Atelier "Analyse des données"

Lecture 2:
Singular Spectrum Analysis (SSA) and the SSA-MTM Toolkit

Michael Ghil
CERES-ERTI, etc.

Based on joint work with many students, post-docs, and colleagues over the years; please see http://www.environnement.ens.fr/ and http://www.atmos.ucla.edu/tcd/ for further details.

Advanced Spectral Methods, Nonlinear Dynamics, and the Nile River

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Motivation

1. Climatic time series have typically broad peaks on top of a continuous, "warm-colored" background ➔ ***Method***

2. Connections to nonlinear dynamics ➔ ***Theory***

3. Need for stringent statistical significance tests ➔ ***Toolkit***

4. Applications to analysis and prediction ➔ ***Examples***

Joint work with: M. R. Allen, M. D. Dettinger, K. Ide, N. Jiang, C. L. Keppene, D. Kondrashov, M. Kimoto, M. E. Mann, J. D. Neelin, M. C. Penland, G. Plaut, A. W. Robertson, A. Saunders, D. Sornette, S. Speich, C. M. Strong, C. Taricco, Y.-d. Tian, Y. S. Unal, R. Vautard, & P. Yiou (on 3 continents).

http://www.atmos.ucla.edu/tcd

Motivation & Outline

1. Data sets in the geosciences are often short and contain errors: this is both an obstacle and an incentive.

2. Phenomena in the geosciences often have both regular (“cycles”) and irregular (“noise”) aspects.

3. Different spatial and temporal scales:
   one person’s noise is another person’s signal.

4. Need both deterministic and stochastic modeling.

5. Regularities include (quasi-)periodicity ➔ spectral analysis via “classical” methods (see SSA-MTM Toolkit).

6. Irregularities include scaling and (multi-)fractality ➔ “spectral analysis” via Hurst exponents, dimensions, etc. (see Multi-Trend Analysis, MTA)

7. Does some combination of the two, + deterministic and stochastic modeling, provide a pathway to prediction?

For details and publications, please visit these two Web sites:

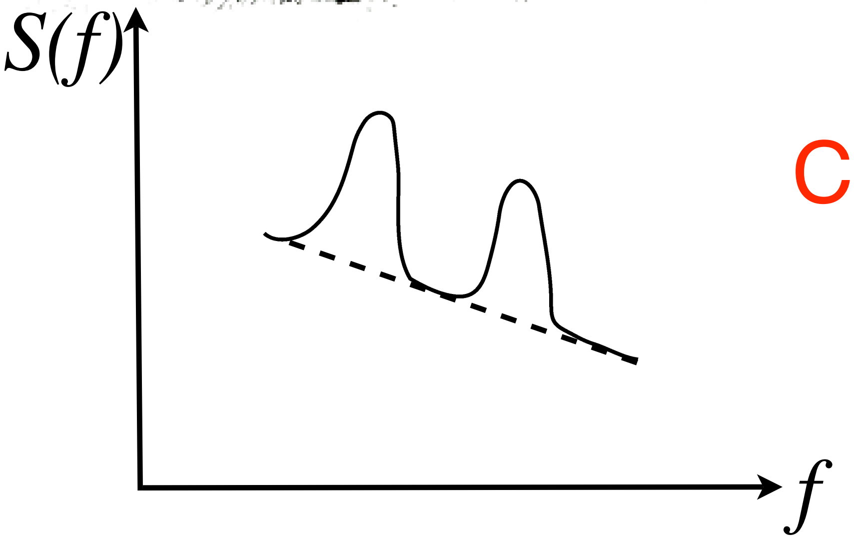
TCD http://www.atmos.ucla.edu/tcd/ ➔ key person – Dmitri Kondrashov!

E2-C2 http://www.ipsl.jussieu.fr/~ypsce/py_E2C2.html

Outline

- Time series analysis
  - The “smooth” and “rough” part of a time series
  - Oscillations and nonlinear dynamics
- Singular spectral analysis (SSA)
  - Principal components in time and space
  - The SSA-MTM Toolkit
- The Nile River floods
  - Longest climate-related, instrumental time series
  - Gap filling in time series
  - NAO and SOI impacts on the Nile River
- Concluding remarks
  - Cautionary remarks (“garde-fous”)
  - References

Spectral Density (Math)/Power Spectrum (Science & Engng.)



Continuous background

+ peaks

- **Wiener-Khinchin (Bochner) Theorem** **Blackman-Tukey Method**

$$R(s) = \lim_{L \to \infty} \frac{1}{2L} \int_{-L}^{L} x(t)x(t+s)dt$$

$$S(f) = \frac{1}{2\pi} \int_{-\infty}^{\infty} R(s)e^{-ifs}ds \equiv \hat{R}(s)$$

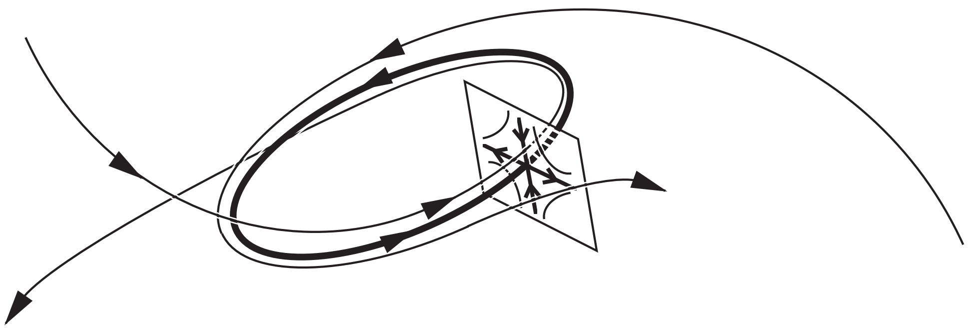
i.e., the **lag-autocorrelation function** & the **spectral density**

are **Fourier transforms** of each other.

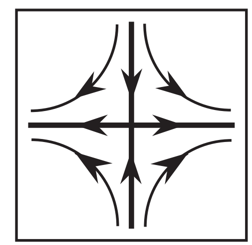
Power Law for Spectrum (cont'd)

- Hypothesis: "***Poles***" correspond to the least unstable periodic orbits

"***unstable limit cycles***"



"***Poincaré section***"



- Major clue to the physics

  that underlies the dynamics

- N.B. Limit cycle not necessarily elliptic, i.e. not

$$(x, y) = (a_f sin(ft), b_f cos(ft))$$

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Spectral density: deterministic signal

- Let f be a 1-D signal, with possibly complex values, such that $f \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$. We define the autocorrelation of the signal by:

$$R_f(\tau) := \int_{\mathbb{R}} f(x)\overline{f(x-\tau)}\mathrm{d}x, \quad \text{for } \tau \in \mathbb{R}. \tag{1}$$

- The power spectral density (PSD) of this signal is given by the positive real function:

$$S_f(\xi) = |\hat{f}(\xi)|^2,$$

where $\hat{f}(\xi)$ represents the Fourier transform of f in ξ. The PSD is often called simply the *spectrum* of the signal. Typically it measures the amount of energy per unit of time (i.e. the power) contained in the signal as a function of the frequency ξ.

- If we introduce the notation $f^s(x) := \overline{f(-x)}$ then $R_f = f * f^s$.
- **Exercise:** Show that the PSD and the autocorrelation are Fourier transforms of each other, up to a multiplicative constant.

Spectral density: random signal

- Let $f(\omega, \cdot)$ be a stationary process, for $\omega \in \Omega$ a probability space. We define the autocorrelation of the signal by:

$$R_f(\tau) := \mathbb{E}(f(\omega, t)f(\omega, t+\tau)), \tag{2}$$

  where the expectation is taken over all the realizations ω. Note that $R_f(\tau)$ is well-defined even if f is not in $L^p(\mathbb{R})$ for any p.
- We assume that $R_f(\cdot)$ is integrable, and that the random process f is ergodic. Under these conditions

$$R_f(\tau) = \lim_{T\to\infty} \frac{1}{T} \int_{-T/2}^{T/2} f(t)f(t+\tau)\mathrm{d}t$$

- We define the truncated Fourier transform, $F_T(\xi) := \int_{-T/2}^{T/2} f(t)e^{-2i\pi\xi t}\mathrm{d}t$, and the truncated power spectral density, $\frac{1}{T}|F_T(\xi)|^2$.
- **Theorem (Wiener-Khinchin):** For all ξ, $\lim_{T\to\infty} \mathbb{E}(\frac{1}{T}|F_T(\xi)|^2)$ exists and is given by

$$\int_{-\infty}^{\infty} R_f(\tau)e^{-2i\pi\xi t}\mathrm{d}\tau; \text{ this limit defines the PSD in this context.}$$

Empirical orthogonal functions of a scalar field (I)

The Karhunen-Loève expansion (I)

- Let $Y(t,x)$ be a random scalar field (we omit the dependence on ω), for $x \in D$ a **spatial domain**. We seek the Karhunen-Loève expansion (or EOF expansion) of Y, namely:

$$Y(t,x) := \sum_k Z_k(t)\varphi_k(x), \tag{3}$$

where $\int_D \varphi_i(x)\varphi_j(x) = \delta_{ij}\lambda_i$, and λ_i is the corresponding eigenvalue.
- The random functions $\{Z_i(t)\}$ are said to be statistically orthogonal if $\mathbb{E}(Z_i(t)Z_j(t)) = \delta_{ij}\lambda_i$; they are found by projecting each realization onto the EOFs: $Z_k(t) := \int_D Y(t,x)\varphi_k(x)\mathrm{d}x$.
- The eigenfunctions are the solutions of the Fredholm integral equation

$$\int_D R(x,y)\varphi_k(y)\mathrm{d}y = \lambda_k\varphi_k(x),$$

where $R(x,y)$ is the autocorrelation of the process $Y(t,x)$.
- It can be shown that there is a countably infinite number of such eigenfunctions and

$$R(x,y) = \sum_k \lambda_k\varphi_k(x)\varphi_k(y).$$

Empirical orthogonal functions of a scalar field (II)

The Karhunen-Loève expansion (II)

- It can be shown that the truncated decomposition $Y_K(t,x) := \sum_{k=1}^{k=K} Z_k(t)\varphi_k(x)$ minimizes the mean integrated squared error:

$$\mathbb{E}\left\{ \int_D [Y(t,x) - Y_K(t,x)]^2 dx \right\} := \sum_{k=K+1}^{\infty} \lambda_k .$$

- The spectral decomposition is optimal in the sense that this error is a minimum compared to K terms of any orthogonal systems (Cohen and Jones, 1969).
- **The discrete analogue:** Given observations of the random field Y for a given time at M locations, we have to estimate $R(x,y)$ and then solve the Fredholm eq. The numerical approximation to this equation is:

$$\sum_{j=1}^{M} R(x_i,x_j)\varphi_k(x_j)\Delta_j = \lambda_k \varphi_k(x_i), \; i = 1, \cdots, M,$$

where Δ_j is the element of area associated with the observation at x_j.

