Empirical Mode Reduction and its Applications to Nonlinear Models in Geosciences

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Joint work with

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Motivation

- Sometimes we have data but no models: empirical approach.
- We want models that are as simple as possible, but not any simpler.

Criteria for a good data-derived model

Capture interesting dynamics: regimes, nonlinear oscillations.

- Intermediate-order deterministic dynamics easy to analyze anallitycaly.
- Good noise estimates.

Linear Inverse Models (LIM)

Penland, C., 1996: A stochastic model of Indo-Pacific sea-surface temperature anomalies. *Physica D*, **98**, 534–558.
Penland, C., and L. Matrosova, 1998: Prediction of tropical Atlantic sea-surface temperatures using linear inverse modeling. *J. Climate*, **11**, 483–496.

Linear inverse model (LIM)

• We aim to use data in order to estimate the two matrices, **B** and **Q**, of the stochastic linear model:

$$dX = BX \cdot dt + d\xi(t), \qquad (1)$$

where **B** is the (constant and stable) dynamics matrix, and **Q** is the lag-zero covariance of the vector white-noise process $d\xi(t)$.
• More precisely, the two matrices **B** and **Q** are related by a fluctuation-dissipation relation:

$$\mathbf{BC}(0) + \mathbf{C}(0)\mathbf{B}^t + \mathbf{Q} = 0, \qquad (2)$$

where $\mathbf{C}(\tau) = \mathrm{E}\{\mathbf{X}(t+\tau)\mathbf{X}(t)\}$ is the lag-covariance matrix of the process $\mathbf{X}(t)$, and $(\cdot)^t$ indicates the transpose.
• One then proceeds to estimate the Green's function $\mathbf{G}(\tau) = \exp(\tau\mathbf{B})$ at a given lag τ_0 from the sample $\mathbf{C}(\tau)$ by

$$\mathbf{G}(\tau_0) = \mathbf{C}(\tau_0)\mathbf{C}^{-1}(0).$$

•Linear inverse models (LIM) are good least-square fits to data, but don't capture all the (nonlinear) processes of interest.

Nonlinear reduced models (MTV)

Majda, A. J., I. Timofeyev, and E. Vanden-Eijnden, 1999: Models for stochastic climate prediction. *Proc. Natl. Acad. Sci. USA*, **96**, 14687–14691.
Majda, A. J., I. Timofeyev, and E. Vanden-Eijnden, 2003: Systematic strategies for stochastic mode reduction in climate. *J. Atmos. Sci*., **60**, 1705–1722.
Franzke, C., and Majda, A. J., 2006: Low-order stochastic mode reduction for a prototype atmospheric GCM. *J. Atmos. Sci.*, **63**, 457–479.

Nonlinear stochastic model (MTV)–I

- Let **z** be a **vector** decomposed into a **slow** ("climate") and a **fast** ("weather") vector of variables, $\mathbf{z} = (\mathbf{x}, \mathbf{y})$.
We model **x** deterministically and **y** stochastically, via the following **quadratic nonlinear dynamics**

$$\frac{d\mathbf{x}}{dt} = L_{11}\mathbf{x} + L_{12}\mathbf{y} + B^1_{11}(\mathbf{x},\mathbf{x}) + B^1_{12}(\mathbf{x},\mathbf{y}) + B^1_{22}(\mathbf{y},\mathbf{y}),$$

$$\frac{d\mathbf{y}}{dt} = L_{21}\mathbf{x} + L_{22}\mathbf{y} + B^2_{11}(\mathbf{x},\mathbf{x}) + B^2_{12}(\mathbf{x},\mathbf{y}) + B^2_{22}(\mathbf{y},\mathbf{y}).$$

- In stochastic modeling, the explicit nonlinear self-interaction for the variable **y**, i.e. $B^2_{22}(\mathbf{y},\mathbf{y})$, is represented by a linear stochastic operator:

$$B^2_{22}(\mathbf{y},\mathbf{y}) \approx -\frac{\Gamma}{\varepsilon}\mathbf{y} + \frac{\sigma}{\sqrt{\varepsilon}}\dot{\mathbf{W}}(t),$$

where Γ and σ are matrices and $\dot{\mathbf{W}}(t)$ is a **vector-valued** white-noise.

