Principal Dynamical Components

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3. Application to the Global Sea-Surface Temperature Field

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This is achieved by transforming to a new set of variables $(m < n)$, the principal components (PCs), which are uncorrelated, and which are ordered so that the first few retain most of the variation present in all of the original variables.

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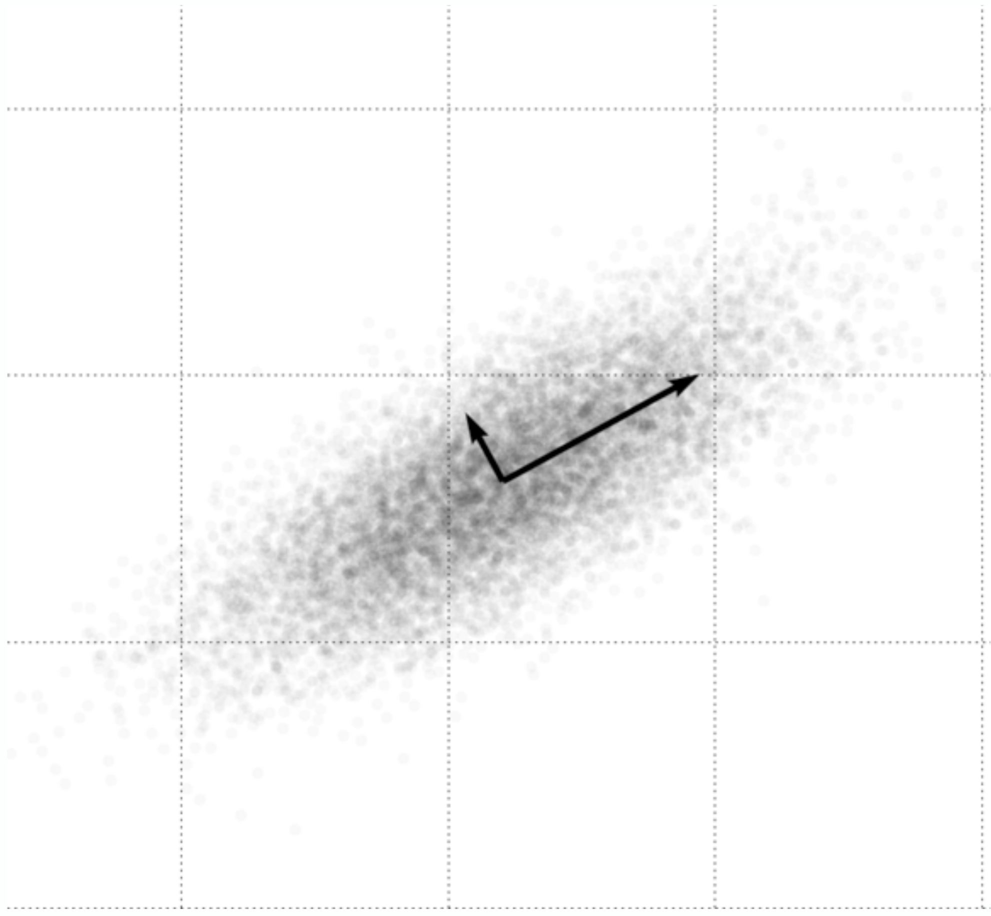

A COUPLE OF EXAMPLES

- Certain analysis considered the grades of $N = 15$ students in $n = 8$ subjects. The first two PCs account for 82,1% of the total variation in the data set. The first one was strongly correlated with humanity subjects and the second one with science subjects.

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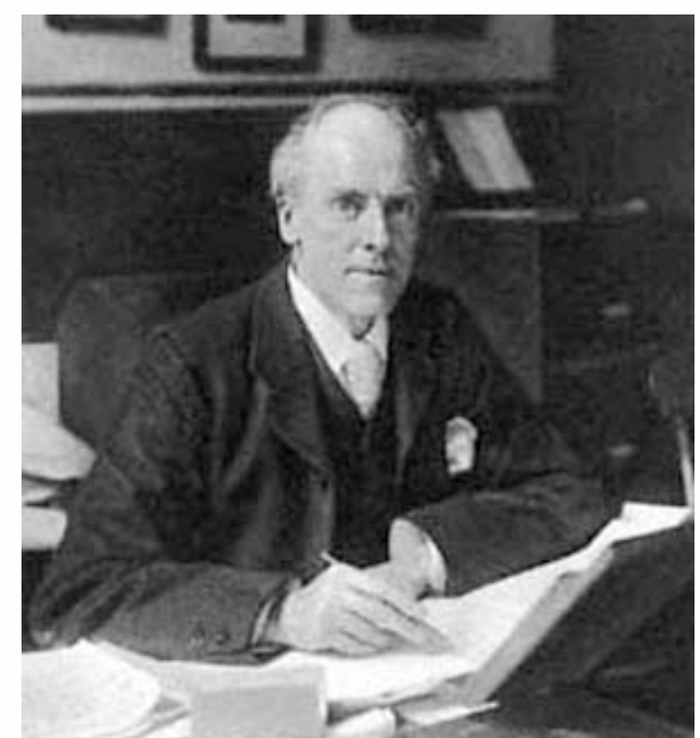
LIII. *On Lines and Planes of Closest Fit to Systems of Points in Space.* *By* KARL PEARSON, *F.R.S., University College, London* *.

(1) IN many physical, statistical, and biological investigations it is desirable to represent a system of points in plane, three, or higher dimensioned space by the "best-fitting" straight line or plane. Analytically this consists in taking



1901

HOW TO OBTAIN THE PC'S

Singular value decomposition

Given a data set $z_1, z_2, \ldots, z_N \in \mathbb{R}^n$ (already subtracted the mean value), the first m PCs are given by $x_j = Q'_x z_j$ where $Q_x \in \mathbb{R}^{n \times m}$ has orthogonal columns such that the predictive uncertainty

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The matrix Q_x consists of the first m columns of U in the singular value decomposition

$$Z' = USV'$$

where $U \in \mathbb{R}^{n \times n}$ and $V \in \mathbb{R}^{N \times N}$ are orthogonal matrices and $S \in \mathbb{R}^{n \times N}$ is diagonal with the eigenvalues of the covariance matrix $Z'Z$ sorted in decreasing order ($Z = [z_1 | \cdots | z_N]$).

AUTORREGRESIVE MODELS (AR(P))

One dimensional AR(p)

For a random process z the AR(p) model is defined as

$$z_j = b + \sum_{i=1}^{p} a_i z_{j-i} + \varepsilon_j,$$

where $a_i, \ldots, a_p$ are the *parameters* of the model, b is a constant, and ε_j is white noise. The process is *stationary* if the roots of the polynomial $x^p - \sum_{i=1}^{p} a_i x^{p-i}$ lie within the unit circle.

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$a_i, \ldots, a_p$ can be estimated by solving the Yule-Walker equations

1927

$$\begin{pmatrix} \gamma_1 \\ \gamma_2 \\ \vdots \\ \gamma_p \end{pmatrix} = \begin{pmatrix} \gamma_0 & \gamma_{-1} & \gamma_{-2} & \cdots \\ \gamma_1 & \gamma_0 & \gamma_{-1} & \cdots \\ \vdots & \vdots & \vdots & \ddots \\ \gamma_{p-1} & \gamma_{p-2} & \gamma_{p-3} & \cdots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_p \end{pmatrix},$$

1931

where $\gamma_m = E[z_{j+m} z_j]$ are the covariance functions.

SOME EXAMPLES OF AR(1) AND AR(2)

VECTOR AR(P)

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Similarly an estimation of the parameters $A_i, \ldots, A_p$ can be calculated solving the Yule-Walker equations (now block matrices).

PRINCIPAL DYNAMICAL COMPONENTS (PDC)

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Given a time series $z_j \in \mathbb{R}^n$ with transition probability $T(z_{j+1}|z_j)$ (Markovian), PDC considers a dimensional reduction of $T(z_{j+1}|z_j)$ in the following way

$$T(z_{j+1}|z_j) = J(z_{j+1})e(y_{j+1}|x_{j+1})d(x_{j+1}|x_j),$$

where

- $x = P_x(z(x,y)) \in \mathbb{R}^m, y = P_y(z(x,y)) \in \mathbb{R}^{n-m}$ (P_x and P_y are projection operators) and $J(z)$ is the Jacobian determinant of the coordinate map $z \to (x,y)$.
- $e(y|x)$ is a probabilistic embedding.
- $d(x_{j+1}|x_j)$ is a reduced dynamical model.