Empirical orthogonal functions of a scalar field (III)

The Karhunen-Loève expansion (III)

- If we let

$$\Gamma_{ij} = R(x_i, x_j)\sqrt{\Delta_i \Delta_j},$$
$$\nu_j^k = \varphi_k(x_i)\sqrt{\Delta_i},$$

then it can be shown that

$$\sum_{j=1}^{p} \Gamma_{ij}\nu_j^k = \lambda_k \nu_i^k;$$

this represents the eigendecomposition of the covariance matrix Γ with eigenvalues $\{\lambda_k\}$. The eigenvectors ν_i^k estimate the eigenfunctions $\varphi_k(x_i)$ at the observation points, multiplied by $\sqrt{\Delta_i}$.

- Singular spectrum analysis of time series extends these ideas from random fields to time series.

Continuous formulation (I)

- We consider here a zero-mean, continuous, infinite and ergodic time series $X(t)$. We introduce the integral operator A, acting on functions $f(t)$ belonging to $H := L^2(-T, T)$ according to:

$$Af(t) := \frac{1}{2T}\int_{-T}^{T} R_X(t-s)f(s)ds,$$

  where $R_X(\tau)$ is the autocorrelation of X at lag τ.
- Since $R_X(\tau)$ is symmetric w.r.t. the origin $\tau = 0$, A is a symmetric non-negative operator. Hilbert-Schmidt theory ensures the existence of a countable set of nonnegative eigenvalues and corresponding eigenfunctions (still called EOFs) of

$$A\varphi = \lambda\varphi.$$

- Each segment of X — having length $2T$ and centered at t — is a function in H that may be expanded w.r.t. the EOF basis. For each t and s, such that $|s| \leq \tau$, provided $\lambda_k > 0$, for all k,

$$X(t+s) = \sum_{k=1}^{\infty} X_k(t)\varphi_k(s).$$

Singular spectrum analysis

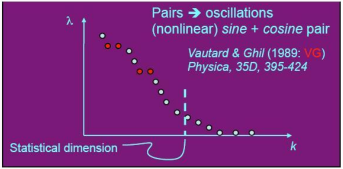
Continuous formulation (II)

- The projection $X_k(t) := \frac{1}{2T}\int_{-T}^{T} X(t+s)\varphi_k(s)ds$ onto the k-th EOF constitutes a zero-mean time series which is called the k-th PC. $X_k(t)$ has variance λ_k, and it represents a filtered version of X, the filter being the moving average weighted by φ_k.
- The PCs are uncorrelated with each other at zero lag, but their cross-covariances are not vanishing for lags $\neq 0$.
- From Mercer's theorem (Riesz & Nagy, 1955) applied to the Hilbert-Schmidt operator A, it follows that the autocorrelation can be expanded as

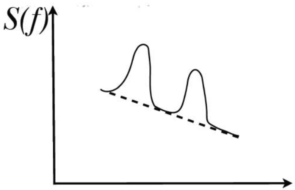
$$R_X(t-s) = \sum_{k=1}^{\infty} \lambda_k \varphi_k(t)\varphi_k(s),$$

  for a.e. t and s in $(-T, T)$. Taking $t = s$ and integrating from $-T$ to T, gives $\sum_{k=1}^{\infty} \lambda_k = R_X(0)$, where $\sigma_X^2 := R_X(0)$ is the total variance of X.

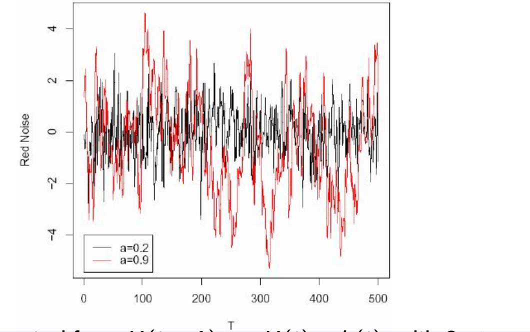
Comparison between the "scree diagram" and the power spectrum



- The equal-eigenvalue pairs correspond to the peaks in the power spectrum.



Red noise



- It is generated from $X(t+1) = aX(t) + b(t)$, with $0 \leq a < 1$ and b is i.i.d. with a Gaussian distribution $\mathcal{N}(0, \sigma)$.
- This process displays more power at low frequencies. Its correlation is $R_X(\tau) = \sigma^2 \frac{a^{|\tau|}}{1-a^2}$ and its power spectrum is:

$$S_X(\xi) = R_X(0) \cdot \frac{1-a^2}{1-2a\cos(2\pi\xi)+a^2} \sim \frac{1}{b^2+c^2\xi^2}$$

Power Spectra & Reconstruction

- **A. Transform pair**:

$$X(t+s) = \sum_{k=1}^{M} a_k(t) e_k(s), e_k(s) - EOF$$

The e_k's are **adaptive filters**,

$$a_k(t) = \sum_{s=1}^{M} X(t+s) e_k(s), a_k(t) - PC$$

the a_k's are **filtered time series**.

B. Power spectra

$$S_X(f) = \sum_{k=1}^{M} S_k(f); \quad S_k(f) = R_k(s); \quad R_k(s) \approx \frac{1}{T} \int_0^T a_k(t) a_k(t+s) dt$$

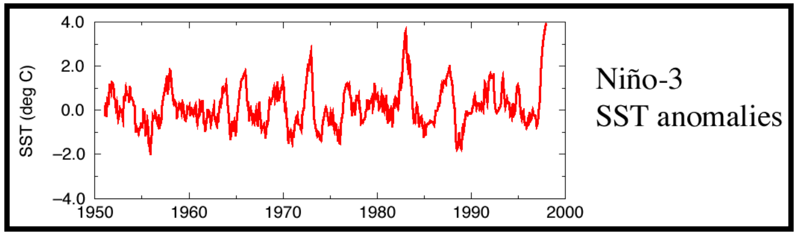
C. Partial reconstruction

$$X^K(t) = \frac{1}{M} \sum_{k \in K} \sum_{s=1}^{M} a_k(t-s) e_k(s);$$

in particular: $K = \{1, 2, ..., S\}$ or $K = \{k\}$ or $K = \{l, l+1; \lambda_l \approx \lambda_{l+1}\}$

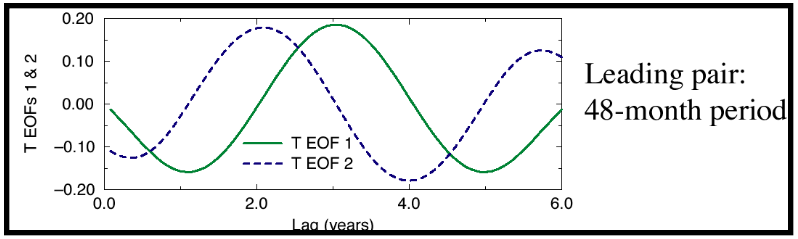
Singular Spectrum Analysis (SSA)

Time series

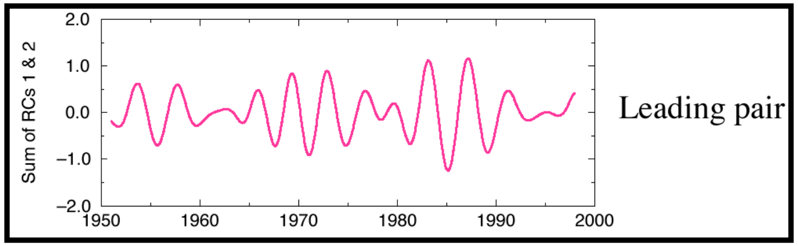


SSA decomposes (geophysical & other) time series into ***Temporal EOFs*** (T-EOFs) and ***Temporal Principal Components*** (T-PCs), based on the series' lag-covariance matrix

T-EOFs



RCs



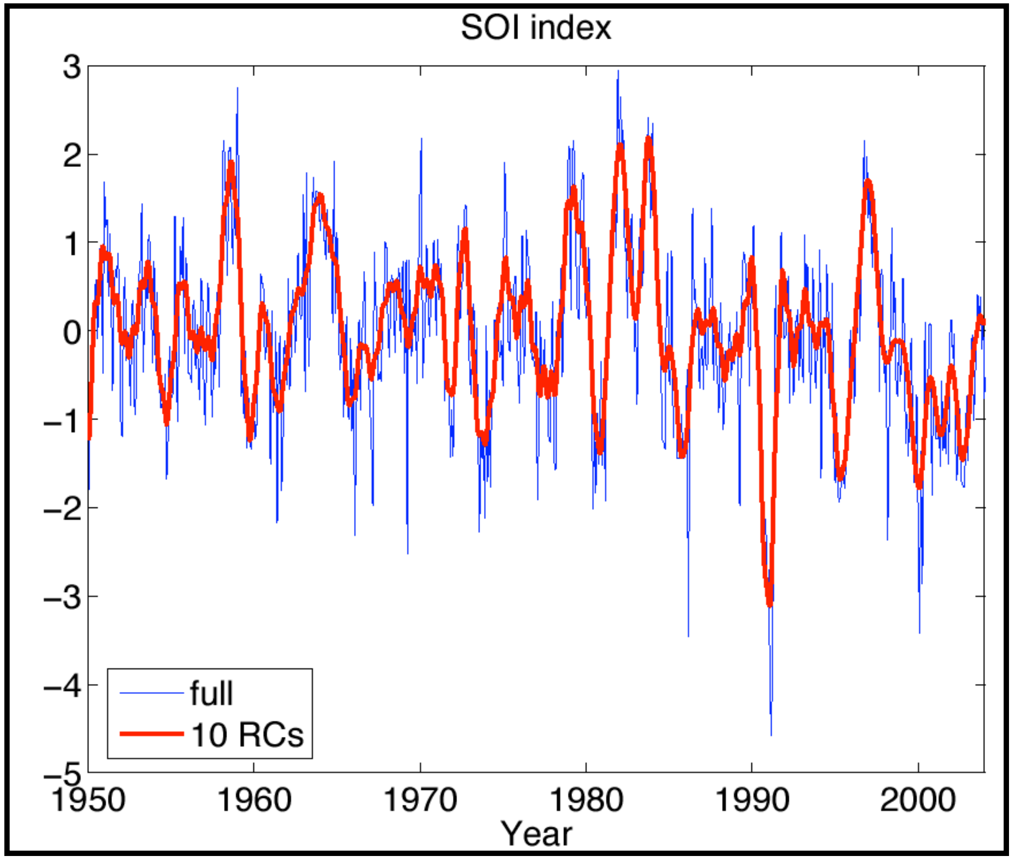
Selected parts of the series can be reconstructed, via ***Reconstructed Components*** (RCs)

