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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.

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 algorithm behind the TMU figure in Chapter 8 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. 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.

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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 MARSS package allows you to easily fit constrained and unconstrained MARSS models to multivariate time-series data via maximum-likelihood using either an EM algorithm or the BFGS algorithm.

A MARSS model, with Gaussian errors, takes the form:

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

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

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

The model includes random variables, parameters and data:

$\mathbf{x}_t$ is a $m \times 1$ column vector of the hidden 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 $\Sigma = \mathbf{Q}$.

$\mathbf{y}_t$ is a $n \times 1$ column vector of the observed data at time t.

$\mathbf{v}_t$ 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 $\Sigma = \mathbf{R}$.

$\mathbf{B}$ 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.

$\boldsymbol{\pi}$ is either a parameter or a fixed prior. It is a $m \times 1$ matrix.

$\mathbf{V}$ is a fixed value. It is a $m \times m$ variance-covariance matrix.

Note that the initial state can either be specified at $t = 1$ ($\mathbf{x}_1$) or $t = 0$ ($\mathbf{x}_0$). The default for the MARSS package is $t = 0$ but $t = 1$ can also be used.

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 inference, and the model is written to explicitly show them for clarity's sake. We include them throughout our discussion, but they can be set to zero easliy if desired.

The meaning of the parameters in the MARSS models depends on the application for which the MARSS model is being used. In the case studies, we show examples of MARSS models used to analyze population count data and animal tracking data, and Appendix A gives a selection of papers from the ecological literature. However, the MARSS package is not specific to population modeling applications. The functions in the MARSS package are generic functions for fitting, bootstrapping, and simulating MARSS models.

1.1 What does the MARSS package do?

The MARSS package is designed to fit unconstrained and constrained MARSS models. A constrained MARSS model is one in which some of the parameters are constrained in the sense that they have fixed, free and/or shared values. For example, let $\mathbf{M}$ and $\mathbf{m}$ be arbitrary matrix and column vector parameters. The MARSS package allows one to specify and fit models where $\mathbf{M}$ and $\mathbf{m}$ have shared values and fixed values. For example,

$$\mathbf{M} = \begin{bmatrix} a & 0.9 & c \\ -1.2 & a & 0 \\ 0 & c & b \end{bmatrix} \text{ and } \mathbf{m} = \begin{bmatrix} d \\ d \\ e \\ 2.2 \end{bmatrix}$$

The MARSS package fits models via maximum-likelihood. Two fitting algorithms are available: an EM algorithm and the BFGS algorithm (via *R* 's optim function). The MARSS is unusual amoung packages for for fitting MARSS models in that it provides an EM algorithm. The EM algorithm gives robust estimation for datasets replete with missing values and for 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. The MARSS package also 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)

Install the MARSS package and then type `library(MARSS)` at the command line to load the package. Read the first 2-4 pages of Chapter 3 then read

through a couple of the examples in Chapter 6. Get your data into a matrix (not dataframe) with time going across the columns and any non-data columns (like year) removed. Replace any missing time steps with a missing value holder (like NA or -99). Write your model down on paper and identify which parameters correspond to **B**, **u**, **Q**, **Z**, **a**, and **R** in the MARSS model (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

MARSS provides maximum-likelihood via an EM algorithm using the Kalman filter/smoother. All code is in native *R* . Thus the model fitting is slow (relatively)[1]. 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 in `optim()` to fit MARSS models.

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).

Data with cycles, from say internal dynamical interactions, are difficult to analyze, and both REML and Kalman-EM approaches will give poor estimates for this type of data. The slope method (Holmes, 2001), is more ad-hoc but is relatively robust to those problems. Holmes et al. (2007) used the slope method in a large study of data from endangered and threatened species; Ellner and Holmes (2008) showed that the slope estimates are close to the theoretical minimum uncertainty. However estimates using the slope method are not easily extended to multi-variate data and it is not a true maximum-likelihood method.

[1] In addition, the Kalman filter/smoother algorithm 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 20-40 times less efficient than more optimal formulations; see also (Kohn and Ansley, 1989; Koopman et al., 1999). However, when possible, MARSS uses the Kalman filter/smoother functions from the KFAS package; the KFAS filter/smoother functions use a more efficient algorithm and are 40-100 times faster.

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[2] 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 ($\boldsymbol{\pi}$ and $\mathbf{V}$) 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 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. 1) The correlation structure in $\mathbf{V}$ (whether the prior is diffuse or not) does match the correlation structure implied by the MARSS model. For example, you specify a diagonal $\mathbf{V}$ (independent states), but the implied distribution has correlations. 2) The correlation structure in $\mathbf{V}$ does not match the structure implied by constraints you placed on $\boldsymbol{\pi}$. For example, you specify that all values in $\boldsymbol{\pi}$ are shared, yet you specify that $\mathbf{V}$ is diagonal (independent). 3) You specify that $\mathbf{V}$=0 and specify that $\boldsymbol{\pi}$ corresponds to $\mathbf{x}_0$, but your model does not "run backwards" robustly so you cannot estimate $\mathbf{x}_0^0$. For example, you have a model with a non-diagonal $\mathbf{B}$ matrix, this model needs the $\mathbf{x}$ to be constrained by data, but $\mathbf{x}_0^0$ has no $\mathbf{y}_0$ to constrain it. You might get around this by specifying your prior as a prior on $\mathbf{x}_1^0$ instead of $\mathbf{x}_0^0$. You can get around these problems sometimes by using a diffuse prior (using `method="BFGS"` and `control$diffuse=TRUE`) but if you do not know the correlation structure of $\mathbf{V}$ then your diffuse prior will still conflict with the model. The other way to get around the problem is to set $\mathbf{V}$=0 (a $m \times m$ matrix of zeros) and estimate $\boldsymbol{\pi}$ only. Now $\boldsymbol{\pi}$ is a fixed but unknown (estimated) parameter, not the mean of a distribution. In this case, $\mathbf{V}$ does not exist in your model (because you set it to zero) and there is no conflict with the model; unfortunately estimating $\boldsymbol{\pi}$ as a parameter and is

[2] referring to the non-parametric bootstrap used in the package

not always robust. Whether to set your prior at $t = 1$ ($\mathbf{x}_1^0$) or at $t = 0$ ($\mathbf{x}_0^0$) will depend on your model.

1.4 Troubleshooting

There are two numerical errors and warnings that you may see when fitting MARSS models: ill-conditioning and degeneracy. 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. MARSS will print warning messages if the algorithm is 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 $\boldsymbol{\pi}$ values in your model[3]. The way our algorithm deals with $\mathbf{V}$ 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.

The second numerical error you may see is a degeneracy warning. 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 degenerate 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 $\boldsymbol{\pi}$. 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 $\boldsymbol{\pi}$. If `control$kf.x0="x10"`, then $\boldsymbol{\pi}$ 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

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

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[4].

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 the 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 diagonal elements of $\mathbf{R}$ or $\mathbf{Q}$ equal to zero). Lastly, the MARSS package allows one to specify a diverse array of models with shared and fixed parameter elements, and there is a one-to-one relationship between the model list in MARSS and the model as you would write it on paper.

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 now has a book also, Dynamic Linear Models with R by Petris et al.

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

[4] 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.

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 case of a 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 the same (or very similar) EM algorithm used in our MARSS package.

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 fit MARSS models using the KFAS functions and the optim() function for maximization using Newton algorithms. 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 $t = 0$.

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 ($\mathbf{Z}$ is the identity matrix). The default has a diagonal observation error matrix ($\mathbf{R}$) and an unconstrained process-error matrix ($\mathbf{Q}$). 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 Kalman-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(data, parList, ...)` 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 `parList`. 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(parList)` This returns simulated data from a MARSS model specified via a list of parameter matrices in `parList` (this is a list with elements `Q`, `R`, `U`, etc). Typically one would pass in `parList` using the `par` element in an marssMLE object (i.e., `MLEobj$par`), but you could also construct the list manually.

`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

The `MARSS()` function is an interface to the core functions and allows users to fit MARSS models using a list to specify the model structure. The MARSS model takes the form

$$\mathbf{x}_t = \mathbf{B}\mathbf{x}_{t-1} + \mathbf{u} + \mathbf{w}_t, \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}) \tag{3.1a}$$

$$\mathbf{y}_t = \mathbf{Z}\mathbf{x}_t + \mathbf{a} + \mathbf{v}_t, \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}) \tag{3.1b}$$

$$\mathbf{x}_0 \sim \text{MVN}(\boldsymbol{\pi}, \mathbf{V}) \text{ or } \mathbf{x}_1 \sim \text{MVN}(\boldsymbol{\pi}, \mathbf{V}) \tag{3.1c}$$

The $\mathbf{y}$ is a $n \times T$ matrix of observations and the $\mathbf{x}$ is a $m \times T$ matrix of hidden states. For example, a $\mathbf{y}$ data matrix of 3 inputs ($n = 3$) measured for 10 time steps would 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. $\mathbf{x}$ might look like (here $m = 2$):

$$\mathbf{x} = \begin{bmatrix} 0.8 & 2.2 & 3 & 2.8 & 3.2 & ... & 7.1 \\ 1.5 & 2.5 & 2.5 & 2.2 & 3.1 & ... & 6 \end{bmatrix}$$

In the process equation, $\mathbf{B}$ is a $m \times m$ matrix, $\mathbf{u}$ and $\mathbf{w}_t$ are $m \times 1$ matrices, and $\mathbf{Q}$ is a $m \times m$ variance-covariance matrix for the $\mathbf{w}_t$ process errors. In the observation equation, $\mathbf{Z}$ is a $n \times m$ matrix. In some applications, $\mathbf{Z}$ is a design matrix of zeros and ones where the row sums equal one. When $\mathbf{Z}$ is a design matrix, it specifies which observation time series, $y_{i,1:T}$, is associated with which hidden state process, $x_{j,1:T}$. $\mathbf{a}$ and $\mathbf{v}_t$ are $n \times 1$ matrices, and $\mathbf{R}$ is a $n \times n$ variance-covariance matrix for the $\mathbf{v}_t$ observation errors.

In the `MARSS()` function, the user specifies the model by passing in a parameter model list:

```
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) )
```

`data` must be a $n \times T$ matrix, that is time goes across columns.

The argument `model` is a list, where the list elements for each model parameter specifies the form of the 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 paramenter are shown. We show the forms using $m = 3$ (the number of hidden state processes) and $n = 3$ (number of observation time series).

3.1 u, a and $\boldsymbol{\pi}$ model structures

u, **a** and $\boldsymbol{\pi}$ 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 $\boldsymbol{\pi}$ because you need to make sure the structure in **V** matches. For example, if you require that all the $\boldsymbol{\pi}$ values are shared (equal) then **V** cannot be a diagonal matrix since that would be saying that the $\boldsymbol{\pi}$ values are independent, which they are clearly not if you force them to be equal.

There are fixed and estimated elements in **u**. `U.model=matrix(list(),m,1)` Here the model is specified as $m \times 1$ list matrix. 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:

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

There are shared elements in **u** but no fixed elements, then **u** can be specified with a character matrix. `U.model=matrix(c(),m,1)`. For example if `U.model=matrix(c("u1","u1","u2"),3,1)`, then **u** in the model has the following structure:

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

Note that `U.model=matrix(list("u1","u1","u2"),3,1)` also works.

Each element of **u** is estimated. `U.model="unequal"` or `U.model="unconstrained"`:

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

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

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

u is fixed `U.model=matrix(list(),m,1)` Here the model is specified as $m \times 1$ numeric (or list) matrix. 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, V model structures

The possible **Q**, **R**, and **V** model structures are identical, except that **R** is $n \times n$ while **Q** and **V** 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 specifing certain common structures. The structures are shown using **Q** as the example.

The most general case. There are fixed and estimated elements in **Q**. `Q.model=matrix(list(),m,m)` Here the model is specified as $m \times m$ list matrix. Each character string in the matrix is the name of one of the **Q** elements to be estimated. 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(..., nrow=m, ncol=m)` Passing in a $m \times m$ numeric matrix, means that **Q** is fixed to the values in the matrix. Note if $m = 1$, you still need to wrap its value in `matrix()` so that its class is 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 **V** model structures. Misspecifying the structure of **V** 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 (**Q**,**R** and **V**), **B** can be specified with a list matrix to allow you to have both fixed and shared elements in the **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 **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 **B** and the variance-covariance matrices, **Z** can be specified with a list matrix to allow you to have both fixed and estimated elements in **Z**. If **Z** is a square matrix, many of the same text shortcuts are available: "diagonal and equal", "diagonal and equal", and "equalvarcov". If **Z** is a design matrix[1], then a special shortcut is available using `factor()` which allows you to specify which **y** rows are associated with which **x** rows. See Chapter 6 and the case studies chapters for more examples.

`Z.model=factor(c(1,1,1))` All **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 **y** corresponds to a different hidden state trajectory. This is the default **Z** model and in this case $n = m$:

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

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

`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")`

`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(..., nrow=n, ncol=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.

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 $\mathbf{x}_0$ 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 MARSS 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 MARSS estimation functions may chug along happily and return a 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 reference and adopt their notation (for the most part).

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 $\boldsymbol{\epsilon}_t \equiv \mathbf{y}_t\text{-}\mathrm{E}(\mathbf{Y}_t)$. 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:

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

where N is the total number of data points, $\boldsymbol{\epsilon}_t$ 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 $\boldsymbol{\epsilon}_t$ and Σ_t in the Equation 5.1. Suppose the value $y_{i,t}$ is missing. First, the corresponding i-th value of $\boldsymbol{\epsilon}_t$ 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 Kalman-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 $\mathbf{V}$.

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 a series of short examples using the MARSS package functions. The examples use the Washington harbor seal dataset (`?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 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
```

6.1 Fitting different MARSS models to a dataset

6.1.1 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 $\mathbf{u}$ 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: 19.11268
AIC: -6.225352   AICc: 3.848722

     Estimate
Q.1   0.03024
Q.2   0.01072
Q.3   0.00690
Q.4   0.00426
Q.5   0.05267
R.1   0.00939
U.1   0.06840
U.2   0.07173
U.3   0.04169
U.4   0.05228
U.5  -0.00288
x0.1  5.98907
x0.2  6.72825
x0.3  6.66751
x0.4  5.83982
x0.5  6.60549
```

```
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 $\mathbf{R}$ and $\mathbf{Q}$), 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 100 interations.

MARSS fit is
Estimation method: BFGS
Estimation converged in 100 iterations.
Log-likelihood: 19.13936
AIC: -6.278712   AICc: 3.795362

     Estimate
Q.1   0.03368
Q.2   0.01124
Q.3   0.00722
Q.4   0.00437
Q.5   0.05600
R.1   0.00849
U.1   0.06837
U.2   0.07152
U.3   0.04187
U.4   0.05233
```

```
U.5  -0.00270
x0.1  5.98432
x0.2  6.72169
x0.3  6.65689
x0.4  5.83529
x0.5  6.60423

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, 23.053 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 86 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, control=list(kf.x0="x10"))
```

6.1.2 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:

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

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

$\mathbf{B}$ 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.