PRINCIPAL DYNAMICAL COMPONENTS (PDC)

We will focus on the case where P_x and P_y are orthogonal projections (therefore $J(z) = 1$) and the embedding and reduced dynamics are given by isotropic Gaussians

$$e(y|x) = \mathcal{N}(0, \sigma^2 I_{n-m}), \quad d(x_{j+1}|x_j) = \mathcal{N}(Ax_j, \sigma^2 I_m).$$

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Therefore, the log-likelihood function is given by

$$L = -\sum_{j=1}^{N-1} \left[\frac{n}{2} \log(2\pi) + n \log(\sigma) + \frac{1}{2\sigma^2} \left(\|x_{j+1} - Ax_j\|^2 + \|y_{j+1}\|^2 \right) \right].$$

Maximazing L over P and A is equivalent to minimizing the cost function

$$c = \frac{1}{N-1} \sum_{j=1}^{N-1} \left(\|x_{j+1} - Ax_j\|^2 + \|y_{j+1}\|^2 \right).$$

LINEAR AND AUTONOMOUS CASE (MARKOVIAN)

For a time series $z \in \mathbb{R}^n$ we look for a m-dimensional submanifold $x = Q'_x z$ such that

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The minimization problem that defines $Q = [Q_x Q_y]$ and A is

$$\min_{Q,A} c = \sum_{j=1}^{N-1} \left\| z_{j+1} - Q \begin{pmatrix} A {Q_x}' z_j \\ 0 \end{pmatrix} \right\|^2 = \sum_{j=1}^{N-1} \left\| \begin{pmatrix} x_{j+1} - A x_j \\ y_{j+1} \end{pmatrix} \right\|^2 .$$

PDC SIMPLEST CASE $n = 2$

Let us call $z = \begin{pmatrix} A \\ P \end{pmatrix}$.We look for a one-dimensional submanifold x of z

$$x = A\cos(\theta) + P\sin(\theta)$$

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The cost function is then

$$\begin{aligned} c(\theta, a) &= \sum_{j=1}^{N-1} \left\| \begin{pmatrix} A_{j+1} - \tilde{A}_{j+1} \\ P_{j+1} - \tilde{P}_{j+1} \end{pmatrix} \right\|^2 = \sum_{j=1}^{N-1} \left\| \begin{pmatrix} x_{j+1} - \tilde{x}_{j+1} \\ y_{j+1} - \tilde{y}_{j+1} \end{pmatrix} \right\|^2 \\ &= \sum_{j=1}^{N-1} \left\| \begin{pmatrix} x_{j+1} - a x_j \\ y_{j+1} \end{pmatrix} \right\|^2 = \sum_{j=1}^{N-1} (y_{j+1})^2 + (x_{j+1} - a x_j)^2 \end{aligned}$$

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By contrast, the corresponding cost function for regular principal components in this 2-dimensional scenario is

$$c_{PCA}(\theta) = \sum_{j=1}^{N} {y_j}^2.$$

SYNTHETIC EXAMPLE

We created data from the dynamical model

$$\begin{aligned} x_{j+1} &= a x_j + 0.3\eta_j^x \\ y_{j+1} &= 0.6\eta_j^y \end{aligned}$$

where $a = 0.6$, $j = 1, \ldots, 999$ and $\eta_j^{x,y}$ are independent samples from a normal distribution.

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Then we rotated the data through the angle $\theta = \frac{\pi}{3}$

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\begin{aligned}
A_j &= x_j \cos(\theta) - y_j \sin(\theta) \\
P_j &= x_j \sin(\theta) + y_j \cos(\theta)
\end{aligned}
$$

and we perform descent over the variables a and θ.

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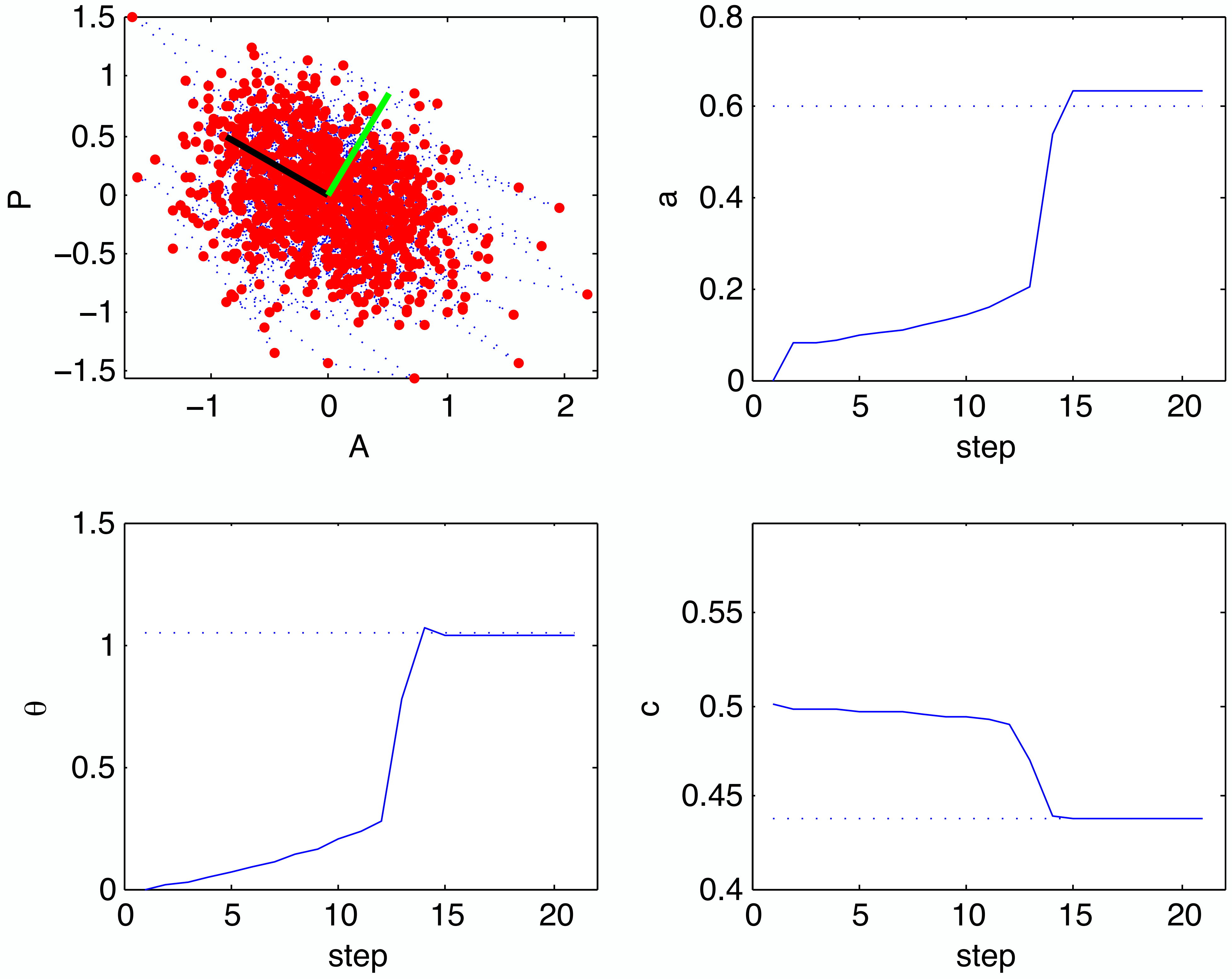

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for $j = 1, \ldots, 999$ and we adopted the values $a_j = \frac{6}{5}\cos^2\left(\frac{2\pi t_j}{T}\right)$ for the dynamics, $b_j = \frac{1}{2}\sin\left(\frac{2\pi t_j}{T}\right)$ for the drift, and $\bar{y}_j = \frac{2}{5}\cos\left(\frac{2\pi t_j}{T}\right)$ for the non-zero mean of y, where $t_j = j$ and $T = 12$.

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Then we rotated the data through

$$\begin{aligned} A_j &= x_j \cos(\theta_j) - y_j \sin(\theta_j), \\ P_j &= x_j \sin(\theta_j) + y_j \cos(\theta_j), \end{aligned}$$

where $\theta_j = \frac{\pi}{6}\sin\left(\frac{2\pi t_j}{T}\right)$.