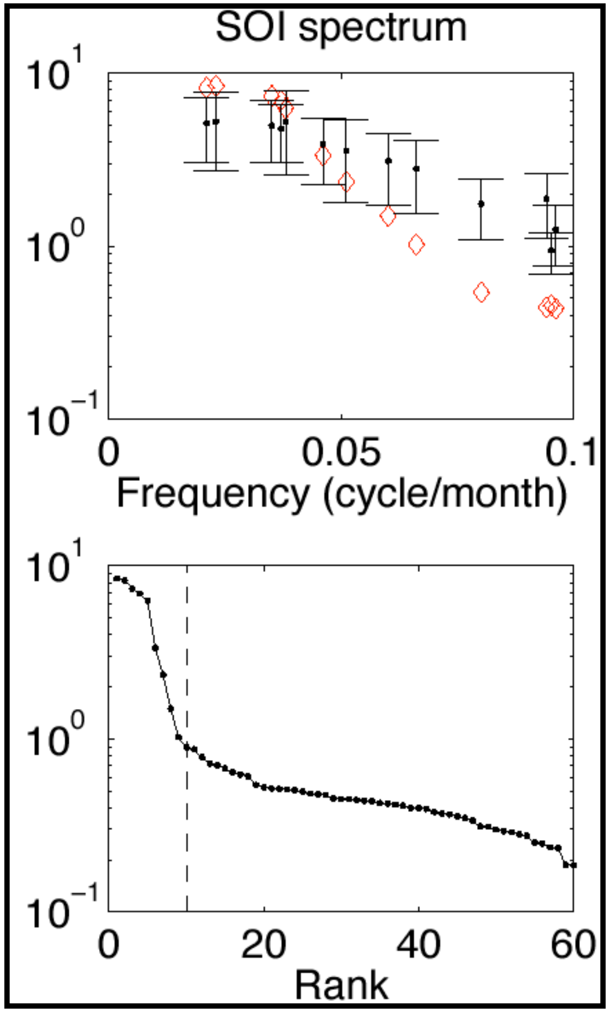
- SSA is good at isolating oscillatory behavior via paired eigenelements.
- SSA tends to lump signals that are longer-term than the window into
  - one or two trend components.

Selected References:

Vautard & Ghil (1989, *Physica* D);
Ghil *et al*. (2002, *Rev. Geophys.)*

Singular Spectrum Analysis (SSA) and M-SSA (cont'd)

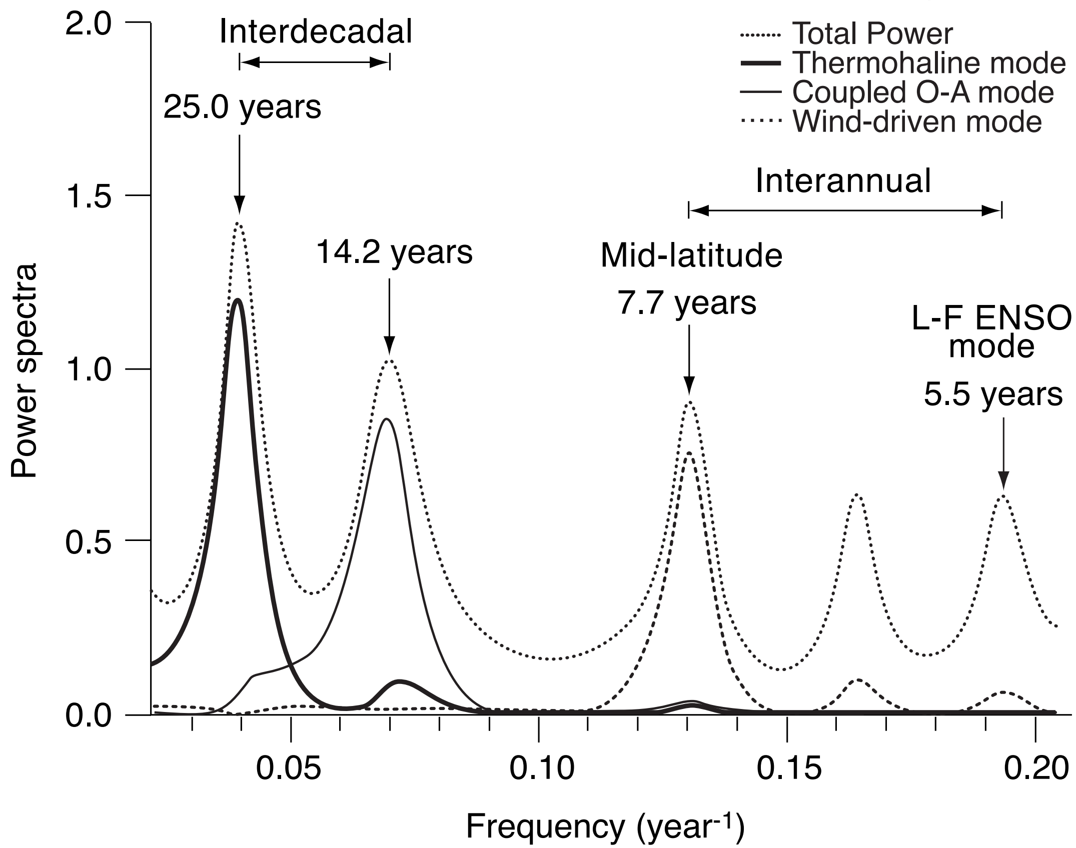




- Break in slope of SSA spectrum distinguishes "***significant***" from "***noise***" EOFs
- Formal Monte-Carlo test (Allen and Smith, 1994) identifies 4-yr and 2-yr ENSO oscillatory modes. A window size of M = 60 is enough to "resolve" these modes in a monthly SOI time series

