



NOAA
FISHERIES

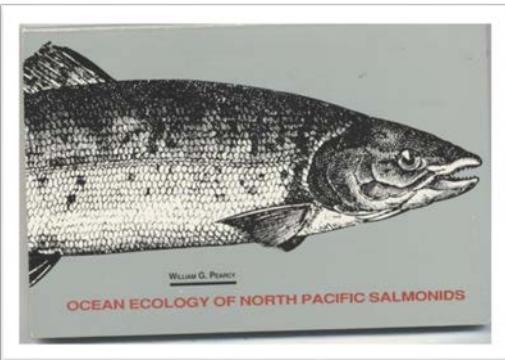
Northwest
Fisheries
Science Center

Inferring and forecasting community responses to climate drivers *using multivariate time-series analysis*

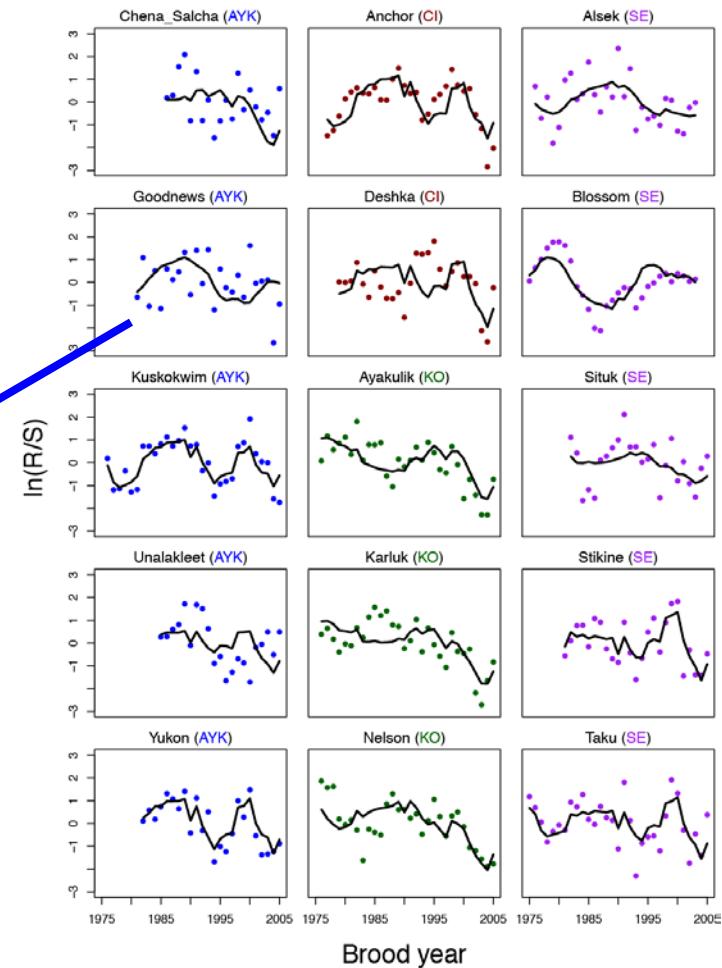
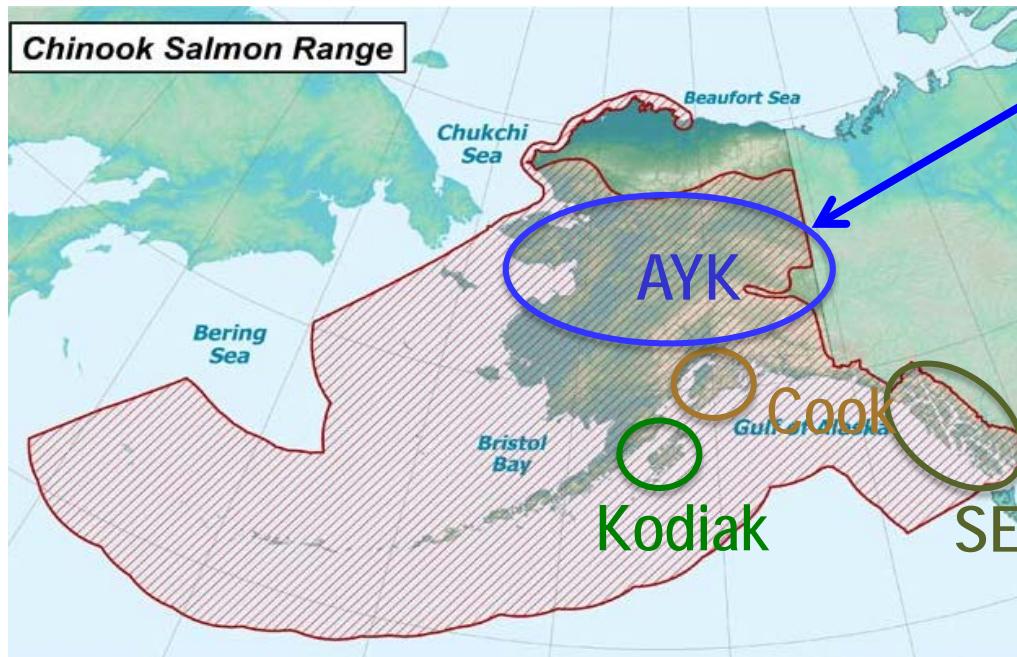
Elizabeth Holmes

NOAA Fisheries/University of Washington
faculty.washington.edu/eeholmes

Multivariate ecological time series



example from work by
Mark Scheuerell,
NWFSC, NOAA



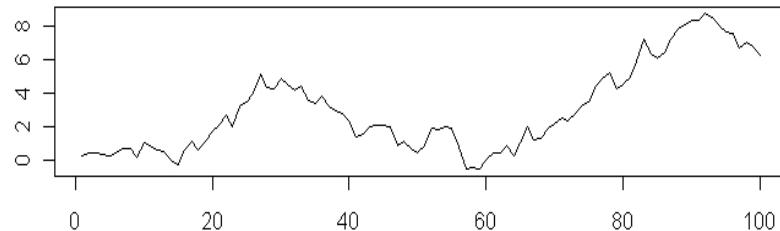
Some problems we have with our data

Multivariate time-series data with

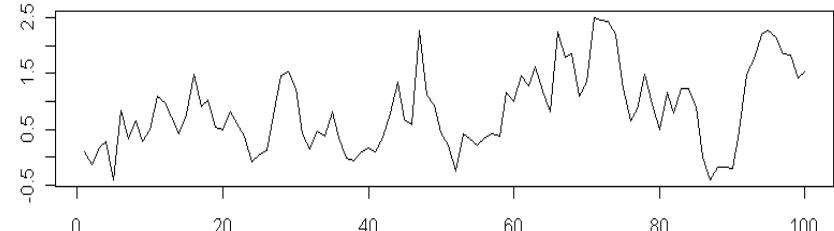
- Lots of gaps (missing data)
- (Unknown) observation error
- Complex (unknown) relationships between observation and underlying process trajectory
- Non-ideal covariate data --- instrumentation changed, multiple time series

The questions we ask often involve random walks

SOME UNDERLYING "HIDDEN" AUTOREGRESSIVE PROCESS

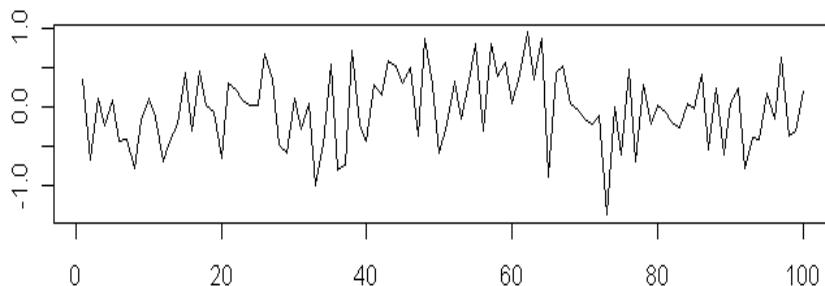


Random walk
 $x(t)=x(t-1)+e(t)$ + u

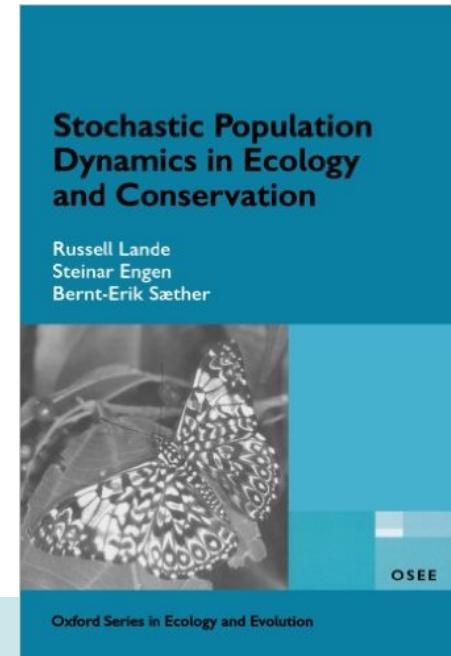


Mean-reverting random walk
 $x(t)=bx(t-1)+e(t)$ + u

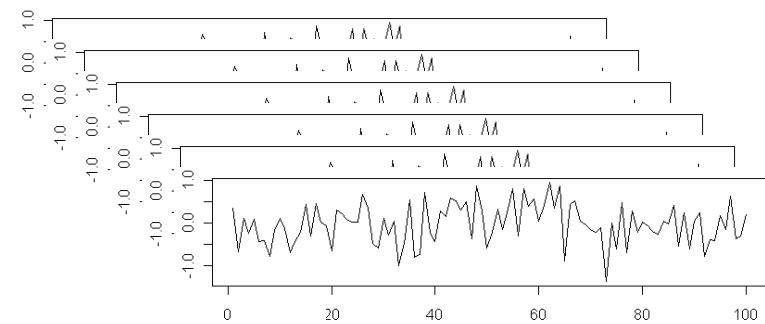
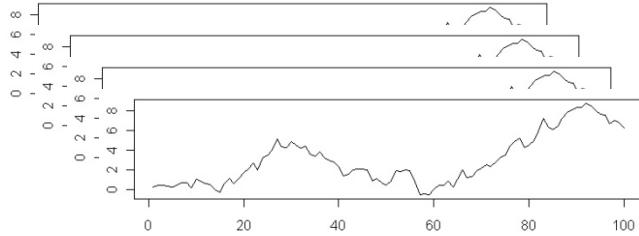
+ OBSERVATION PROCESS



White or autocorrelated noise
 $x(t)=e(t)$ + u



Our problems are multivariate



hidden random walks that we want to estimate or ‘understand’

Multivariate autoregressive “random walk”

observations

Multivariate with noise

Multivariate auto-regressive state-space (MARSS) models

Process

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

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

Observation

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

$$\mathbf{y}_t = \mathbf{Z}_t \mathbf{x}_t + \mathbf{a}_t + \mathbf{D}_t \mathbf{d}_t + \mathbf{v}_t, \quad \mathbf{v}_t \sim MVN(0, \mathbf{R}_t)$$

A talk in two parts

Part I: Development of a new expectation-maximization algorithm for fitting *constrained* MARSS models

$$\begin{aligned}\log L(\mathbf{y}, \mathbf{x}; \Theta) = & -\sum_1^T \frac{1}{2} (\mathbf{y}_t - \mathbf{Z}\mathbf{x}_t - \mathbf{a})^\top \mathbf{R}^{-1} (\mathbf{y}_t - \mathbf{Z}\mathbf{x}_t - \mathbf{a}) - \sum_1^T \frac{1}{2} \log |\mathbf{R}| \\ & - \sum_1^T \frac{1}{2} (\mathbf{x}_t - \mathbf{B}\mathbf{x}_{t-1} - \mathbf{u})^\top \mathbf{Q}^{-1} (\mathbf{x}_t - \mathbf{B}\mathbf{x}_{t-1} - \mathbf{u}) - \sum_1^T \frac{1}{2} \log |\mathbf{Q}| \\ & - \frac{1}{2} (\mathbf{x}_0 - \boldsymbol{\xi})^\top \boldsymbol{\Lambda}^{-1} (\mathbf{x}_0 - \boldsymbol{\xi}) - \frac{1}{2} \log |\boldsymbol{\Lambda}| - \frac{n}{2} \log 2\pi\end{aligned}$$

Part II: Using MARSS models to study the effect of climate variation versus species interactions on native fishes in a desert river



NOAA FISHERIES

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Parameter estimation for constrained MARSS models

x are hidden states

$$\mathbf{x}_t = \boxed{\mathbf{B}_t} \mathbf{x}_{t-1} + \boxed{\mathbf{u}_t} + \boxed{\mathbf{C}_t} \mathbf{c}_t + \mathbf{w}_t, \mathbf{w}_t \sim \text{MVN}(0, \boxed{\mathbf{Q}_t})$$
$$\mathbf{y}_t = \boxed{\mathbf{Z}_t} \mathbf{x}_t + \boxed{\mathbf{a}_t} + \boxed{\mathbf{D}_t} \mathbf{d}_t + \mathbf{v}_t, \mathbf{v}_t \sim \text{MVN}(0, \boxed{\mathbf{R}_t})$$

c and d are 'inputs'

y are data (w or w/o missing values)

$$\begin{bmatrix} \psi & 0 & 3 + \chi \\ 0 & \psi & \psi + 2\chi \\ 2 & \theta & 0 \end{bmatrix}$$

$$\begin{bmatrix} \psi \\ \psi \\ 2 \end{bmatrix}$$

$$\boxed{\begin{bmatrix} \psi & \chi & 0 \\ \chi & \psi & 0 \\ 0 & 0 & \theta \end{bmatrix}}$$

Linear constraints on matrix elements

$$\begin{bmatrix} \psi & 0 & 3 + \chi \\ 0 & \psi & \psi + 2\chi \\ 2 & \theta & 0 \end{bmatrix}$$

$$\begin{bmatrix} \psi & \chi & 0 \\ \chi & \psi & 0 \\ 0 & 0 & \theta \end{bmatrix}$$

$$c + \alpha_1 \beta_1 + \alpha_2 \beta_2 + \dots$$

Models that can be written with a constrained MARSS form

- **Multivariate auto-regressive process**
 - stochastic exponential growth, random walk movement
 - Gompertz density-dependent growth
- **Multi-site data**
 - Combining multiple time series with collection methods that have changed over time
- **Estimation of species interaction matrices (“MAR” modeling)**
- **Linear dynamical models**
 - a multivariate regression model where the coefs are random walks
- **Dynamic factor analysis**
 - similar to PCA but for time-series data
 - describe a large number (100s) of time series with a smaller set (1-5) of ‘trend’ time series
- **AR-p models**
- **Multivariate-response linear regression**

Related to 'shrinkage estimation'

Statistical Applications in Genetics and Molecular Biology

Volume 4, Issue 1

2005

Biometrika (2010), 0, 0, pp. 1–24

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A Shrinkage Approach to Large Covariance Matrix Estimation: Implications for Functional

Sparse Estimation of a Covariance Matrix

BY JACOB BIEN AND ROBERT TIBSHIRANI

Departments of Statistics and Health Research & Policy, Stanford University, Sequoia Hall, 4305-4065, U.S.A.