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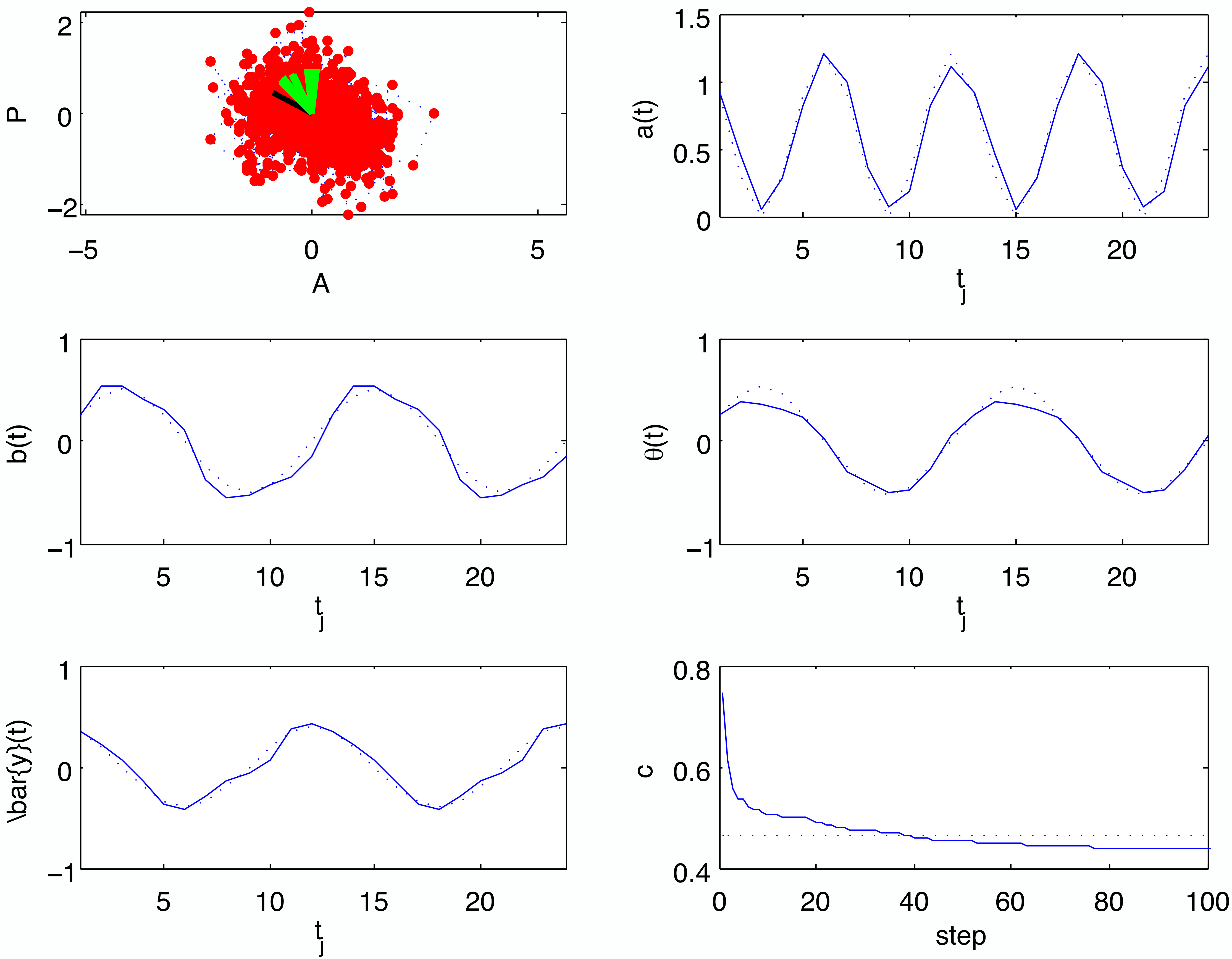

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Take $n = 2$, $m = 1$, and $r = 3$, the order of the Non-Markovian process. We created data from the dynamical model

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Then, as before, we define

$$\begin{aligned} A_j &= x_j \cos(\theta) - y_j \sin(\theta), \\ P_j &= x_j \sin(\theta) + y_j \cos(\theta), \end{aligned}$$

with $\theta = \frac{\pi}{3}$, and provide the A_j and P_j as data for the principal dynamical component routine.

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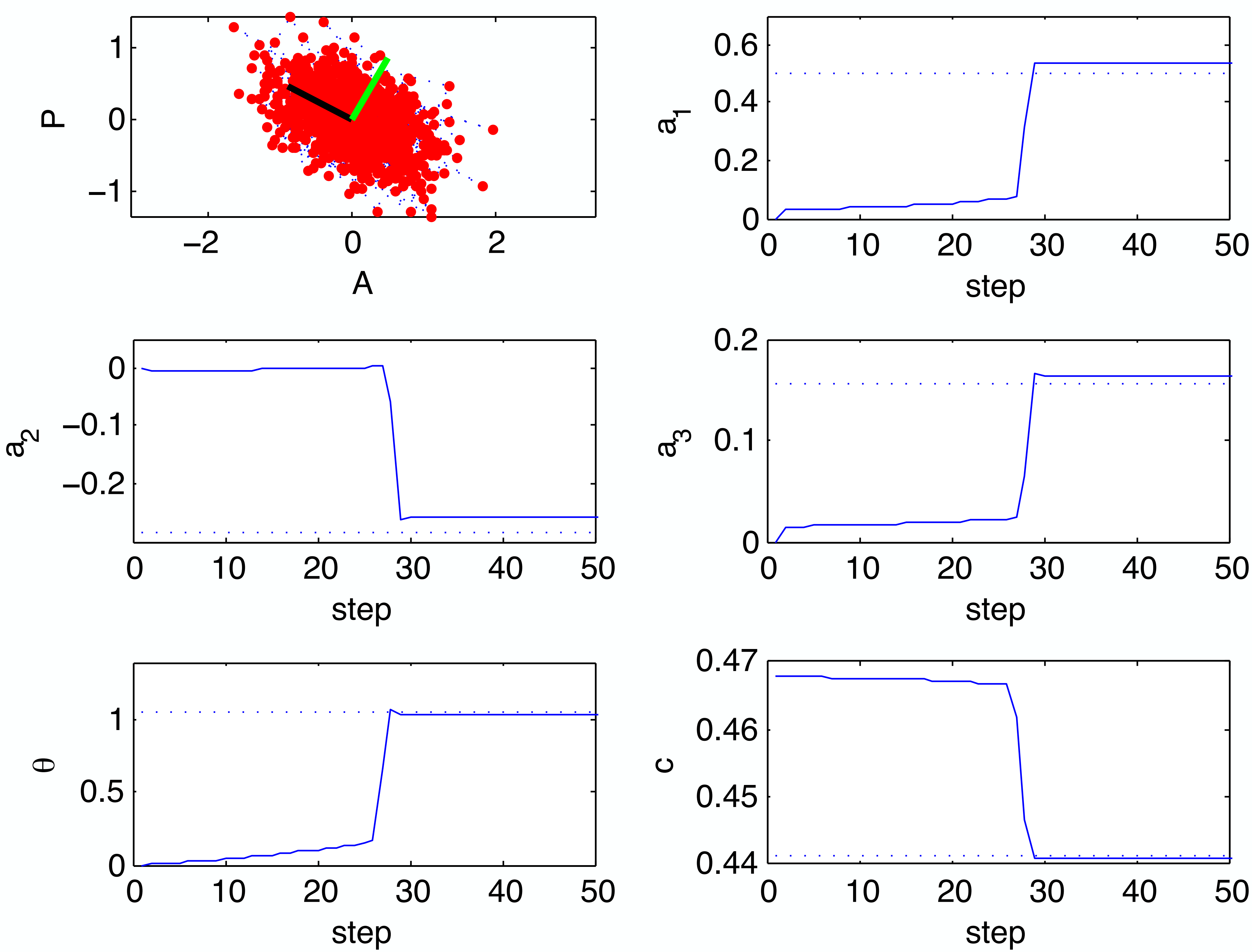

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- The ocean is not an isolated player in climate dynamics: it interacts with the atmosphere and the continents, and is also affected by external conditions, like solar radiation or human-related release of CO_2 into the atmosphere. The latter are examples of slowly varying external trends that fit naturally into our non-autonomous setting.

