 blocked at iter=X. logLik was lower in attempt to set 0 diagonals on X

This is a warning not an error. What is happening is that one of the variances (in **Q** or **R**) is getting small and the EM algorithm is attempting to set the value to 0 (because `control$degen.allow=TRUE`). But when it tried to do this, the new likelihood with the variance equal to 0 was lower and the variance was not set to 0.

A model with a variance minuscule and a model with the same variance equal to 0 are not the same model. In the first, a stochastic process with small variance exists but in the second, the analogous process is deterministic. And in the first case, you can get a situation where the likelihood term L(x|mean=mu,sigma=0) appears. That term will be infinite when x=mu. So in the model with variance minuscule, you will get very large likelihood values as the variance term gets smaller and smaller. In the analogous model with that variance set to 0, that likelihood term does not appear so the likelihood does not go to infinity.

This is not an error nor pathological behavior; the models are fundamentally different. Nonetheless, this will pose a dilemma when you want to chose the best model based on maximum likelihood. The model with minuscule variance will have infinite likelihood but the same behavior as the one with variance 0. In our experience, this dilemma arises when one has a lot of missing data near the beginning of the time series and is affected by how you specify the prior on the initial state. Try setting the prior at $t = 0$ versus $t = 1$. Try using a diffuse prior. You absolutely want to compare estimates using the BFGS and EM algorithms in this case, because the different algorithms differ in their ability to find the maximum in this strange case. Neither is uniformly better or worse. It seems to depend on which variance (**Q** or **R**) is going to zero.

Warning: kf returned error at iter=X in attempt to set 0 diagonals for X

This is a warning that the EM algorithm tried to set one of the diagonals of element X to 0 because `allow.degen` is TRUE and element X is going to zero. However when this was tried, the Kalman filter returned an error. Typically, this happens when both **R** and **Q** elements are both trying to be set to 0. If the maximum-likelihood estimate is that both **R** and **Q** are zero, it probably means that your MARSS model is not a very good description of the data.

Warning: At iter=X attempt to set 0 diagonals for R blocked for elements where corresponding rows of A or Z are not fixed.

You have `control$degen.allow=TRUE` and one of the **R** diagonal elements is getting very small. MARSS attempts to set these **R** elements to 0, but if row i of **R** is 0, then the corresponding i rows of **a** and **Z** must be fixed. This is for the EM algorithm. It might work with the BFGS algorithm, or might spit out garbage without telling you. Always be a suspect, when the EM and BFGS behavior is different. That is a good sign that something is wrong with how your model describes the data. It's not a problem with the algorithms per se; rather for certain pathological models, the algorithms behave differently from each other.

Stopped at iter=X in MARSSkem. XYZ is not invertable.

There are a series of checks in MARSS that check if matrix inversions are possible before doing the inversion. These errors crop up most often when **Q** or **R** are getting very small. At some point, they can get so small that inversions become unstable. If this error is given, then the output will be the last parameter estimates before the error. Try setting `control$allow.degen=FALSE`. Sometimes the error occurs when a diagonal element of **Q** or **R** is being set to 0. You will also have to set `control$maxit` to something smaller because the EM algorithm will not stop since the problematic diagonal element will walk slowly and inexorably to 0.

C

Package MARSS: Object structures

Model objects: class marssm

Objects of class 'marssm' specify Multivariate Autoregressive State Space (MARSS) models. The `model` component of an ML estimation object (class marssMLE; see below) is a marssm object. These objects have the following components:

data An optional matrix (not dataframe), in which each row is a time series (time across columns).

fixed A list with 8 matrices Z, A, R, B, U, Q, x0, V0, specifying which elements of each parameter are fixed.

free A list with 8 matrices Z, A, R, B, U, Q, x0, V0, specifying which elements of each parameter are to be estimated.

M An array of dim $n \times n \times T$ (an $n \times n$ missing values matrix for each time point). Each matrix is diagonal with 0 at the i,i value if the i-th value of **y** is missing, and 1 otherwise.

miss.value Specifies missing value representation in the data.