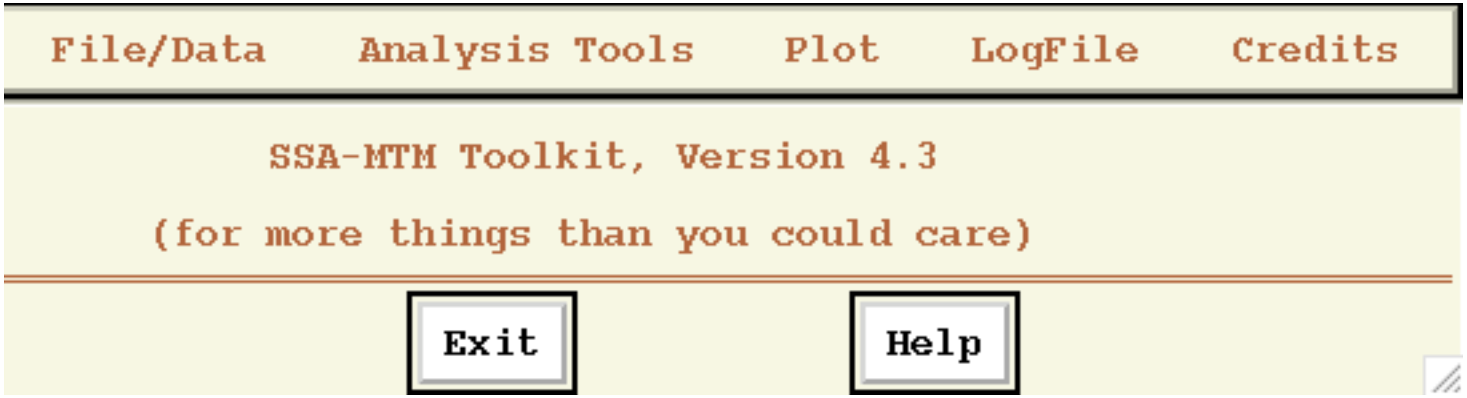
SSA (prefilter) + (low-order) MEM

- "Stack" spectrum

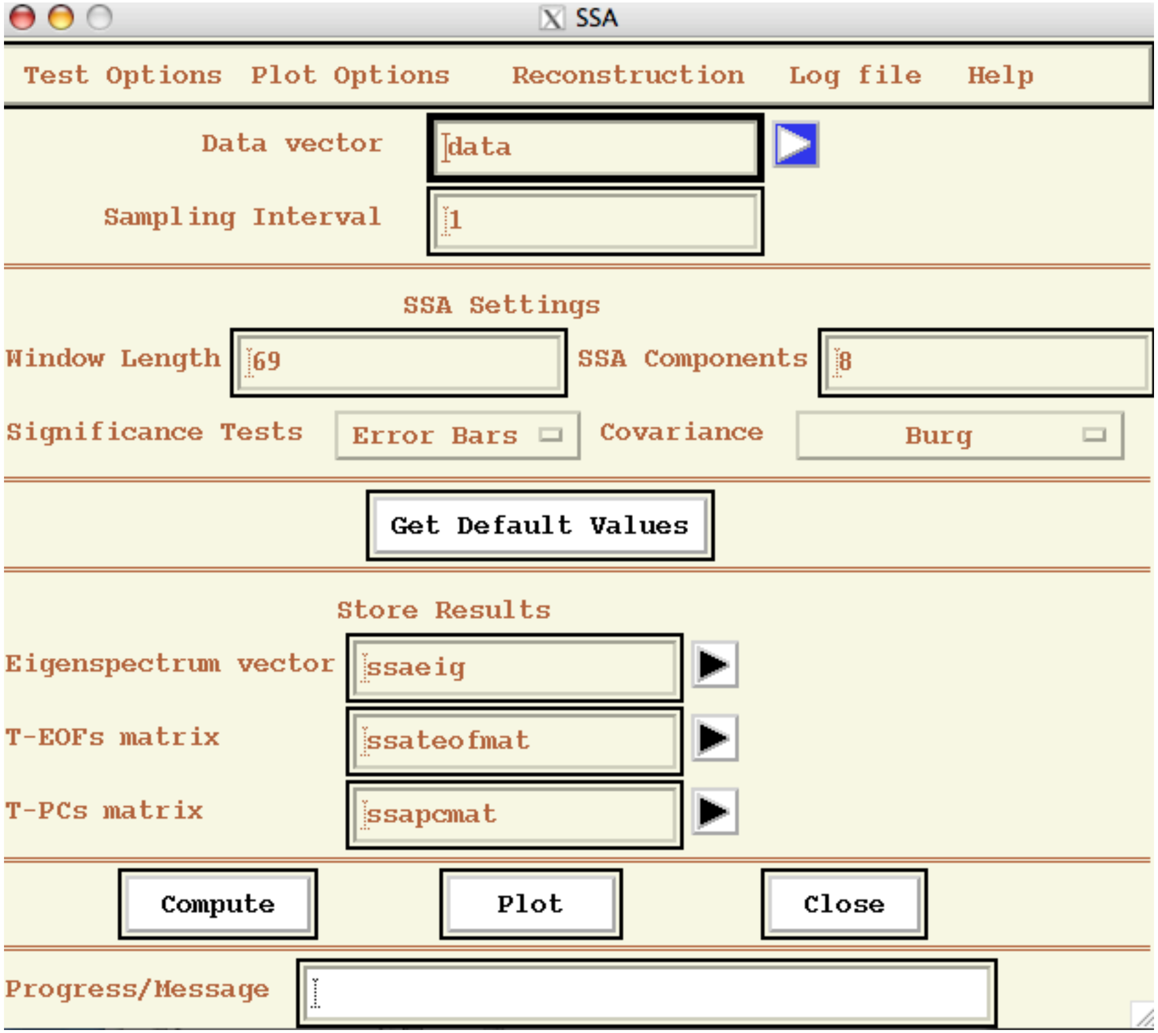


In good agreement with MTM peaks of **Ghil & Vautard (1991, *Nature*)** for the Jones *et al.* (1986) temperatures & stack spectra of Vautard *et al.* (1992, *Physica D*) for the IPCC "consensus" record (both global), to wit 26.3, 14.5, 9.6, 7.5 and 5.2 years.

Peaks at 27 & 14 years also in Koch sea-ice index off Iceland (Stocker & Mysak, 1992), etc.
Plaut, Ghil & Vautard (1995, *Science*)



- Ported to Sun, Dec, SGI, PC Linux, and Mac OS X
- Graphics support for IDL and Grace
- Precompiled binaries are available at www.atmos.ucla.edu/ tcd/ssa
- Includes ***Blackman-Tukey FFT***, ***Maximum Entropy Method***, ***Multi-Taper Method (MTM)***, ***SSA and M-SSA***.
- Spectral estimation, decomposition, reconstruction & prediction.
- Significance tests of "**oscillatory modes**" vs. "**noise.**"



- **Free!!!**
- Data management with ***named vectors & matrices.***
- ***Default values*** button.

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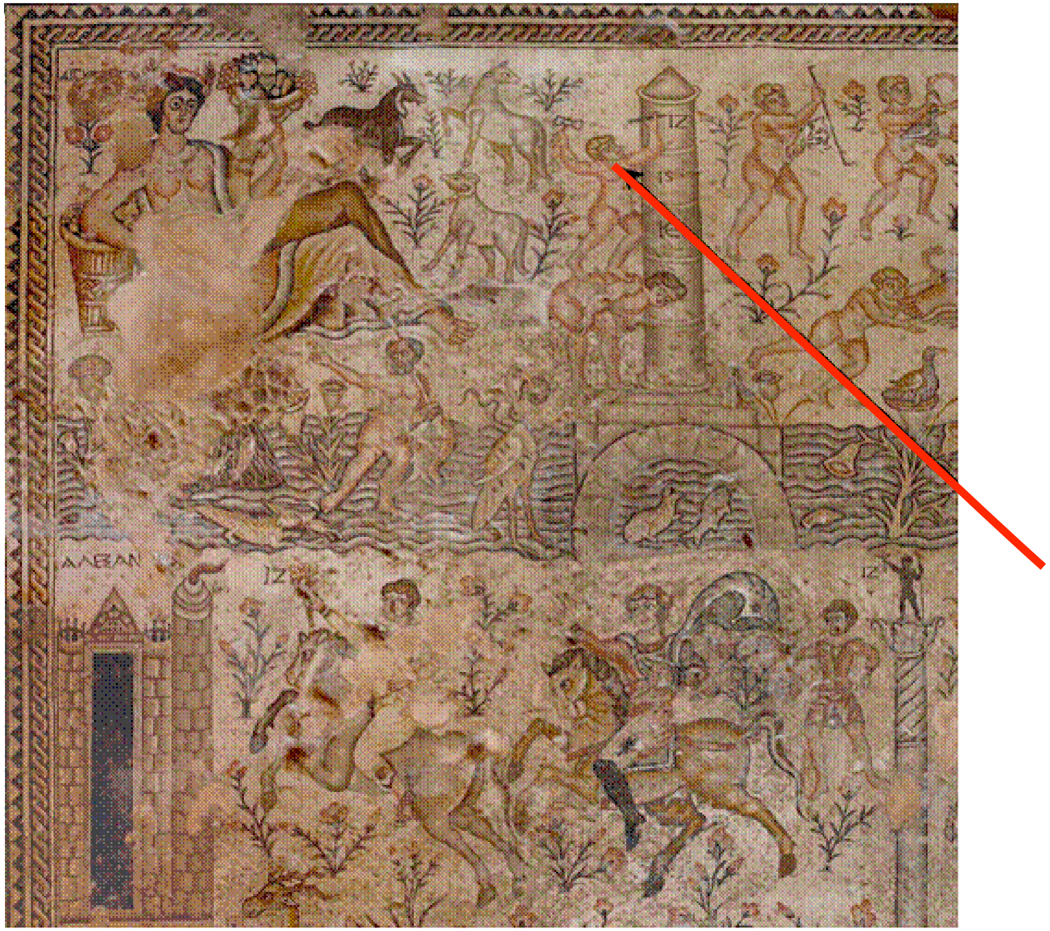
The Nile River Records Revisited:

How good were Joseph's predictions?

Michael Ghil, ENS & UCLA
Yizhak Feliks, IIBR & UCLA,
Dmitri Kondrashov, UCLA

Why are there data missing?



Hard Work

- Byzantine-period mosaic from Zippori, the capital of Galilee (1st century B.C. to 4th century A.D.); photo by Yigal Feliks, with permission from the Israel Nature and Parks Protection Authority)

What to do about gaps?

- Most of the advanced ***filling-in*** methods are different flavors of ***Optimal Interpolation*** (**OI**: Reynolds & Smith, 1994; Kaplan 1998).

Drawbacks: they either (i) require error statistics to be specified *a priori*; or (ii) derive it **only** from the interval of dense data coverage.

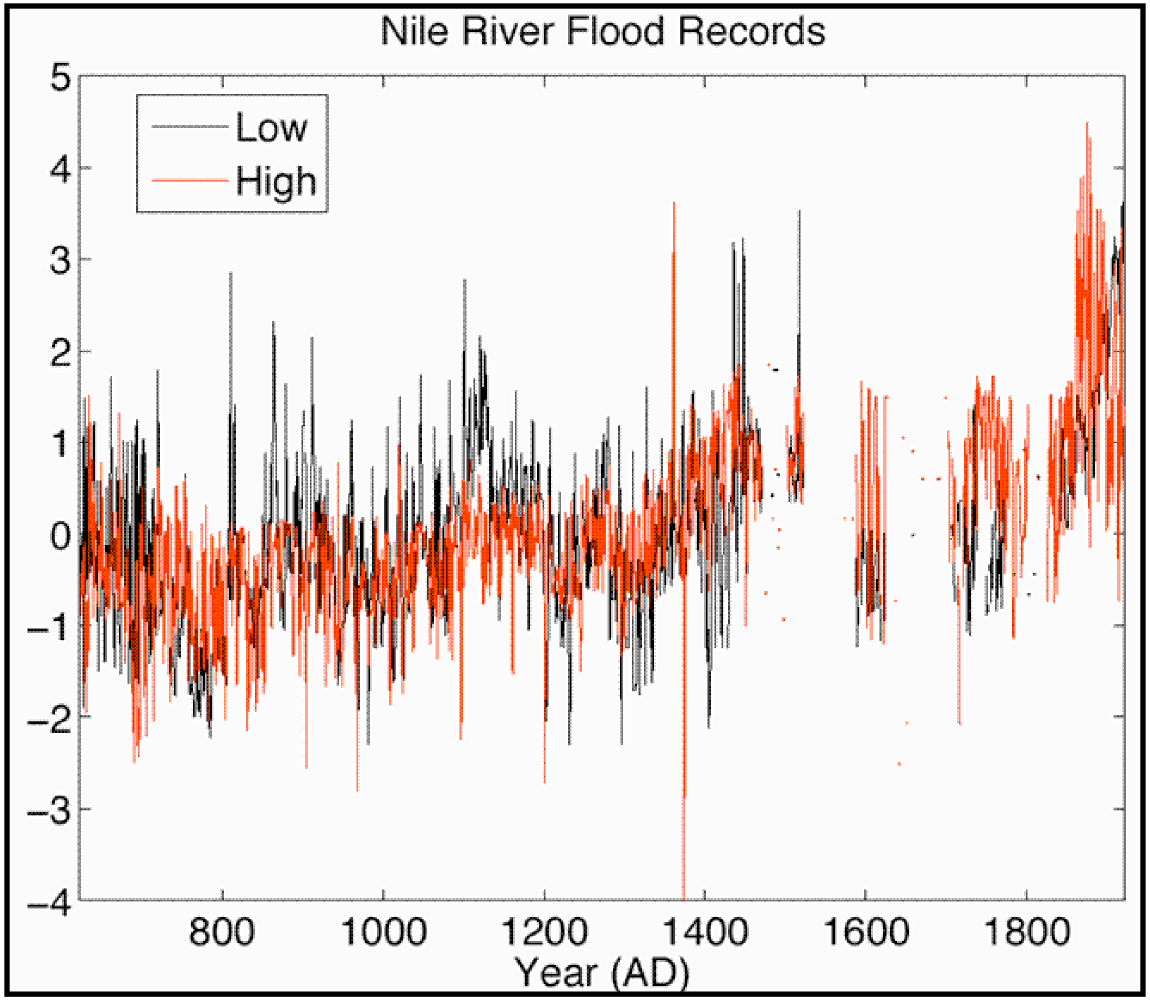
EOF Reconstruction (Beckers & Rixen, 2003): (i) iteratively compute **spatial-covariance** matrix using **all the data**; (ii) determine via cross-validation "**signal**" EOFs and use them to fill in the missing data; accuracy is similar to or better than **OI** (Alvera-Azcarate *et al*. 2004).