6.1.3 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 $\mathbf{B}$ 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 ($\mathbf{B}$,$\mathbf{Q}$,$\mathbf{R}$, and $\mathbf{V}$).

6.1.4 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.

6.1.5 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)))
```

6.1.6 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 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: 3.575237
AIC: 8.849526   AICc: 11.17211

     Estimate
A.2   0.80614
A.3   0.28714
A.4  -0.54169
A.5  -0.61899
Q.1   0.00458
R.1   0.04512
U.1   0.04763
x0.1  6.38185

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)`.

6.1.7 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: 16.65824
AIC: -9.316477   AICc: -3.937167

     Estimate
A.2   0.79435
A.3   0.27418
A.4  -0.53862
A.5  -0.61053
Q.1   0.00607
R.1   0.03217
R.2   0.03506
R.3   0.01361
R.4   0.01095
R.5   0.19662
U.1   0.05276
x0.1  6.26683

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

6.1.8 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 $\boldsymbol{\pi}$). `"diagonal and equal"` can be used as a shortcut for all square matrices (**B**,**Q**,**R**, and **V**).

6.2 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.

6.3 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.

6.3.1 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: 7.940938
AIC: 0.1181231   AICc: 2.440704

       ML.Est Std.Err    low.CI  up.CI
A.2   0.79560 0.06146  0.675148 0.9161
A.3   0.27505 0.06247  0.152604 0.3975
A.5  -0.06879 0.08871 -0.242666 0.1051
Q.1   0.00794 0.00435 -0.000581 0.0165
R.1   0.03399 0.00645  0.021350 0.0466
U.1   0.04315 0.01460  0.014532 0.0718
x0.1  6.17126 0.14647  5.884190 6.4583
x0.2  6.20511 0.15805  5.895335 6.5149

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.

6.3.2 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: 7.940938
AIC: 0.1181231   AICc: 2.440704

       ML.Est Std.Err  low.CI  up.CI Est.Bias Unbias.Est
A.2   0.79560 0.09546  0.6341 0.9255  0.01372    0.80932
A.3   0.27505 0.04596  0.1807 0.3086  0.01296    0.28801
A.5  -0.06879 0.07100 -0.1373 0.0486 -0.02365   -0.09244
Q.1   0.00794 0.00538  0.0000 0.0143  0.00182    0.00977
```

```
R.1   0.03399 0.00488  0.0278 0.0406  0.00141    0.03540
U.1   0.04315 0.01278  0.0259 0.0633 -0.00260    0.04056
x0.1  6.17126 0.15792  5.9596 6.4102 -0.03075    6.14050
x0.2  6.20511 0.19329  5.7782 6.4167  0.13973    6.34484

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

6.4 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         Q.1         R.1
0.79559952  0.27504984 -0.06878883  0.00794155  0.03398797
       U.1        x0.1        x0.2
0.04315203  6.17125597  6.20511352
```

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

```
parvec.new=parvec
parvec.new["Q.1"]=0.02; parvec.new["U.1"]=0.05
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 data and the parameters as a list.

```
kf=MARSSkf(dat, kem.new$par, miss.value=NA)
kf$logLik
```

```
[1] 5.943587
```

6.5 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: 11.67847
AIC: 2.643054   AICc: 63.30972

     Estimate
Q.1  1.89e-02
Q.2  1.03e-05
Q.3  8.24e-06
Q.4  3.05e-05
R.1  1.22e-02
U.1  9.79e-02
U.2  1.09e-01
U.3  9.28e-02
U.4  1.11e-01
x0.1 5.96e+00
x0.2 6.73e+00
x0.3 6.60e+00
x0.4 5.71e+00

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

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

```
Success! Parameters converged at 182 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 182 iterations.
Log-likelihood: 11.71475
AIC: 2.570491   AICc: 63.23716

     Estimate
Q.1    0.0189
Q.2    0.0000
Q.3    0.0000
Q.4    0.0000
R.1    0.0123
U.1    0.0979
U.2    0.1088
U.3    0.0924
U.4    0.1108
x0.1   5.9645
x0.2   6.7285
x0.3   6.6011
x0.4   5.7093

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

So three of the four $\mathbf{Q}$ 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 $\mathbf{Q}$ and one u value in $\mathbf{u}$:

```
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: 11.18711
AIC: -8.374226   AICc: 0.9591069
```

```
     Estimate
Q.1    0.0000
R.1    0.0194
U.1    0.1030
x0.1   6.0579
x0.2   6.7664
x0.3   6.5293
x0.4   5.7430

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.

6.6 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"`).

6.7 Data simulation

6.7.1 Simulated data from a fitted MARSS model

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

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

```
MARSSkf(sim.data[,,2], kem.sim.1$par, miss.value=NA)$logLik
```

```
[1] -67.27261
```

There are no missing values in our simulated data, but we still need to pass `miss.value` into `MARSSkf()`.

6.7.2 Simulated data from a user-built MARSS model

This shows you how to build up a model from scratch and simulate from that using `MARSSsimulate()`.

```
nsim = 20              # number of simulations
burn = 10              # length of burn in period
tSteps = 25
m=3                    #number of hidden state trajectories
B = diag(1,m);
A = array(0, dim=c(m,1))
Z = diag(1,m)
U = array(0.01, dim=c(m,1))
Q = diag(0.3, m)       #independent process errors
R = diag(0.01, m)      #independent obs errors
x0 = array(10, dim=c(m,1)) #initial conditions, really x_1
V0 = array(0,dim=c(m,m))   #leave this 0
the.par.list =
    list(Z=Z, A=A, R=R, B=B, U=U, Q=Q, x0=x0, V0=V0 )
# simulate data
sim = MARSSsimulate(the.par.list,nsim=nsim,tSteps=burn+tSteps)
# take off the burn
obs = sim$sim.data[,(burn+1):(burn+tSteps),] #m x T x nsim
```

We could also use `MARSSboot()` to create simulated data. However, `MARSSboot()` is designed to take a marssMLE object such as would be returned from `MARSS()`.

6.8 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: 7.940938
AIC: 0.1181231   AICc: 2.440704   AICbp(param): 472.7519

     Estimate
A.2   0.79560
A.3   0.27505
A.5  -0.06879
Q.1   0.00794
R.1   0.03399
U.1   0.04315
x0.1  6.17126
x0.2  6.20511

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

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.

8

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

8.1 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 σ^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, which is the same as the Gompertz model (Equation 3.1) 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:

$$x_t = x_{t-1} + u + w_t \qquad \text{where } w_t \sim \mathrm{N}(0, \sigma^2) \tag{8.1}$$

$$y_t = x_t + v_t \qquad \text{where } v_t \sim \mathrm{N}(0, \eta^2) \tag{8.2}$$

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 $\mathbf{Q}$ and $\mathbf{R}$ for the respective variance-covariance matrices.

8.2 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 8.1:

```
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 8.2 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
```

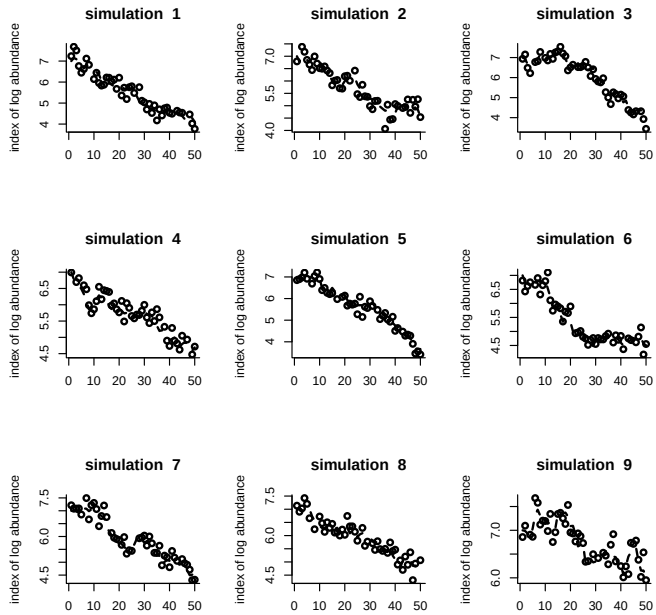

Fig. 8.1. Plot of nine simulated population time series with process and observation error. Circles are observation and the dashed line is the true population size.

Stochastic population trajectories show much variation, so it is best to look at a few simulated data sets at once. In Figure 8.1, nine simulations from the identical parameters are shown.

Example 8.1 (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 8.1 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))
```

8.3 Maximum-likelihood parameter estimation

8.3.1 Model with process and observation error

We put the simulated data through the Kalman-EM algorithm in order to estimate the parameters, u, σ^2, and η^2, and 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 8.1 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    -0.06717738 0.006180181 0.07288993
sim 2    -0.04517142 0.017932005 0.07003728
sim 3    -0.06911082 0.049417585 0.02638645
sim 4    -0.04678197 0.017297776 0.03446797
sim 5    -0.07156920 0.012044579 0.03917218
sim 6    -0.04523284 0.020796139 0.04522111
sim 7    -0.05735080 0.021471497 0.04753658
sim 8    -0.04612468 0.000000000 0.06892213
sim 9    -0.01662074 0.019171074 0.04505914
mean sim -0.05168221 0.018256760 0.04996586
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 a process with no environment variation and only observation error.

The Kalman-EM algorithm also gives an estimate of the true population size with observation error removed. This is in `kem$states`. Figure 8.2 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!

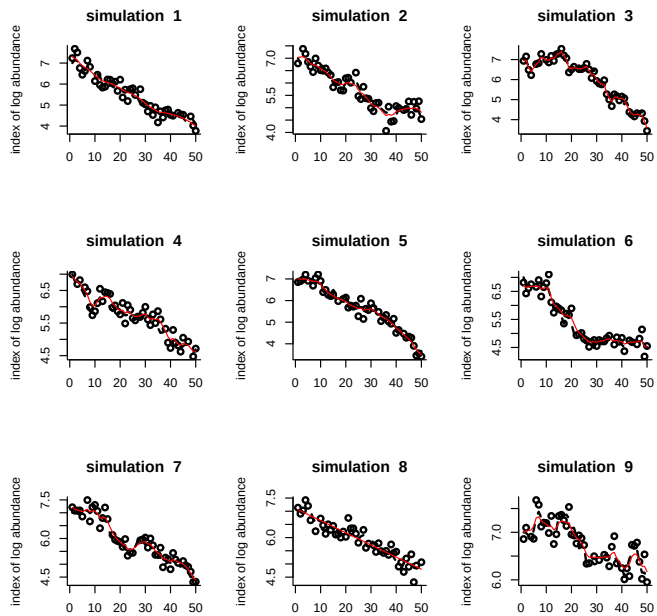

Fig. 8.2. The circles are the observed population sizes with error. The dashed lines are the true population sizes. The solid thin lines are the estimates of the true population size from the Kalman-EM algorithm. When the process error variance is 0, these lines are straight.

8.3.2 Model with no observation error

We used the Kalman-EM algorithm 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; 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 8.3. 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 8.2 using the process-error only model:

```
             den91.U    den91.Q
sim 1    -0.06364191 0.14749333
sim 2    -0.05912175 0.17813633
sim 3    -0.06844952 0.10790059
sim 4    -0.06196102 0.08688776
sim 5    -0.07091310 0.09809145
sim 6    -0.05631026 0.12135370
sim 7    -0.02992288 0.13479950
sim 8    -0.02456301 0.14427782
sim 9    -0.01724823 0.10579143
mean sim -0.05023685 0.12497021
true     -0.05000000 0.02000000
```

Notice that the u estimates are similar to those from the Kalman-EM algorithm, 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 8.2 (The variability in parameter estimates)

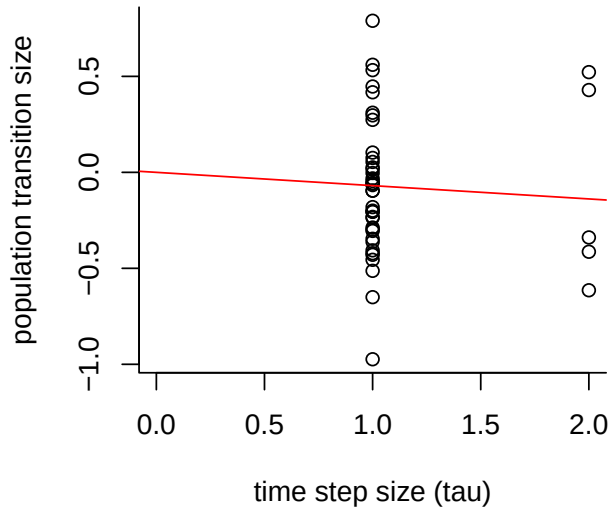

Fig. 8.3. The regression of $log(N_{t+\tau}) - log(N_t)$ against τ. The slope is the estimate of u and the variance of the residuals is the estimate of σ^2.

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 Kalman-EM estimates to the estimates using a process error only model (i.e. ignoring the observation error).