The matrices in `fixed` and `free` work as pairs to specify the fixed and free elements for each parameter. See Chapter 4. The dimensions for `fixed` and `free` matrices are as follows, where n is the number of observation time series and m is the number of state processes:

Z n x m
B m x m
U m x 1
Q m x m
A n x 1
R n x n
x0 m x 1
V0 m x m

Use `is.marssm()` to check whether an marssm object is correctly specified. The MARSS package includes an `as.marssm()` method to convert objects of class popWrap (see next section) to objects of class marssm.

Wrapper objects: class popWrap

Wrapper objects of class popWrap contain specifications and options for estimation of a MARSS model. A popWrap object has the following components:

data A matrix (not dataframe) of observations (rows) × time (columns).
m Number of hidden state processes (number of rows in **x**).
model Either a list with 8 string elements Z, A, R, B, U, Q, x0, V0 (see below for details), or string `"use fixed/free"`.
fixed If `model[[elem]]="use fixed/free"`, a list with 8 matrices Z, A, R, B, U, Q, x0, V0.
free If `model[[elem]]="use fixed/free"`, a list with 8 matrices Z, A, R, B, U, Q, x0, V0.
inits A list with 8 matrices Z, A, R, B, U, Q, x0, V0, specifying initial values for parameters. Dimensions are given in the class 'marssm' section.
miss.value Specifies missing value representation (default is NA).
method The method used for estimation: 'kem' for EM, 'BFGS' for quasi-Newton.
control List of estimation options. For the EM algorithm, these include the elements `minit, maxit, abstol, allow.degen, safe` and `trace`. For Monte Carlo initialization, these include the elements `MCInit`, `numInits`, `numInitSteps` and `boundsInits`. See class marssMLE section for details.

Component `model` is a convenient way to specify model structure for certain common cases. If `model="use fixed/free"`, both `fixed` and `free` must be provided. See the class marssm section for how to specify fixed and free matrices. The function `MARSS()` calls `popWrap()` to create a popWrap object, then `is.marssm()` to coerce this object to class marssm for the estimation function.

The `popWrap()` function calls `checkPopWrap()` to check user inputs from `MARSS()`. Valid model structures are below.

A String 'unconstrained'='unequal', 'equal', 'scaling' or 'zero'. May also be a $m \times 1$ numeric matrix specifying a fixed **a** matrix. Specified as a list matrix to allow fixed and estimated elements.
B String 'identity', 'zero', 'unconstrained', 'diagonal and unequal', 'diagonal and equal', or 'equalvarcov'. May also be a numeric matrix specifying a fixed **B** matrix or a list matrix with fixed and estimated elements.
Q String 'identity', 'zero', 'unconstrained', 'diagonal and unequal', 'diagonal and equal', or 'equalvarcov'. May also be a numeric matrix specifying a fixed **Q** matrix or a list matrix with fixed and estimated elements.

R String 'identity', 'zero', 'unconstrained', 'diagonal and unequal', 'diagonal and equal', or 'equalvarcov'. May also be a numeric matrix specifying a fixed **R** matrix or a list matrix with fixed and estimated elements.

V0 String 'identity', 'zero', 'unconstrained', 'diagonal and unequal', 'diagonal and equal', or 'equalvarcov'. May also be a numeric matrix specifying a fixed Λ matrix or a list matrix with fixed and estimated elements.

U String 'unconstrained'='unequal', 'equal', or 'zero'. May also be a $m \times 1$ numeric matrix specifying a fixed **u** matrix. Specified as a list matrix to allow fixed and estimated elements.

x0 String 'unconstrained'='unequal', 'equal', or 'zero'. May also be a $m \times 1$ numeric matrix specifying a fixed π. Specified as a list matrix to allow fixed and estimated elements.

Z A vector of class factor specifying which **y** time series correspond to which state time series (in **x**) or a numeric $n \times m$ matrix specifying the **Z** matrix. The string 'identity' can be used to specify a $n \times n$ identity matrix and string 'ones' may be used to specify a column vector of n ones. A list matrix is used to specify a combination of fixed and estimated elements.