July

Multi-Target Shrinkage Estimation for Covariance Matrices

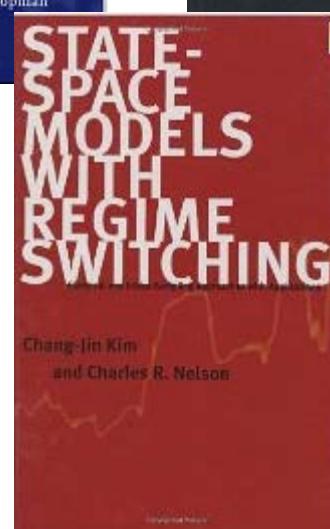
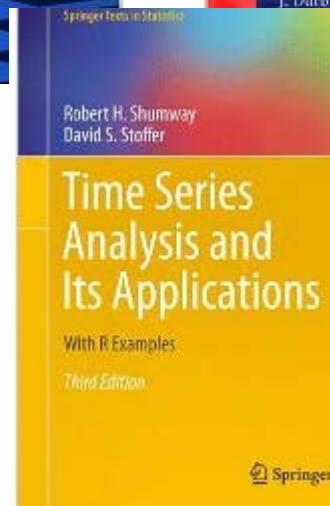
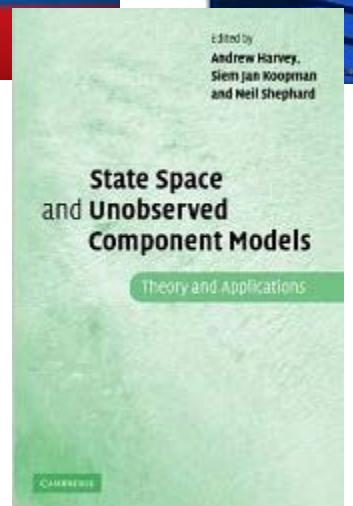
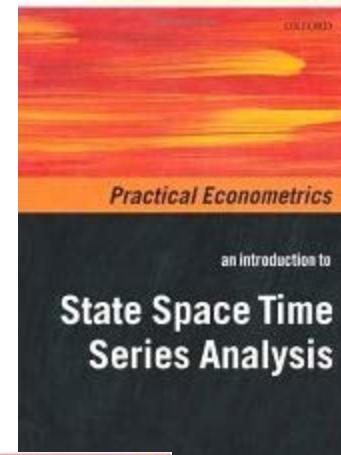
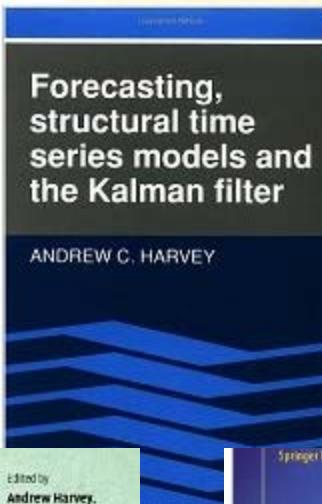
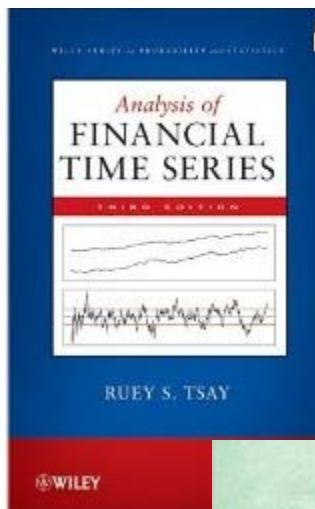
Tomer Lancewicki, Member, IEEE, and Mayer Aladjem

Abstract—Covariance matrix estimation is problematic when the number of samples is relatively small compared to the number of variables. One way to tackle this problem is the use of shrinkage estimators that offer a compromise between the sample covariance matrix and a well-chosen target (also known as the "target") with the aim of minimizing mean-squared error (MSE). In this paper, we propose a multi-target shrinkage estimator that minimizes MSE for covariance matrices that exploits the structure of the target matrix.

It can be hard to impose these constraints---in a general way

MARSS models are widely used in economics, finance and engineering

though perhaps with different names, e.g. VARSS, DLM, or simply state-space



If MARSS models have such a history, why not just use existing algorithms?

Existing methods could deal with

- Some types of MARSS models with missing data
- observation error
- time-varying parameters

Deriving algorithms is fun and captivating. I didn't really need any more justification than that for putting years of effort into this!

Goal

- Develop a general robust algorithm for constrained MARSS models based on Expectation-Maximization algorithms

Holmes, E. E. 2010, 2012. Derivation of the EM algorithm for constrained and unconstrained multivariate autoregressive state-space (MARSS) models.

Finding MLE parameters for *constrained* MARSS models:

Joint likelihood of y (data) and x (hidden states) given a set of parameters

$$\begin{aligned} \mathbb{E}_{\mathbf{X}, \mathbf{Y}} [\log \mathbf{L}(\mathbf{Y}, \mathbf{X}; \Theta); \mathbf{Y}(1) = \mathbf{y}(1), \Theta_j] &= \Psi = \\ &- \frac{1}{2} \sum_1^T \left(\mathbb{E}[\mathbf{Y}_t^\top \mathbf{R}^{-1} \mathbf{Y}_t] - \mathbb{E}[\mathbf{Y}_t^\top \mathbf{R}^{-1} \mathbf{Z} \mathbf{X}_t] - \mathbb{E}[(\mathbf{Z} \mathbf{X}_t)^\top \mathbf{R}^{-1} \mathbf{Y}_t] - \mathbb{E}[\mathbf{a}^\top \mathbf{R}^{-1} \mathbf{Y}_t] - \mathbb{E}[\mathbf{Y}_t^\top \mathbf{R}^{-1} \mathbf{a}] \right. \\ &\quad \left. + \mathbb{E}[(\mathbf{Z} \mathbf{X}_t)^\top \mathbf{R}^{-1} \mathbf{Z} \mathbf{X}_t] + \mathbb{E}[\mathbf{a}^\top \mathbf{R}^{-1} \mathbf{Z} \mathbf{X}_t] + \mathbb{E}[(\mathbf{Z} \mathbf{X}_t)^\top \mathbf{R}^{-1} \mathbf{a}] + \mathbb{E}[\mathbf{a}^\top \mathbf{R}^{-1} \mathbf{a}] \right) - \frac{T}{2} \log |\mathbf{R}| \\ &- \frac{1}{2} \sum_1^T \left(\mathbb{E}[\mathbf{X}_t^\top \mathbf{Q}^{-1} \mathbf{X}_t] - \mathbb{E}[\mathbf{X}_t^\top \mathbf{Q}^{-1} (\mathbf{B} \mathbf{X}_{t-1})] - \mathbb{E}[(\mathbf{B} \mathbf{X}_{t-1})^\top \mathbf{Q}^{-1} \mathbf{X}_t] \right. \\ &\quad \left. - \mathbb{E}[\mathbf{u}^\top \mathbf{Q}^{-1} \mathbf{X}_t] - \mathbb{E}[\mathbf{X}_t^\top \mathbf{Q}^{-1} \mathbf{u}] + \mathbb{E}[(\mathbf{B} \mathbf{X}_{t-1})^\top \mathbf{Q}^{-1} \mathbf{B} \mathbf{X}_{t-1}] \right. \\ &\quad \left. + \mathbb{E}[\mathbf{u}^\top \mathbf{Q}^{-1} \mathbf{B} \mathbf{X}_{t-1}] + \mathbb{E}[(\mathbf{B} \mathbf{X}_{t-1})^\top \mathbf{Q}^{-1} \mathbf{u}] + \mathbf{u}^\top \mathbf{Q}^{-1} \mathbf{u} \right) - \frac{T}{2} \log |\mathbf{Q}| \\ &- \frac{1}{2} \left(\mathbb{E}[\mathbf{X}_0^\top \mathbf{V}_0^{-1} \mathbf{X}_0] - \mathbb{E}[\boldsymbol{\xi}^\top \boldsymbol{\Lambda}^{-1} \mathbf{X}_0] - \mathbb{E}[\mathbf{X}_0^\top \boldsymbol{\Lambda}^{-1} \boldsymbol{\xi}] + \boldsymbol{\xi}^\top \boldsymbol{\Lambda}^{-1} \boldsymbol{\xi} \right) - \frac{1}{2} \log |\boldsymbol{\Lambda}| - \frac{n}{2} \log \pi \end{aligned}$$

log L(y,x;Θ) = f(y, x, Θ)

Idea is to find the Θ that maximizes the **log L(y;Θ)**

Newton-based method

- The Kalman filter will give you the marginal likelihood
- Write a function to compute the marginal likelihood $L(y; Q)$, or there are a number of R packages that do this. I use KFAS.
- Maximize that using a Newton-type algorithm. You could use `optim()`.
- You can do this in a few lines of code.

Works great for lots of problems. But for many big multivariate problems it doesn't work so great.

How do you deal with constrained variance-covariance matrices?

Expectation-Maximization algorithm

Joint likelihood of y and x is $\log L(y, x; \Theta) = f(y, \textcolor{red}{x}, \Theta)$

The EM algorithm maximizes the expected value of the joint likelihood

$$E_{XY}[\log L(Y, X; \Theta); Y(1) = y(1), \Theta_j]$$

1. Start with Θ_1
2. Compute the expectations involving X and Y conditioned on Θ_1 and the data
3. Put those in $E_{XY}[\log L(Y, X; \Theta); Y(1) = y(1), \Theta_j]$
4. Maximize that (3) with respect to Θ to get Θ_2
 - *This is the hard part.*
 - Take the partial derivative of (3) wrt Θ and solve for Θ
5. Repeat until convergence

We need to take the partial derivative of the expectation of the LL wrt parameters: u, R, Q, B, a, Z

$$E_{\mathbf{X} \mathbf{Y}}[\log \mathbf{L}(\mathbf{Y}, \mathbf{X}; \Theta); \mathbf{Y}(1) = \mathbf{y}(1), \Theta_j] = \Psi =$$

$$\begin{aligned} & -\frac{1}{2} \sum_1^T \left(E[\mathbf{Y}_t^\top \mathbf{R}^{-1} \mathbf{Y}_t] - E[\mathbf{Y}_t^\top \mathbf{R}^{-1} \mathbf{Z} \mathbf{X}_t] - E[(\mathbf{Z} \mathbf{X}_t)^\top \mathbf{R}^{-1} \mathbf{Y}_t] - E[\mathbf{a}^\top \mathbf{R}^{-1} \mathbf{Y}_t] - E[\mathbf{Y}_t^\top \mathbf{R}^{-1} \mathbf{a}] \right. \\ & \quad \left. + E[(\mathbf{Z} \mathbf{X}_t)^\top \mathbf{R}^{-1} \mathbf{Z} \mathbf{X}_t] + E[\mathbf{a}^\top \mathbf{R}^{-1} \mathbf{Z} \mathbf{X}_t] + E[(\mathbf{Z} \mathbf{X}_t)^\top \mathbf{R}^{-1} \mathbf{a}] + E[\mathbf{a}^\top \mathbf{R}^{-1} \mathbf{a}] \right) - \frac{T}{2} \log |\mathbf{R}| \\ & -\frac{1}{2} \sum_1^T \left(E[\mathbf{X}_t^\top \mathbf{Q}^{-1} \mathbf{X}_t] - E[\mathbf{X}_t^\top \mathbf{Q}^{-1} \mathbf{B} \mathbf{X}_{t-1}] - E[(\mathbf{B} \mathbf{X}_{t-1})^\top \mathbf{Q}^{-1} \mathbf{X}_t] \right. \\ & \quad \left. - E[\mathbf{u}^\top \mathbf{Q}^{-1} \mathbf{X}_t] - E[\mathbf{X}_t^\top \mathbf{Q}^{-1} \mathbf{u}] + E[(\mathbf{B} \mathbf{X}_{t-1})^\top \mathbf{Q}^{-1} \mathbf{B} \mathbf{X}_{t-1}] \right. \\ & \quad \left. + E[\mathbf{u}^\top \mathbf{Q}^{-1} \mathbf{B} \mathbf{X}_{t-1}] + E[(\mathbf{B} \mathbf{X}_{t-1})^\top \mathbf{Q}^{-1} \mathbf{u}] + \mathbf{u}^\top \mathbf{Q}^{-1} \mathbf{u} \right) - \frac{T}{2} \log |\mathbf{Q}| \\ & -\frac{1}{2} \left(E[\mathbf{X}_0^\top \mathbf{V}_0^{-1} \mathbf{X}_0] - E[\boldsymbol{\xi}^\top \boldsymbol{\Lambda}^{-1} \mathbf{X}_0] - E[\mathbf{X}_0^\top \boldsymbol{\Lambda}^{-1} \boldsymbol{\xi}] + \boldsymbol{\xi}^\top \boldsymbol{\Lambda}^{-1} \boldsymbol{\xi} \right) - \frac{1}{2} \log |\boldsymbol{\Lambda}| - \frac{n}{2} \log \pi \end{aligned}$$