Example 8.2 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

  #Kalman-EM 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    -0.0813 -0.06931 0.02377 0.0511  0.1190
sim 2    -0.0542 -0.03817 0.01483 0.0596  0.1415
sim 3    -0.0244  0.00412 0.00000 0.0864  0.1899
sim 4    -0.0658 -0.05747 0.04150 0.0395  0.1212
sim 5    -0.0696 -0.03456 0.00000 0.0795  0.1475
sim 6    -0.0292 -0.03026 0.03778 0.0375  0.1202
sim 7    -0.0657 -0.03899 0.00811 0.0568  0.1150
sim 8    -0.0283 -0.01664 0.00626 0.0361  0.0824
sim 9    -0.0536 -0.05016 0.02414 0.0408  0.1012
mean sim -0.0525 -0.03683 0.01738 0.0541  0.1264
true     -0.0500 -0.05000 0.02000 0.0500  0.0200
```

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).*

8.4 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:

$$\Pi(x_d, t_e) = \pi(u) \times \Phi\left(\frac{-x_d + |u|t_e}{\sqrt{\sigma^2 t_e}}\right) + \exp(2x_d|u|/\sigma^2)\Phi\left(\frac{-x_d - |u|t_e}{\sqrt{\sigma^2 t_e}}\right) \quad (8.3)$$

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 8.4 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 Kalman-EM 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 Kalman-EM 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.

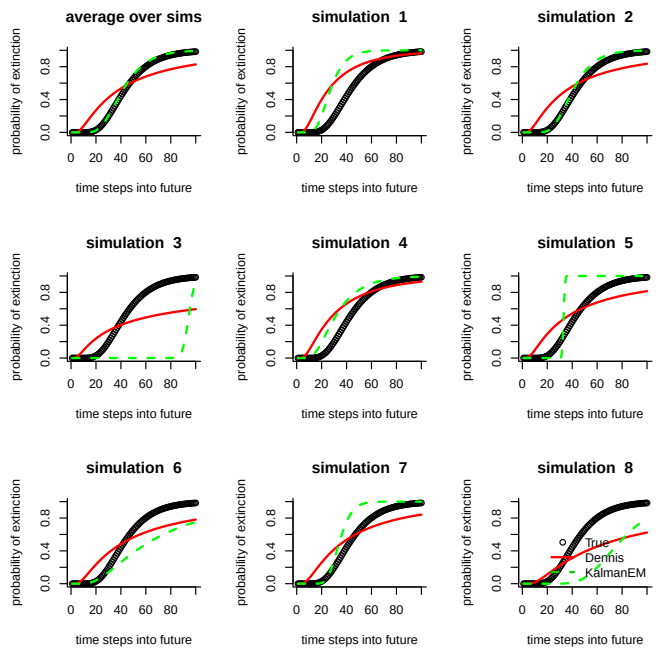

Fig. 8.4. Plot of the true and estimated probability of declining 90% in different time horizons for nine simulated population time series with observation error. The plot may look like a step-function if the σ^2 estimate is very small (<1e-4 or so).

Example 8.3 (The effect of parameter values on risk estimates)

In this example, you will recreate Figure 8.4 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 8.2 code before running the Example 8.3 code.

Example 8.3 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)

  #Kalman-EM 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 8.2 code. Then run the Example 8.3 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 8.2 code.)*

4. *How does changing the rate of decline (*`sim.u`*) change the estimates of risk? Rerun the Example 8.2 code using a lower u; this will create a new matrix of parameter estimates. Then run the Example 8.3 code. Do the estimates seem better of worse for rapidly declining populations?*

5. *Rerun the Example 8.2 code using fewer number of years (*`nYr` *smaller) and increase* `fracmiss`*. Then run the Example 8.3 code. The graphs will start to look peculiar. Why do you think it is doing that? Hint: look at the estimated parameters.*

8.5 Certain and uncertain regions

From Example 8.3, 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 8.3, 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 8.5 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.

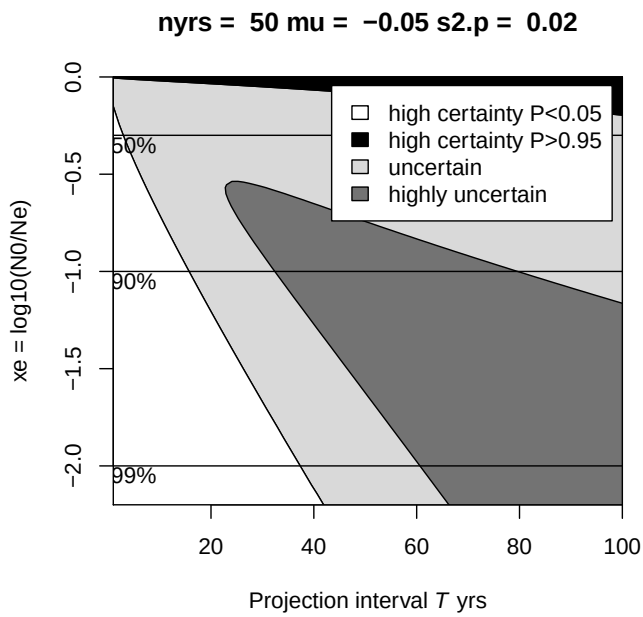

Fig. 8.5. This figure shows your region of high uncertainty (dark grey). In this region, the minimum 95% confidence intervals (meaning if you had no observation error) span 80% of the 0 to 1 probability. That is, you are uncertain if the probability of a specified decline is close to 0 or close to 1. 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 8.4 (Uncertain and certain regions)

Use the Example 8.4 code to re-create Figure 8.5 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 8.4 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)
```

8.6 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 8.6 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 8.5 (Risk figures for different species)

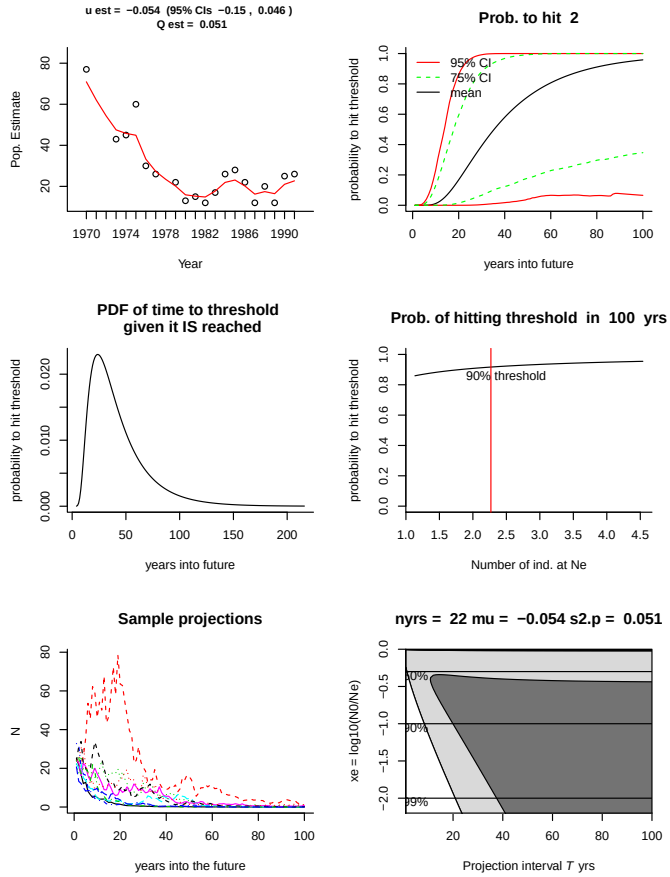

Fig. 8.6. Risk figure using data for the critically endangered African Wild Dog (data from Ginsberg et al. 1995). This population went extinct after 1992.

Use the Example 8.5 code to re-create Figure 8.6. 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 Sharp-tailed 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)
```

8.7 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 8.1 and 8.2
- 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 8.3 and code from Example 8.3)
- 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.

8.8 Comments

Data with cycles, from age-structure or predator-prey interactions, are difficult to analyze and the Kalman-EM algorithm used in the MARSS package will give poor estimates for this type of data. The slope method (Holmes, 2001) is 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).

9

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

9.1 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 9.1 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

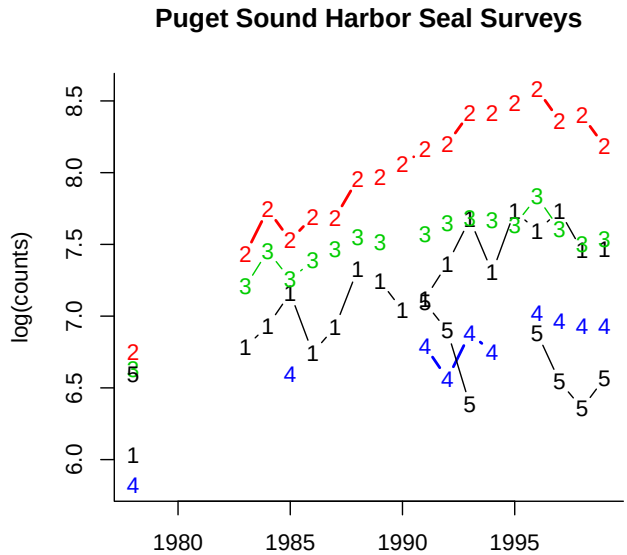

Fig. 9.1. Plot of the of the count data from the five harbor seal regions (Jeffries et al. 2003). Each region is an index of the total harbor seal population, but the bias (the difference between the index and the true population size) for each region is unknown.

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 (`years`) are in row 1 of `dat` and the logged data are in the rest of the rows. 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.

9.2 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

$$\mathbf{x}_t = \mathbf{B}\mathbf{x}_{t-1} + \mathbf{u} + \mathbf{w}_t, \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}) \tag{9.1}$$

$$\mathbf{y}_t = \mathbf{Z}\mathbf{x}_t + \mathbf{a} + \mathbf{v}_t, \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}) \tag{9.2}$$

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

9.2.1 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:

$$n_t = \exp(u + w_t)n_{t-1}, \tag{9.3}$$

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:

$$x_t = x_{t-1} + u + w_t, \text{ where } w_t \sim \text{N}(0, q) \tag{9.4}$$

$x_t = \log n_t$. 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.

9.2.2 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:

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} x_t + \begin{bmatrix} 0 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \end{bmatrix} \tag{9.5}$$

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 $\mathbf{R}$ ($\mathbf{v} \sim \text{MVN}(0, \mathbf{R})$), 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 th total population.

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

$$\mathbf{R} = \begin{bmatrix} r_1 & 0 & 0 & 0 & 0 \\ 0 & r_2 & 0 & 0 & 0 \\ 0 & 0 & r_3 & 0 & 0 \\ 0 & 0 & 0 & r_4 & 0 \\ 0 & 0 & 0 & 0 & r_5 \end{bmatrix} \tag{9.6}$$

$\mathbf{Z}$ 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 $n \times 1$:

$$\mathbf{Z} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \tag{9.7}$$

9.2.3 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()`. `model` is a list which specifies the model structure for $\mathbf{Z}$, $\mathbf{u}$, $\mathbf{Q}$, etc. The function call will now look like:

```
kem = 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 9.5). 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 (9.5) 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.

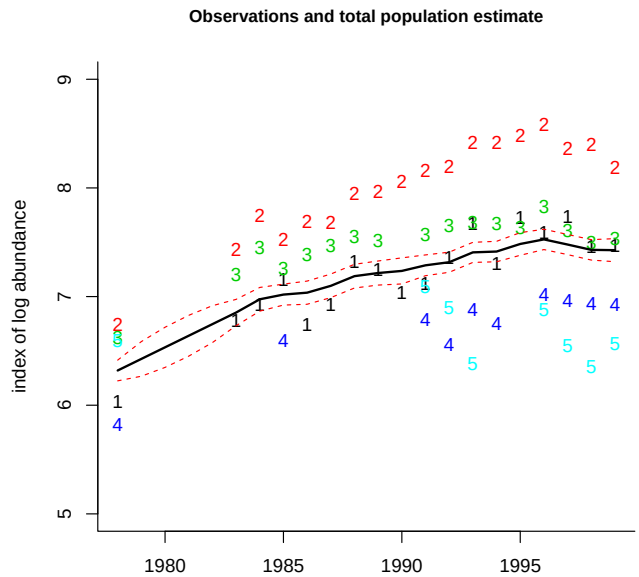

Fig. 9.2. Plot of the estimate of "log total harbor seals in Puget Sound" (minus the unknown bias for time series 1) against the data. The estimate of the total seal count has been scaled relative to the first time series. The 95% confidence intervals on the population estimates are the dashed lines. These are not the confidence intervals on the observations, and the observations (the numbers) will not fall between the confidence interval lines.

9.2.4 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 9.2) 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 9.2 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 9.1 (Fit the single population model)

Analyze the harbor seal data using the single population model (Equations 9.4 and 9.5). The code for Example 9.1 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 9.1 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$states,type="l",lwd=2)
title("Observations and total population estimate",cex.main=.9)
#show params
kem1$par
kem1$logLik
kem1$AIC
```

9.3 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 9.1:

```
print(kem1$par$R, digits=3)
```

```
         SJF:1  SJI:2 EBays:3 PSnd:4  HC:5
SJF:1   0.0322 0.0000  0.0000  0.000 0.000
SJI:2   0.0000 0.0351  0.0000  0.000 0.000
EBays:3 0.0000 0.0000  0.0136  0.000 0.000
```

```
PSnd:4  0.0000 0.0000  0.0000  0.011 0.000
HC: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] -9.316477  8.849526
```

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

[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.

[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.

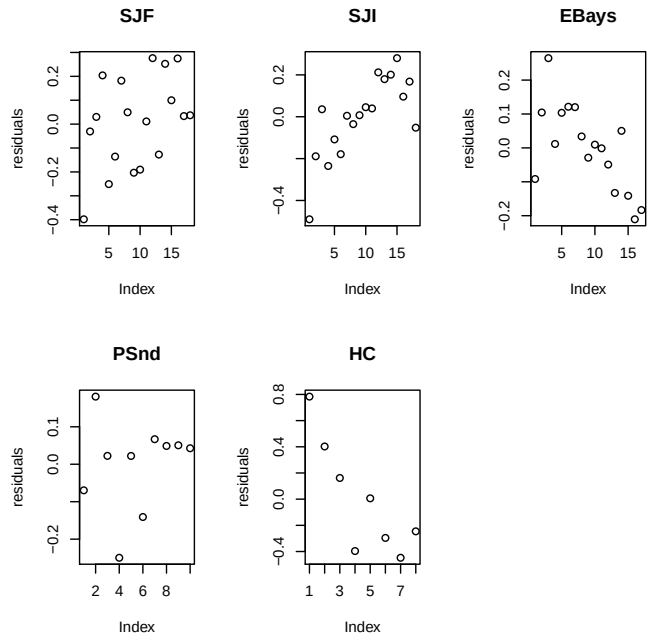

Fig. 9.3. Residuals for the model with a single population. The plots of the residuals should not have trends with time, but they do... This is an indication that the single population model is inconsistent with the data. The code to make this plot is given in the script file for this case study.

Example 9.2 (Fit a model with shared observation variances)

Analyze the data using the same population model as in Example 9.1, but constrain the $\mathbf{R}$ *matrix so that all five census regions have the same observation variance. The Example 9.2 code shows you how to do this. It also shows you how to make the diagnostics figure (Figure 9.3).*

Example 9.2 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 parameters
kem2$par$U       #population growth rate
kem2$par$Q       #process variance
kem2$par$R[1,1]  #observation variance
kem2$logLik #log likelihood
c(kem1$AIC,kem2$AIC)
#plot residuals
plotdat = t(dat)
matrix.of.biases = matrix(kem2$par$A,
  nrow=nrow(plotdat),ncol=ncol(plotdat),byrow=T)
xs = matrix(kem2$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))
```

9.4 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:

$$\begin{bmatrix} x_{n,t} \\ x_{s,t} \end{bmatrix} = \begin{bmatrix} x_{n,t-1} \\ x_{s,t-1} \end{bmatrix} + \begin{bmatrix} u \\ u \end{bmatrix} + \begin{bmatrix} w_{n,t} \\ w_{s,t} \end{bmatrix} \tag{9.8}$$