ML estimation objects: class marssMLE

Objects of class marssMLE specify maximum-likelihood estimation for a MARSS model, both before and after fitting. A minimal marssMLE object contains components `model, start` and `control`, which must be present for estimation by functions like `MARSSkem()`.

model MARSS model specification (an object of class 'marssm').

start List with 7 matrices A, R, B, U, Q, x0, V0, specifying initial values for parameters. Dimensions are given in the class marssm section.

control A list specifying estimation options. For `method="kem"`, these are

- *minit* Minimum number of iterations in the maximization algorithm.
- *maxit* Maximum number of iterations in the maximization algorithm.
- *abstol* Optional tolerance for log-likelihood change. If log-likelihood decreases less than this amount relative to the previous iteration, the EM algorithm exits.
- *trace* A positive integer. If not zero, a record will be created of each variable the maximization iterations. The information recorded depends on the maximization method.
- *safe* If TRUE, `MARSSkem()` will rerun `MARSSkf()` after each individual parameter update rather than only after all parameters are updated.
- *MCInit* Use Monte Carlo initialization?
- *numInits* Number of random initial value draws.
- *numInitSteps* Number of iterations for each initial value draw.
- *boundsInits* Bounds on the uniform distributions from which initial values will be drawn. (Note that bounds for the covariance matrices Q and R, which require positive values, are specified in logs.)

silent Suppresses printing of progress bar and convergence information.

`MARSSkem()` appends the following components to the marssMLE' object:

method A string specifying the estimation method ('kem' for estimation by `MARSSkem()`).
par A list with 8 matrices of estimated parameter values Z, A, R, B, U, Q, x0, V0. If there are fixed elements in the matrices, the corresponding elements in `$par` are set to the fixed values.
kf A list containing Kalman filter/smoother output. See Chapter 2
numIter Number of iterations required for convergence.
convergence Convergence status.
logLik the exact Log-likelihood. See Section 5.2.
errors any error messages
iter.record record of the parameter values at each iteration (if `control$trace=1`)

Several functions append additional components to the 'marssMLE' object passed in. These include:

`MARSSaic` Appends `AIC, AICc, AICbb, AICbp`, depending on the AIC flavors requested.
`MARSShessian` Appends `Hessian, gradient, parMean` and `parSigma`.
`MARSSparamCIs` Appends `par.se, par.bias, par.upCI` and `par.lowCI`.

D

Package MARSS: The top-level MARSS functions and the base functions

Package MARSS includes functions for estimating Multivariate Autoregressive State Space models, obtaining confidence intervals for parameters, and calculating Akaike's Information Criterion (AIC) for model selection. To make the package both flexible and easy to use, it is designed in two levels. At the base level, the programmer can interact directly with the estimation functions, using two kinds of R objects: objects of the model specification class 'marssm', and objects of estimation classes such as 'marssMLE'. At the user level, the `MARSS()` function allows model estimation with just one function call, hiding the details for ease of use. Users create models in an intuitive way using either list matrices or text strings; the `MARSS()` function then converts these constraints into the object structures required by the estimation functions, performing error checking as necessary.

The two-level package structure allows new users convenient access to the underlying functions, while maintaining flexibility to incorporate different applications and algorithms. Developers can use the base object types to write new functions for their own modeling applications.

To use `MARSS()`, the user specifies a model by supplying the model argument to `MARSS()`, using the method argument to specify an estimation method. Optionally, the user may provide initial values for the free parameters, and specify estimation options; for details see the `MARSS()` help file. The function returns an object containing the model, parameter values and estimation details. The user may pass the returned object to `MARSSboot()`, which generates bootstrap parameter estimates, or to `MARSSaic()`, which calculates various versions of AIC for model selection.

Figure C.1 shows the underlying base level operations `MARSS()` performs. The function creates a wrapper object of class 'popWrap'. It then calls the `as.marssm()` method for 'popWrap' to create a marssm object from the model structures provided. This model object, initial values and control information are the minimal information required by the estimation functions, and are combined into an object of class appropriate for the estimation method. The estimation function adds to this object the estimated parameter values, esti-

mation details, and other function-specific components, and then returns the augmented object.