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

Solve for the u that maximizes the $E[LL]$ ψ

$$\Psi = -\mathbf{a}^\top \mathbf{u} - \mathbf{u}^\top \mathbf{a} + \mathbf{u}^\top \mathbf{u}$$

$$\frac{\partial \Psi}{\partial \mathbf{u}} = -\frac{\partial \mathbf{a}^\top \mathbf{u}}{\partial \mathbf{u}} - \frac{\partial \mathbf{u}^\top \mathbf{a}}{\partial \mathbf{u}} + \frac{\partial \mathbf{u}^\top \mathbf{u}}{\partial \mathbf{u}}$$

$$\frac{\partial \Psi}{\partial \mathbf{u}} = -2\mathbf{a}^\top + 2\mathbf{u}^\top$$

$$\mathbf{u} = \mathbf{a}$$

$$\mathbf{u} = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix}$$

$$\mathbf{u} = \begin{bmatrix} u_1 \\ u_1 \\ u_2 \\ u_2 \\ u_2 \end{bmatrix}$$

$$\mathbf{u} = \begin{bmatrix} 1 \\ 0 \\ u_1 \\ u_1 \\ u_2 \end{bmatrix}$$

$$\mathbf{u} = \begin{bmatrix} u_1 \\ u_1 + u_2 \\ u_2 \\ 3 + u_2 + u_3 \\ 4 \end{bmatrix}$$

$$\mathbf{u} = \begin{bmatrix} u_1 \\ u_1 + u_2 \\ u_2 \\ 3 + u_2 + u_3 \\ 4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 3 \\ 4 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} = \mathbf{f} + \mathbf{Du}$$

$$\Psi = -\text{constant} - \mathbf{a}^\top \mathbf{D} \mathbf{u} - \mathbf{u}^\top \mathbf{D}^\top \mathbf{a} + \mathbf{u}^\top \mathbf{D}^\top \mathbf{D} \mathbf{u}$$

$$\frac{\partial \Psi}{\partial \mathbf{u}} = -2\mathbf{a}^\top \mathbf{D} + 2\mathbf{u}^\top \mathbf{D}^\top \mathbf{D}$$

$$\mathbf{u}^\top = \mathbf{a}^\top \mathbf{D} (\mathbf{D}^\top \mathbf{D})^{-1}$$

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

Solve for the B that maximizes the $E[LL]$ ψ

$$\Psi = -\mathbf{a}^\top \mathbf{B} \mathbf{b} - \mathbf{b}^\top \mathbf{B}^\top \mathbf{a} + \mathbf{c}^\top \mathbf{B}^\top \mathbf{B} \mathbf{c}$$

$$\frac{\partial \Psi}{\partial \mathbf{B}} = -\frac{\partial \mathbf{a}^\top \mathbf{B} \mathbf{b}}{\partial \mathbf{B}} - \frac{\partial \mathbf{b}^\top \mathbf{B}^\top \mathbf{a}}{\partial \mathbf{B}} + \frac{\partial \mathbf{c}^\top \mathbf{B}^\top \mathbf{B} \mathbf{c}}{\partial \mathbf{B}}$$

$$\frac{\partial \Psi}{\partial \mathbf{B}} = -2\mathbf{b}\mathbf{a}^\top + 2\mathbf{c}\mathbf{c}^\top \mathbf{B}^\top$$

$$\mathbf{B}^\top = (\mathbf{c}\mathbf{c}^\top)^{-1} \mathbf{b}\mathbf{a}^\top$$

$$\mathbf{B} = \begin{bmatrix} b_1 & b_2 \\ b_3 & b_4 \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} b_1 & 0 \\ 0 & b_2 \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} b_1 & b_2 \\ b_3 & b_1 \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} 1 & b_1 \\ 0 & b_1 + b_2 \end{bmatrix}$$

Write the log likelihood in vec form

$$\Psi = -\mathbf{a}^\top \mathbf{B} \mathbf{b} - \mathbf{b}^\top \mathbf{B}^\top \mathbf{a} + \mathbf{c}^\top \mathbf{B}^\top \mathbf{B} \mathbf{c}$$

$$\vec{\mathbf{b}} = \text{vec}(\mathbf{B})$$

$$\Psi = \text{vec}(\Psi) = \text{vec}(-\mathbf{a}^\top \mathbf{B} \mathbf{b} - \mathbf{b}^\top \mathbf{B}^\top \mathbf{a} + \mathbf{c}^\top \mathbf{B}^\top \mathbf{B} \mathbf{c})$$

$$\Psi = -\mathbf{d}^\top \vec{\mathbf{b}} - \vec{\mathbf{b}}^\top \mathbf{d} + \vec{\mathbf{b}}^\top \mathbf{C} \vec{\mathbf{b}}$$

$$\mathbf{d} = (\mathbf{b}^\top \otimes \mathbf{a}^\top)$$

$$\mathbf{C} = (\mathbf{c}^\top \otimes \mathbf{I})^\top (\mathbf{c}^\top \otimes \mathbf{I})$$

$$\boxed{\begin{aligned}\mathbf{B} &= \begin{bmatrix} 1 & b_1 \\ 0 & b_1 + b_2 \end{bmatrix} \\ \vec{\mathbf{b}} &= \begin{bmatrix} 1 \\ b_1 \\ 0 \\ b_1 + b_2 \end{bmatrix}\end{aligned}}$$

This leads to a simple solution for linear constraints within parameter matrices

$$\mathbf{B} = \begin{bmatrix} 1 & b_1 \\ 0 & b_1 + b_2 \end{bmatrix}$$

$$\vec{\mathbf{b}} = \begin{bmatrix} 1 \\ b_1 \\ 0 \\ b_1 + b_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 0 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \mathbf{f} + \mathbf{D}\mathbf{b}$$

$$\partial\Psi\partial\mathbf{b} = -\text{constant} - \mathbf{d}^\top \mathbf{D}\mathbf{b} - \mathbf{b}^\top \mathbf{D}^\top \mathbf{d} + \mathbf{b}^\top \mathbf{D}^\top \mathbf{C}\mathbf{D}\mathbf{b}$$

Solve for \mathbf{b} that maximizes Ψ .

$$\mathbf{b}^\top = \mathbf{d}^\top \mathbf{D} (\mathbf{D}^\top \mathbf{C}\mathbf{D})^{-1}$$

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

Solving for constrained variances Q (and R) follow the same steps as for B

We don't need the 'trace' trick to pull the \mathbf{Q}^{-1} out, because the `vec()` does that

$$\text{vec}(\mathbf{a}^\top \mathbf{Q}^{-1} \mathbf{b}) = (\mathbf{b}^\top \otimes \mathbf{a}^\top) \text{vec}(\mathbf{Q}^{-1}) = \mathbf{c}^\top \mathbf{D} \mathbf{q}'$$

The estimate has the familiar form

$$\mathbf{q}^\top = \mathbf{d}^\top \mathbf{D} (\mathbf{D}^\top \mathbf{D})^{-1}$$

Works for all legal forms (that I've come up) of variance-covariance matrices

$$\mathbf{Q} = \begin{bmatrix} q_1 & 0 & 0 & 0 & 0 \\ 0 & f_1 & 0 & 0 & 0 \\ 0 & 0 & q_2 & 0 & 0 \\ 0 & 0 & 0 & f_2 & 0 \\ 0 & 0 & 0 & 0 & q_2 \end{bmatrix} \quad \mathbf{Q} = \begin{bmatrix} \alpha & \beta & \beta & \beta \\ \beta & \alpha & \beta & \beta \\ \beta & \beta & \alpha & \beta \\ \beta & \beta & \beta & \alpha \end{bmatrix}$$

$$\mathbf{Q} = \begin{bmatrix} \mathbb{B}_1 & 0 & 0 \\ 0 & \mathbb{B}_2 & 0 \\ 0 & 0 & \mathbb{B}_3 \end{bmatrix} \quad \mathbf{Q} = \begin{bmatrix} \mathbb{E}_1 & \mathbb{C}_{1,2} & \mathbb{C}_{1,3} \\ \mathbb{C}_{1,2} & \mathbb{E}_2 & \mathbb{C}_{2,3} \\ \mathbb{C}_{1,3} & \mathbb{C}_{2,3} & \mathbb{E}_3 \end{bmatrix}$$

$$\mathbf{q}^\top = \mathbf{d}^\top \mathbf{D} (\mathbf{D}^\top \mathbf{D})^{-1}$$

$$\mathbf{Q} = \begin{bmatrix} \mathbb{F} & 0 & 0 & 0 \\ 0 & \mathbb{G}_1 & 0 & 0 \\ 0 & 0 & \mathbb{G}_2 & 0 \\ 0 & 0 & 0 & \mathbb{G}_3 \end{bmatrix}$$

Expectation-Maximization algorithm

Advantage?

- 1) It can make certain types of model fitting problems tractable by being considerably faster and more stable
- 2) Very insensitive to initial conditions. EM algorithms are very good at getting close to the maximum.
- 3) Very flexible---within the MARSS structure
- 4) One algorithm for many different MARSS models.

Expectation-Maximization algorithm

Disdvantages?

- 1) Locked into the MARSS structure
 - 1) Especially bad when your data have zeros and you want ‘zeros’ model
- 2) MVN errors
- 3) Getting a profile of the likelihood is painful (relative to Bayesian approach)
- 4) E-M algorithms are really slow. If a Newton-esque method works (I use BFGS), it is much faster.

MARSS R package on CRAN

CRAN - Package MARSS - Windows Internet Explorer

Google “MARSS cran” or “time series task view cran”

MARSS: Multivariate Autoregressive State-Space Modeling

The MARSS package provides maximum-likelihood parameter estimation for constrained and unconstrained linear multivariate data. Fitting is primarily via an Expectation-Maximization (EM) algorithm, although fitting via the BFGS algorithm (using the op model (DLM) and vector autoregressive model (VAR) model. Functions are provided for parametric and innovations bootstraps (AICb), confidence intervals via the hessian approximation and via bootstrapping and calculation of auxiliary residuals for detection of outliers for parameter estimation for a variety of applications, model selection, dynamic factor analysis, outlier and shock detection, and at the R command line to open the MARSS user guide.

Version: 2.7

Depends: [MASS](#), [mvtnorm](#), [nlme](#), [time](#), [KFAS](#)

Published: 2011-10-23

Author: Eli Holmes, Eric Ward, and Kellie Wills, NOAA, Seattle, USA

Maintainer: Eli Holmes <eli.holmes at noaa.gov>

License: [GPL-2](#)

In views: [TimeSeries](#)

CRAN checks: [MARSS results](#)

Downloads:

Package source: [MARSS 2.7.tar.gz](#)

MacOS X binary: [MARSS 2.7.tgz](#)

Windows binary: [MARSS 2.7.zip](#)

Reference manual: [MARSS.pdf](#)

Vignettes: [EM Derivation](#)
[Quick Start Guide](#)
[User Guide](#)
[Changes between versions](#)

Old sources: [MARSS archive](#)

E. E. Holmes and E. J. Ward

Analysis of multivariate time-series using the MARSS package

version 2.7

October 21, 2011

Mathematical Biology Program
Northwest Fisheries Science Center, Seattle, WA

Developed with support by the Comparative
Analysis of Marine Ecosystem Organizations
(CAMEO) Program

Assessing marine plankton community structure from long-term monitoring data with multivariate autoregressive (MAR) models: a comparison of fixed station versus spatially distributed sampling data

Lindsay P. Scheef¹, Daniel E. Pendleton², Stephen Scheuerell³, and David G. Johns⁴

¹National Center for Ecological Analysis & Synthesis

²Northwest Fisheries Science Center, NOAA Fisheries

³Channel Islands National Marine Sanctuary, Santa

⁴Sir Alister Hardy Foundation for Ocean Science, Ply-

Abstract

We examined how marine plankton interactions, as analyzed by multivariate autoregressive analysis of time-series, differ based on data collected at a fixed station (the English Channel) and four similar time-series sites distributed across the North Sea.

The results show that the interactions between phytoplankton and zooplankton, and between the two groups, differ significantly between the fixed station and the distributed sites. The interactions between phytoplankton and zooplankton were more complex at the distributed sites than at the fixed station. The interactions between the two groups were more complex at the distributed sites than at the fixed station. The interactions between the two groups were more complex at the distributed sites than at the fixed station.