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:

$$\begin{bmatrix} w_{n,t} \\ w_{s,t} \end{bmatrix} \sim MVN\left(\begin{bmatrix} 0 \\ 0 \end{bmatrix}, \begin{bmatrix} q & 0 \\ 0 & q \end{bmatrix} \right) \tag{9.9}$$

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

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_{n,t} \\ x_{s,t} \end{bmatrix} + \begin{bmatrix} 0 \\ a_2 \\ 0 \\ a_4 \\ a_5 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \end{bmatrix} \tag{9.10}$$

9.4.1 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: 11.52836
AIC: -7.056721   AICc: -4.73414

     Estimate
A.2   0.79879
A.4  -0.75590
A.5  -0.81696
Q.1   0.00812
R.1   0.02928
U.1   0.05036
x0.1  6.06203
x0.2  6.83393

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

Figure 9.4 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 9.3 (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,* u *and* q*. The Example 9.3 code shows how to set the* `MARSS()` *arguments for this case.*

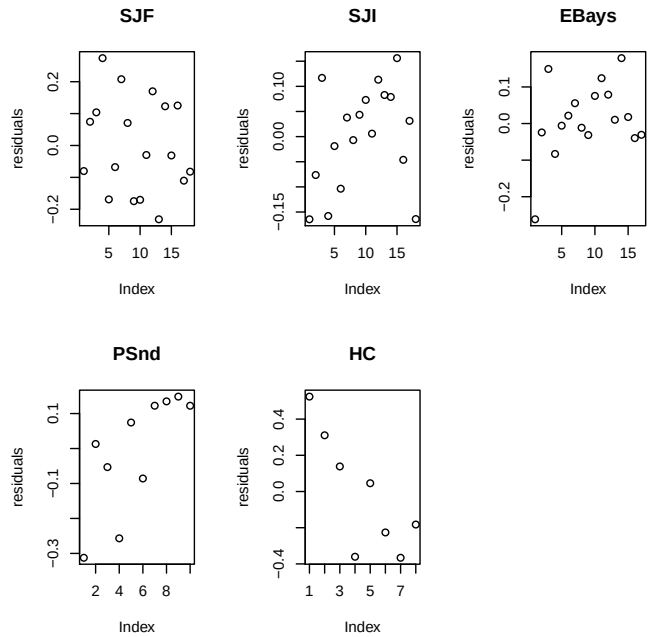

Fig. 9.4. The residuals for the analysis with a north and south subpopulation. The plots of the residuals should not have trends with time. Compare with the residuals for the analysis with one subpopulation.

Example 9.3 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(kem3$par$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))
```

9.5 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 9.4 (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 9.4 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 9.4 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 9.5 (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:

$$\begin{bmatrix} x_{n,t} \\ x_{s,t} \end{bmatrix} = \begin{bmatrix} x_{n,t-1} \\ x_{s,t-1} \end{bmatrix} + \begin{bmatrix} u_n \\ u_s \end{bmatrix} + \begin{bmatrix} w_{n,t} \\ w_{s,t} \end{bmatrix}, \begin{bmatrix} w_{n,t} \\ w_{s,t} \end{bmatrix} \sim \text{MVN}\left(0, \begin{bmatrix} q_n & 0 \\ 0 & q_s \end{bmatrix}\right) \quad (9.11)$$

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_{n,t} \\ x_{s,t} \end{bmatrix} + \begin{bmatrix} 0 \\ a_2 \\ 0 \\ a_4 \\ a_5 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \end{bmatrix} \quad (9.12)$$

Example 9.6 (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:

$$\begin{bmatrix} x_{p,t} \\ x_{h,t} \end{bmatrix} = \begin{bmatrix} x_{p,t-1} \\ x_{h,t-1} \end{bmatrix} + \begin{bmatrix} u_p \\ u_h \end{bmatrix} + \begin{bmatrix} w_{p,t} \\ w_{h,t} \end{bmatrix}, \begin{bmatrix} w_{p,t} \\ w_{h,t} \end{bmatrix} \sim \text{MVN}\left(0, \begin{bmatrix} q & c \\ c & q \end{bmatrix}\right) \quad (9.13)$$

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_{p,t} \\ x_{h,t} \end{bmatrix} + \begin{bmatrix} 0 \\ a_2 \\ a_3 \\ a_4 \\ 0 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \end{bmatrix} \quad (9.14)$$

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 9.7 (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 specifiy 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 estimates from a plane have the same variance as do 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)
```

9.6 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.]

10

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

10.1 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 10.1). 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 10.1). 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.

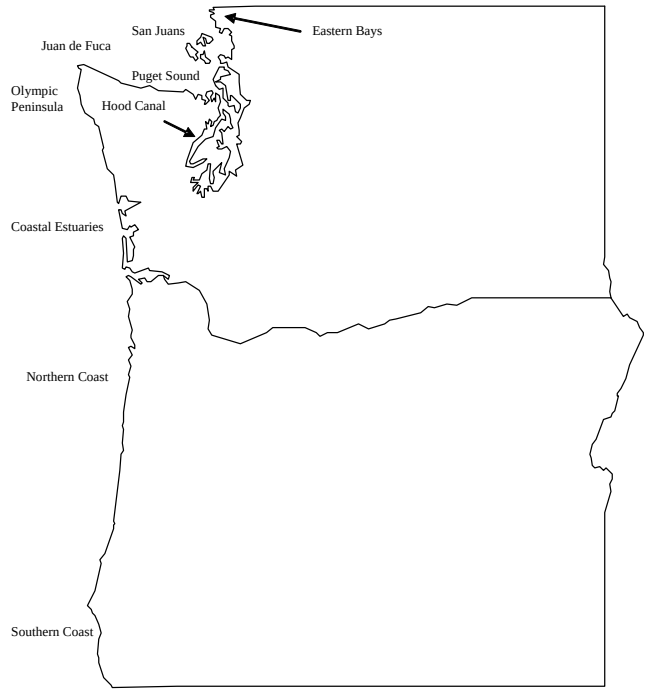

Fig. 10.1. Map of spatial distribution of 9 harbor seal sites in Washington and Oregon.

10.2 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.

10.2.1 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.

$$
\begin{array}{r}
\\ \\ \\ \\ \\ \\ \\ \\ \\
\end{array}
\begin{array}{c}
\text{H 1 and 2} \\ \mathbf{Z} \\ \begin{array}{cc} \text{subpop} & \text{subpop} \\ 1 & 2 \end{array} \\
\begin{bmatrix} \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{bmatrix}
\end{array}
\begin{array}{c}
\text{H 3 and 4} \\ \mathbf{Z} \\ \begin{array}{cc} \text{subpop} & \text{subpop} \\ 1 & 2 \end{array} \\
\begin{bmatrix} \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{bmatrix}
\end{array}
\begin{array}{c}
\text{H 5} \\ \mathbf{Z} \\ \begin{array}{c} \text{subpop} \\ 1 \end{array} \\
\begin{bmatrix} \\ \\ \\ \\ \\ \\ \\ \\ \\ \end{bmatrix}
\end{array}
$$

```
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=`

10.2.2 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=`

10.2.3 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.

10.2.4 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 10.1. Table to fill out for the five hypotheses from the first analysis (Section 10.2). 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"`.

10.3 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

10.3.1 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:

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

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

10.3.2 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.

10.3.3 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 10.2. Table to fill out for the four hypotheses from the second analysis (Section 10.3). 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							

10.3.4 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.

11

Case Study 4: Dynamic factor analysis (DFA) using MARSS

11.1 Dynamic factor analysis

In this case study, we use MARSS to do dynamic factor analysis (DFA) to look for a common set of underlying state processes that explain a set of time series (Harvey, 1989, sec. 8.5). Zuur et al. (2003) show a number of examples of using DFA to analyze fisheries catch data and zoobenthic abundances. This is conceptually different that what we have been doing in the previous case studies. Here we are trying to explain a set of n time series using linear combinations of a set of m hidden random walks.

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

$$\begin{aligned} \mathbf{x}_t &= \mathbf{x}_{t-1} + \mathbf{w}_t \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}) \\ \mathbf{y}_t &= \mathbf{Z}\mathbf{x}_t + \mathbf{a} + \mathbf{v}_t \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}) \\ \mathbf{x}_0 &\sim \text{MVN}(\boldsymbol{\pi}, \mathbf{V}) \end{aligned} \tag{11.1}$$

The $\mathbf{x}$'s are the hidden random walks (or trends) and $\mathbf{Z}\mathbf{x}_t$ is a linear combination of these. The objective is to estimate $\mathbf{Z}$ and $\mathbf{x}$. The $\mathbf{Z}$ matrix gives the factor loadings.

We will start by using a data set with six time series, thus $n = 6$. We will fit a model with three hidden random walks (or trends), thus $m = 3$. If we write out the model parameter matrices, this DFA model looks like so,

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

$$
\begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \\ y_{6,t} \end{bmatrix} = \begin{bmatrix} \gamma_{11} & \gamma_{12} & \gamma_{13} \\ \gamma_{21} & \gamma_{22} & \gamma_{23} \\ \gamma_{31} & \gamma_{32} & \gamma_{33} \\ \gamma_{41} & \gamma_{42} & \gamma_{43} \\ \gamma_{51} & \gamma_{52} & \gamma_{53} \\ \gamma_{61} & \gamma_{62} & \gamma_{63} \end{bmatrix} \mathbf{x}_t + \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \\ v_{6,t} \end{bmatrix} \tag{11.2}
$$

The **B** and **u** matrices have been added because MARSS will need values for these.

11.1.1 Constraints to ensure identifiability

If **Z**, **A** and **Q** are not constrained, then the DFA model above is not identifiable (Harvey, 1989, sec 4.4). Harvey (1989, sec. 8.5.1) suggests the following constraints to make the model identifiable:

- The **Q** matrix is constrained to be the identity matrix (a $m \times m$ diagonal matrix with 1s on the diagonal).
- In the first $m-1$ rows of **Z**, the j-th column in the i-th row is set to zero if $j > i$.
- The **a** vector is constrained such that the first m values are zero.

Zuur et al. (2003), however, note that with Harvey's third 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 use a different type of constraint on the **a** parameter. Constrain each x time-series in $\mathbf{x}$ to have a mean of zero across $t = 1$ to $t = T$. This means that you replace your 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. $\bar{\mathbf{x}}$ is the mean $\mathbf{x}_t$ value across t for $t = 1$ to T (the mean is across t not m). With this approach, you estimate all the **a** elements (none are set to zero) and they represent the average level of $\mathbf{y}_t$ relative to $\mathbf{Z}(\mathbf{x}_t - \bar{\mathbf{x}})$. Forcing the hidden state trajectories to have a mean of zero is implemented in the `MARSS()` function using the control value `demean.states=TRUE`.

Using these constraints, the DFA model becomes

$$\mathbf{x}_t = \begin{bmatrix} x_{1,t} \\ x_{2,t} \\ x_{3,t} \end{bmatrix} = \mathbf{I}_m \begin{bmatrix} x_{1,t-1} \\ x_{2,t-1} \\ x_{3,t-1} \end{bmatrix} + \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} w_{1,t} \\ w_{2,t} \\ w_{3,t} \end{bmatrix}, \mathbf{w}_t \sim \text{MVN}(0, \mathbf{I}_m)$$

$$\mathbf{y}_t = \begin{bmatrix} y_{1,t} \\ y_{2,t} \\ y_{3,t} \\ y_{4,t} \\ y_{5,t} \\ y_{6,t} \end{bmatrix} = \begin{bmatrix} \gamma_{11} & 0 & 0 \\ \gamma_{21} & \gamma_{22} & 0 \\ \gamma_{31} & \gamma_{32} & \gamma_{33} \\ \gamma_{41} & \gamma_{42} & \gamma_{43} \\ \gamma_{51} & \gamma_{52} & \gamma_{53} \\ \gamma_{61} & \gamma_{62} & \gamma_{63} \end{bmatrix} \mathbf{x}_t + \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \\ v_{3,t} \\ v_{4,t} \\ v_{5,t} \\ v_{6,t} \end{bmatrix}, \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}) \quad (11.3)$$

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

Here $\mathbf{I}_m$ is the $m \times m$ identity matrix[1]. Following Zuur et al. (2003), we set the initial state to have a zero mean and a diagonal variance-covariance matrix with a large variance.

11.2 The data

For this case study, we will analyze the Lake Washington plankton data that are loaded in the MARSS package. This is a 33-year time series of monthly counts of 13 plankton species along with temperature, phosporous, and pH data. We want to load in the data and then extract the subset of columns that are the phytoplankton species abundances.

```
data(lakeWAplankton)   #load the data
#Select out only the columns of abundance data
phytoplankton = c("Cryptomonas","Diatom", "Green",
   "bluegreen","Unicells","Otheralgae")
dat.spp = lakeWAplankton[,phytoplankton]
#we will use the data from 1977 onward
dat.spp.1977 = dat.spp[181:396,]
#Transpose so time goes across columns
dat.spp.1977 = t(dat.spp.1977)
```

It is normal in this type of analysis to standardize each time series by substracting its mean and dividing by its standard deviation:

$$\mathbf{y}_t^* = \Sigma^{-1}(\mathbf{y}_t - \bar{\mathbf{y}}) \quad (11.4)$$

[1] a diagonal matrix with 1s on the diagonal and 0s on the off-diagonal

where Σ 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

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

Figure 11.1 shows the data.

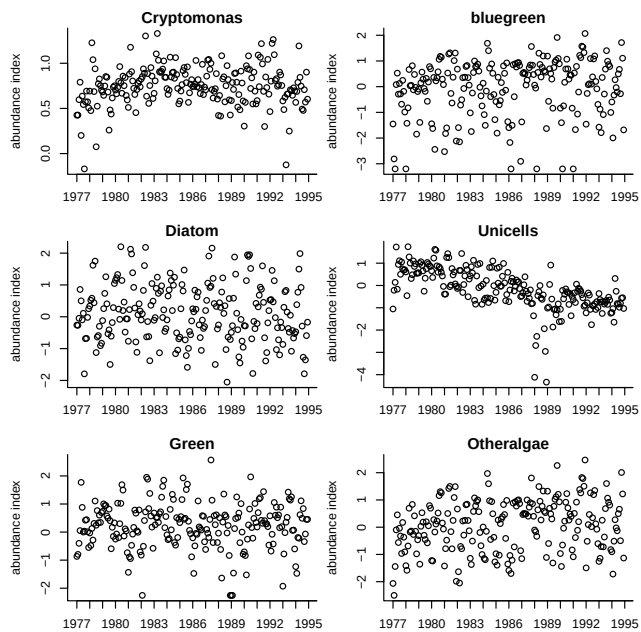

Fig. 11.1. Plot of the phytoplankton data.

11.3 Setting up the model

Notice when setting up the model structure for MARSS, that the parameter matrices have a one-to-one correspondence to the model as you would write it on paper (Equation 11.3). If a parameter matrix has a combination of fixed and

estimated values, then you specify that using `matrix(list(), rows, cols)`. 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(
"gam11",   0,      0,
"gam21","gam22",   0,
"gam31","gam32","gam33",
"gam41","gam42","gam43",
"gam51","gam52","gam53",
"gam61","gam62","gam63")
Z = matrix(Z.vals,6,3,byrow=TRUE)
```

When specifying the list values, spacing and carriage returns were added to help show the correspondence with the **Z** matrix in Equation 11.3. 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 0s). Notice that the 0s 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 not a fixed numeric value.

```
print(Z)
```

```
     [,1]    [,2]    [,3]
[1,] "gam11" 0       0
[2,] "gam21" "gam22" 0
[3,] "gam31" "gam32" "gam33"
[4,] "gam41" "gam42" "gam43"
[5,] "gam51" "gam52" "gam53"
[6,] "gam61" "gam62" "gam63"
```

The parameter **A** is set up similarly.

```
A.vals = list("a1","a2","a3","a4","a5","a6")
A = matrix(A.vals,6,1)
```

The **Q** and **B** matrices are set to be the identity matrix using `diag()`.