Drawbacks: uses **only** spatial correlations **=>** cannot be applied to very **gappy** data.

We propose ***filling in*** **gaps by applying iterative SSA (or M-SSA):**

Utilize both spatial and temporal correlations of data => can be used for highly **gappy** data sets; simple and easy to implement!

Historical records are full of “gaps”....



Annual maxima and minima of the water level at the nilometer on Rodah Island, Cairo.

SSA (M-SSA) Gap Filling

Main idea: utilize both spatial and temporal correlations to iteratively compute self-consistent lag-covariance matrix; M-SSA with $M = 1$ is the same as the EOF reconstruction method of Beckers & Rixen (2003)

Goal: keep "signal" and truncate "noise" — usually a few leading EOFs correspond to the dominant oscillatory modes, while the rest is noise.

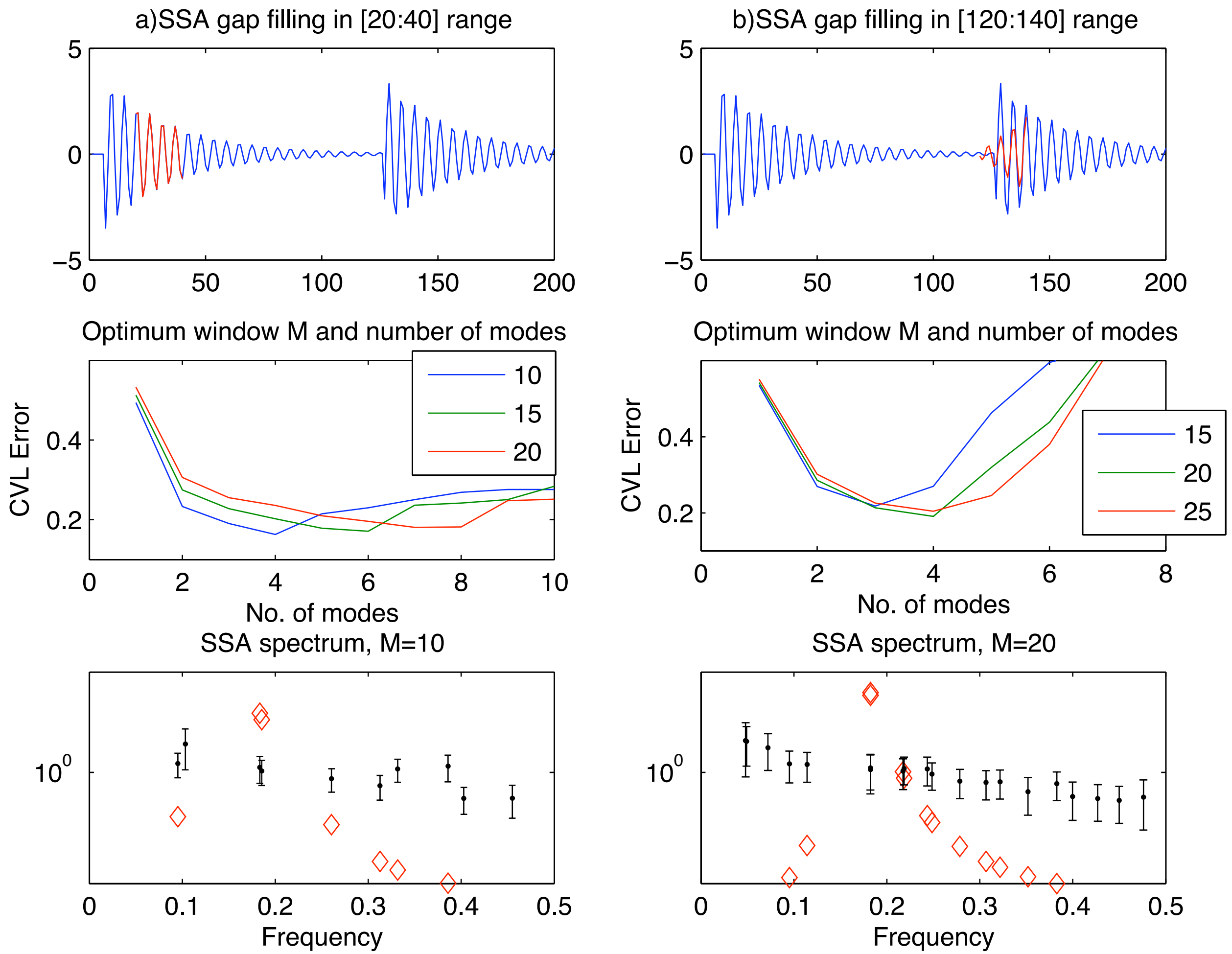
(1) for a given window width M: center the original data by computing the unbiased value of the mean and set the missing-data values to zero.

(2) start iteration with the first EOF, and replace the missing points with the reconstructed component (RC) of that EOF; repeat the SSA algorithm on the new time series, until convergence is achieved.

(3) repeat steps (1) and (2) with two leading EOFs, and so on.

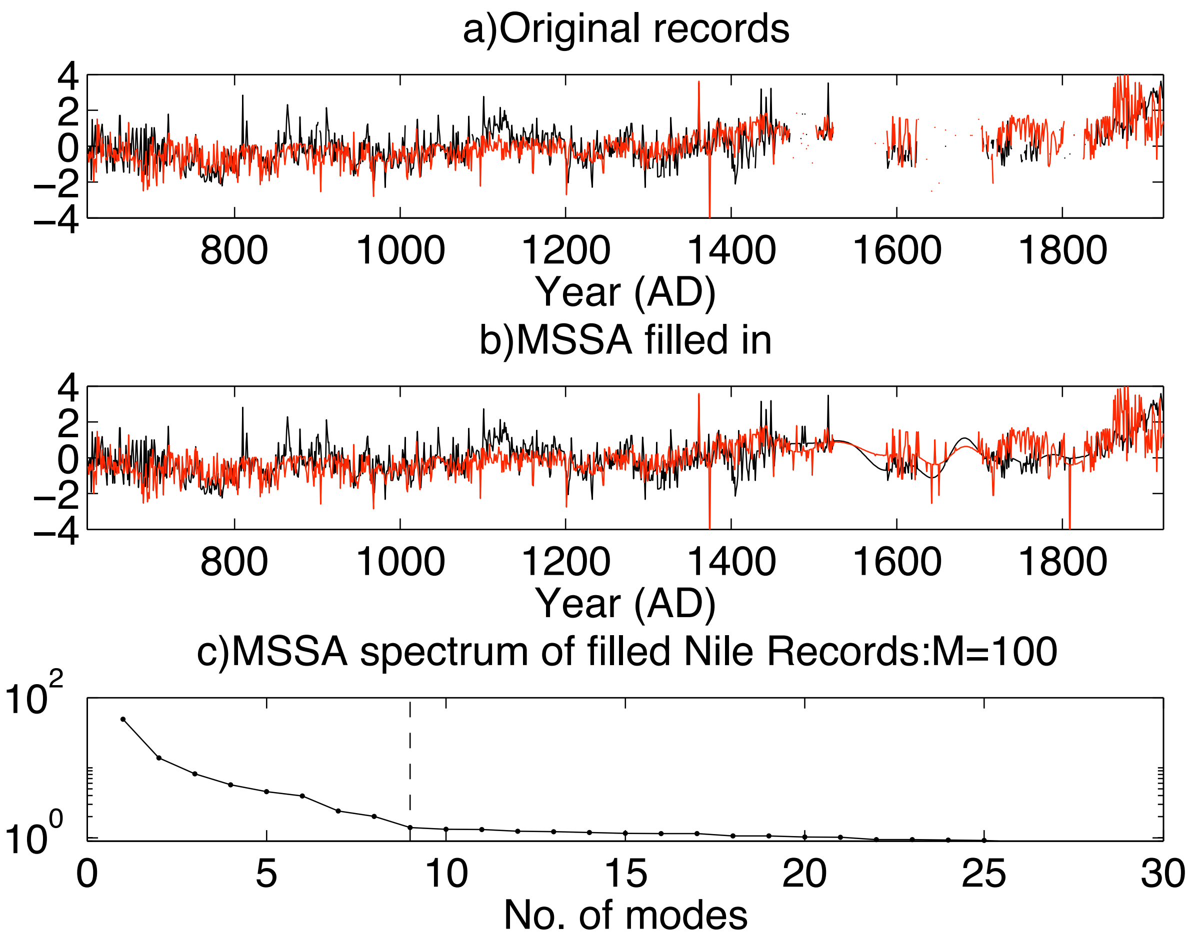
(4) apply cross-validation to optimize the value of M and the number of dominant SSA (M-SSA) modes K to fill the gaps: a portion of available data (selected at random) is flagged as missing and the RMS error in the reconstruction is computed.