Global Change Biology (2008) 14, 1947–1958, doi: 10.1111/j.1365-2486.2008.01616.x

Sixty years of environmental change in the world's largest freshwater lake – Lake Baikal, Siberia

STEPHANIE E. HAMPTON^{*}, LYUBOV R. IZMEST'eva[†], MARIANNE V. MOORE[‡], STEPHEN L. KATZ[§], BRIAN DENNIS[¶] and EUGENE A. SILOW[†]

^{*}National Center for Ecological Analysis & Synthesis, University of California – Santa Barbara, Santa Barbara, CA 93101, USA,

[†]Scientific Research Institute of Biology, Irkutsk State University, Irkutsk, 664003, Russia, [‡]Department of Biological Sciences,

Wellesley College, Wellesley, MA 02481, USA, [§]Northwest Fisheries Science Center, NOAA Fisheries, Seattle, WA 98112, USA,

[¶]Departments of Statistics and Fish and Wildlife Resources, University of Idaho, Moscow, ID 83844, USA

OnlineOpen: This article is available free online at www.blackwell-synergy.com

Abstract

High-resolution data collected over the past 60 years by a single family of Siberian scientists on Lake Baikal reveal significant warming of surface waters and long-term changes in the basal food web of the world's largest, most ancient lake. Attaining depths over 1.6 km, Lake Baikal is the deepest and most voluminous of the world's great lakes. Increases in average water temperature (1.21 °C since 1946), chlorophyll *a* (300% since

Global Change Biology

Global Change Biology (2012) 18, 2498–2508, doi: 10.1111/j.1365-2486.2012.02702.x

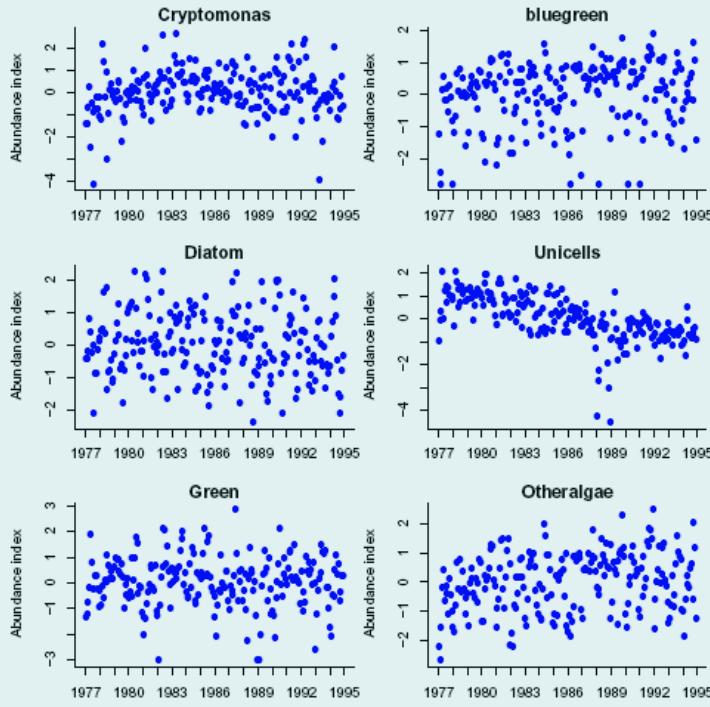
Climate shifts the interaction web of a marine plankton community

TESSA B. FRANCIS^{*}, MARK D. SCHEUERELL^{*}, RICHARD D. BRODEUR[†], PHILLIP S. LEVIN^{*}, JAMES J. RUZICKA[‡], NICK TOLIMIERI^{*} and WILLIAM T. PETERSON[†]

^{*}National Oceanic and Atmospheric Administration, Northwest Fisheries Science Center, 2725 Montlake Blvd. E, Seattle, WA 98112, USA [†]National Oceanic and Atmospheric Administration, Northwest Fisheries Science Center, Hatfield Marine Science Center, Oregon Institute of Marine Resources Studies, Oregon

bed, yet accurate predictions about ecosystem biotic responses in a food-web context to support. Here we conduct time-series analyses with abundance in the Northern California Current zooplankton community interactions. Autoregression vs. cool ocean climate conditions. Negative major warm phase during the time series, altered zooplankton communities. Local environmental (El Niño/Southern Oscillation) were associated secondary environmental correlates of zooplankton during the warm phase for upwelling as a covariate simultaneous quantitation of community zooplankton community structure varies with

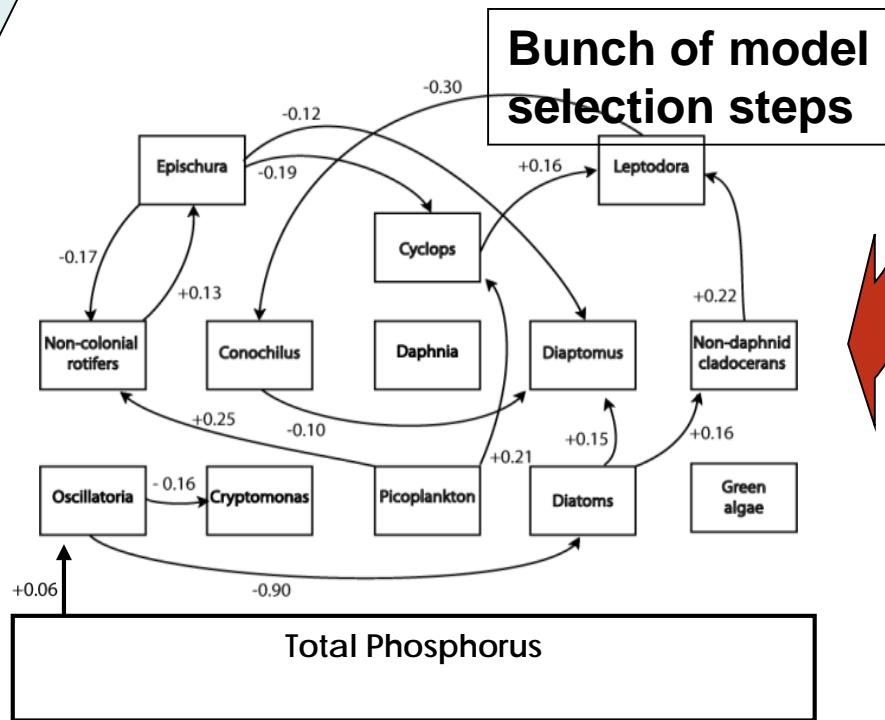
Estimating species interaction strengths from time-series data



Time series of abundance for the species/groups in the community plus time series of covariates

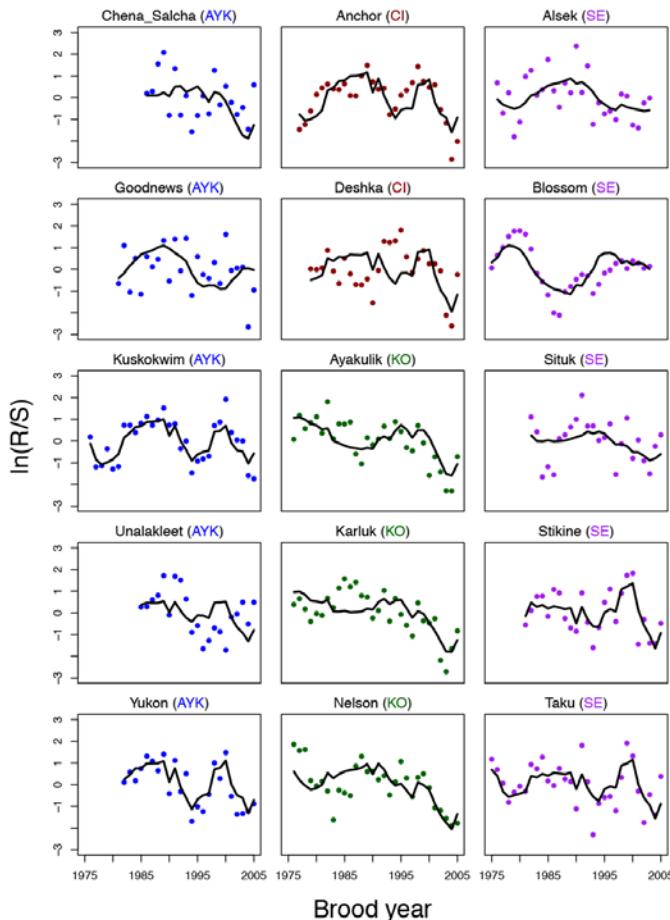
“MAR”

$$\mathbf{x}_t = \mathbf{B}\mathbf{x}_{t-1} + \mathbf{u} + \mathbf{C}\mathbf{f}_t + \mathbf{w}_t$$

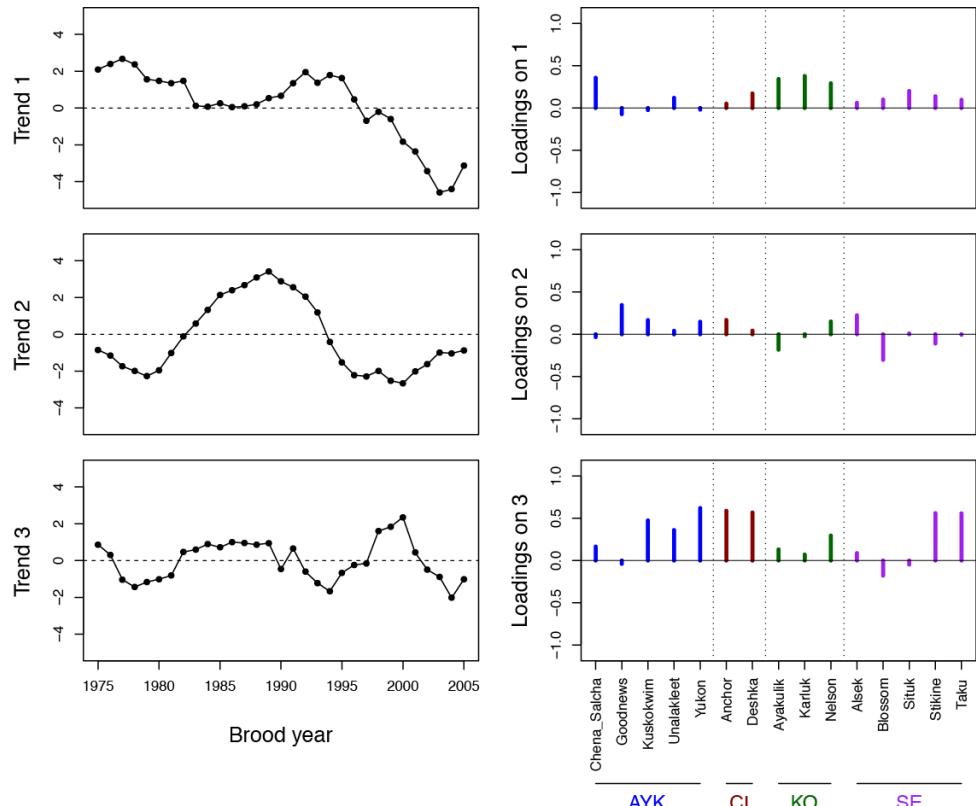


Dynamic Factor Analysis: PCA for time series"

Lot of time series



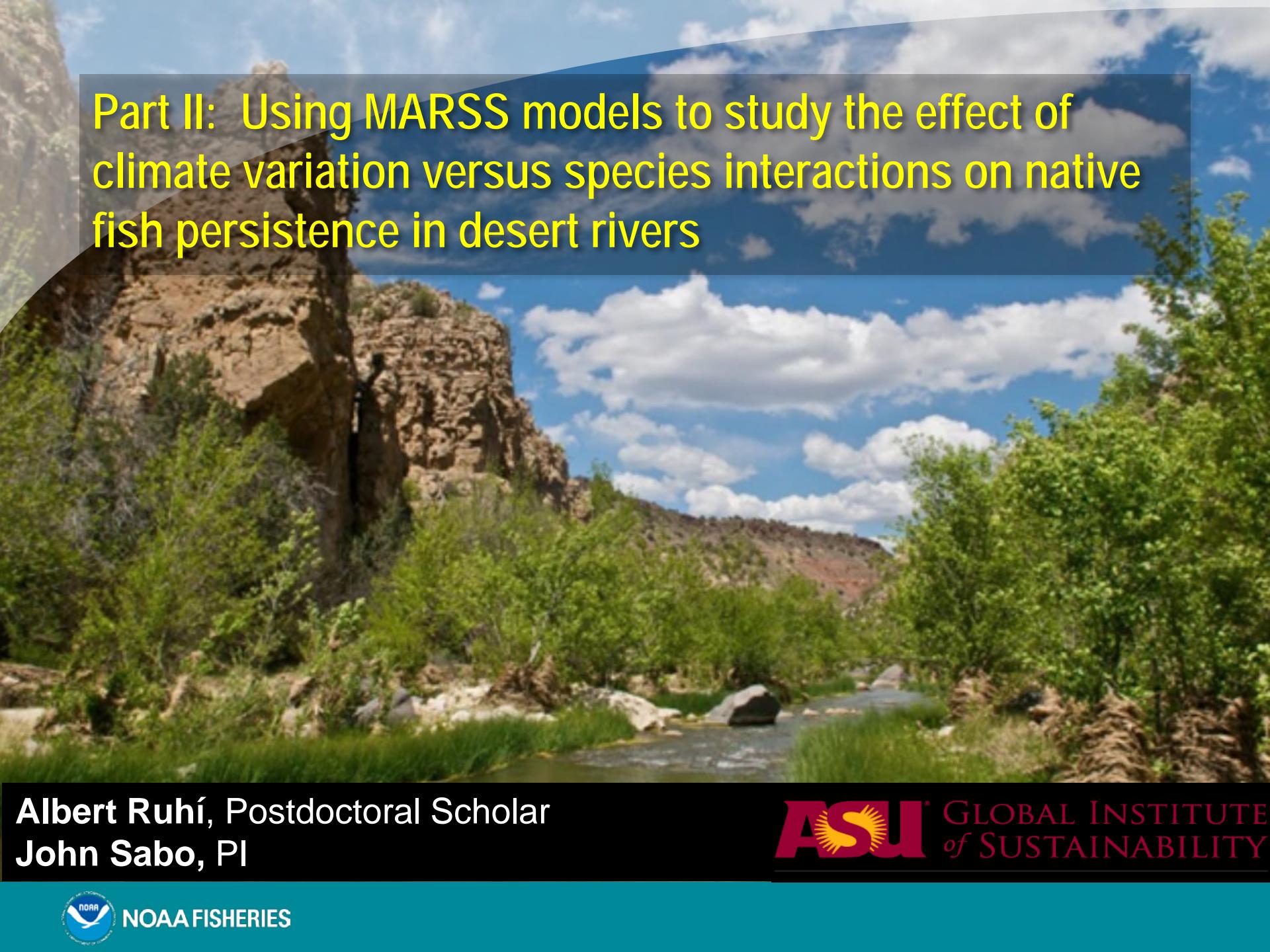
Reduce to a few hidden drivers with weighting



NOAA FISHERIES

Mark Scheuerell, NWFSC, NOAA

Part II: Using MARSS models to study the effect of climate variation versus species interactions on native fish persistence in desert rivers

A scenic view of a desert river flowing through a rocky landscape under a blue sky with white clouds. The river is surrounded by green shrubs and large, light-colored rock formations. The water is clear and reflects the surrounding environment.