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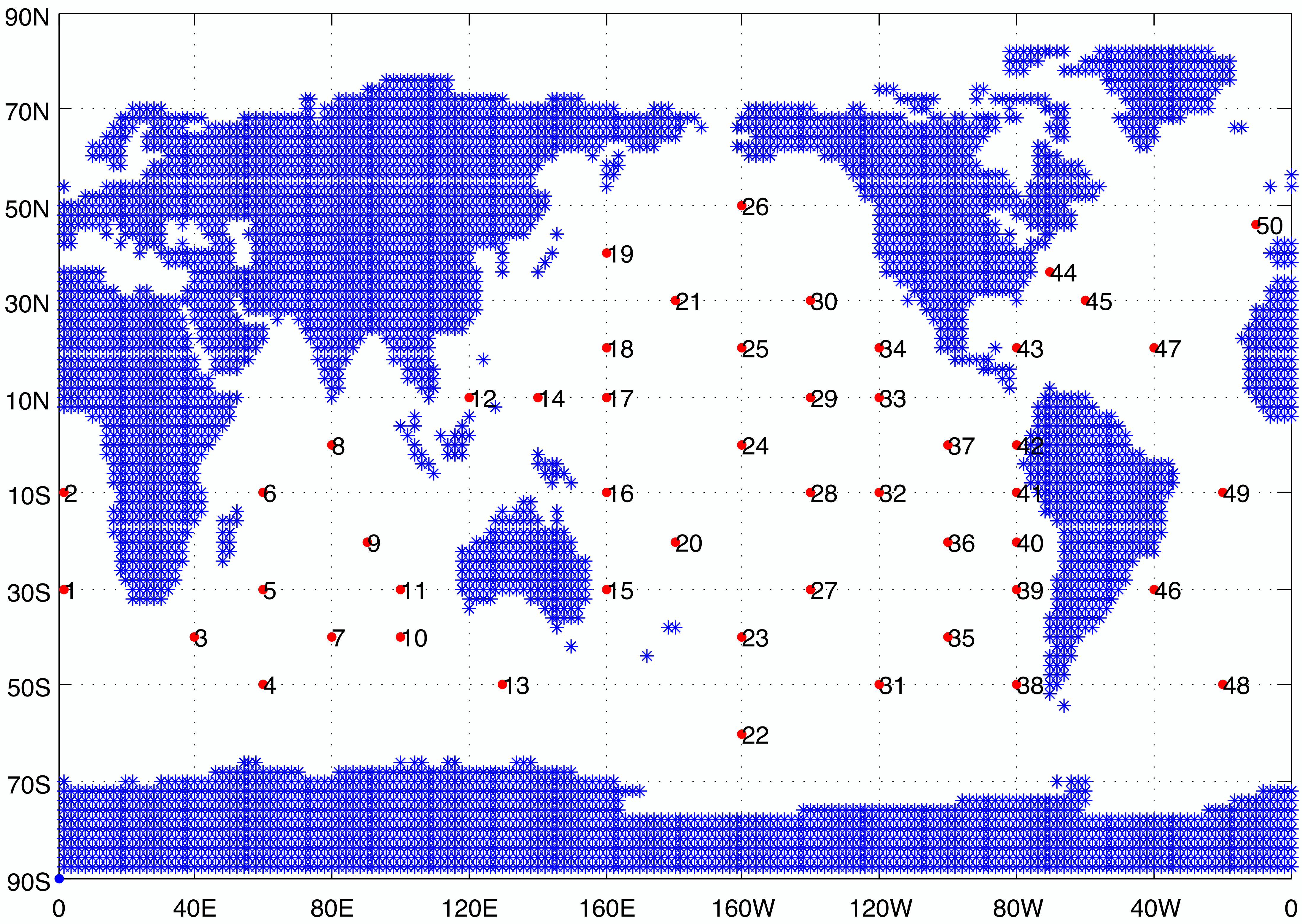
- Even within the ocean, the surface temperature does not evolve alone: it is carried by currents, and it interacts through mixing with lower layers of the ocean. One way to account for unobserved variables is to make the model non-Markovian.

50 POINTS IN THE OCEAN



$$\Rightarrow n = 50 \text{ and } N = 1858$$

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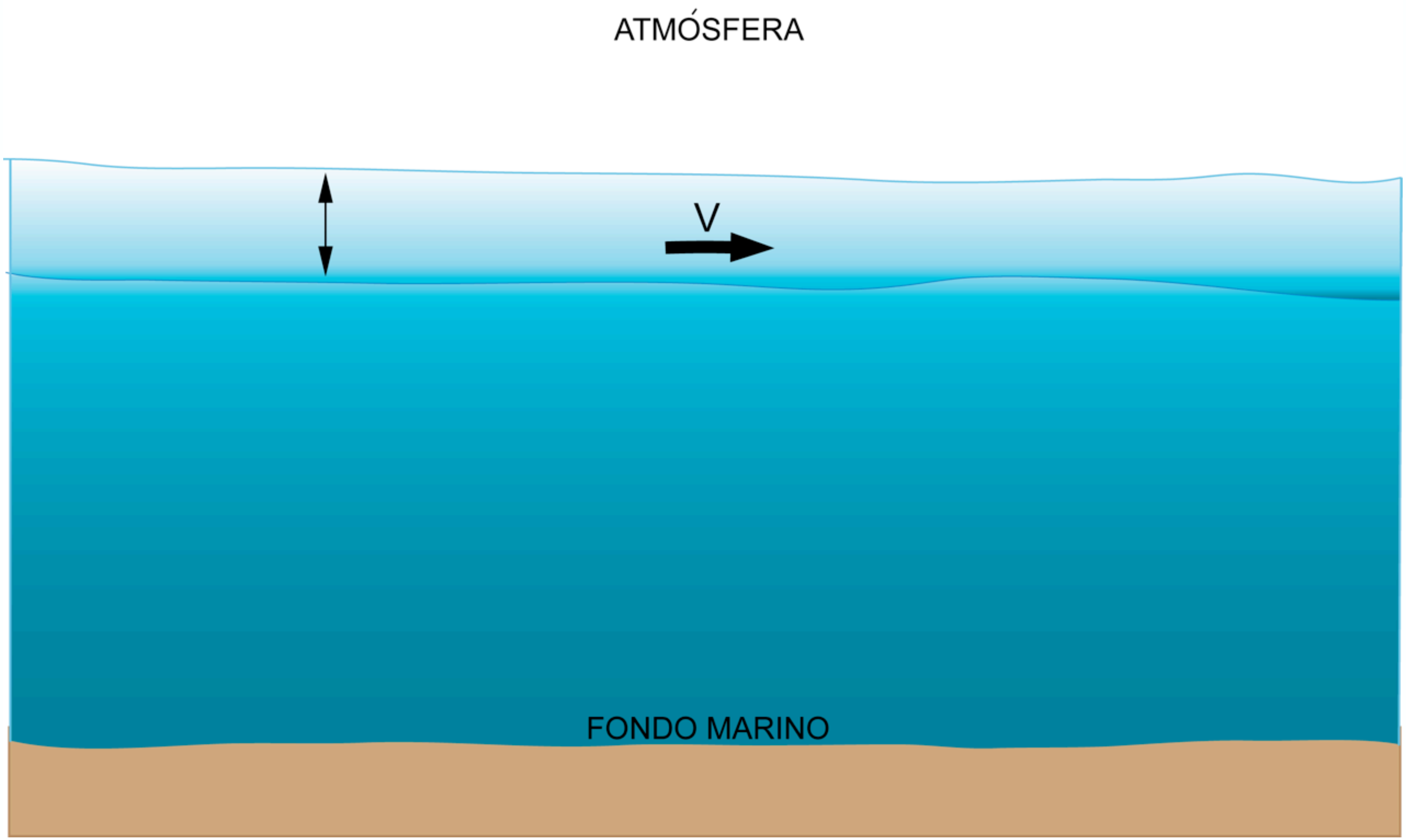
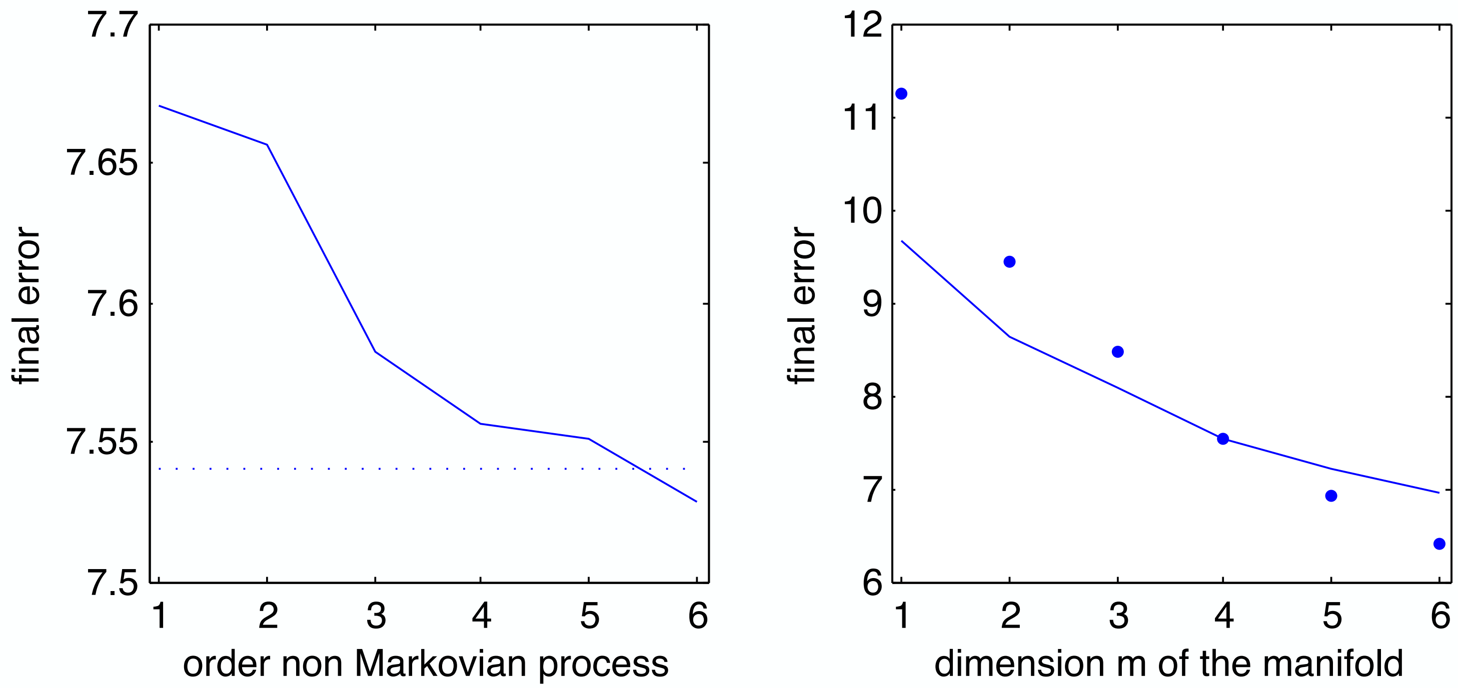