Synthetic I: Gaps in Oscillatory Signal



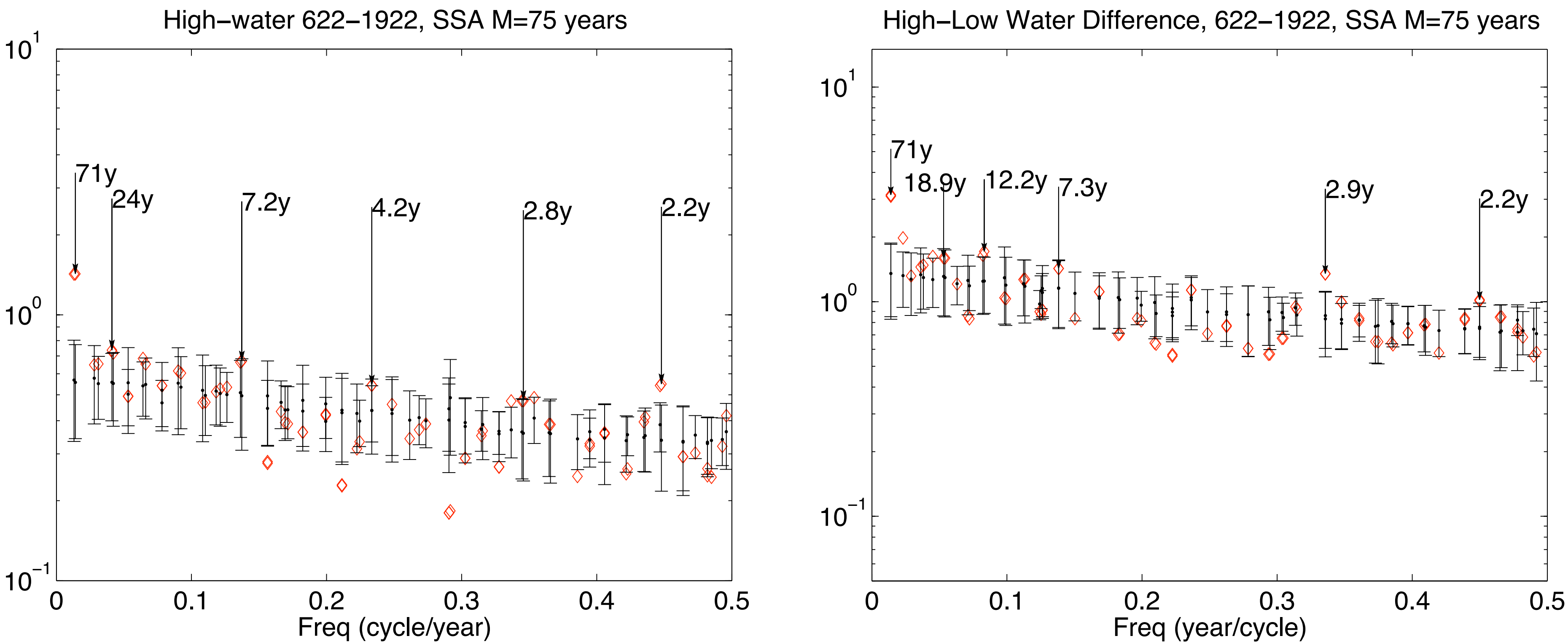
- Very good gap filling for smooth modulation; OK for sudden modulation.

Nile River Records



- High level
- Low level

MC-SSA of Filled-in Records



SSA results for the extended Nile River records;
arrows mark highly significant peaks (at 95%), in both SSA and MTM.

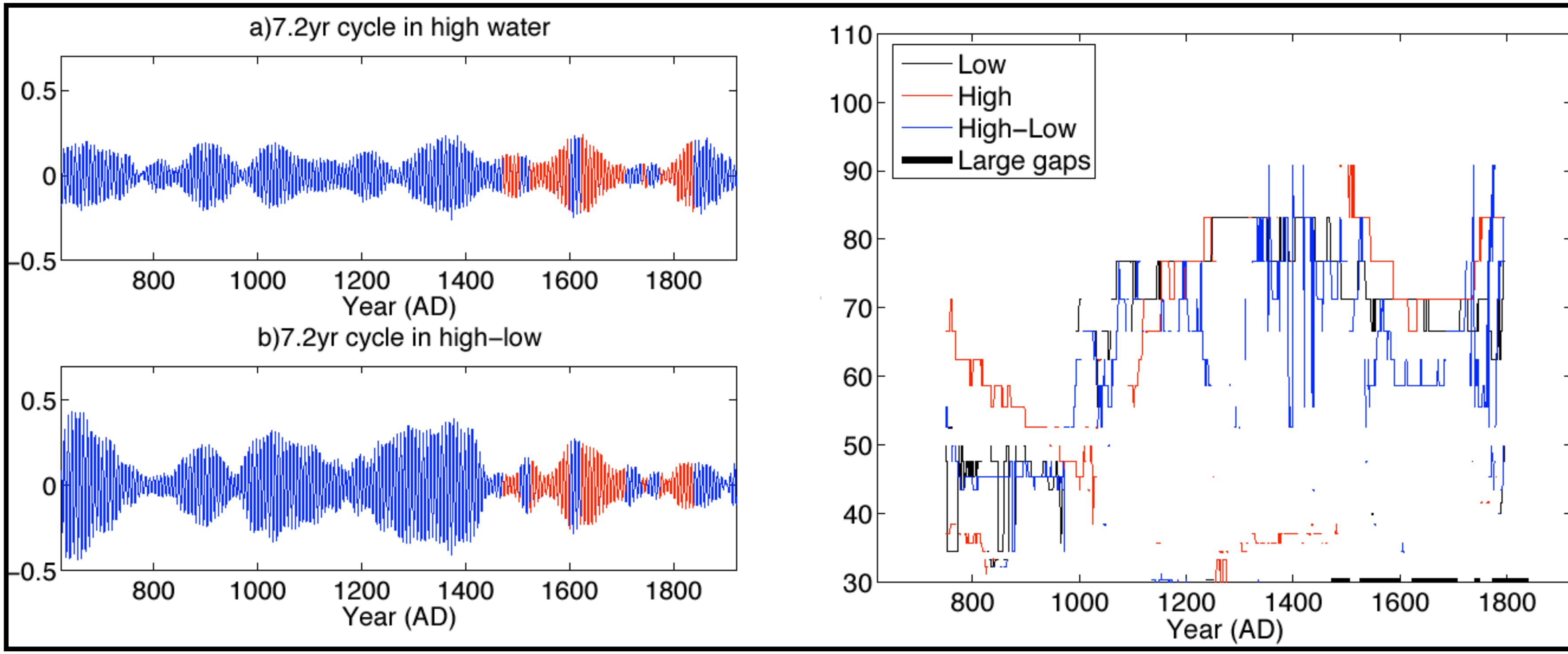
Table 1a: Significant oscillatory modes in short records (A.D. 622–1470)

Periods	Low	High	High-Low
40–100yr	**64** (9.3%)	**64** (6.9%)	**64** (6.6%)
20–40yr		[32]	
10–20yr	**12.2** (5.1%), **18.0** (6.7%)		**12.2** (4.7%), **18.3** (5.0%)
5–10yr	**6.2** (4.3%)	**7.2 (4.4%)**	**7.3 (4.4%)**
0–5yr	**3.0** (2.9%), **2.2** (2.3%)	**3.6** (3.6%), **2.9** (3.4%), **2.3** (3.1%)	**2.9** (4.2%),

Table 1b: Significant oscillatory modes in extended records (A.D. 622–1922)

Periods	Low	High	High-Low
40–100yr	**64** (13%)	**85** (8.6%)	**64** (8.2%)
20–40yr		**23.2** (4.3%)	
10–20yr	[12], **19.7** (5.9%)		**12.2** (4.3%), **18.3** (4.2%)
5–10yr	[6.2]	**7.3** (4.0%)	**7.3** (4.1%)
0–5yr	**3.0** (4%), **2.2** (3.3%)	**4.2** (3.3%), **2.9** (3.3%), **2.2** (2.9%)	[4.2], **2.9** (3.6%), **2.2** (2.6%)

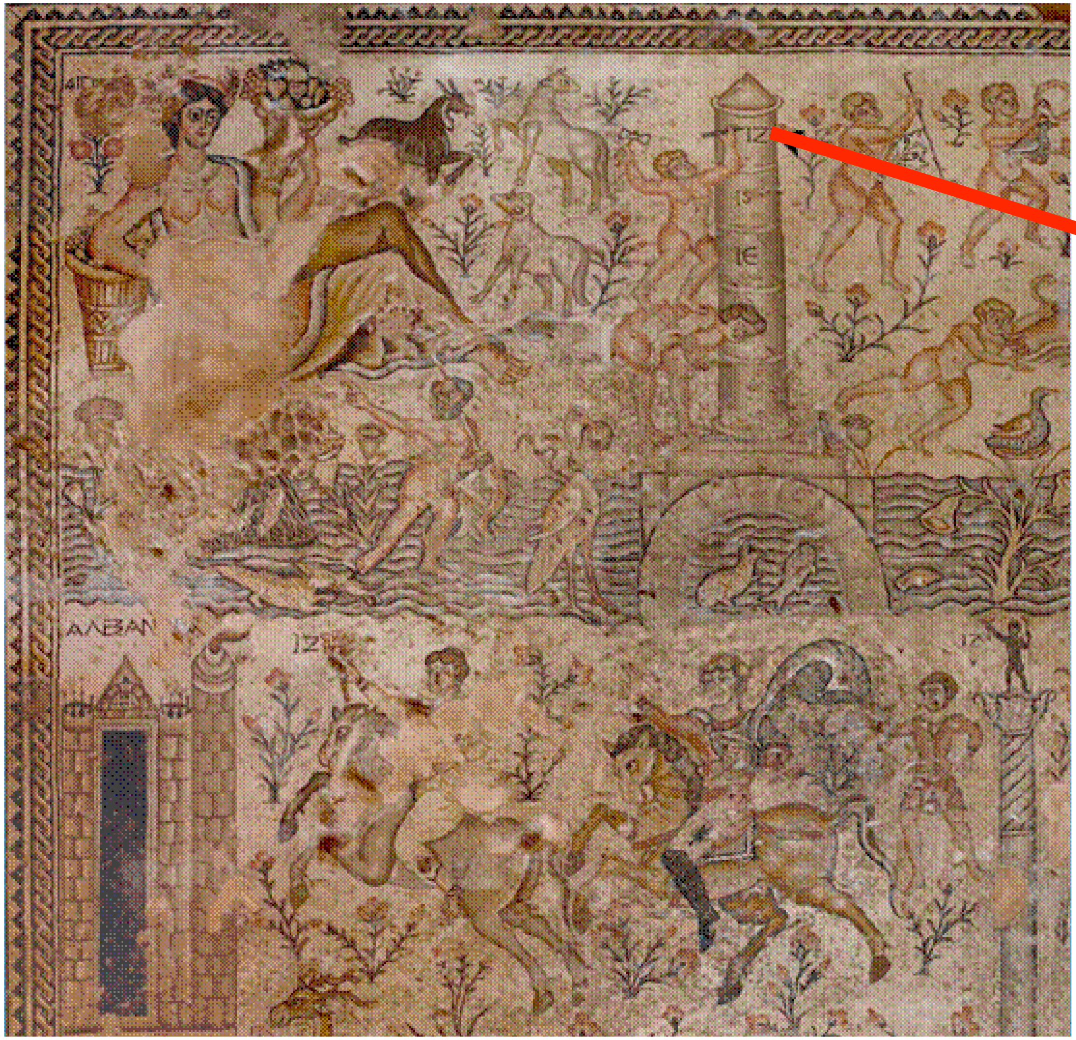
Significant Oscillatory Modes



SSA reconstruction of the 7.2-yr mode in the extended Nile River records: (a) high-water, and (b) difference. Normalized amplitude; reconstruction in the large gaps in red.

Instantaneous frequencies of the oscillatory pairs in the low-frequency range (40–100 yr). The plots are based on multi-scale SSA [Yiou *et al*., 2000]; local SSA performed in each window of width $W = 3M$, with $M = 85$ yr.