Albert Ruhí, Postdoctoral Scholar
John Sabo, PI

8 non-native species



catfish



carp



bullhead



Red shiner



mosquitofish



5 native species



Longfin dace



Desert sucker



Sonora sucker



**Roundtail
chub**

Photo Credit: USFWS

"Poor" but highly endemic, imperiled, and invaded fish communities
(Olden & Poff 2006; Olden et al. 2006; Jaeger et al. 2014; Pool & Olden 2012)

These systems are prone to large discharge variation: flash flood and droughts



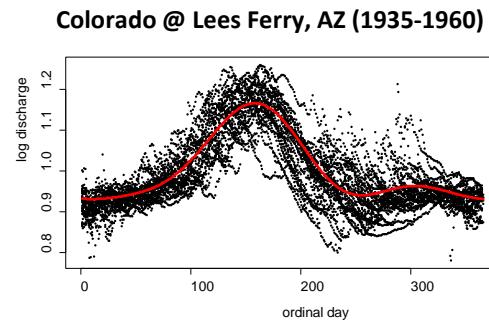
The American Southwest is experiencing increases in extreme low water events

- Increasing human appropriation of freshwater resources and associated low & zero flows
- Expanding climatic droughts caused by global warming

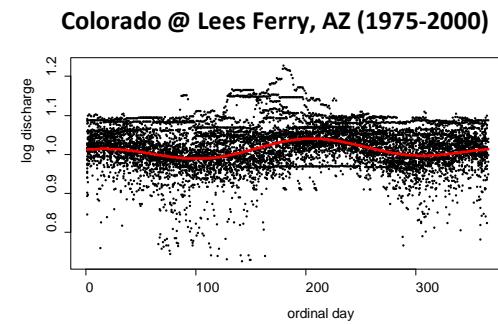
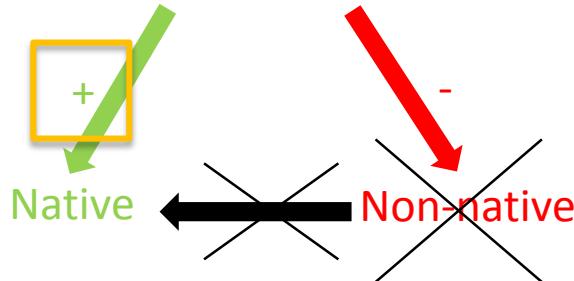


What predicts the persistence of native fish in desert rivers: presence of non-natives or extreme water events

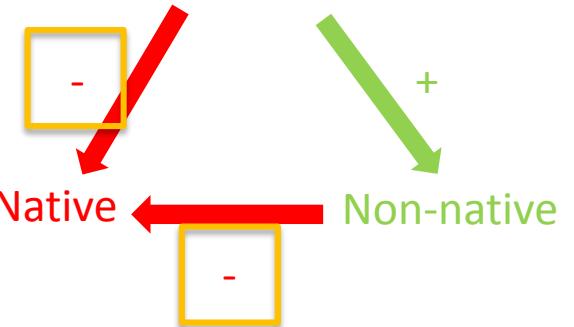
The presence of non-natives confounds detection of the effect of flow



Natural hydrograph



Altered hydrograph



Direct effects of flow or flow-mediated effects of non-natives?

Anomalous droughts, not invasion, decrease persistence of native fishes in a desert river

Albert Ruhí¹, Elizabeth E. Holmes², John N. Rinne³ & John L. Sabo^{1,4}

^① Global Institute of Sustainability, Arizona State University, Tempe AZ;

^② Northwest Fisheries Science Center, NOAA Fisheries Service, Seattle WA;

^③ Southwest Forest Science Complex, Rocky Mountain Research Station, Flagstaff AZ;

^④ School of Life Sciences, Arizona State University, Tempe AZ



Upper Verde River (AZ)

7 sites

(Rocky Mountain Research Station, USDA Forest Service)

Sullivan Lake to Sycamore Creek

Fish monitored yearly for 15 years (1994-2008)

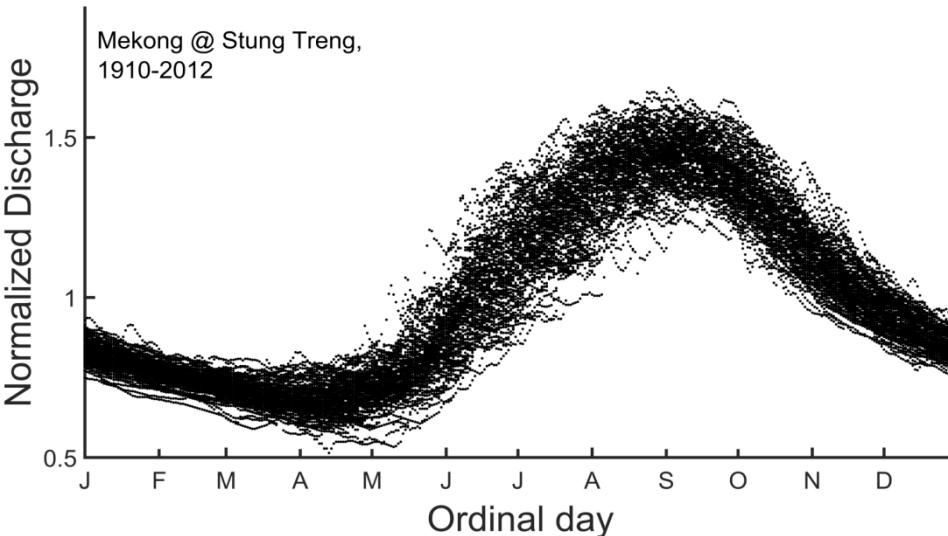
Daily discharge (USGS station 09504000, "Verde River near Clarkdale, AZ") for 45 years (1966-2010)

...ideal setting to study the abiotic and biotic factors that influence fish assemblage structure in desert rivers

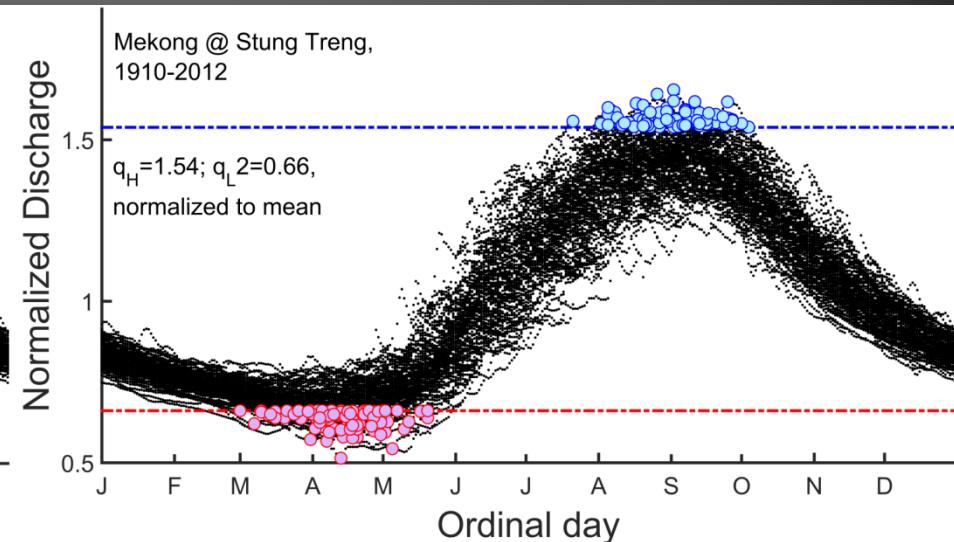
(e.g. Stefferud & Rinne, 1995; Rinne & Stefferud, 1996)

Methods: What is DFFT?

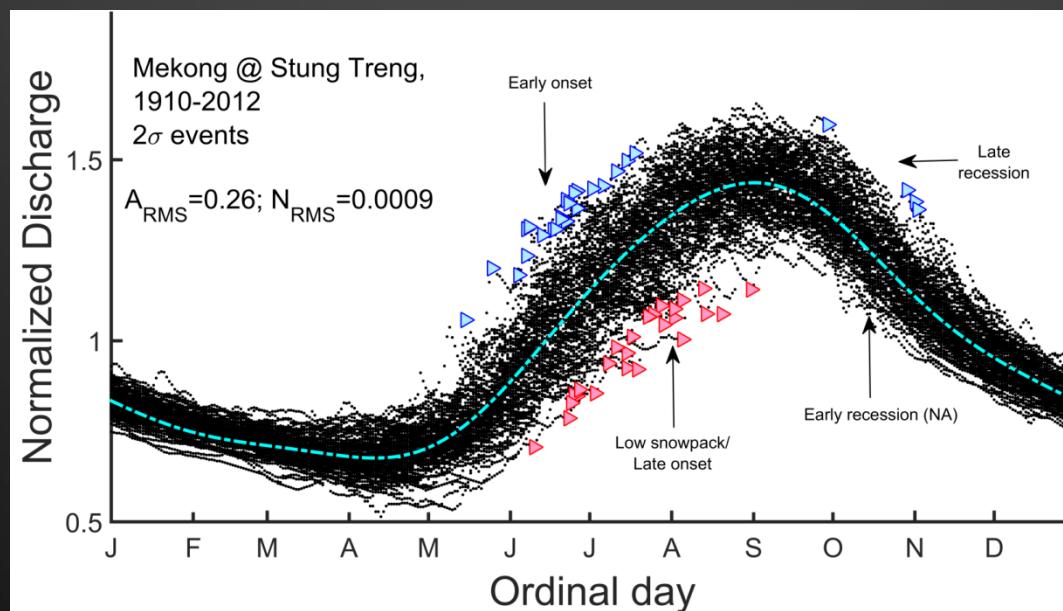
100-year hydrograph



Extreme events (Q_2)

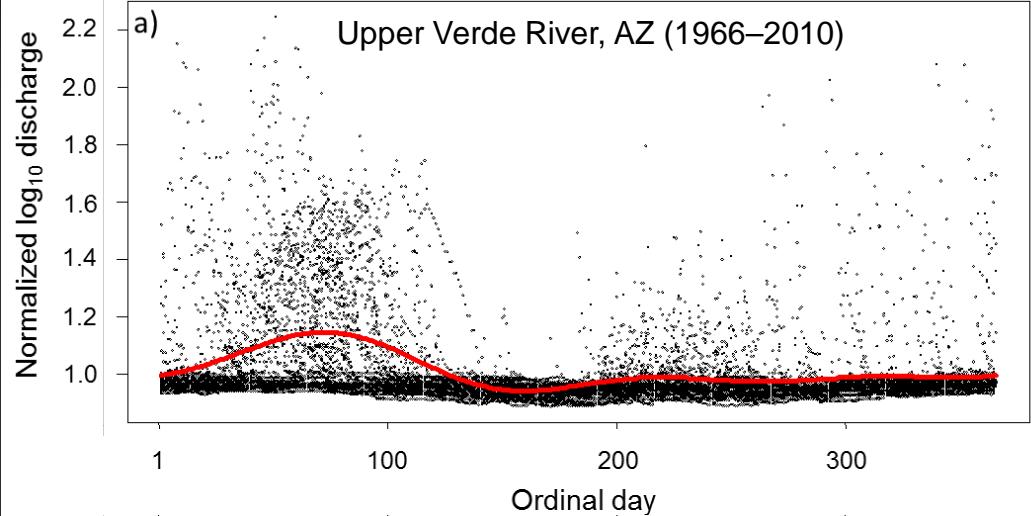


Spectral anomalies (2σ)