CHOICE OF DIMENSION AND ORDER

Predictive uncertainty as a function of the dimension m of the reduced dynamical manifold and the order r of the process.



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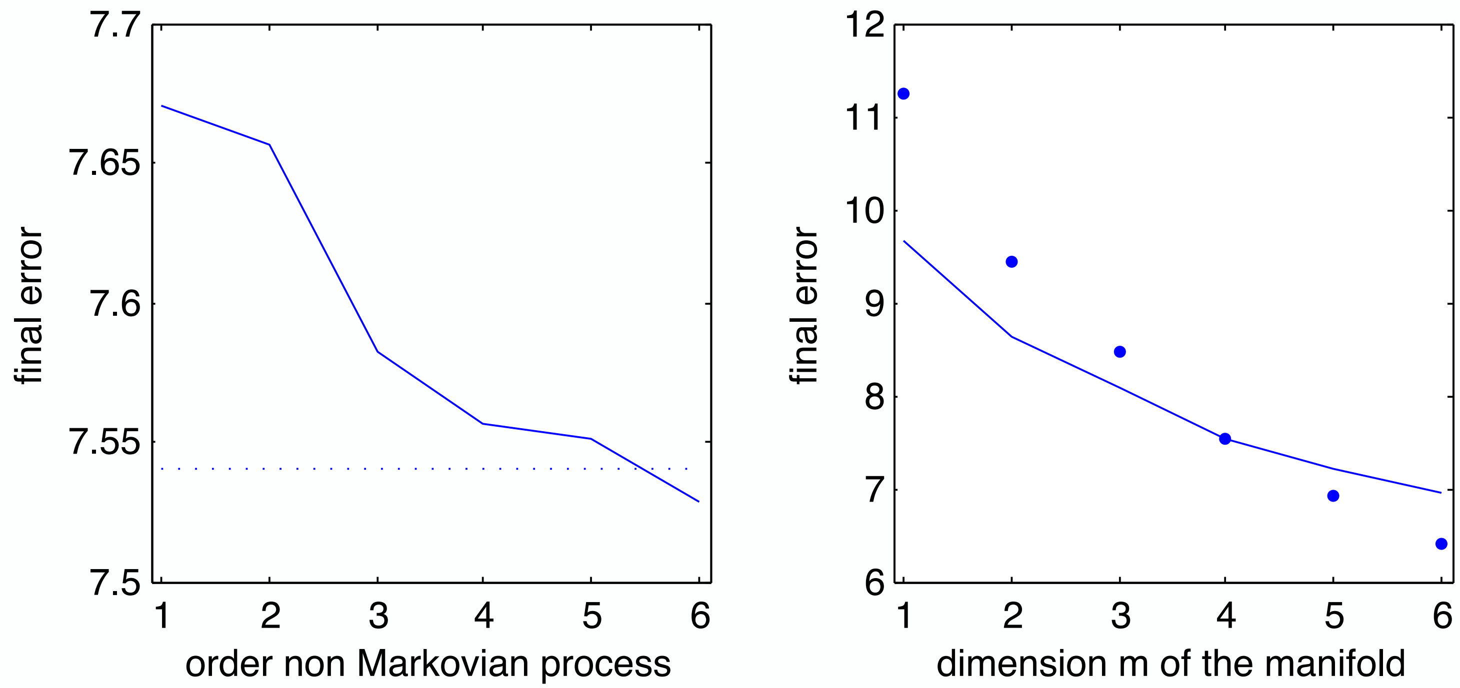
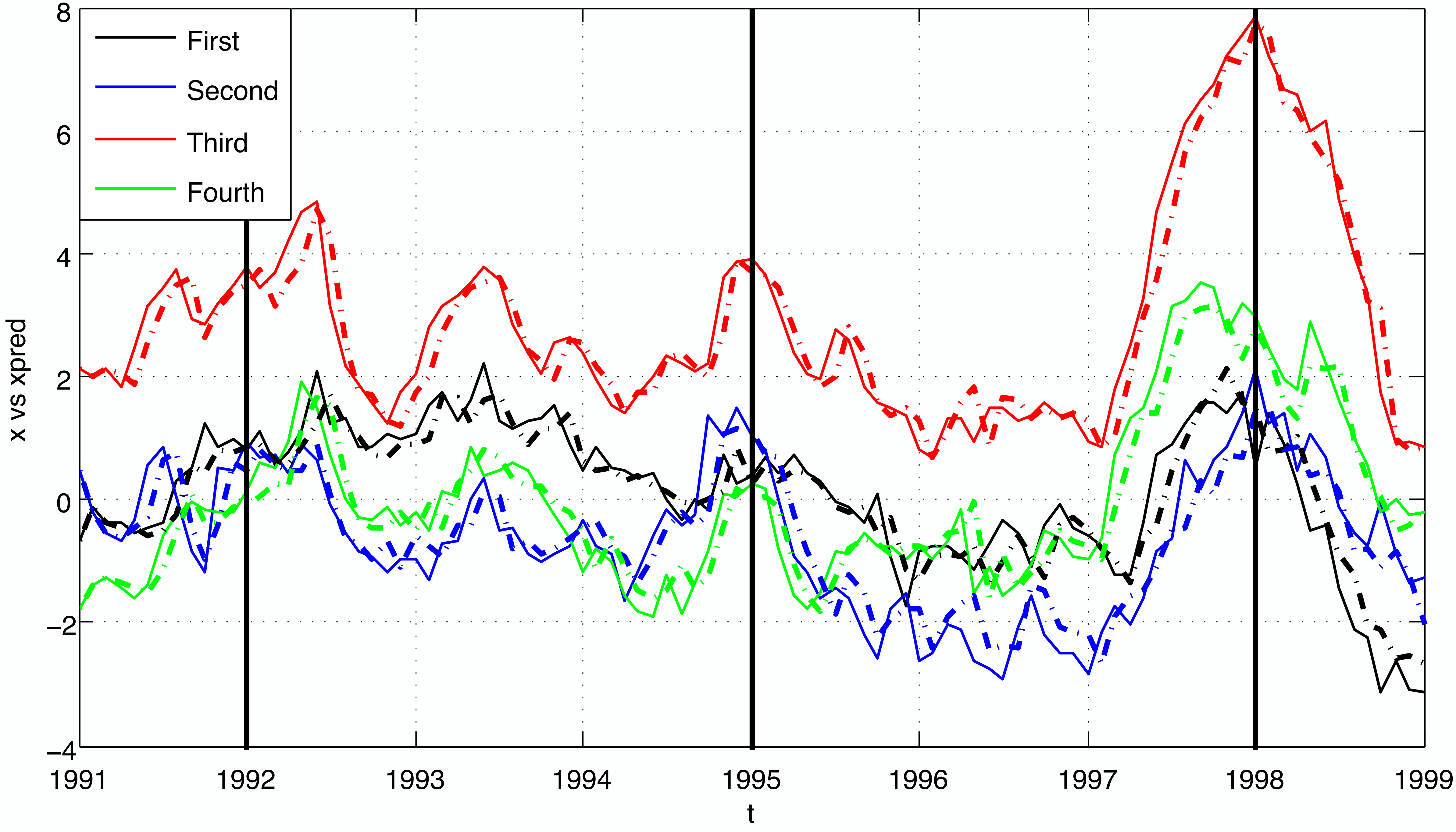
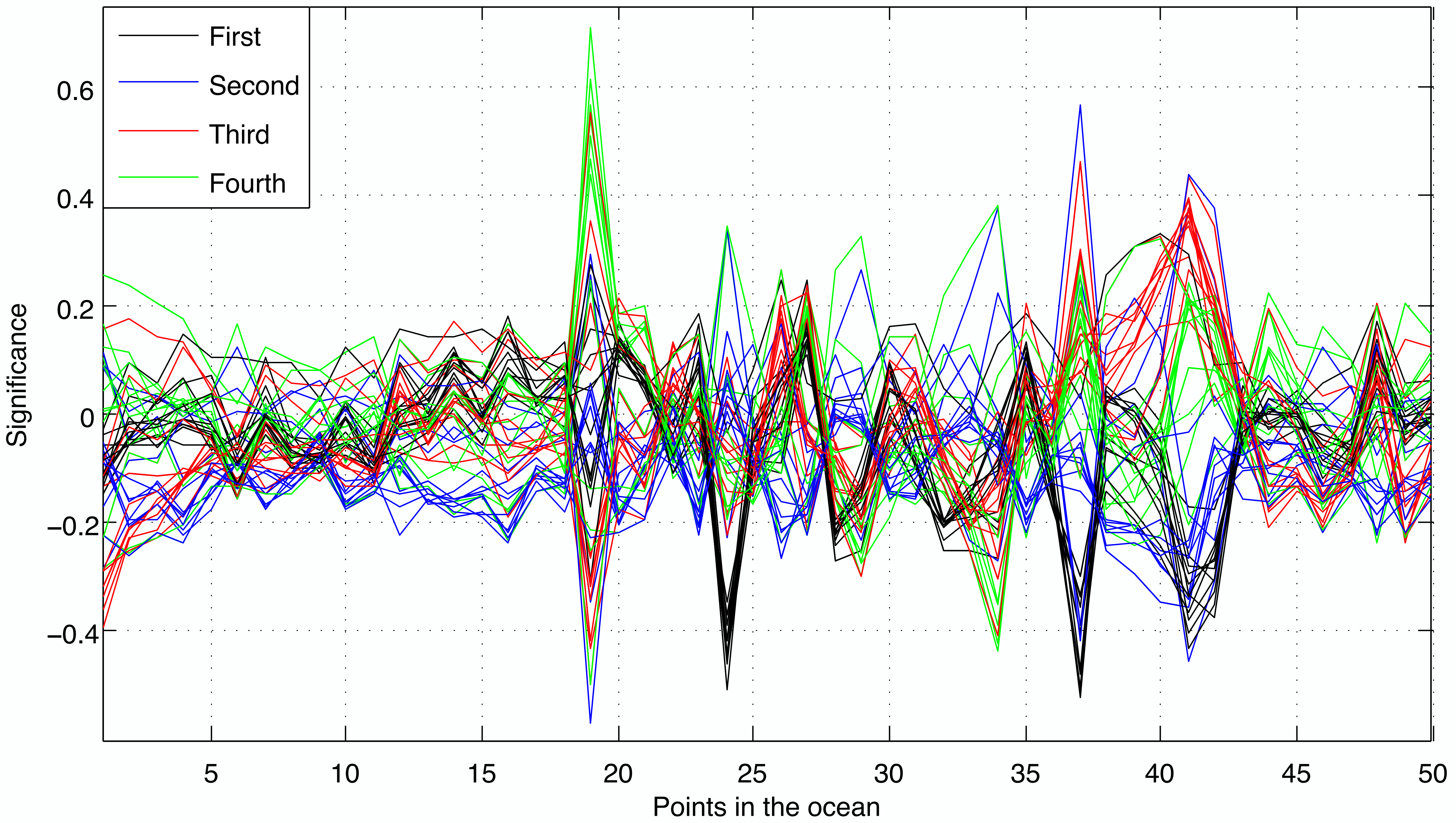