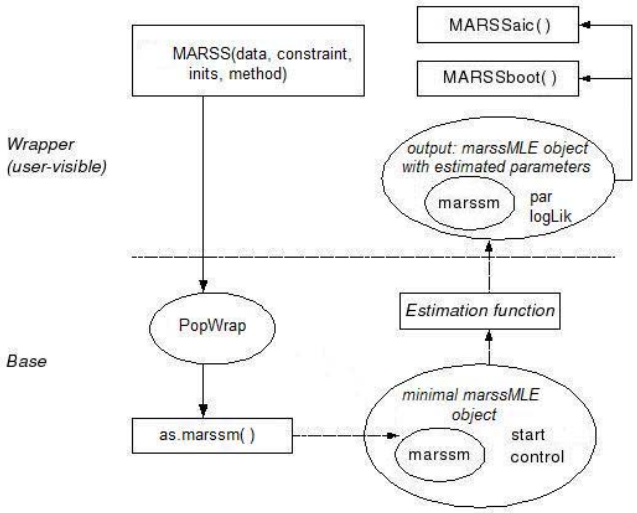

Fig. D.1. Two-level structure of the MARSS package. Rectangles represent functions; ovals represent objects.

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Index

animal tracking, 127
  kftrack, 133

bootstrap
  innovations, 13, 30, 31
  MARSSboot function, 13
  parametric, 13, 30, 31

confidence intervals, 80
  Hessian approximation, 13, 80
  MARSSparamCIs function, 13
  non-parametric bootstrap, 13
  parametric bootstrap, 13, 80
covariates, 53, 154, 157

density-independent, 63
diagnostics, 91

error
  observation, 64
  process, 63, 64
errors
  degenerate, 7
  ill-conditioned, 6
estimation, 67
  BFGS, 36
  Dennis method, 68
  EM, 12, 29, 67
  Kalman filter, 12, 27
  Kalman smoother, 12, 27
  maximum-likelihood, 67, 68
  Newton methods, 30
  quasi-Newton, 12, 36
  REML, 5

extinction, 63
  diffusion approximation, 72
  uncertainty, 76

functions
  as.marssm, 184
  checkPopWrap, 184
  is.marssm, 13, 184
  is.marssMLE, 12
  MARSS, 11, 35, 38, 40, 41, 184
  MARSSaic, 12, 30, 31, 50, 186
  MARSSboot, 13, 30, 49
  MARSShessian, 13, 186
  MARSSkem, 12, 29, 30, 185, 186
  MARSSkf, 12, 27, 28, 46
  MARSSkfas, 28
  MARSSmcinit, 12, 30
  MARSSoptim, 12
  MARSSparamCIs, 5, 13, 30, 44, 186
  MARSSsimulate, 13, 31, 50
  MARSSvectorizeparam, 13, 45
  optim, 12
  popWrap, 184
  summary, 13, 43

initial conditions
  setting for BFGS, 37

KFAS package, 5

likelihood, 12, 28, 50
  and missing values, 29
  innovations algorithm, 28
  MARSSkf function, 50

missing value modifications, 28
multimodal, 30
troubleshooting, 6, 30

MA(q), 59
MAR(p), 57
MARSS model, 1, 127
DFA example, 111
multivariate example, 83, 103, 127
print, 43
summary, 43
univariate example, 63
missing values, 5
and AICb, 31
and parametric bootstrap, 30
likelihood correction, 29
model selection, 31, 103
AIC, 31, 89, 91, 100, 101, 106, 110
AICc, 31, 100
bootstrap AIC, 31, 100
bootstrap AIC, AICbb, 31, 50
bootstrap AIC, AICbp, V, 31, 50, 100
MARSSaic function, 12, 50
model specification
in MARSS, 15
in marssm objects, 23

objects
marssm, 11, 13, 183
marssMLE, 11, 185, 186
popWrap, 184
outliers, 135

prior, 2, 19, 34
diffuse, 139, 140
troubleshooting, 5, 37, 140, 148, 178, 181

simulation, 31, 50, 64
MARSSsimulate function, 13, 50
standard errors, 13
structural breaks, 135