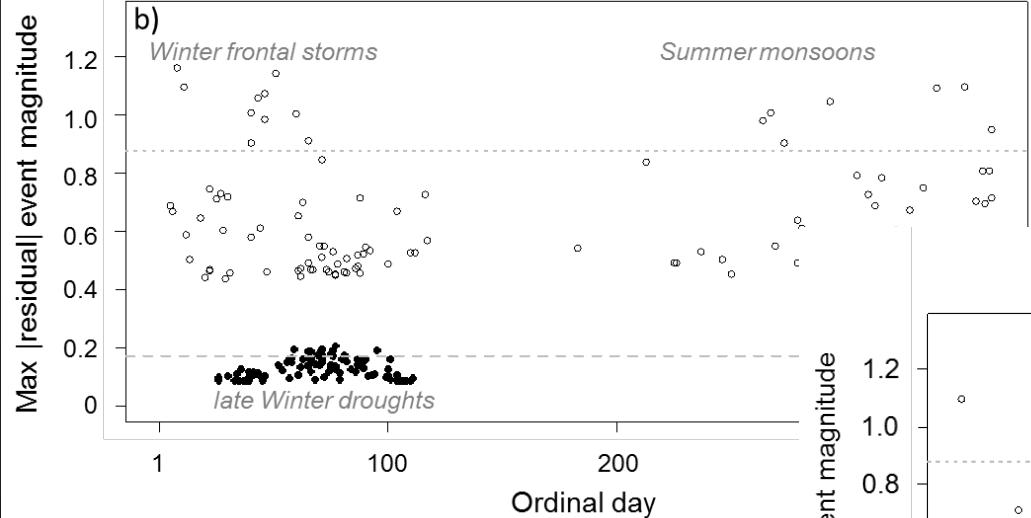


Discrete Fast Fourier Transform (DFFT) to extract characteristic signals (freq., phase, amplitude) and identify anomalous high and low flows

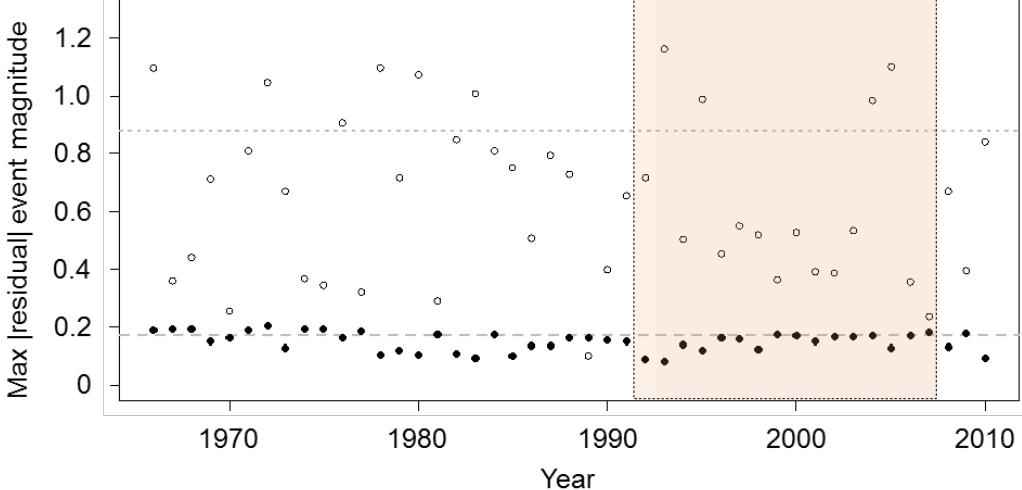
(after Sabo & Post 2008)

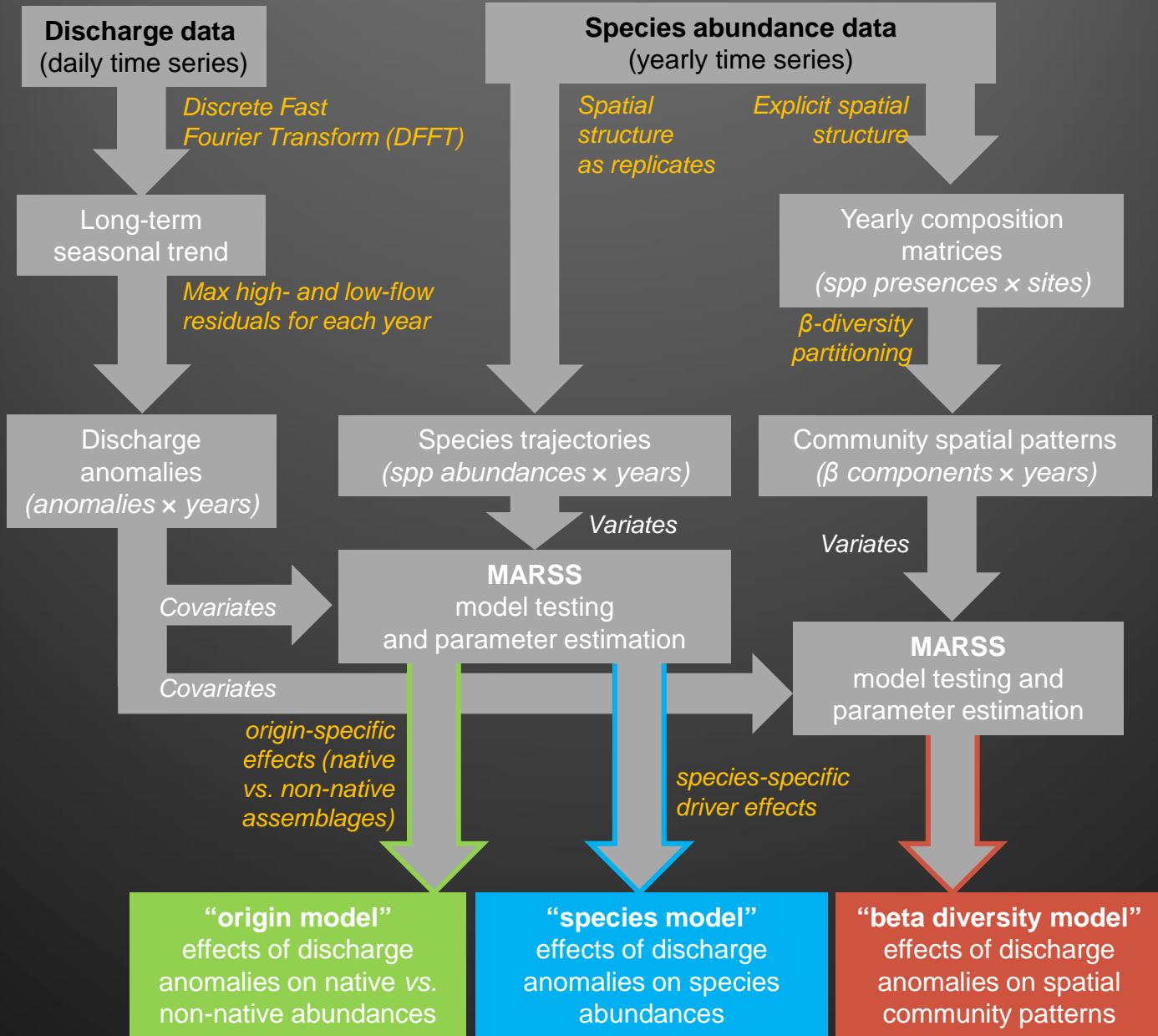


'Discharge' R package



Fish data





Written in matrix form:

The effect of species 1 on species 2

$$\begin{bmatrix} x_{1,t} \\ x_{2,t} \\ x_{3,t} \end{bmatrix} = \begin{bmatrix} 1 + \alpha_{1,1} & \alpha_{1,2} & \alpha_{1,3} \\ \alpha_{2,1} & 1 + \alpha_{2,2} & \alpha_{2,3} \\ \alpha_{3,1} & \alpha_{3,2} & 1 + \alpha_{3,3} \end{bmatrix} \begin{bmatrix} x_{1,t-1} \\ x_{2,t-1} \\ x_{3,t-1} \end{bmatrix} + \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} + \begin{bmatrix} c_{1,1} & c_{1,2} \\ c_{2,1} & c_{2,2} \\ c_{3,1} & c_{3,2} \end{bmatrix} \begin{bmatrix} v_{1,t-1} \\ v_{2,t-1} \end{bmatrix} + \begin{bmatrix} w_1 \\ w_2 \\ w_3 \end{bmatrix}$$

B = interaction matrix

covariate effect

Environmental variation (not from covariates)

Methods: What is a MARSS model?

Multivariate Autoregressive State-Space model

- Extensively used in econometrics
(in ecology mainly in fisheries, rev. in Hampton et al. 2013 Ecology)
- Rely on theory about temporal correlation patterns that emerge from environmental drivers and species interactions (Ives et al. 2003 Ecol Monogr)

In the matrix form:

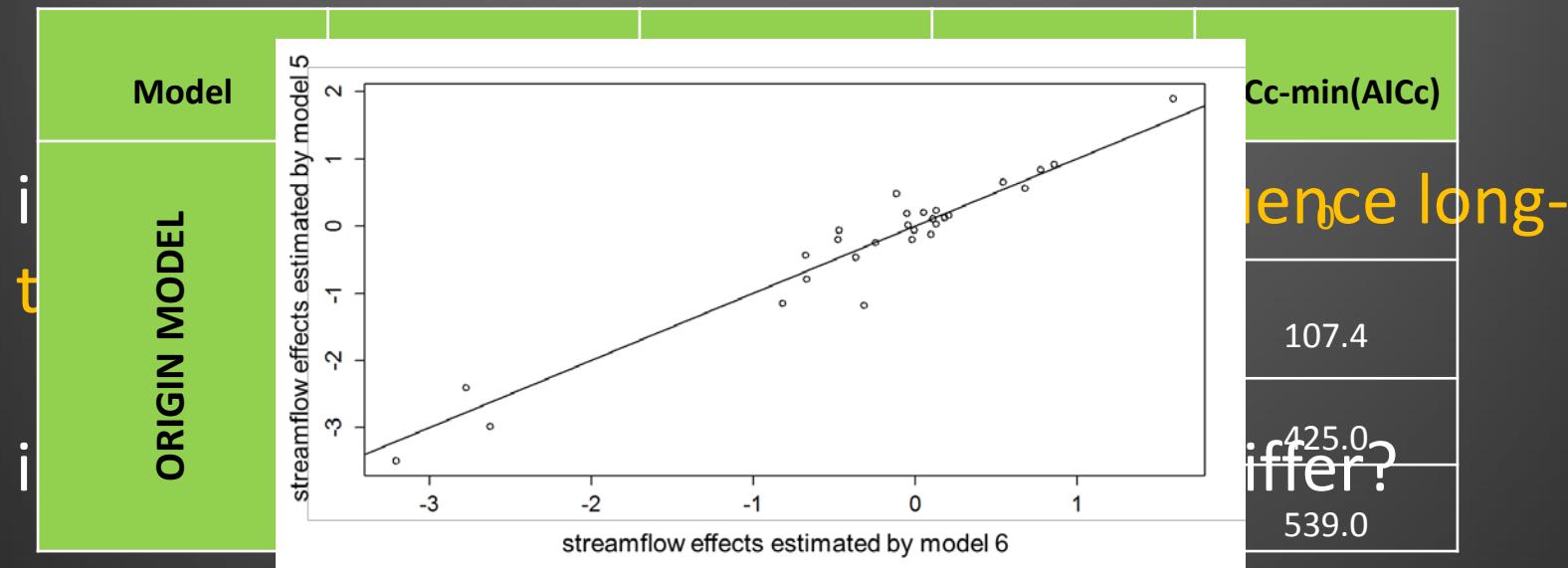
$$\begin{aligned} \mathbf{x}_t &= \mathbf{B}\mathbf{x}_{t-1} + \mathbf{C}\mathbf{c}_{t-1} + \mathbf{w}_t, \\ \mathbf{y}_t &= \mathbf{Z}\mathbf{x}_t + \mathbf{v}_t, \end{aligned}$$

where $\mathbf{w}_t \sim \text{MVN}(0, \mathbf{Q}_t)$ (Process model)
where $\mathbf{v}_t \sim \text{MVN}(0, \mathbf{R}_t)$ (Observation model)

covariate data
covariate effects! (interesting)
“true” abundances
“last year”
“true” abundances
spp interactions
this year
“true” abundances
this year
observed abundances
this year

‘MARSS’ R-package (Holmes et al. 2014)