Therefore, we pick $r = 3$ and $m = 4$.

REAL AND PREDICTED DYNAMICAL COMPONENTS



POINTS OF SIGNIFICANCE: 19, 24, 37, 41



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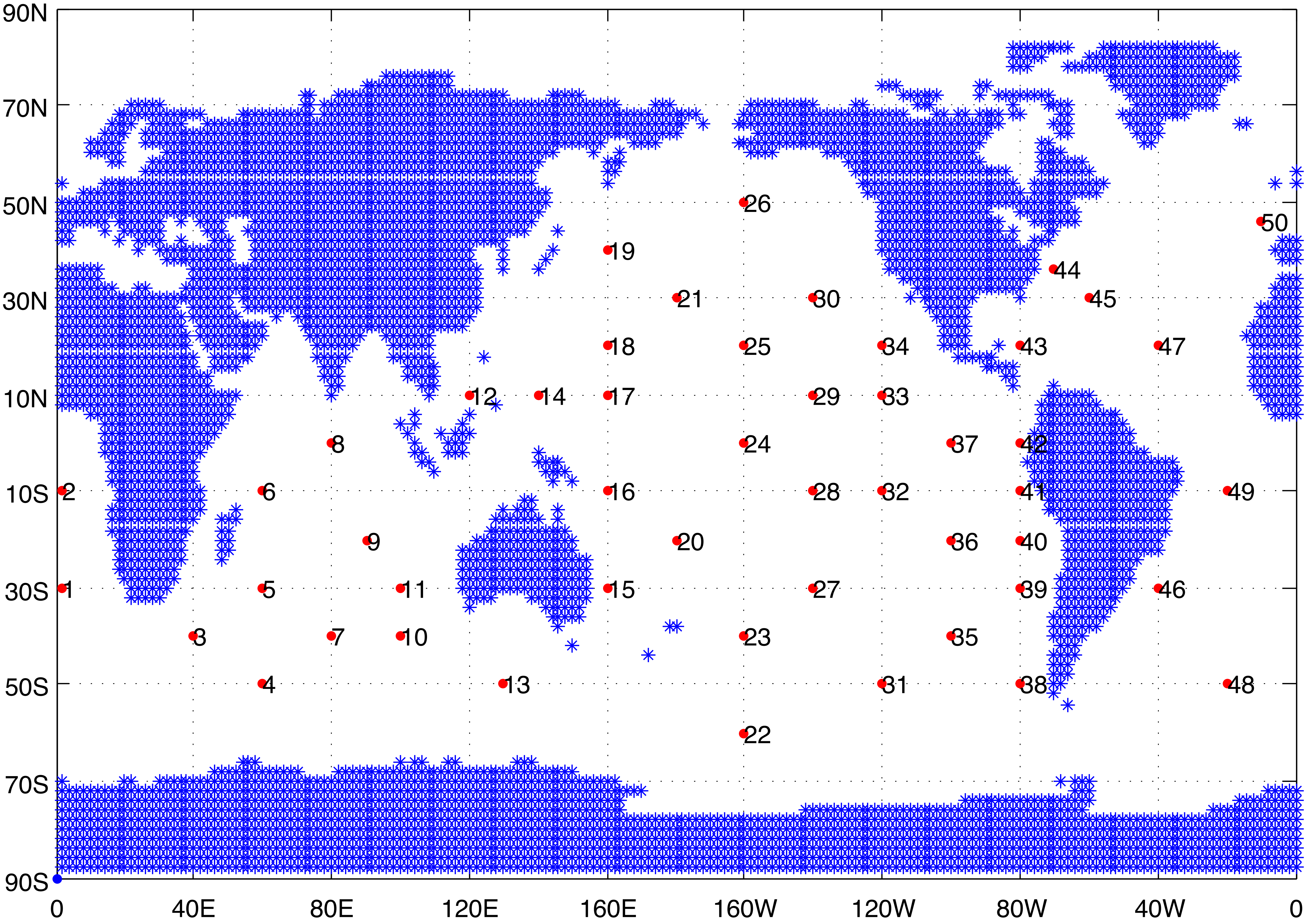