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

For our first analysis, we will assume that **R** is diagonal (no covariances) and each time series of phytoplankton is allowed to have a different observation variance. Thus **R** is a diagonal matrix that looks like so:

$$\begin{bmatrix} r_{11} & 0 & 0 & 0 & 0 & 0 \\ 0 & r_{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & r_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & r_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & r_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & r_{66} \end{bmatrix} \tag{11.5}$$

Each of the r_{ii} values is a different parameter to be estimated. We can 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,6,6,byrow=TRUE)
```

This is what **R** 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"
```

Alternatively, MARSS has a shorthand for this structure because it is very commonly used:

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

The parameters $\boldsymbol{\pi}$ (termed `x0` in MARSS) and **u** are set to be a matrix of zeros. Either of the following can be used:

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

There are shorthands for many of the common parameter matrix structures. Type ?MARSS at the *R* command line to see a list of the shorthand for each parameter matrix.

The **V** matrix (termed `V0` in MARSS) is a diagonal matrix with 5 along the diagonal:

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

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

```
dfa.model = list( Z=Z, A=A, R=R, B=B, U=U, Q=Q, x0=x0, V0=V0)
```

11.4 Fitting the model

We can now pass the DFA model list to `MARSS()` to estimate the **Z** matrix. The output is not shown since it is voluminous.

```
kemz.3 = MARSS(dat.z.scored, model=dfa.model,
  control=list(demean.states=TRUE) )
```

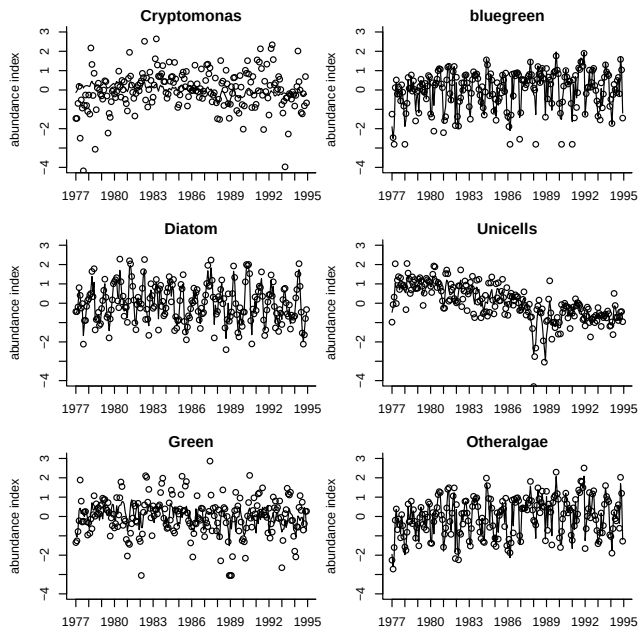

Fig. 11.2. Plot of the fits to the phytoplankton data.

11.5 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 which 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 parameters **R** and **a** stay the same but we need to change the other parameters because m is different.

```
m=2
n=6
Q=B=diag(1,m)
x0 = U = matrix(0,m,1)
V0 = diag(5,m)
#Set up Z as a list matrix
Z = matrix(list(),n,m)
#replace all the Z values with "1" to "12" sequentially
Z[,] = as.character(1:(m*n))
#Set the correct i,j values in Z to numeric 0
for(i in 1:(m-1)) Z[i,(i+1):m]=0
dfa.model = list( Z=Z, A=A, R=R, B=B, U=U, Q=Q, x0=x0, V0=V0)
```

The **Z** matrix specification looks a little odd because we need to create a list matrix with characters and numeric values (the 0s). You need to be careful that you do not end up with a character matrix (instead list matrix) with the 0s given as "0". If you do that, MARSS will interpret the "0" as names of a **Z** parameter that needs to be estimated. You can copy and paste this code to the R command line and check that the parameters have the correct structure.

Now we can fit the model and compare the AICc values (output not shown).

```
dat = dat.z.scored
kemz.2=MARSS(dat,model=dfa.model,control=list(demean.states=TRUE))
print(c(kemz.3$AICc, kemz.2$AICc))
```

Now let's test a suite of models. We will test one to six underlying trends (m 1 to 6) and four structures for the **R** matrix (diagonal and unequal, diagonal and equal, unconstrained, and equal variance and equal covariance). The following code builds our model matrices; you could also write out each matrix as we did in the first example, but this code allows us to build and run all the models.

```
#Set up the model
levels.R = c("diagonal and unequal", "diagonal and equal",
     "unconstrained")
model.data = data.frame()
dat = dat.z.scored
n=dim(dat)[1]
for( R in levels.R ){
for(m in 1:(n-1))
{
Z = matrix(list(),n,m)
```

```
Z[,] = as.character(1:(m*n))
if(m>1){
  for(i in 1:(m-1)) Z[i,(i+1):m]=0
}
x0 = U = matrix(0,m,1)
Q = B = diag(1,m)
V0 = diag(5,m)
dfa.model = list( Z=Z, A=A, R=R, B=B, U=U, Q=Q, x0=x0, V0=V0)
kemz=MARSS(dat,model=dfa.model,control=list(demean.states=TRUE))
model.data=rbind(model.data,data.frame(R=R,m=m,logLik=kemz$logLik,
   AICc=kemz$AICc, K=kemz$num.params, stringsAsFactors=FALSE))
assign(paste("kemz",m,R,sep="."),kemz)
}
}
```

Table 11.1. The model fits.

R	m	logLik	AICc	K
unconstrained	4	-1455.45	3004.22	45.00
unconstrained	3	-1459.99	3006.86	42.00
unconstrained	5	-1455.24	3008.10	47.00
unconstrained	2	-1469.74	3017.83	38.00
diagonal and unequal	4	-1512.44	3086.36	30.00
diagonal and unequal	5	-1532.05	3129.77	32.00
diagonal and unequal	3	-1547.93	3151.05	27.00
diagonal and equal	5	-1592.27	3239.73	27.00
diagonal and unequal	2	-1597.73	3242.32	23.00
diagonal and equal	4	-1601.50	3254.03	25.00
diagonal and equal	3	-1614.45	3273.69	22.00
unconstrained	1	-1611.01	3289.80	33.00
diagonal and unequal	1	-1644.37	3325.28	18.00
diagonal and equal	2	-1688.60	3413.73	18.00
diagonal and equal	1	-1770.42	3567.12	13.00

11.6 Using a varimax rotation to determine the trend loadings

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, however the different possible solutions are equivalent. The different solutions 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 equivalent solutions:

$$\begin{aligned} \mathbf{y}_t &= \mathbf{Z}\mathbf{x}_t + \mathbf{a} + \mathbf{v}_t \\ \mathbf{x}_t &= \mathbf{x}_{t-1} + \mathbf{w}_t \end{aligned} \tag{11.6}$$

and

$$\begin{aligned} \mathbf{y}_t &= \mathbf{Z}\mathbf{H}^{-1}\mathbf{x}_t + \mathbf{a} + \mathbf{v}_t \\ \mathbf{H}\mathbf{x}_t &= \mathbf{H}\mathbf{x}_{t-1} + \mathbf{H}\mathbf{w}_t \end{aligned} \tag{11.7}$$

There are many ways of doing factor rotations, and a common approach is the varimax rotation which seeks a rotation matrix $\mathbf{H}$ that tries to create 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 $(0.8, 0.1, 0.2)$, 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 $(0.8, 0.2, 0.2)$ and less like $(0.2, 0.2, 0.2)$.

The varimax rotation is easy to compute in *R* since *R* has a built in function for this.

```
b=sort(model.data$AICc,index.return=TRUE)
best.model=model.data[b$ix[1],]
fitname=paste("kemz",best.model$m,best.model$R,sep=".")
best.fit=get(fitname)
Zrot = varimax(best.fit$par$Z)$loadings #Z%*%H^{-1}
```

11.7 Discussion

These models can take a long time to converge. Make sure to try different inits values and force the algorithm to run a long time by using `control=list(minit=big, maxit=x)`, where "x" is a big. 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.

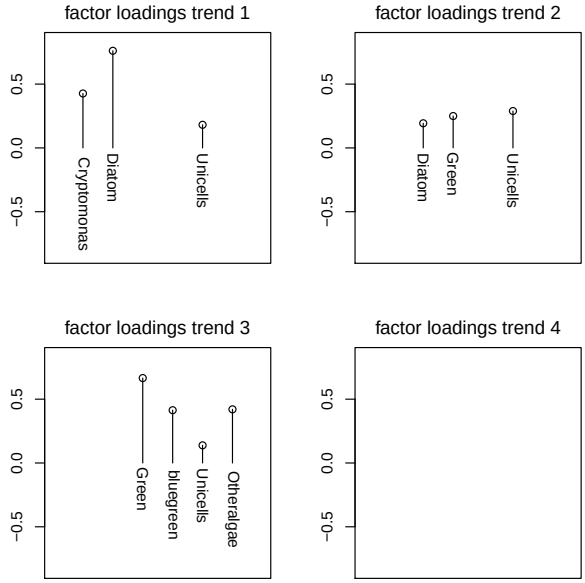

Fig. 11.3. Plot of the factor loadings (after varimax rotation) to the phytoplankton data. Factor loadings that are less than 0.1 are not plotted. Why is the trend 4 plot blank? It turns out that after the varimax rotation, the loadings on trend 4 are close to 0. The loadings on the other 3 trends are close to those from the model with $m = 3$ (instead of $m = 4$). This suggests that we choose the model with $m = 3$ (2nd row in table) instead of $m = 4$.

12

Case Study 5: Using state-space models to analyze noisy animal tracking data

12.1 A simple random walk model of animal movement

A simple random walk model of movement with drift (directional movement) but no correlation is

$$x_{1,t} = x_{1,t-1} + u_1 + w_{1,t}, \quad w_{1,t} \sim \mathrm{N}(0, \sigma_1^2) \tag{12.1}$$

$$x_{2,t} = x_{2,t-1} + u_2 + w_{2,t}, \quad w_{2,t} \sim \mathrm{N}(0, \sigma_2^2) \tag{12.2}$$

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:

$$y_{1,t} = x_{1,t} + v_{1,t}, \quad v_{1,t} \sim \mathrm{N}(0, \eta_1^2) \tag{12.3}$$

$$y_{2,t} = x_{2,t} + v_{2,t}, \quad v_{2,t} \sim \mathrm{N}(0, \eta_2^2), \tag{12.4}$$

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 12.2 and 12.4 written as a MARSS model (in matrix form):

$$\begin{bmatrix} x_{1,t} \\ x_{2,t} \end{bmatrix} = \begin{bmatrix} x_{1,t-1} \\ x_{2,t-1} \end{bmatrix} + \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} + \begin{bmatrix} w_{1,t} \\ w_{2,t} \end{bmatrix}, \ \mathbf{w}_t \sim \mathrm{MVN}\left(0, \begin{bmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{bmatrix}\right) \tag{12.5}$$

$$\begin{bmatrix} y_{1,t} \\ y_{2,t} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_{1,t} \\ x_{2,t} \end{bmatrix} + \begin{bmatrix} v_{1,t} \\ v_{2,t} \end{bmatrix}, \ \mathbf{v}_t \sim \mathrm{MVN}\left(0, \begin{bmatrix} \eta_1^2 & 0 \\ 0 & \eta_2^2 \end{bmatrix}\right) \tag{12.6}$$

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

$$\mathbf{x}_t = \mathbf{x}_{t-1} + \mathbf{u} + \mathbf{w}_t, \quad \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}) \tag{12.7}$$

$$\mathbf{y}_t = \mathbf{Z}\mathbf{x}_t + \mathbf{v}_t, \quad \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}). \tag{12.8}$$

The $\mathbf{Z}$ matrix is a 2×2 identity matrix.

12.2 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 12.1) 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.

12.3 Estimate locations from bad tag data

12.3.1 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,]
```

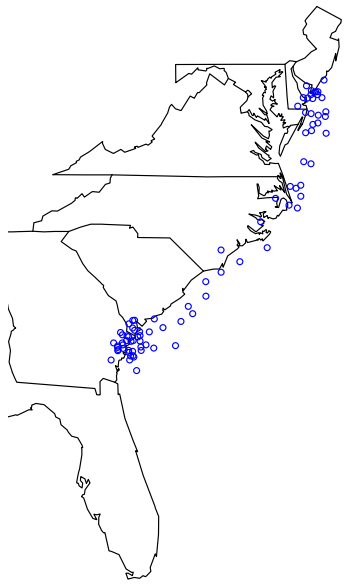

Fig. 12.1. Plot of the tag data from the turtle Big Mama. Errors in the location data make it seem that Big Mama has been moving overland.

```
   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 12.6, $\mathbf{Z}$ 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))
```

12.3.2 Compare state estimates to the real positions

The real locations (from which `loggerheadNoisy` was produced by adding noise) are in `loggerhead`. In Figure 12.2, 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.

12.3.3 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])
```

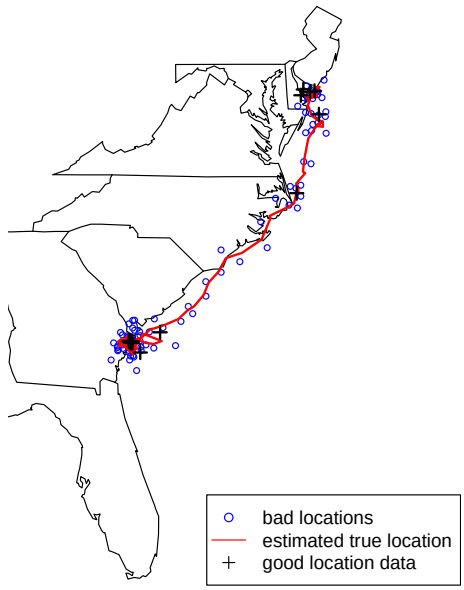

Fig. 12.2. Plot of the estimated track of the turtle Big Mama versus the good location data (before we corrupted it with noise).