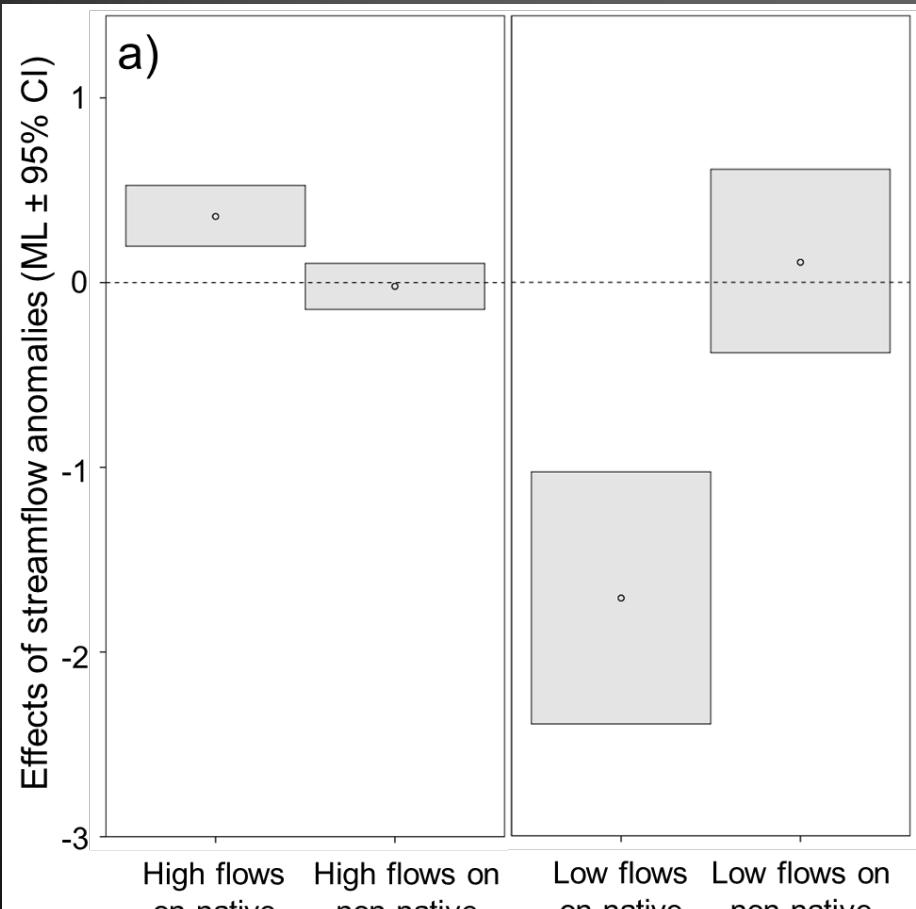
Model selection: ‘origin’ and ‘species’ models



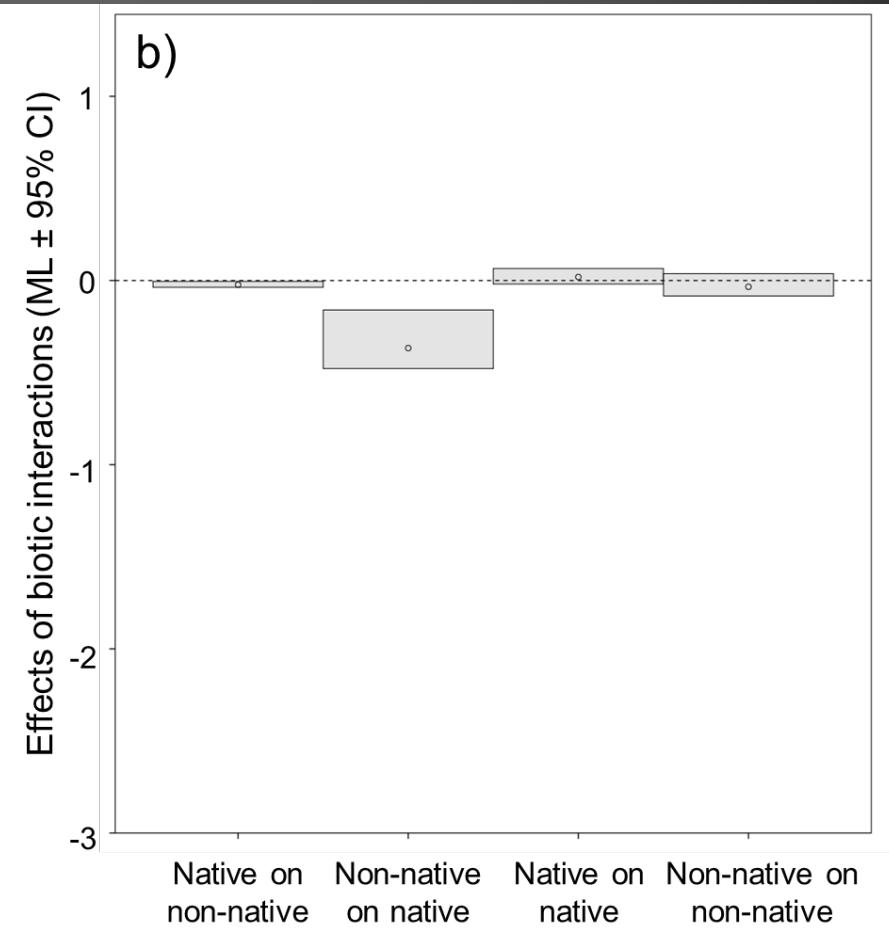
Model	Biotic interactions	Obs. errors	AICc	AICc-min(AICc)
SPECIES MODEL	5 YES, species-specific	species-specific	1104.2	133.5
	6 none	species-specific	1104.6	133.9
	7 YES, species-specific	constant	1559.3	588.6
	8 none	constant	1538.2	567.5

Origin model

Abiotic drivers

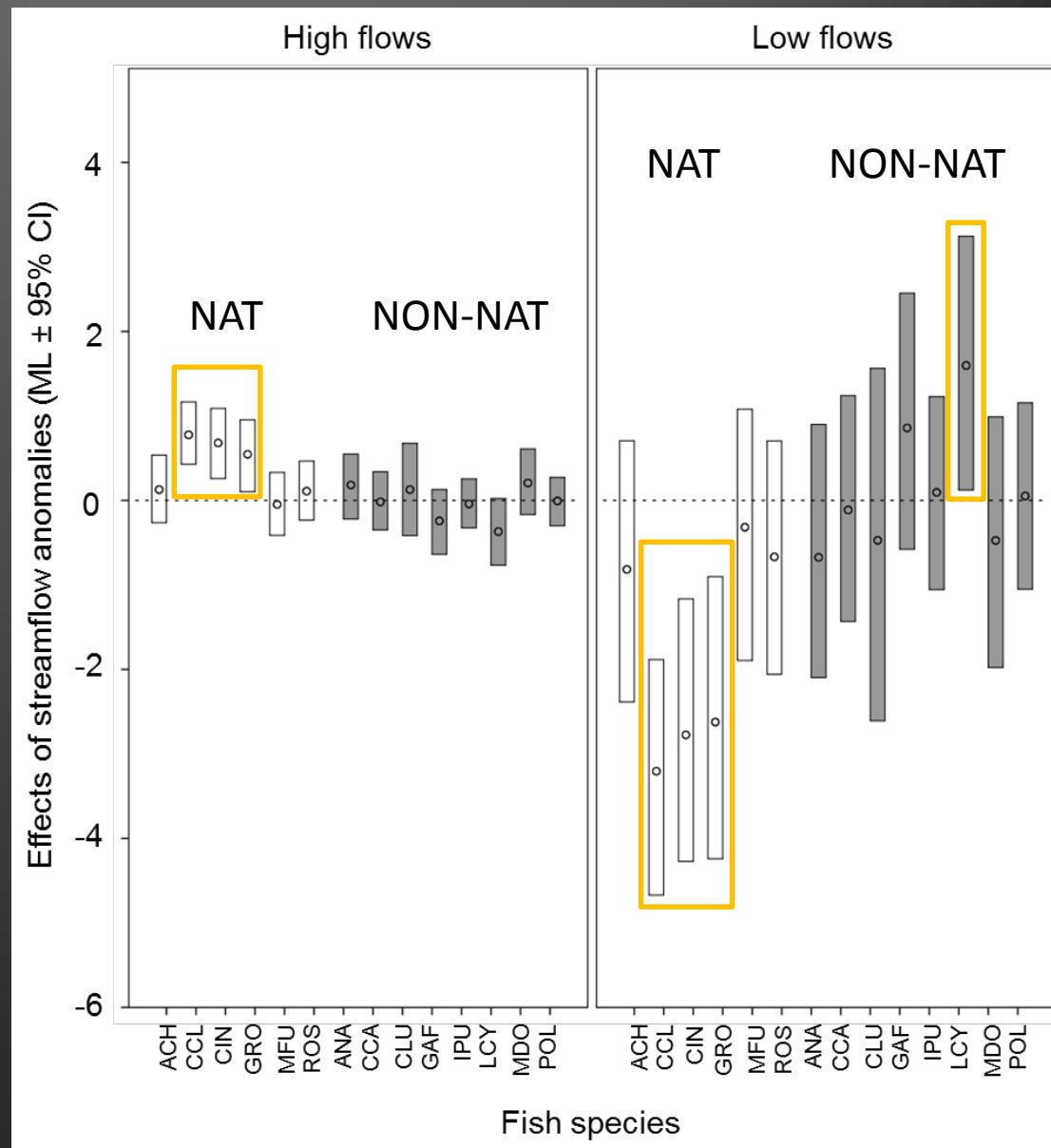


Biotic drivers



Species model (only abiotic)

Code	English name	Latin name	FUni
ACH	Longfin dace	<i>Agosia chrysogaster</i>	0.78
CCL	Desert sucker	<i>Catostomus clarki</i>	0.82
CIN	Sonora sucker	<i>Catostomus insignis</i>	1.00
GRO	Roundtail chub	<i>Gila robusta</i>	0.90
MFU	Spike dace	<i>Meda fulgida</i>	0.86
ROS	Speckled dace	<i>Rhinichthys osculus</i>	0.91
ANA	Yellow bullhead	<i>Ameiurus natalis</i>	0.86
CCA	Common carp	<i>Cyprinus carpio</i>	0.78



Trait differences between NAT and NON-NAT

(iii) Were differences in responses between the native and the non-native assemblage explained by differences in their biological traits?

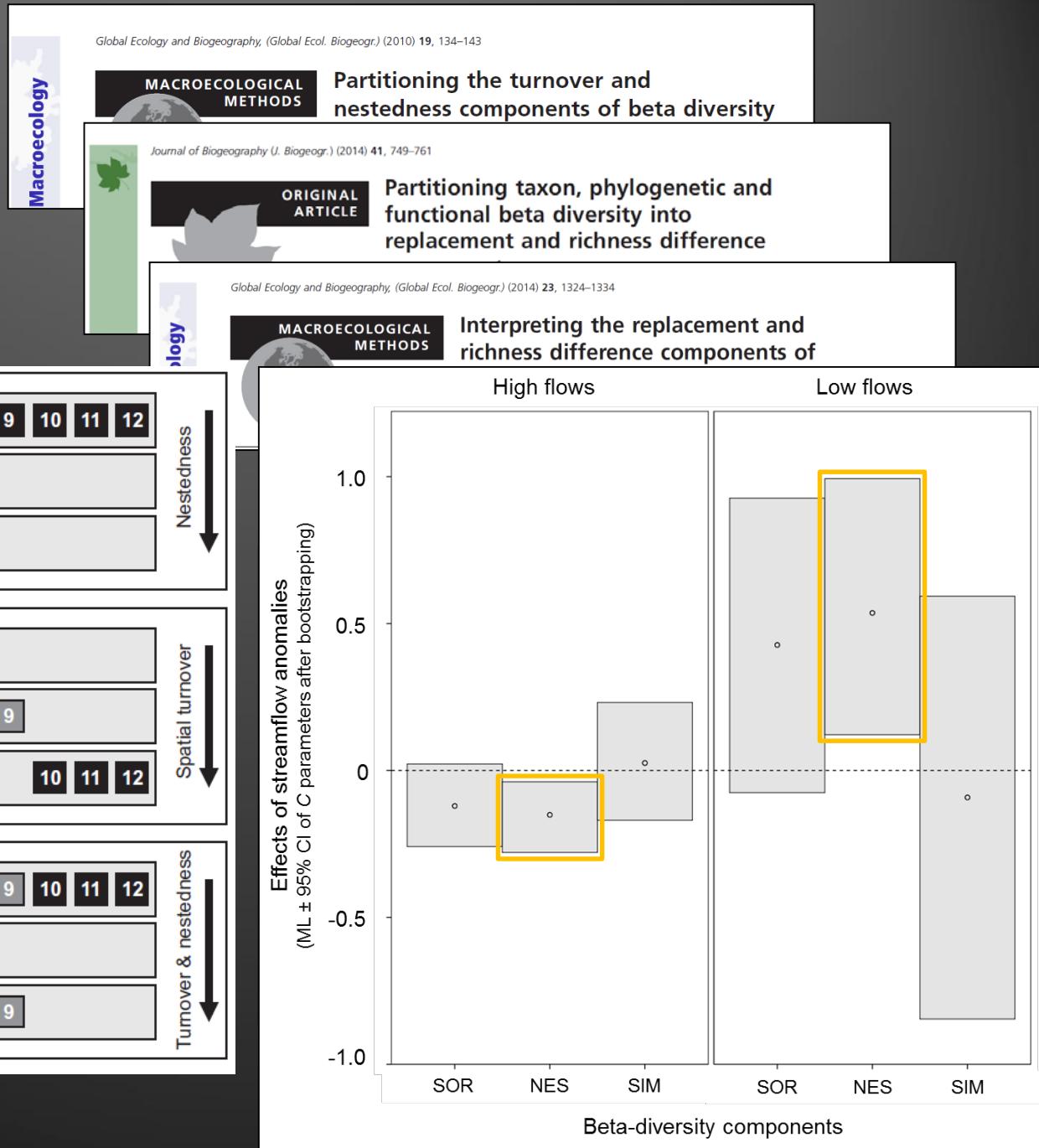
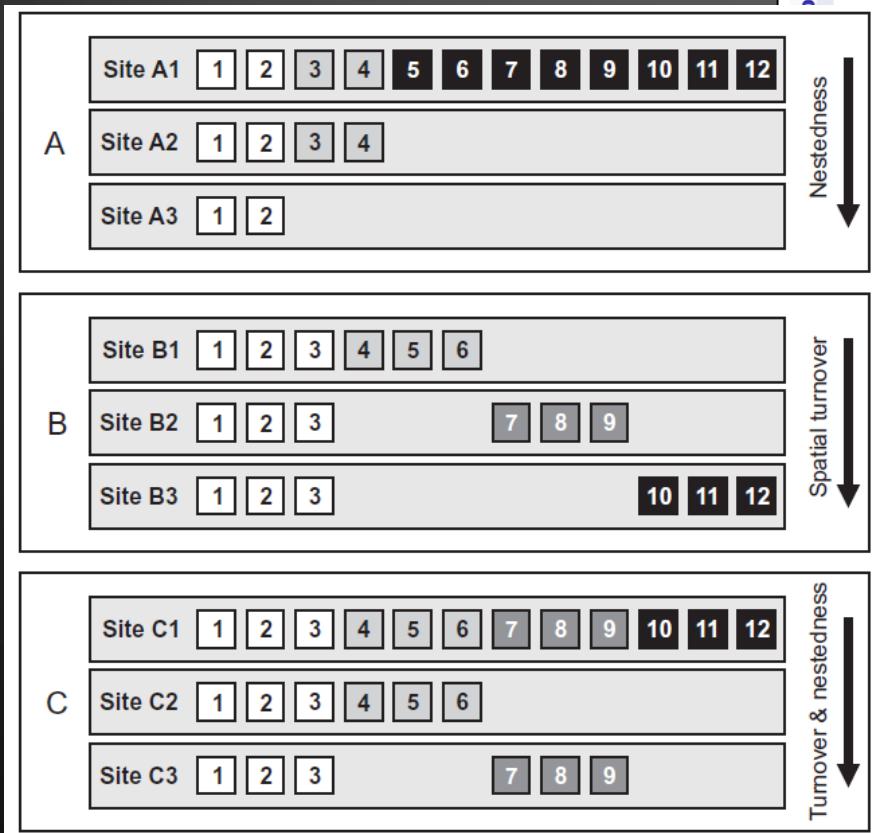
SIMPER (SIMilarity PERcentages) test, native vs. non-native species