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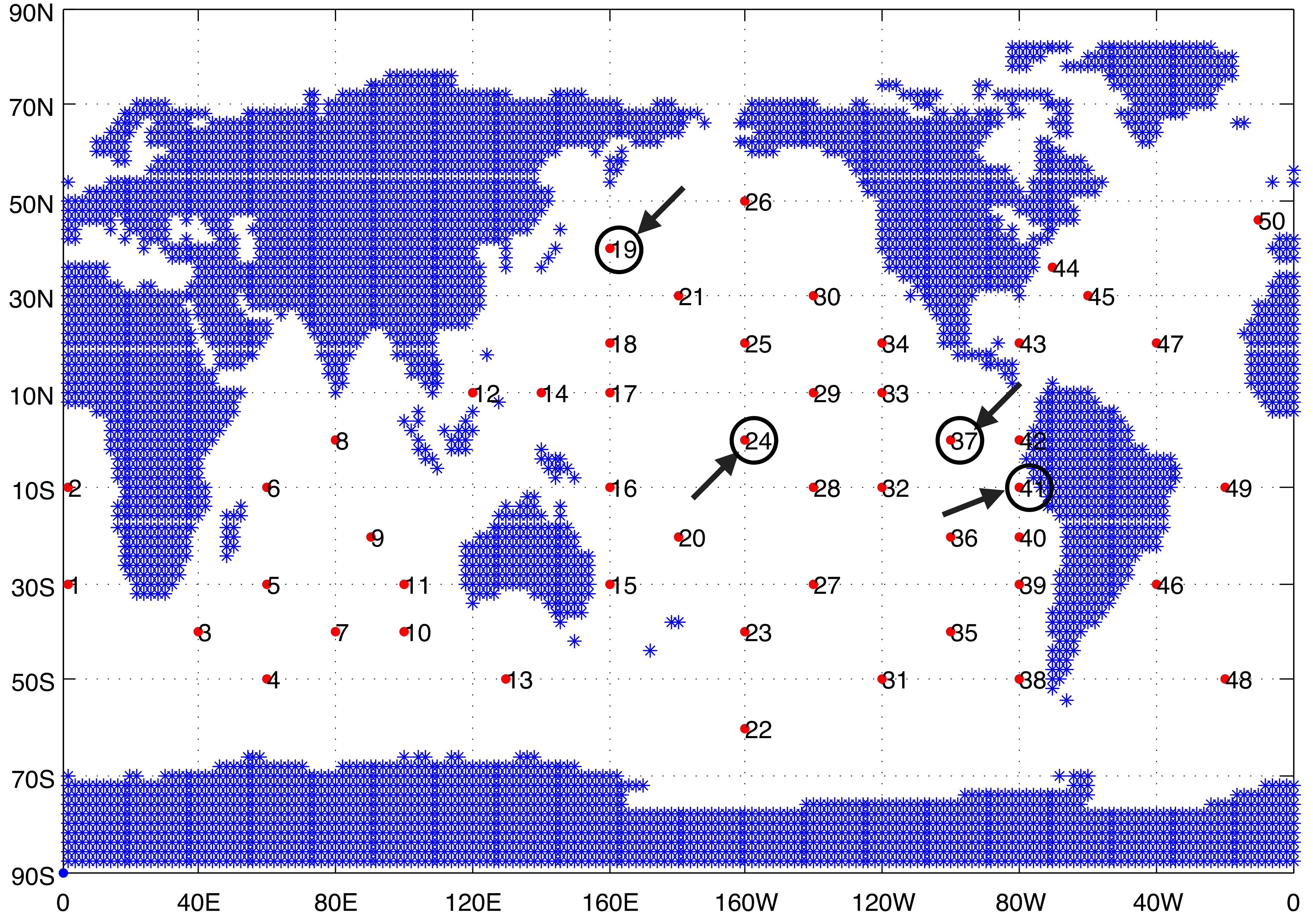
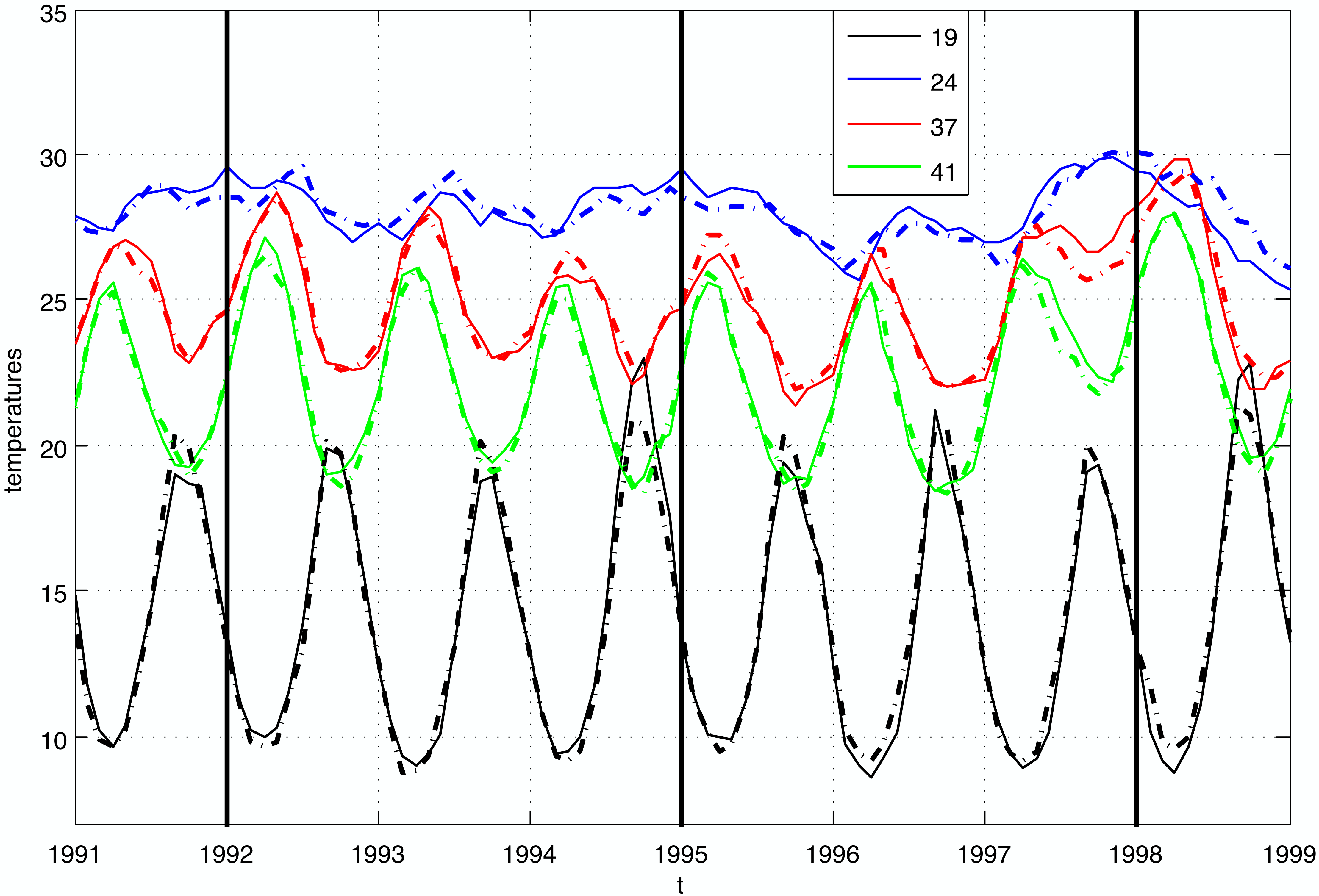
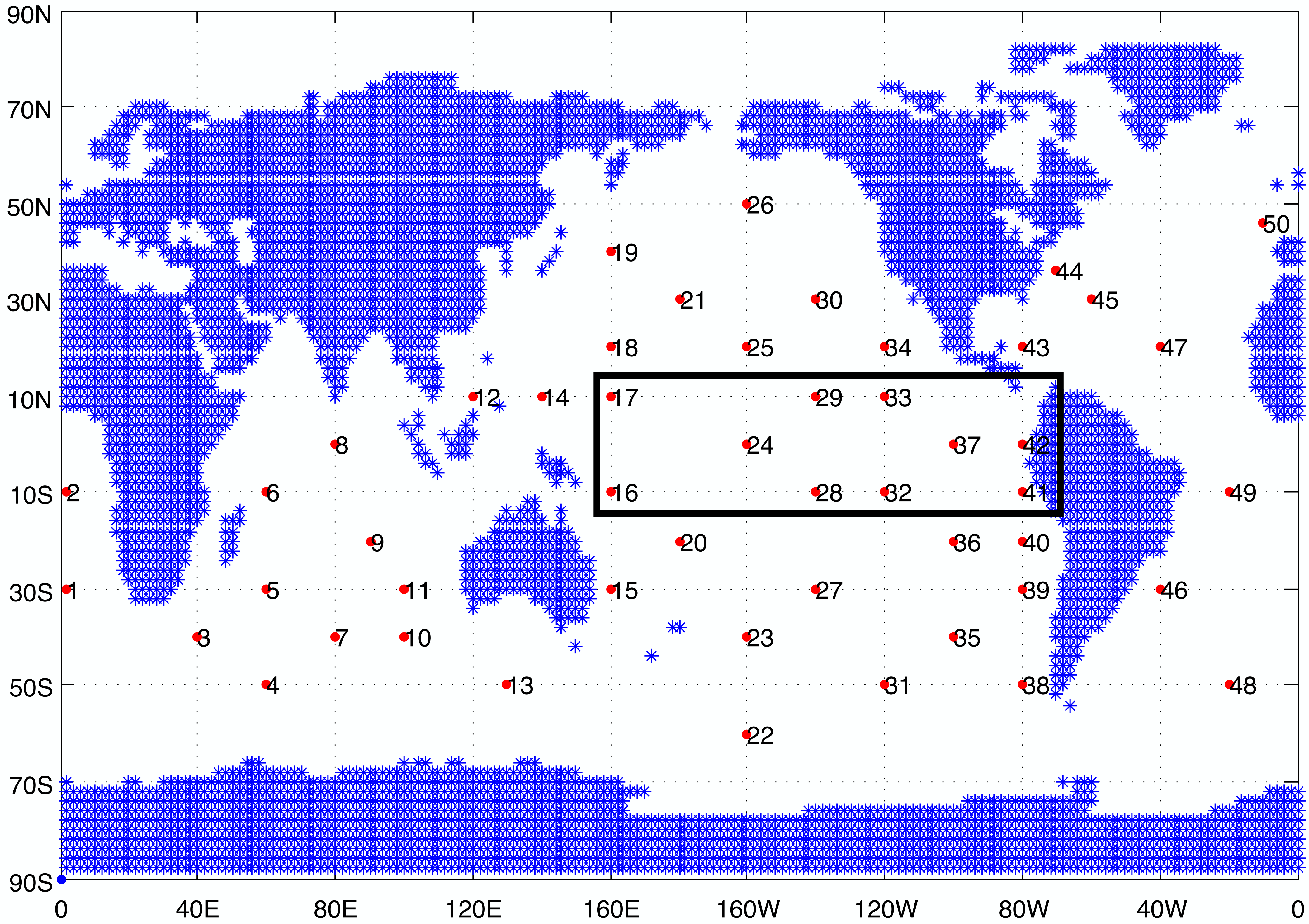