`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 12.3). Repeat the analysis done for "Big Mama" for each of the other turtles and fill out the speed table (Table 12.1).

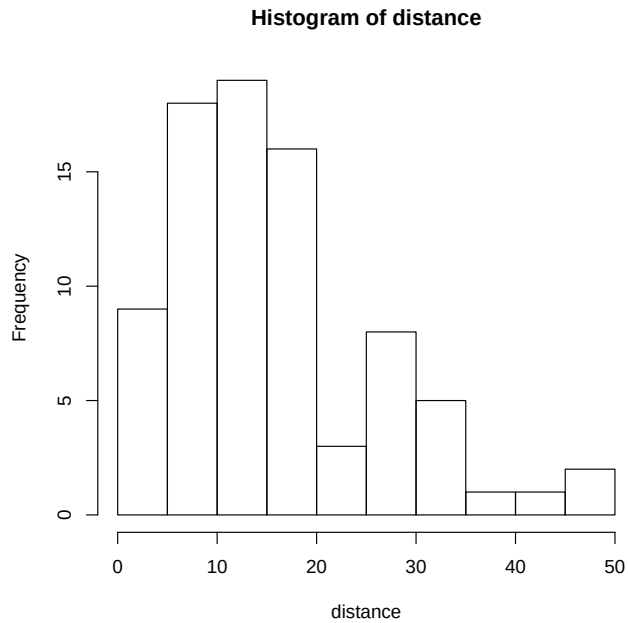

Fig. 12.3. Histogram of the miles traveled per day for Big Mama. Compare this to the estimate of miles traveled per day if you had not accounted for measurement errors. See the script file, `Case_Study_5.R`, for the code to do this.

12.4 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 12.1. 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		

12.5 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")
```

13

Case Study 6: Detection of outliers and structural breaks using MARSS

13.1 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 13.1 shows the data. To see all the *R* code behind the figures in the chapter, type `RShowDoc("Case_study_6.R",package="MARSS")`.

13.2 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.

13.2.1 Flat level model

We will start by modeling these data as a simple average river flow with variability around this level.

$$y_t = a + v_t \text{ where } v_t \sim \text{N}(0, r) \tag{13.1}$$

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.

$$\begin{gathered} x_t = 1 \times x_{t-1} + 0 + w_t \text{ where } w_t \sim \text{N}(0, 0) \\ y_t = 0 \times x_t + a + v_t \text{ where } v_t \sim \text{N}(0, r) \\ x_0 = 0 \end{gathered} \tag{13.2}$$

```
#load the datasets package
library(datasets)
data(Nile)   #load the data
plot(Nile,ylab="Flow volume",xlab="Year")
```

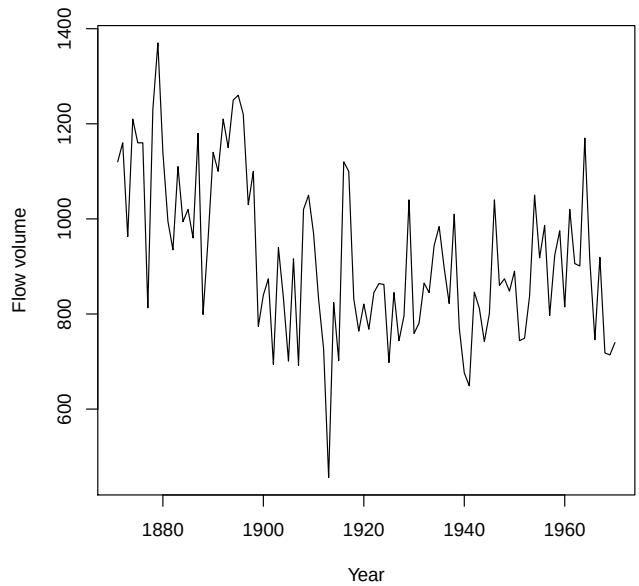

Fig. 13.1. The Nile River flow volume 1871 to 1970 (included dataset in *R*).

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:

$$\begin{aligned} x_t &= 1 \times x_{t-1} + 0 + w_t \text{ where } w_t \sim \text{N}(0,0) \\ y_t &= 1 \times x_t + 0 + v_t \text{ where } v_t \sim \text{N}(0,r) \\ x_0 &= a \end{aligned} \tag{13.3}$$

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.
```

13.2.2 Linear trend in flow model

Figure 13.2 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:

$$\begin{aligned} x_t &= 1 \times x_{t-1} + u + w_t \text{ where } w_t \sim \mathrm{N}(0,0) \\ y_t &= 1 \times x_t + 0 + v_t \text{ where } v_t \sim \mathrm{N}(0,r) \\ x_0 &= a \end{aligned} \tag{13.4}$$

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 13.2 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).

13.2.3 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 $t-1$.

$$\begin{aligned} x_t &= x_{t-1} + w_t \text{ where } w_t \sim \mathrm{N}(0, q) \\ y_t &= x_t + v_t \text{ where } v_t \sim \mathrm{N}(0, r) \\ x_0 &= \pi \end{aligned} \tag{13.5}$$

As before, y_t is the river flow volume at year t. With all the MARSS parameters shown, the model is:

$$
\begin{aligned}
x_t &= 1 \times x_{t-1} + 0 + w_t \text{ where } w_t \sim \mathrm{N}(0, q) \\
y_t &= 1 \times x_t + 0 + v_t \text{ where } v_t \sim \mathrm{N}(0, r) \\
x_0 &= \pi
\end{aligned}
\tag{13.6}
$$

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 $\mathbf{R}$ and $\mathbf{Q}$ 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 $\mathbf{Z}$, $\mathbf{A}$, $\mathbf{B}$ and $\mathbf{U}$, the following shortcuts could be used:

```
Z=B="ones"
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 interations.

MARSS fit is
Estimation method: BFGS
Estimation converged in 13 iterations.
Log-likelihood: -637.7462
AIC: 1281.492   AICc: 1281.742

      Estimate
Q.q       1238
R.r      15352
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_0 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:

```
kem.2.koop=MARSS(dat, model=mod.nile.2,
  control=list(kf.x0="x10",diffuse=TRUE), inits=kem.2em$par, method="BFGS")
```

```
Success! Converged in 12 interations.

MARSS fit is
Estimation method: BFGS
Estimation converged in 12 iterations.
Log-likelihood: -637.6043
AIC: 1281.209   AICc: 1281.459

      Estimate
Q.q       1271
R.r      15309
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 `control$diffuse=TRUE` specification means to use a true diffuse prior (variance is infinite). When using a diffuse prior make sure that **V** 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 **V** 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 **V** is specified as a diagonal variance-covariance matrix but `MLEobj$kf$VtT[,,1]` is not diagonal.

13.3 Observation and state residuals

Figure 13.2 shows the MARSS fits to the data. From these model fits, auxiliary residuals can be computed which contain information about whether the 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), **?** and Penzer (2001) for discussions of using auxiliary residuals for detection of outliers and structural breaks.

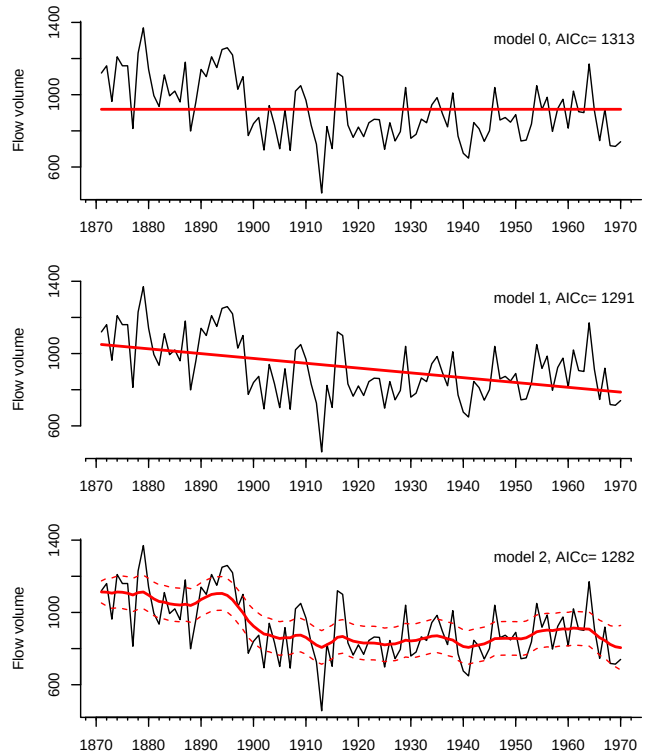

Fig. 13.2. The Nile River flow volume with the model estimated flow rates (solid lines). The bottom model is a stochastic level model, and the 2 standard deviations for the level are also shown. The other two models are deterministic level models so the state is not stochastic and does not have a standard deviation.

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 $\hat{y}_t$:

$$\begin{aligned} \hat{x}_t &= \mathrm{E}(x_t|\hat{\theta}, y_1^T) \\ \hat{y}_t &= \mathrm{E}(y_t|\hat{\theta}, y_1^T) \\ &= \mathrm{E}(x_t|\hat{\theta}, y_1^T) + \mathrm{E}(w_t|\hat{\theta}, y_1^T) = \hat{x}_t \end{aligned} \tag{13.7}$$

where $\hat{\theta}$ are the maximum-likelihood estimates of the parameters. The $\hat{y}_t$ equation comes directly from equation (13.5).

13.3.1 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:

$$\begin{aligned} \hat{v}_t &= y_t - \hat{y}_t \\ e_t &= \frac{1}{\sqrt{\mathrm{var}(\hat{v}_t)}}\hat{v}_t \end{aligned} \tag{13.8}$$

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 13.5). 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 13.3 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).

13.3.2 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:

[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.

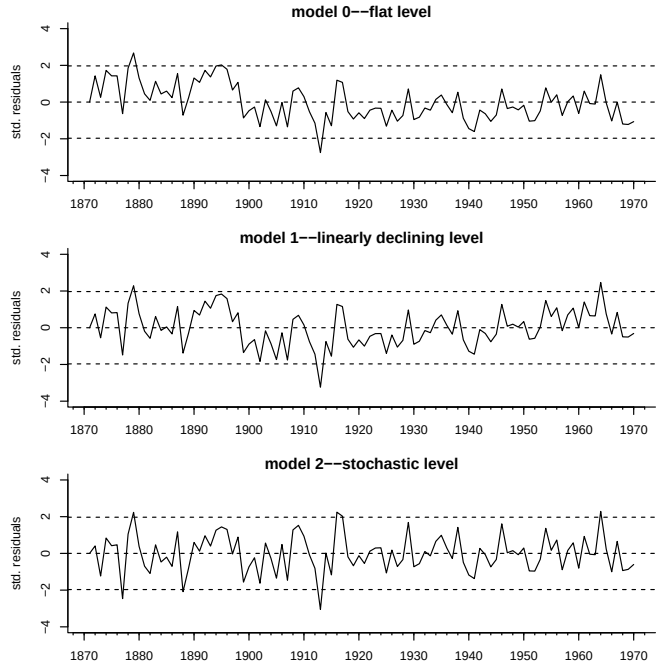

Fig. 13.3. The standardized observation residuals from models 0, 1, and 2. These residuals are the standardized $\hat{v}_t$. The dashed lines are the 95% CIs for a t-distribution.

$$\begin{aligned} \hat{w}_t &= \hat{x}_t - \hat{x}_{t-1} \\ f_t &= \frac{1}{\sqrt{\mathrm{var}(\hat{w}_t)}}\hat{w}_t \end{aligned} \tag{13.9}$$

These state residuals do not show simple changes in the average level; x_t is clearly changing in Figure 13.2, bottom panel. Instead we are looking for "breaks" or sudden changes in the level. The bottom panel of Figure 13.4 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.

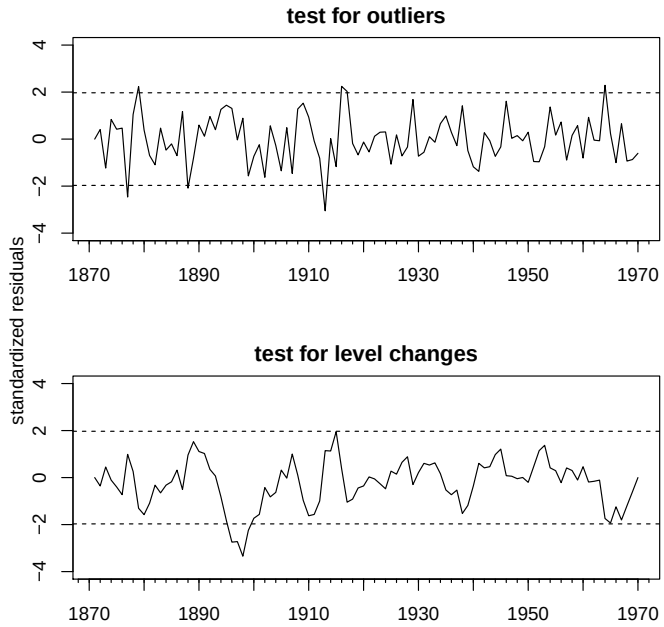

Fig. 13.4. Top panel, the standardized observation residuals. Bottom panel, the standardized state residuals. This replicates Figure 12 in Koopman et al. (1999).

14

Case Study 7: Estimation of species interaction strengths with and without covariates

14.1 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; Beisner et al., 2003; Hampton et al., 2008, 2006; Hampton and Schindler, 2006; Klug and Cottingham, 2001). These models are based on a process model of the form

$$\mathbf{x}_t = \mathbf{B}\mathbf{x}_{t-1} + \mathbf{u} + \mathbf{w}_t \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}) \tag{14.1}$$

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:

$$\mathbf{y}_t = \mathbf{Z}\mathbf{x}_t + \mathbf{a} + \mathbf{v}_t \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}) \tag{14.2}$$

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.

[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).

14.2 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.