How good were Joseph's predictions?



Pretty good!

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  - Oscillations and nonlinear dynamics
- Singular spectral analysis (SSA)
  - Principal components in time and space
  - The SSA-MTM Toolkit
- The Nile River floods
  - Longest climate-related, instrumental time series
  - Gap filling in time series
  - NAO and SOI impacts on the Nile River
- Concluding remarks
  - Cautionary remarks ("garde-fous")
  - References

Significance tests ("garde-fous") in SSA

To check a spectral feature, e.g., an oscillatory pair:

1. Find pair for given data set $\{X_n: n = 1,2, \ldots N\}$ and window width M.
2. Apply statistical significance tests (MC-SSA, etc.).
3. Check robustness of pair by changing M, sampling interval τ_s, etc.
3. Apply additional methods (MTM, wavelets, etc.) and their tests to $\{X_n\}$.
4. Obtain additional time series pertinent to the same phenomenon $\{Y_m\}$, etc.
5. Apply steps (1)–(3) to these data sets.
6. Use multi-channel SSA (M-SSA) and other multivariate methods to check mutual dependence between $\{X_n\}$, $\{Y_m\}$, etc.
7. Based on steps (1)–(6), try to provide a physical explanation of the mode.
8. Use (7) to predict an as-yet-unobserved feature of the data sets.
9. If this new feature is found in new data, go on to next problem.
10. If not, go back to an earlier step of this list.

(*) **Ghil, M.**, M. R. Allen, M. D. Dettinger, K. Ide, D. Kondrashov, M. E. Mann, A. W. Robertson, A. Saunders, Y. Tian, F. Varadi, and P. Yiou, 2002: Advanced spectral methods for climatic time series, *Rev. Geophys.*, **40**(1), pp. **3**.1–**3**.41, doi: 10.1029/2000RG000092.

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Reserve slides

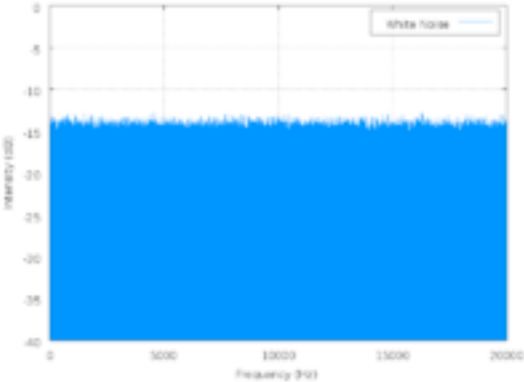
Diapos de réserve

Singular

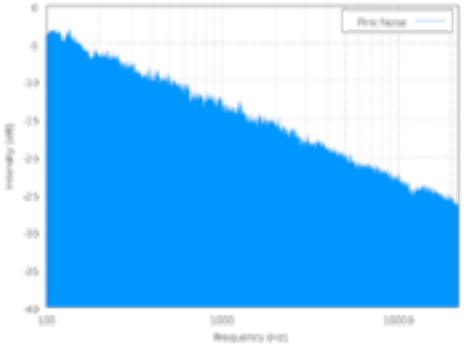
Spectrum

Analysis

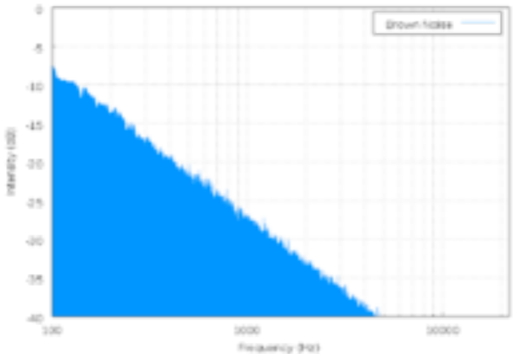
Noise "colors"



White noise, $S \sim f^{0}$



Pink (or 1/*f*) noise, $S \sim f^{-1}$



Red (or Brown) noise, $S \sim f^{-2}$

Blue noise, $S \sim f^{+1}$

SSA for Southern Oscillation Index (SOI)

SOI = mean monthly values of Δp_s (Tahiti – Darwin)

Results ("undigested") from 1933–1988 time interval (*)

1. For $18 < M < 60$ months, singular spectra show a clear break at $5 < S < 17$ (= "deterministic" part; $M - S$ = "noise");
2. 3 pairs of EOFs stand out:
   EOFs 1 + 2 (27%), 3 + 4 (19.7%), and 9 + 10 (3%);
3. the associated periods are ~
   60 mos. ("ENSO"), 30 mos. (QBO"), and 5.5 mos. (?!)

(*) E. M. ("Gene") Rasmusson, X. Wang, and C.F. Ropelewski, 1990: The biennial component of ENSO variability. *J. Marine Syst.*, **1**, 71–96.

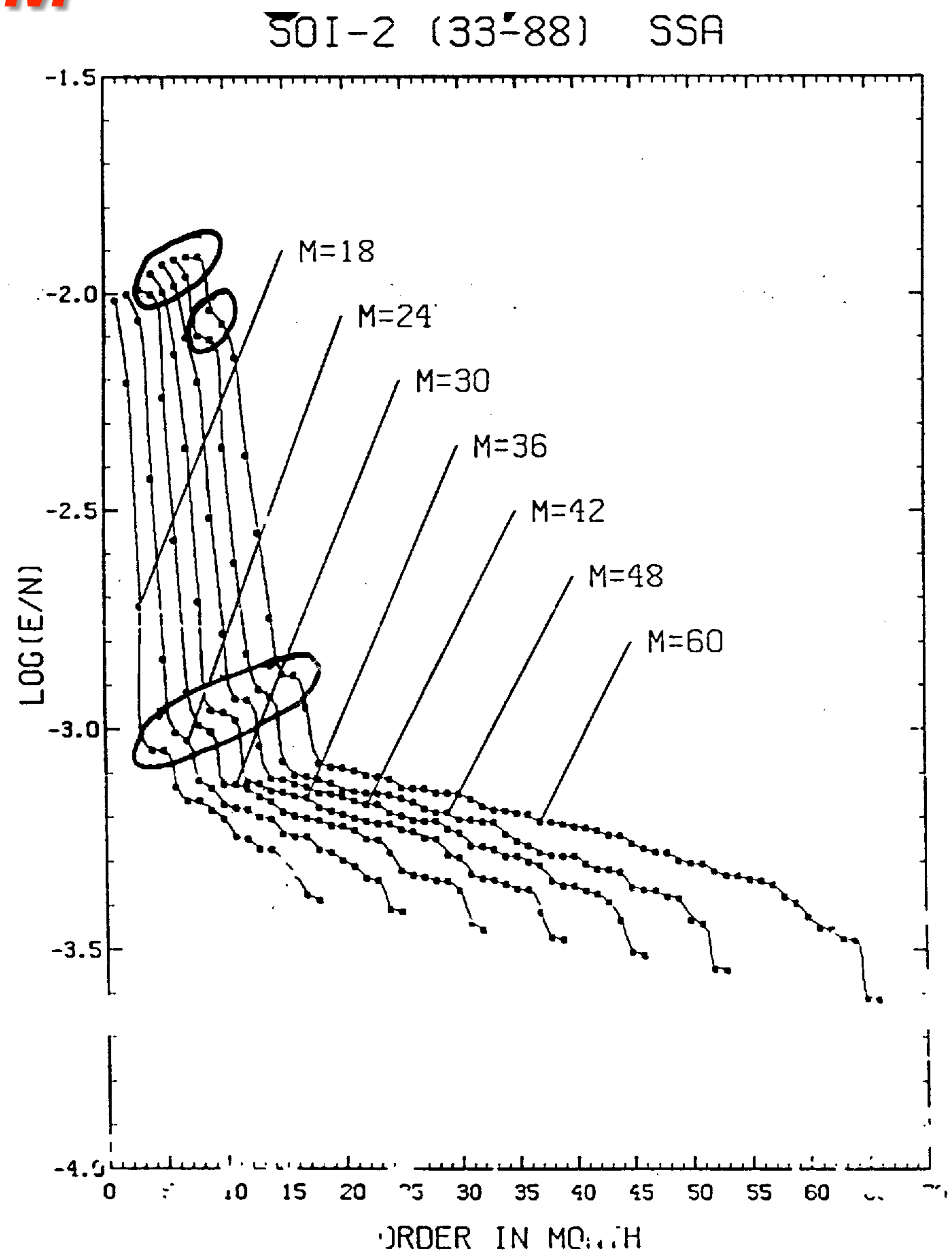
Variable window size *M*

Sampling interval – $\tau_s = 1$ month

Window width $M\tau_s$:

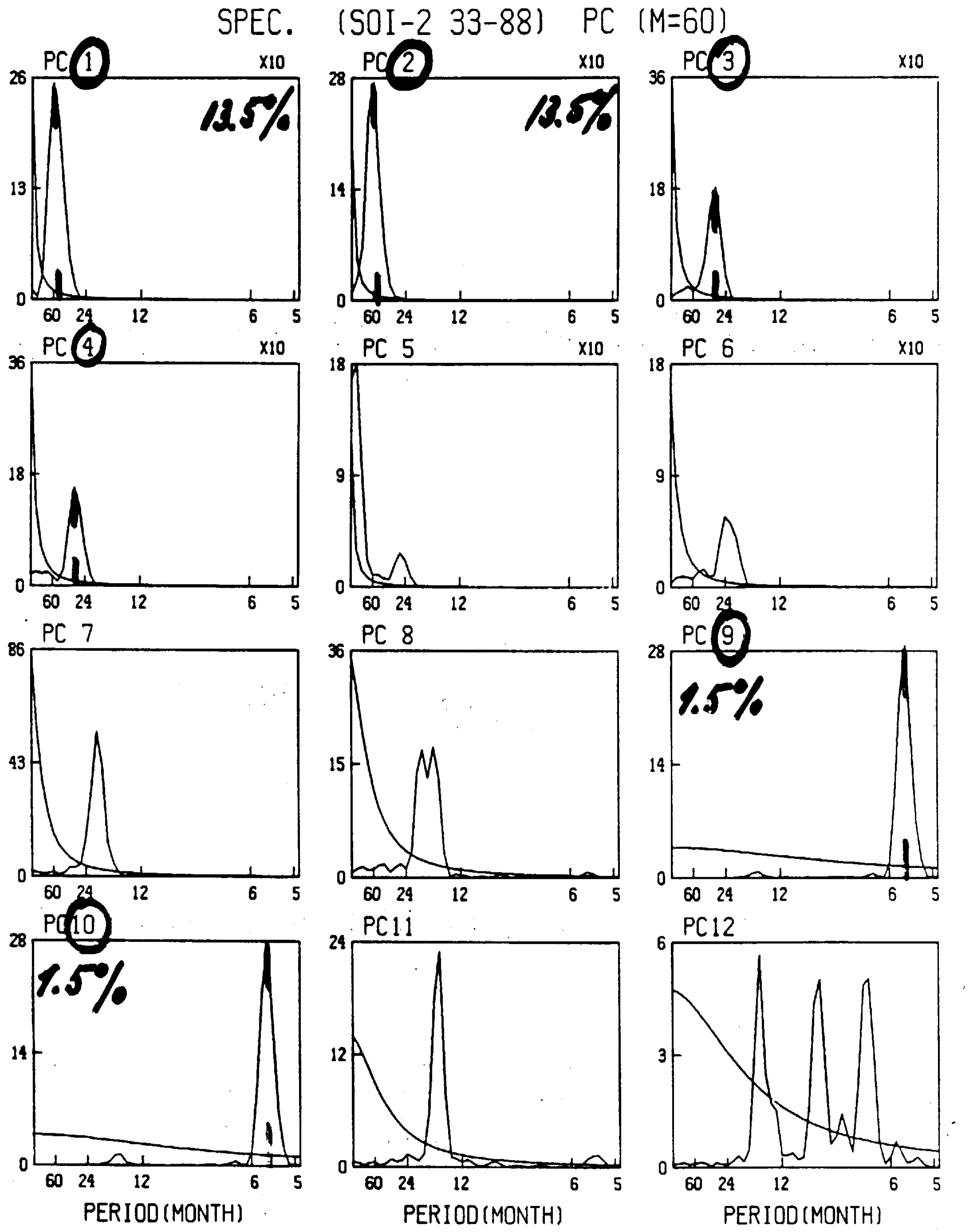
$18\tau_s < \tau_w < 60\tau_s$ or

1.5 yr $< \tau_w <$ 5 yr.



Spectral peaks
(*M* = 60)

Each principal component (PC) is Fourier analyzed separately; individual variance indicated as well.

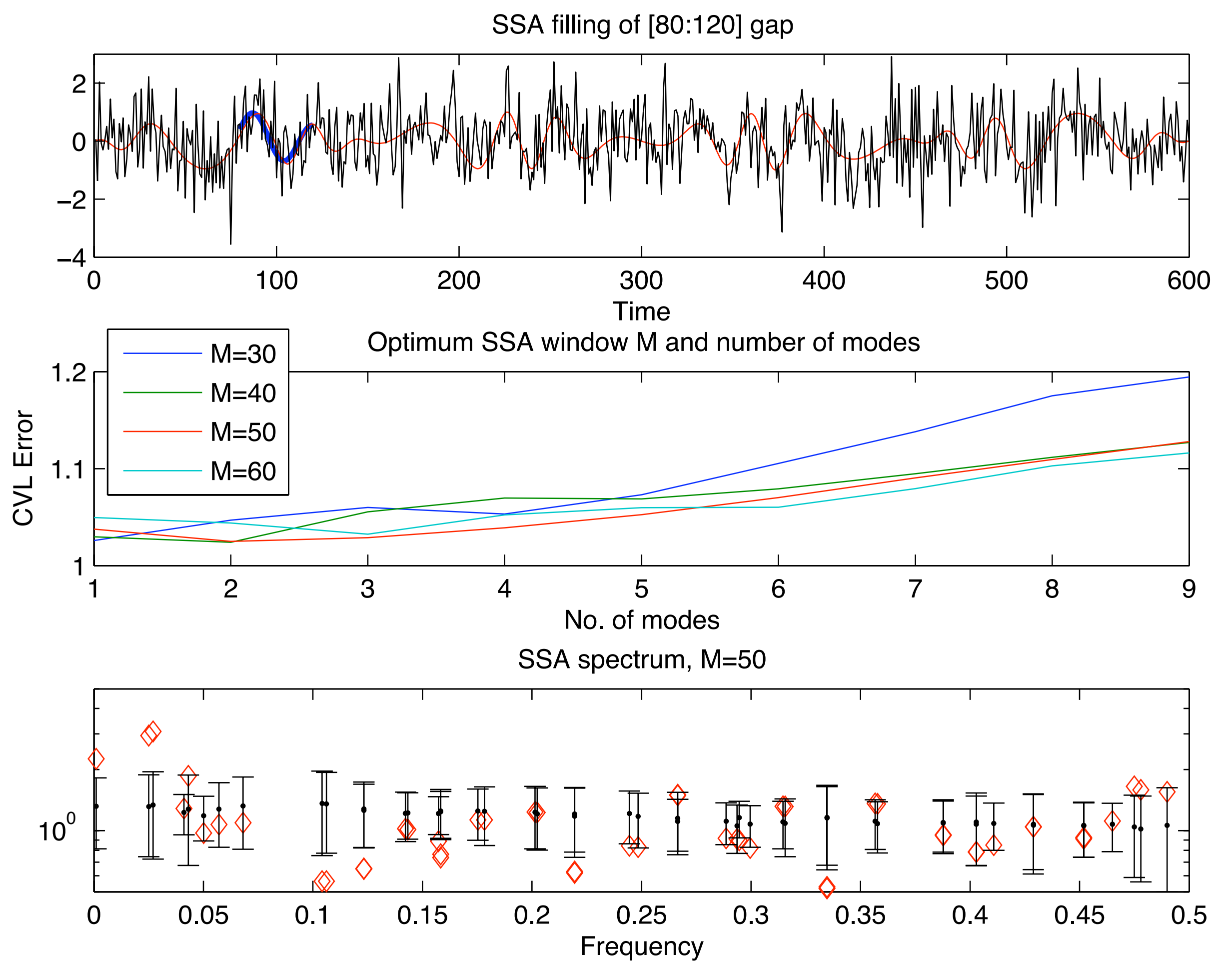


PCs (1+2) – period = 60 months, low-frequency or “ENSO” or quasi-quadrennial (QQ) component;

PCs (3+4) – period = 30 months quasi-biennial (QB) component;

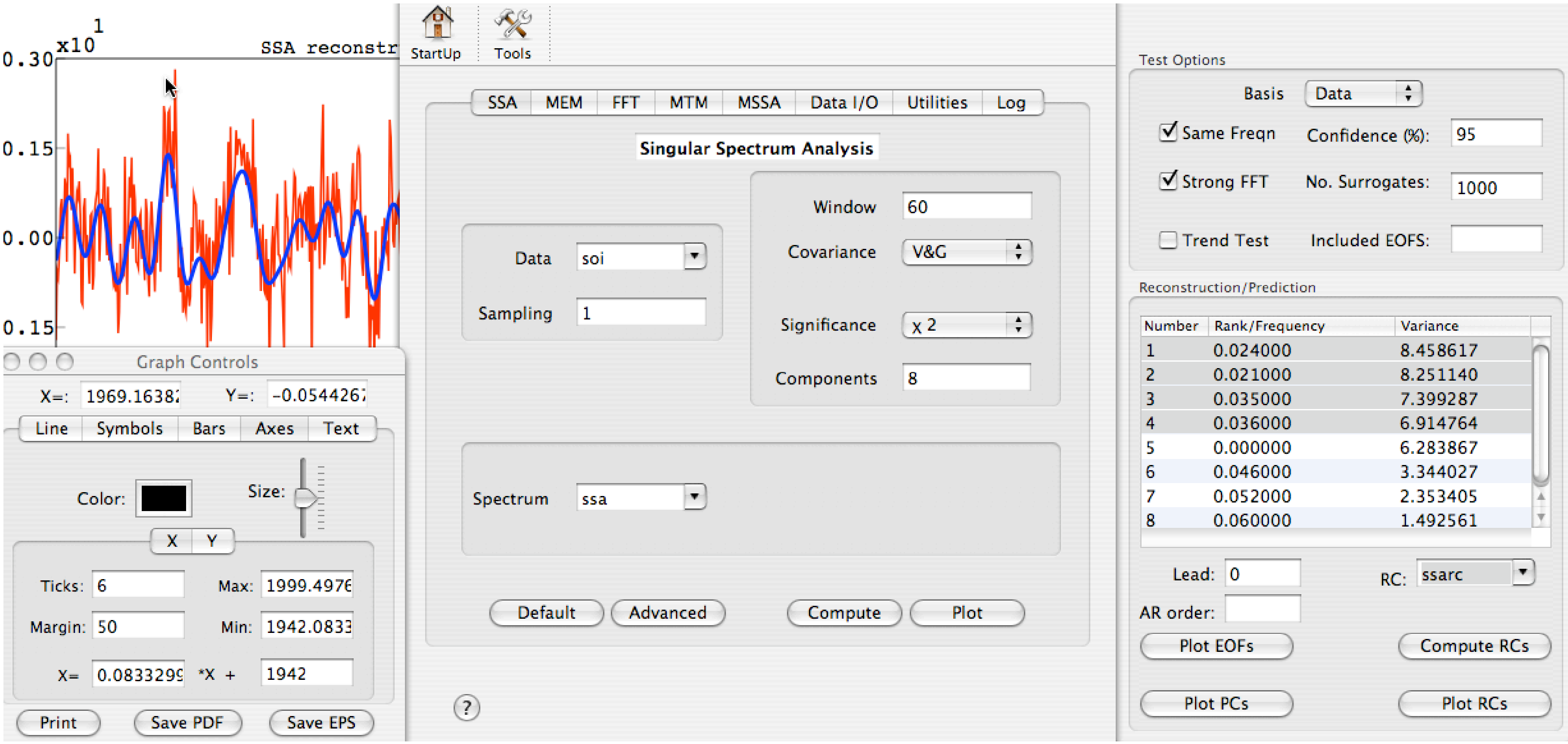
PCs (9+10) – period = 5.5 months

Synthetic II: Gaps in Oscillatory Signal + Noise



$$x(t) = sin(\frac{2\pi}{300}t) * cos(\frac{2\pi}{40}t + \frac{\pi}{2} sin\frac{2\pi}{120}t)$$

kSpectra Toolkit for Mac OS X



- **$$ ... but: *Project files*, *Automator WorkFlows*, *Spotlight* and more!**
- **www.spectraworks.com**

Un peu de bibliographie

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The Nile River Basin initiative will greatly modify the flow along the longest & best-documented river system in the world …