Based on the Fish Traits database (Frimpong & Angermeier 2009)

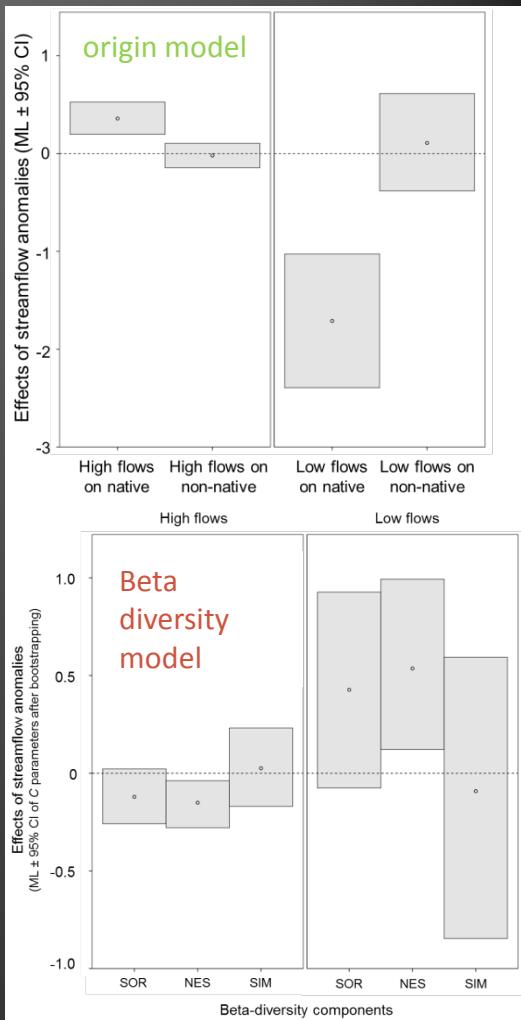
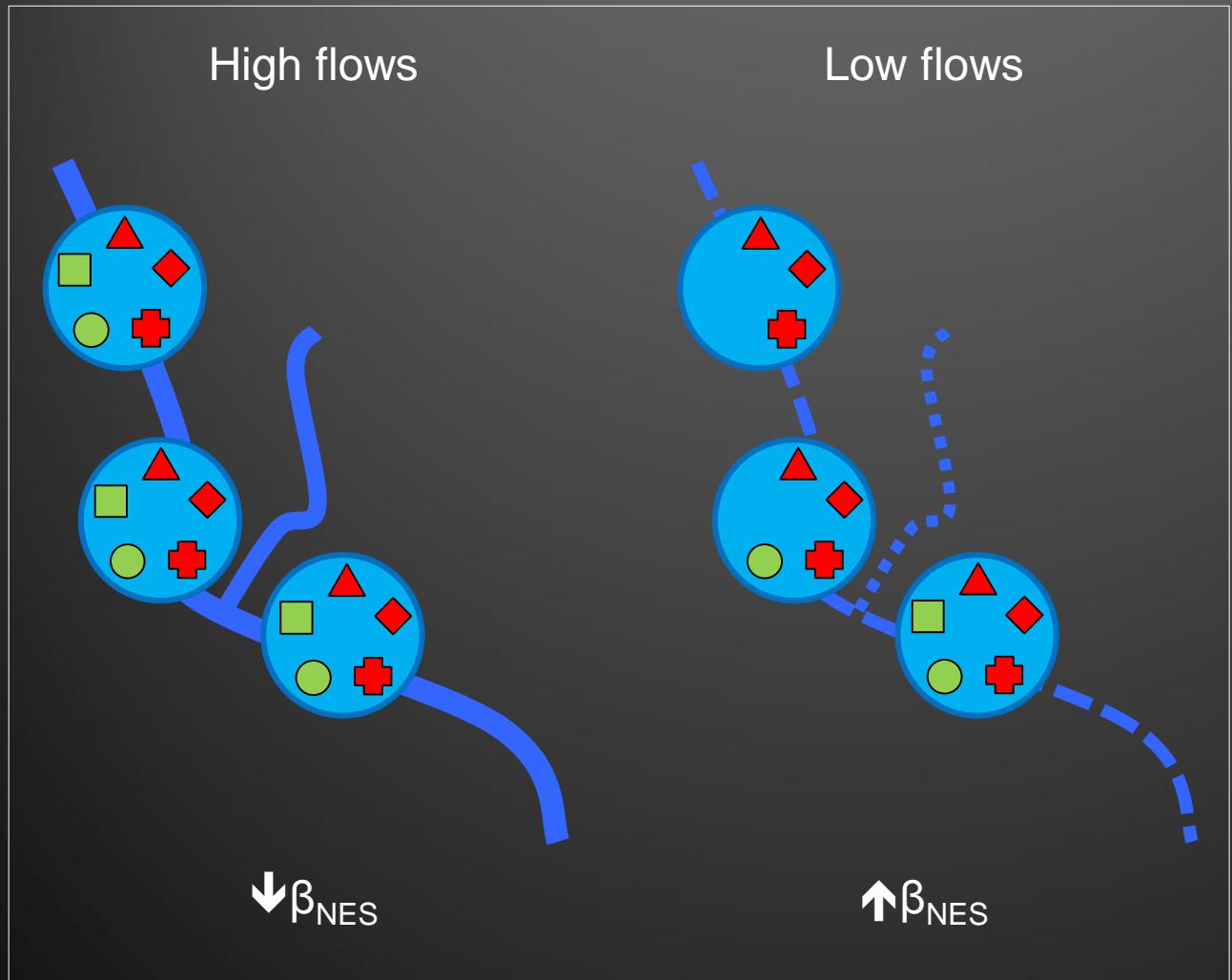
Trait type	Trait	Native	Non-native	Diss/SD	Contrib%
body size	Max total length	4.12	9.41	1.17	3.02
	preference for lentic systems	2.08	10.94	1.62	3.88
habitat preference	preference for moderate current	11.11	4.17	1.20	2.63
	preference for clay or silt substrate	4.76	8.93	1.02	3.08
life history	length of the spawning season	8.15	6.38	1.24	2.00
	longevity	4.90	8.82	1.10	2.41
trophic ecology	serial or batch spawner	9.52	5.36	1.01	3.19
	fishes and large macroinvertebrates	2.78	10.42	1.11	4.12
	detritus	9.52	5.36	1.03	3.18

Spatial patterns: beta diversity model

beta diversity partitioning (after Baselga 2010)



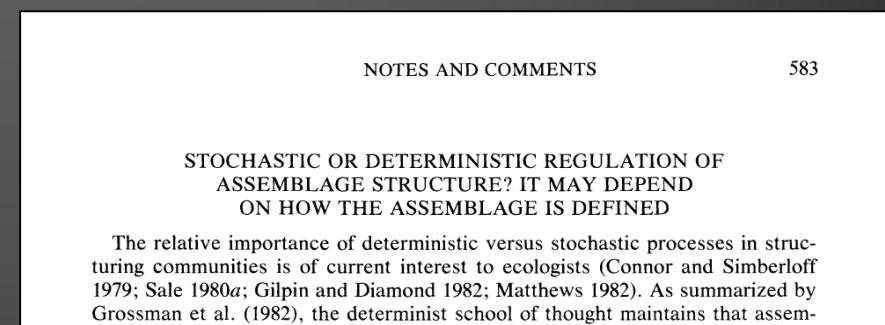
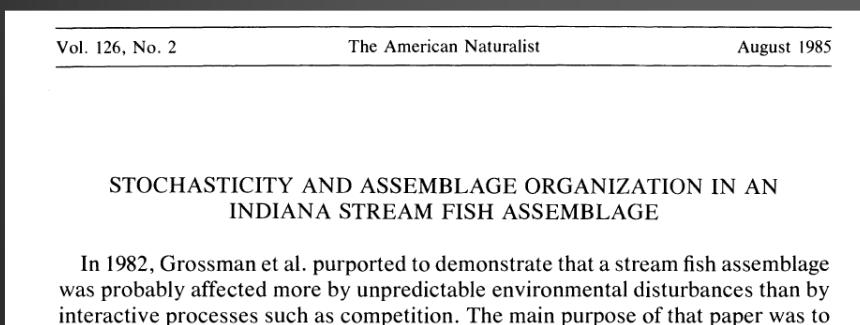
Beta diversity model



Non-natives
Natives

Ongoing debate: deterministic or stochastic?

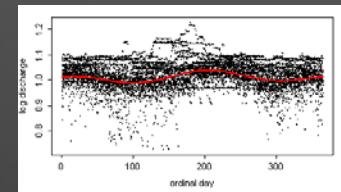
- “Classical” fish studies: biotic = deterministic, abiotic = stochastic...
(e.g., Grossman 1982, Rahel et al. 1984, Grossman et al. 1985, Moyle & Vondracek 1985...)



- ...false dichotomy? Communities increasingly driven by discharge variation as the stochastic component of environmental variation increases (Grossman & Sabo 2010)
- Environmental variation is key and may underlie the commonly-observed negative co-variation between native and non-native faunas in highly variable environments

Implications

- ✓ Non-natives as a symptom of hydrologic alteration
(i.e. “passengers, not drivers” of native decline)
[e.g. similar to Cottonwood vs. Saltcedar, Stromberg et al. 2007 GEB]
- ✓ Invasion may not be addressed without better water management



Hydrological alteration



Is this a Southwest-wide pattern?

A different approach to parameter estimation for hidden state problems: Expectation-Maximization algorithms

Holmes, E. E. 2013. Derivation of the EM algorithm for **constrained** and unconstrained multivariate autoregressive state-space (MARSS) models. Technical Report. arXiv:1302.3919 [stat.ME]

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

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

$$\alpha + \beta_1 p_1 + \beta_2 p_2 + \dots$$

What's the point?

- 1) It can make **multivariate AR state-space** model fitting problems tractable by being considerably faster and more stable
- 2) For many of the problems we work on, other approaches grind to a halt

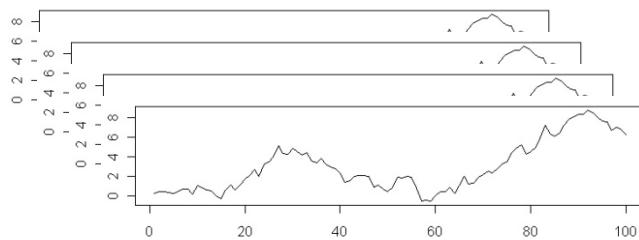
MARSS model

Multivariate
autoregressive
“random walk”

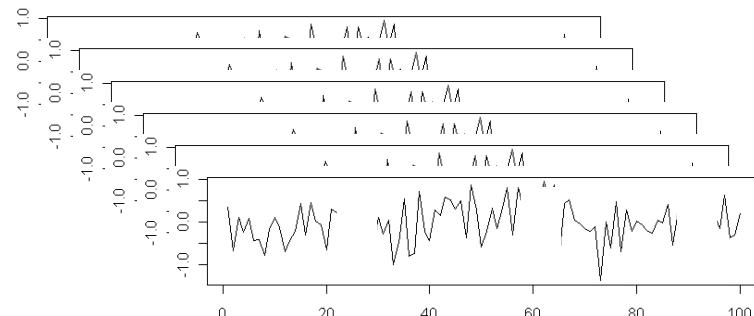
$$\mathbf{x}_t = \mathbf{B}\mathbf{x}_{t-1} + \mathbf{u} + \mathbf{w}_t, \text{ where } \mathbf{w}_t \sim MVN(0, \mathbf{Q})$$

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

Multivariate
with noise



hidden



observe

written out....

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

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

“We have not succeeded in answering all our problems. The answers we have found only serve to raise a whole set of new questions. In some ways we feel we are as confused as ever, but we believe we are confused on a higher level and about more important things.”

Earl C. Kelley, 1951, ‘The Workshop Way of Learning’