14.2.1 Load in and plot the data

```
royale.dat = log(t(isleRoyal[,2:3]))
```

14.2.2 Fit the model to the wolf-moose data

The naive way to fit the model is to use Equations 14.2 and 14.1 "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. This a well-known problem, and you will need to find a way to fix $\mathbf{u}$ 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 $\mathbf{u}$ 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 $\mathbf{x}$ is treated as being at $t = 0$. If we are estimating the $\mathbf{B}$ matrix, we need to set this to be at $t = 1$ so that the initial $\mathbf{x}$ is constrained by the data at $t = 1$[2]. The reason is that we

[2] If there are many missing values at $t = 1$, we might still have problems and have to adjust accordingly.

```
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")
```

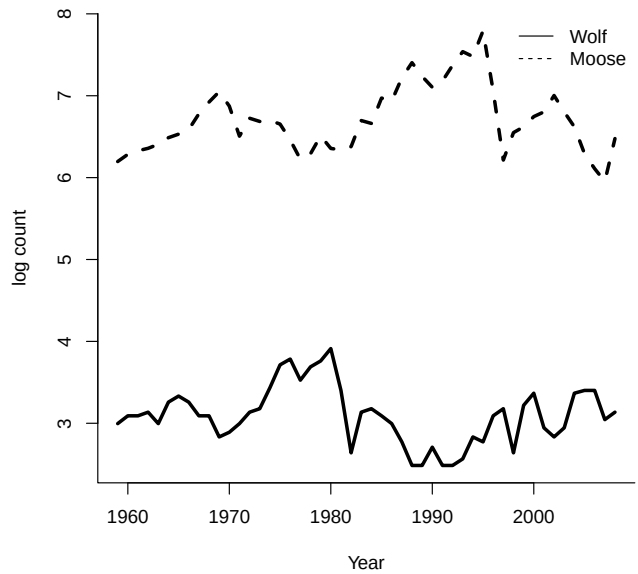

Fig. 14.1. Plot of the Isle Royale wolf and moose data.

need to estimate the initial $\mathbf{x}$. Even if we use a prior on the initial $\mathbf{x}$, we are still estimating its value. A model with a non-diagonal $\mathbf{B}$ matrix, does not "run backwards" well and the estimation of the initial $\mathbf{x}$ will run in circles. If we constrain it by data (at $t = 1$), we avoid this problem. So we will set `control$kf.x0="x10"`.

The other setting we want to change is `allow.degen`. This sets the diagonals of $\mathbf{Q}$ or $\mathbf{R}$ to zero if they are heading towards zero. When the initial $\mathbf{x}$ is at $t = 1$, this can have non-intuitive (not wrong but puzzling; see Appendix B) consequences if $\mathbf{R}$ is going to zero. So, we will set `control$allow.degen=FALSE` and manually set $\mathbf{R}$ to 0 if needed.

```
royale.model.1=list(Z=factor(c("Wolf","Moose")), B="unconstrained",
      Q="diagonal and unequal", R="diagonal and unequal",U="zero")
cntl.list=list(kf.x0="x10",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: -83.32606
AIC: 186.6521   AICc: 189.124

      Estimate
B.1   0.694642
B.2  -0.275035
B.3  -0.068210
B.4   0.632706
Q.1   0.452057
Q.2   0.279783
R.1   0.001760
R.2   0.000368
x0.1 -0.283219
x0.2 -1.261685

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

Convergence warnings
 Warning: the  R.1  parameter value has not converged.
 Warning: the  R.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=factor(c("Wolf","Moose")), B="unconstrained",
    Q="diagonal and unequal", R="zero", U="zero")
kem.2=MARSS(z.royale.dat, model=royale.model.2, control=cntl.list)
```

14.2.3 Look at the estimated interactions

The estimated **B** matrix is `kem.2$par$B`.

```
rownames(kem.2$par$B)=colnames(kem.2$par$B)=rownames(royale.dat)
print(kem.2$par$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 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.

14.2.4 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**.

14.3 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 14.2 shows the data. What you can see from the figure is that the data are only collected in the summer.

14.3.1 Load in the plankton data

```
# only use the plankton, daphnia, & non-daphnia
plank.dat = ivesDataByWeek[,3:6]
#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.

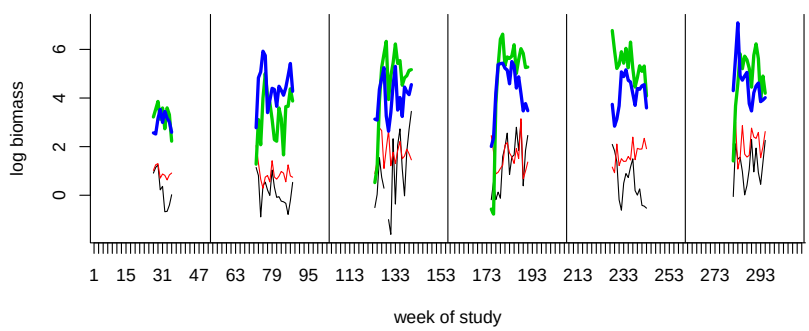

Fig. 14.2. Plot of the plankton data. Zooplankton are the thicker lines. Phytoplankton are the thinner lines.

14.3.2 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=factor(rownames(d.plank.dat))
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)
```

14.3.3 Fit the plankton model and look at the estimated B matrix

The call to fit the model is standard with the addition of setting `kf.x0`.

```
kem.plank.0 = MARSS(d.plank.dat, model=plank.model.0, control=list(kf.x0="x10"))
```

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 = kem.plank.0$par$B[1:4,1:4]
rownames(B.0) = colnames(B.0) = c("LP","SP","D","NP")
B.0[B.0==0]=NA
print(B.0,digits=2,na.print="--")
```

```
       LP   SP       D     NP
LP  0.834 0.10 -0.0024  0.075
SP  0.016 0.77  0.0134 -0.029
D   0.120 0.39  0.6045  0.469
NP -0.012 0.44 -0.1780  0.957
```

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    NP
LP 0.48 -0.39    --    --
SP   --  0.25 -0.17 -0.11
D    --    --  0.74  0.00
NP   --  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 aprior 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, control=list(kf.x0="x10"))
```

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.

14.3.4 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 (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,
    control=list(kf.x0="x10"))
```

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     NP
LP  0.535 0.014  0.082 0.1199
SP -0.157 0.846  0.065 0.0043
D   0.138 0.351  0.654 0.3760
NP  0.045 0.303 -0.154 0.8895
```

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,
     control=list(kf.x0="x10"))
```

Now we are getting closer to the Ives et al. estimates:

```
     LP     SP      D    NP
LP 0.75 -0.303     --    --
SP   --  0.748 -0.015 0.033
D    --     --  0.885    --
NP   --  0.059     -- 0.665
```

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,
    control=list(kf.x0="x10"))
```

As you can see from Table 14.1, 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.

14.3.5 Adding covariates

The standard way that you will see covariate data, denoted $\mathbf{z}_t$, added to a MARSS model is the following:

$$\begin{aligned} \mathbf{x}_t &= \mathbf{B}\mathbf{x}_{t-1} + \mathbf{u} + \mathbf{C}\mathbf{z}_t + \mathbf{w}_t, \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}) \\ \mathbf{y}_t &= \mathbf{Z}\mathbf{x}_t + \mathbf{a} + \mathbf{v}_t, \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}) \end{aligned} \tag{14.3}$$

Now, $\mathbf{z}_t$ is the covariate data[3], like temperature, at time t and $\mathbf{C}$ is the (linear) effect of $\mathbf{z}_t$ on $\mathbf{x}_t$. Keep in mind that this is the data, not the actual covariate value, although in the standard covariate model, we treat the covariate data as the true value of the covariate.

The difficulty with this approach is that is 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. You cannot have missing values in your covariate data, again unlikely. 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.

MARSS instead deals with covariates by including them in $\mathbf{y}_t$ and modeling them with their own state process(es) in $\mathbf{x}_t$. This is the approach that Ives et al. used in their state-space model and solves the difficulties listed above.

The MARSS model with covariates looks like:

$$\begin{aligned} \begin{bmatrix} \mathbf{x}_t \\ \mathbf{x}'_t \end{bmatrix} &= \begin{bmatrix} \mathbf{B} & \mathbf{C} \\ 0 & \mathbf{B}' \end{bmatrix} \begin{bmatrix} \mathbf{x}_{t-1} \\ \mathbf{x}'_{t-1} \end{bmatrix} + \begin{bmatrix} \mathbf{u} \\ \mathbf{u}' \end{bmatrix} + \mathbf{w}_t, \ \mathbf{w}_t \sim \text{MVN}\left(0, \begin{bmatrix} \mathbf{Q} & 0 \\ 0 & \mathbf{Q}' \end{bmatrix}\right) \\ \begin{bmatrix} \mathbf{y}_t \\ \mathbf{z}_t \end{bmatrix} &= \begin{bmatrix} \mathbf{Z} & 0 \\ 0 & \mathbf{Z}' \end{bmatrix} \begin{bmatrix} \mathbf{x}_t \\ \mathbf{x}'_t \end{bmatrix} + \begin{bmatrix} \mathbf{a} \\ \mathbf{a}' \end{bmatrix} + \mathbf{v}_t, \ \mathbf{v}_t \sim \text{MVN}\left(0, \begin{bmatrix} \mathbf{R} & 0 \\ 0 & \mathbf{R}' \end{bmatrix}\right) \end{aligned} \tag{14.4}$$

If we wanted to replicate Equation 14.3, we would set $\mathbf{Z}' = \mathbf{I}$, $\mathbf{R}' = 0$, $\mathbf{B}' = \mathbf{I}$, $\mathbf{u}' = 0$, $\mathbf{a}' = 0$ and $\mathbf{Q}' = \mathbf{I}$. The $\mathbf{I}$'s are identity matrices[4]. $\mathbf{R}'$ is set to zero, so $\mathbf{x}'_t$ will be equal to $\mathbf{z}_t$, and we set $\mathbf{Q}'$ equal to something big (like $\mathbf{I}$) to give the state process enough flexibility so that $\mathbf{x}'_t$ can equal exactly $\mathbf{z}_t$.

The MARSS model with covariates is written concisely as

$$\begin{aligned} \mathbf{x}_t &= \mathbf{B}^\sharp\mathbf{x}_{t-1} + \mathbf{u}^\sharp + \mathbf{w}_t, \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}^\sharp) \\ \mathbf{y}_t &= \mathbf{Z}^\sharp\mathbf{x}_t + \mathbf{a}^\sharp + \mathbf{v}_t, \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}^\sharp) \end{aligned} \tag{14.5}$$

[3] In Ives et al., $\mathbf{z}_t$ is termed $\mathbf{U}_t$.

[4] diagonal matrix with 1s on the diagonal. The size of the matrix is implicit here to remove clutter.

where the parameters with the $^\sharp$ are defined as follows:

$$\mathbf{B}^\sharp = \begin{bmatrix} \mathbf{B} & \mathbf{C} \\ 0 & \mathbf{B}' \end{bmatrix}, \mathbf{u}^\sharp = \begin{bmatrix} \mathbf{u} \\ \mathbf{u}' \end{bmatrix}, \mathbf{Q}^\sharp = \begin{bmatrix} \mathbf{Q} & 0 \\ 0 & \mathbf{Q}' \end{bmatrix}$$
$$\mathbf{Z}^\sharp = \begin{bmatrix} \mathbf{Z} & 0 \\ 0 & \mathbf{Z}' \end{bmatrix}, \mathbf{a}^\sharp = \begin{bmatrix} \mathbf{a} \\ \mathbf{a}' \end{bmatrix}, \mathbf{R}^\sharp = \begin{bmatrix} \mathbf{R} & 0 \\ 0 & \mathbf{R}' \end{bmatrix} \tag{14.6}$$

14.3.6 Set up the MARSS model with covariates

First we need to add the logged covariates to our data matrix.

```
#transpose to make time go across columns
covariates = t(log(ivesDataByWeek[,7:8]))
d.covariates = (covariates-apply(covariates,1,mean,na.rm=TRUE))
plank.dat.covar = rbind(plank.dat,covariates)
d.plank.dat.covar = rbind(d.plank.dat,d.covariates)
```

Next make the $\mathbf{B}^\sharp$ matrix. Some elements are estimated and others are fixed at 0.

```
B=matrix(list(0),6,6)
diag(B)=list("B11","B22","B33","B44",1,1)
B[1,2]="B12";B[2,3]="B23"; B[2,4]="B24"
B[4,2]="B42";
B[,5]=list("C11","C12",0,0,"B55",0)
B[,6]=list(0,0,"C32","C42",0,"B66")
print(B)
```

```
     [,1]  [,2]  [,3]  [,4]  [,5]  [,6]
[1,] "B11" "B12" 0     0     "C11" 0
[2,] 0     "B22" "B23" "B24" "C12" 0
[3,] 0     0     "B33" 0     0     "C32"
[4,] 0     "B42" 0     "B44" 0     "C42"
[5,] 0     0     0     0     "B55" 0
[6,] 0     0     0     0     0     "B66"
```

Now we have a $\mathbf{B}$ matrix that looks like that in Equation 14.6.

Then we set up the $\mathbf{R}^\sharp$ matrix. In their state-space model, Ives et al. allowed the fish data to have observation errors but set the observation error variance of the phosporous to 0 since that was experimental manipulated. Their $\mathbf{R}^\sharp$ looks like so

$$\begin{bmatrix} 0.04 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0.04 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0.16 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.16 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.36 \end{bmatrix}$$

So,

```
R=diag(c(0.04,0.04,0.16,0.16,0,0.36))
```

Last, we need to set up the $\mathbf{Q}^\sharp$ matrix. $\mathbf{Q}^\sharp$ is a variance-covariance matrix, and we need the proper sharing of values in the lower and upper triangle.

```
Q=matrix(list(0),6,6);
diag(Q)=list("11","22","33","44","55","66")
Q[1,2:4]=list("12","13","14")
Q[2:4,1]=list("12","13","14")
Q[2,3:4]=list("23","24")
Q[3:4,2]=list("23","24")
Q[4,3]="34"
Q[3,4]="34"
print(Q)
```

```
     [,1] [,2] [,3] [,4] [,5] [,6]
[1,] "11" "12" "13" "14" 0    0
[2,] "12" "22" "23" "24" 0    0
[3,] "13" "23" "33" "34" 0    0
[4,] "14" "24" "34" "44" 0    0
[5,] 0    0    0    0    "55" 0
[6,] 0    0    0    0    0    "66"
```

14.3.7 Fit the model with covariates

After specification of the model parameters, the fitting is standard. $\mathbf{u}$ is 0 since we have demeaned the data and covariates. $\mathbf{a}$ is 0 because we have only one time series of data per state process (row in $\mathbf{x}$). The default $\mathbf{Z}$ is the identity matrix, which is what we need, so we don't need to specify that.