OBSERVED AND PREDICTED TEMPERATURES

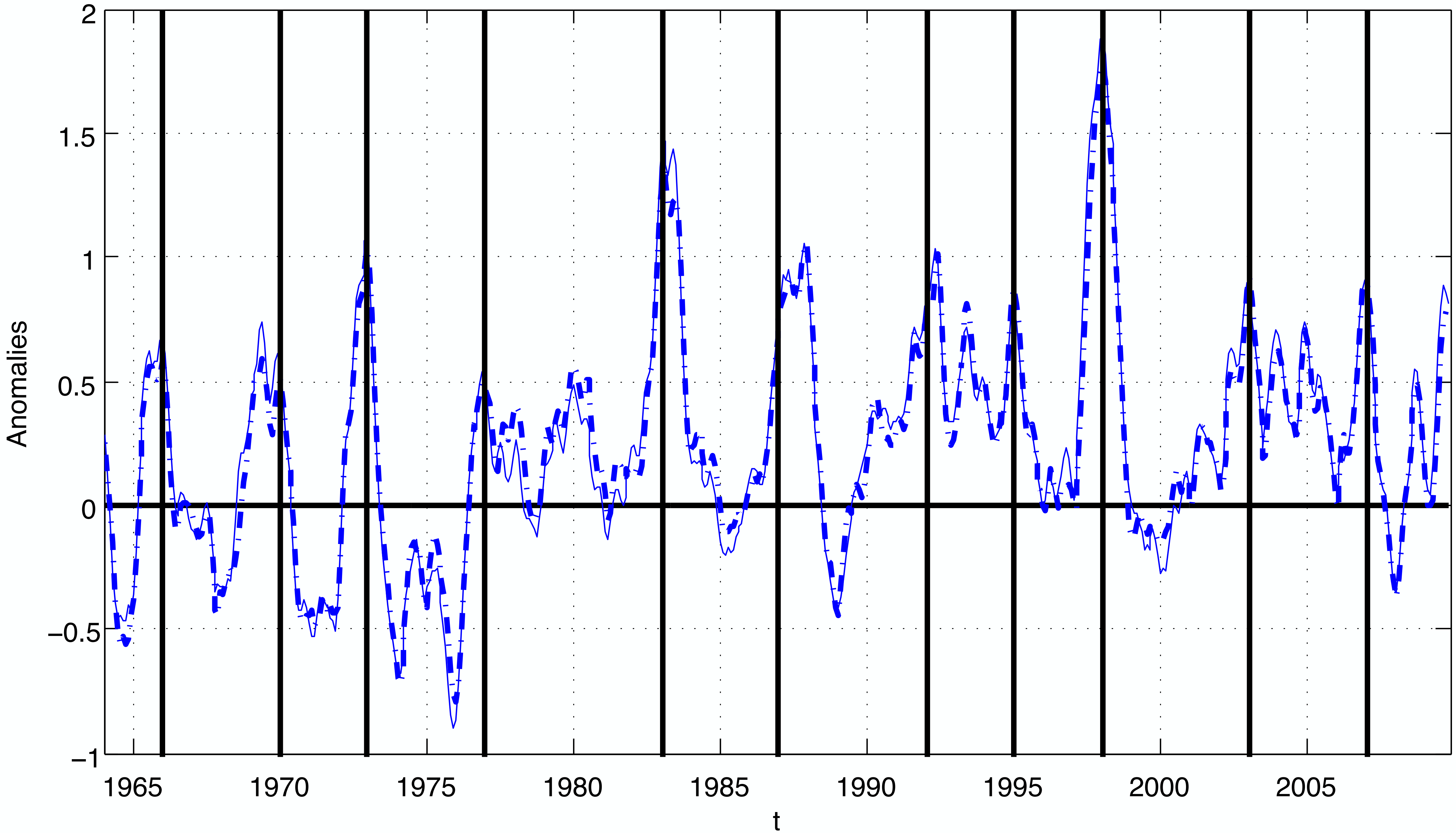


ANOMALIES

We consider three-month mean SST anomaly in the following El Niño region:



ANOMALIES



2
1.5
1
0.5
0
−0.5
−1
Anomalies
1965
1970
1975
1980
1985
1990
1995
2000
2005
t

CONCLUSIONS

- This new methodology allows a dimensional reduction of time series seeking a low-dimensional manifold x and a dynamical model $x_{j+1} = D(x_j, x_{j-1}, \ldots, t)$ that minimize the predictive uncertainty of the series. We have tested on synthetic data and with a real application on sea-surface temperature over the ocean.

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- An interesting question is future prediction. For the case of sea-surface temperatures, after 3 months the prediction is not good. This happens because there are many variables inside that may modify significantly the model. Nevertheless, the prediction could work for other models where there is not so much volatility in the data.

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- M. D. de la Iglesia and E. G. Tabak, *Principal dynamical components*, Comm. Pure Appl. Math. **66** (2013), no. 1, 48–82


THANK YOU