```
plank.model.4=list(B=B,U="zero",Q=Q,R=R,A="zero")
kem.plank.4=MARSS(d.plank.dat.covar,model=plank.model.4,
    control=list(kf.x0="x10"))
```

This is the new $\mathbf{B}$ matrix using covariates.

```
     LP     SP      D     NP
LP 0.59 -0.709     --     --
SP   --  0.121 -0.045 -0.092
D    --     --  0.908     --
NP   --  0.077     --  0.711
```

Now we are getting are getting close to Ives et al.'s estimates. Compare model 4 in Table 14.1 to the first column.

Table 14.1. 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.

	Ives et al.	Model 0	Model 1	Model 2	Model 3	Model 4
B11	0.48	0.83	0.54	0.75	0.64	0.59
B22	0.25	0.77	0.85	0.75	0.53	0.12
B33	0.74	0.60	0.65	0.88	0.90	0.91
B44	0.60	0.96	0.89	0.66	0.71	0.71
B12	-0.39	0.10	0.01	-0.30	-0.33	-0.71
B23	-0.17	0.01	0.06	-0.02	-0.03	-0.05
B24	-0.11	0.44	0.30	0.06	0.07	-0.09
B42	0.10	-0.03	0.00	0.03	0.03	0.08
C11	0.25					0.31
C21	0.25					0.31
C32	-0.14					-0.04
C42	-0.04					-0.01

14.3.8 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

$$\begin{aligned} \mathbf{x}_t^+ &= \mathbf{B}^+\mathbf{x}_{t-1}^+ + \mathbf{u}^+\mathbf{w}_t, \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}^+) \\ \mathbf{y}_t^+ &= \mathbf{Z}^+\mathbf{x}_t^+ + \mathbf{a}^+ + \mathbf{v}_t, \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}^+) \end{aligned} \tag{14.7}$$

where the + matrices are stacked matrices from the different sites (1 and 2):

$$\begin{aligned} \begin{bmatrix} \mathbf{x}_{1,t} \\ \mathbf{x}_{2,t} \end{bmatrix} &= \begin{bmatrix} \mathbf{B} & 0 \\ 0 & \mathbf{B} \end{bmatrix} \begin{bmatrix} \mathbf{x}_{1,t-1} \\ \mathbf{x}_{2,t-1} \end{bmatrix} + \begin{bmatrix} \mathbf{u} \\ \mathbf{u} \end{bmatrix} + \mathbf{w}_t, \ \mathbf{w}_t \sim \text{MVN}\left(0, \begin{bmatrix} \mathbf{Q} & \mathbf{q} \\ \mathbf{q} & \mathbf{Q} \end{bmatrix}\right) \\ \begin{bmatrix} \mathbf{y}_{1,t} \\ \mathbf{y}_{2,t} \end{bmatrix} &= \begin{bmatrix} \mathbf{Z} & 0 \\ 0 & \mathbf{Z} \end{bmatrix} \begin{bmatrix} \mathbf{x}_{1,t} \\ \mathbf{x}_{2,t} \end{bmatrix} + \begin{bmatrix} \mathbf{a} \\ \mathbf{a} \end{bmatrix} + \mathbf{v}_t, \ \mathbf{v}_t \sim \text{MVN}\left(0, \begin{bmatrix} \mathbf{R} & 0 \\ 0 & \mathbf{R} \end{bmatrix}\right) \end{aligned} \tag{14.8}$$

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.

15

Case Study 8: Combining data from multiple time series

15.1 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:

$$\mathbf{x}_t = \mathbf{B}\mathbf{x}_{t-1} + \mathbf{u} + \mathbf{w}_t \text{ where } \mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}) \tag{15.1}$$

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,

$$\mathbf{y}_t = \mathbf{Z}\mathbf{x}_t + \mathbf{a} + \mathbf{v}_t \text{ where } \mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}) \tag{15.2}$$

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.

15.2 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.

15.2.1 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)
```

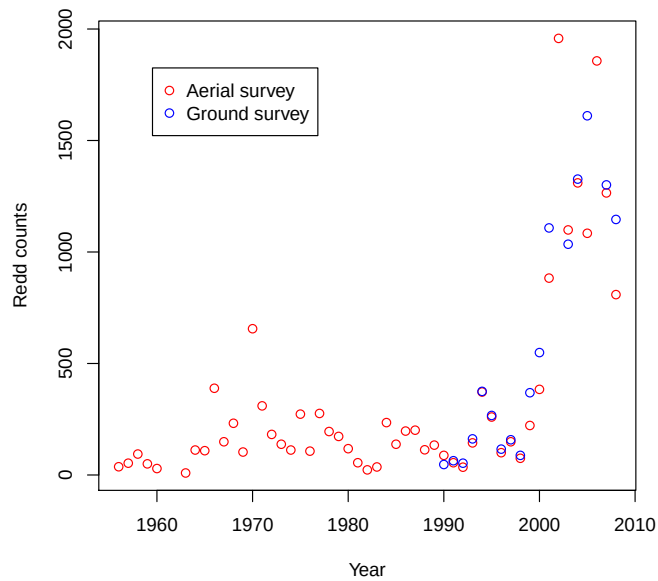

Fig. 15.1. The two time series look to be pretty close to one another in the years there is overlap.

15.2.2 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 the
# same 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 15.2).

15.3 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

```
# Code for plotting the fit from the best model
plot(okanaganRedds[,1], logRedds[1,],
xlab = "Year", ylab="Redd counts",main="", col="red", ylim=c(0,8))
points(okanaganRedds[,1], logRedds[2,], col="blue")
lines(okanaganRedds[,1], c(kem1$states), lty=1, lwd=2)
lines(okanaganRedds[,1], c(kem1$states + 2*kem1$states.se), lty=1, lwd=1, col="grey40")
lines(okanaganRedds[,1], c(kem1$states - 2*kem1$states.se), lty=1, lwd=1, col="grey40")
```

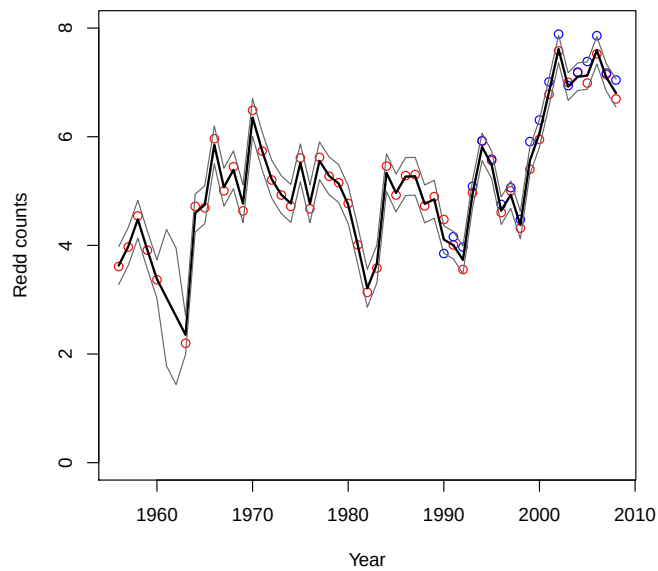

Fig. 15.2. The data support the hypothesis that the two time series are from the same population.

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.

15.3.1 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
```

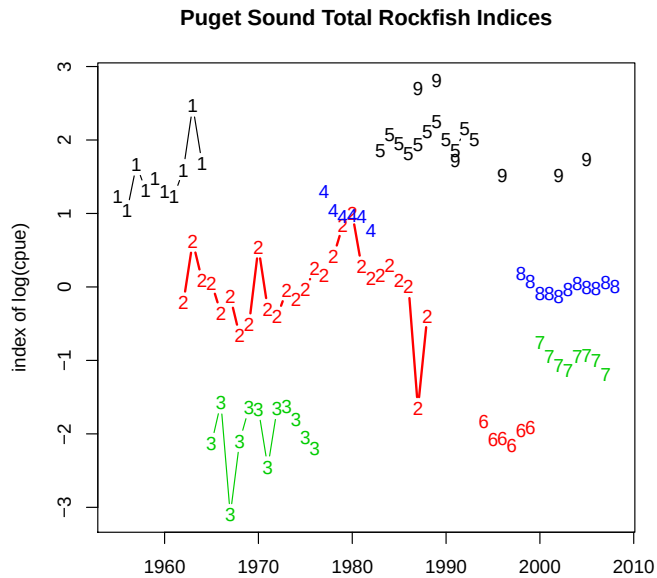

Fig. 15.3. Plot of the catch per unit effort data for Puget Sound total rockfish. Each time series has been given an arbitrary bias (up or down) to purposefully mask any trend in the data that you might pick out by eye – for teaching purposes not for analysis purposes.

15.3.2 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)
```

15.3.3 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)
```

15.4 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.

15.4.1 Read in and look at the data

Figure 15.4 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
```

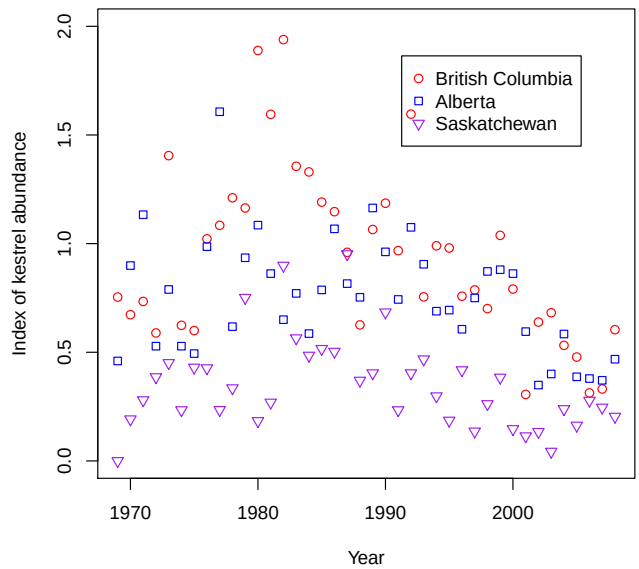

Fig. 15.4. The kestrel data.

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"
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] 23.13703
```

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] 19.34036
```

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] 12.50069
```

This last model was superior to the others, improving the AICc value compared to model 1 by 8 units. Figure 15.5 shows the fits for this model.

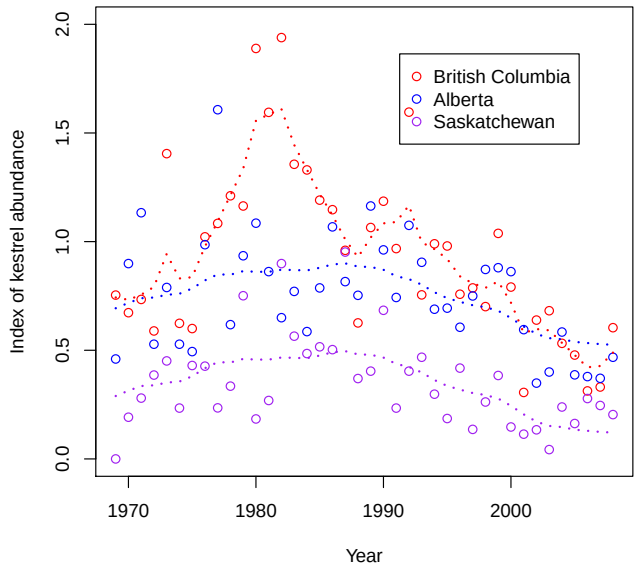

Fig. 15.5. Plot model 4 fits to the kestrel data.

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, New York, New York, USA.

Harvey, A. C. 1989. Forecasting, structural time series models and the Kalman filter. Cambridge University Press, Cambridge, UK.

Durbin, J., and S. J. Koopman. 2001. Time series analysis by state space methods. Oxford University Press, Oxford.

Kim, C. J. and Nelson, C. R. (1999), State space models with regime switching, MIT Press, Cambridge, Massachusetts.

King, R., G. Olivier, B. Morgan, and S. Brooks. 2009. Bayesian analysis for population ecology.

Giovanni, P., S. Petrone, and P. Campagnoli. 2009. Dynamic linear models in R.

Pole, A., M. West, and J. Harrison. 1994. Applied Bayesian forecasting and time series analysis.

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.

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 otherhand $|\mathbf{B}| < 1$, 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, $\boldsymbol{\pi}$ and $\mathbf{V}$. If, say, you try to specify a vague prior on $\mathbf{x}_0$ (or $\mathbf{x}_1$) with $\boldsymbol{\pi}$ equal to zero and $\mathbf{V}$ 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 $\mathbf{V}$ 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 $\mathbf{V}$ 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 $\boldsymbol{\pi}$ and $\mathbf{V}$ by setting `x0="unconstrained"` and `V0="unconstrained"` in the model specification. Estimating both $\boldsymbol{\pi}$ and $\mathbf{V}$ 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 `control$kf.x0="x10"`, so that $\boldsymbol{\pi}$ refers to $t = 1$ not $t = 0$. Then estimate $\boldsymbol{\pi}$ and fix $\mathbf{V} = 0$.

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 $\mathbf{V}$ goes to zero, the update steps for $\boldsymbol{\pi}$ 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. Like so, `MARSS(kem.MLE$model$data,model=kem.MLE$model,inits=kem.MLE$par, method="BFGS")`. `kem.MLE` is the output from your EM algorithm fits.

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. 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 fine as it means that the values converged but the parameters are such that there are slight numerical fluctuations. 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.

Stopped at iter=xx in MARSSkem: solution became unstable. R (or Q) update is not positive definite

This is generally 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.

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 miniscule 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). That term will be infinite when x=mu. So in the model with variance miniscule, 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 miniscule 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 Kalman-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 **V** 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 $\boldsymbol{\pi}$. 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.

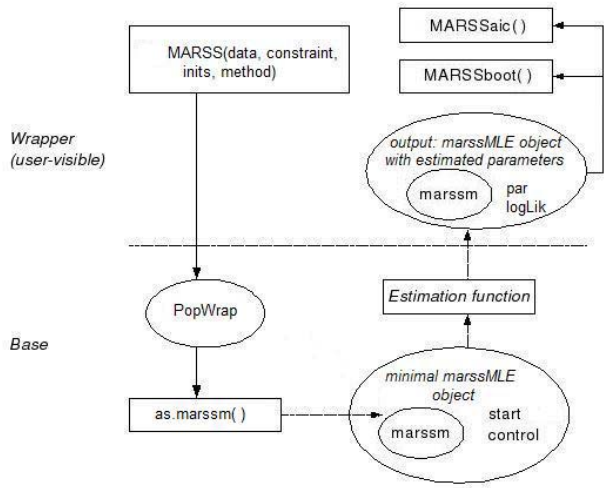

Fig. D.1. Two-level structure of the MARSS package. Rectangles represent functions; ovals represent objects.

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