Nonlinear stochastic model (MTV)–II

- The parameter ε measures the ratio of the correlation time of the weather and the climate variables, respectively, and $\varepsilon \ll 1$ corresponds to this ratio being very small.
- Using the scaling $t \to \varepsilon t$, we derive the stochastic climate model:

$$\frac{d\mathbf{y}}{dt} = \frac{1}{\varepsilon}(L_{11}\mathbf{x} + L_{12}\mathbf{y} + B^1_{11}(\mathbf{x},\mathbf{x}) + B^1_{12}(\mathbf{x},\mathbf{y})),$$

$$\frac{d\mathbf{y}}{dt} = \frac{1}{\varepsilon}(L_{21}\mathbf{x} + L_{22}\mathbf{y} + B^2_{11}(\mathbf{x},\mathbf{x}) + B^2_{12}(\mathbf{x},\mathbf{y})) - \frac{\Gamma}{\varepsilon^2}\mathbf{y} + \frac{\sigma}{\varepsilon}\dot{\mathbf{W}}(t).$$

- In practice, the climate variables are determined by a variety of procedures, including leading-order empirical orthogonal functions (EOFs), zonal averaging in space, low-pass and high-pass time filtering, or a combination of these procedures.

- MTV model coefficients are predicted by the theory.
- Relies on scale separation between the resolved (slow) and unresolved (fast) modes
- Their estimation requires very long libraries of the full model's evolution.
- Difficult to separate between the slow and fast dynamics (MTV).

Key ideas

- Nonlinear dynamics: $$\dot{\mathbf{x}} = \mathbf{L}\mathbf{x} + \mathbf{N}(\mathbf{x}).$$
- Discretized, quadratic:

$$dx_i = (\mathbf{x}^{\mathrm{T}}\mathbf{A}_i\mathbf{x} + \mathbf{b}_i^{(0)}\mathbf{x} + c_i^{(0)})\,dt + dr_i^{(0)}; \qquad 1 \le i \le I.$$

- Multi-level modeling of red noise:

$$\begin{aligned}
dx_i &= (\mathbf{x}^{\mathrm{T}}\mathbf{A}_i\mathbf{x} + \mathbf{b}_i^{(0)}\mathbf{x} + c_i^{(0)})\,dt + r_i^{(0)}\,dt,\\
dr_i^{(0)} &= \mathbf{b}_i^{(1)}[\mathbf{x}, \mathbf{r}^{(0)}]\,dt + r_i^{(1)}\,dt,\\
dr_i^{(1)} &= \mathbf{b}_i^{(2)}[\mathbf{x}, \mathbf{r}^{(0)}, \mathbf{r}^{(1)}]\,dt + r_i^{(2)}\,dt,\\
&\dots\\
dr_i^{(L)} &= \mathbf{b}_i^{(L)}[\mathbf{x}, \mathbf{r}^{(0)}, \mathbf{r}^{(1)}, \dots, \mathbf{r}^{(L)}]\,dt + dr_i^{(L+1)}; \qquad 1 \le i \le I.
\end{aligned}$$

Nomenclature

Response variables:

$$\{y^{(n)}\}\ (1 \le n \le N) \equiv \{y^{(1)}, \ldots, y^{(N)}\}$$

Predictor variables:

$$\{x^{(n)}\}\ (1 \le n \le N) \equiv \{x^{(1)}, \ldots, x^{(N)}\}$$

- Each $y^{(n)}$ is *normally distributed* about $\widehat{y}^{(n)}$
- Each $x^{(n)}$ is *known exactly. Parameter set* $\{a_p\}$:

$$\widehat{y} = f(x;\, a_1, \ldots, a_P)$$ – known dependence of *f* on $\{x^{(n)}\}$ and $\{a_p\}$.

REGRESSION: Find $\{a_p\}\ (1 \le p \le P)$

LIM extension #1

- Do a least-square fit to a *nonlinear function of the data*:

J response variables: $y_i^{(n)} \equiv (x_i^{(n+1)} - x_i^{(n)})/\Delta t$

Predictor variables (example – quadratic polynomial of *J* original predictors):

$$\widehat{y}_i = a_{0,\,i} + \sum_{j=1}^{J} a_{j,\,i} x_j + \sum_{j=1}^{J} \sum_{k \geq j} \tilde{a}_{jk,\,i} x_j x_k$$

Note: Need to find many more regression coefficients than for LIM; in the example above $P = J + J(J+1)/2 + 1 = O(J^2)$.

Regularization

- *Caveat*: If the number *P* of regression parameters is comparable to (*i.e.*, it is not much smaller than) the number of data points, then the least-squares problem may become ill-posed and lead to unstable results (overfitting) ==> One needs to transform the predictor variables to *regularize* the regression procedure.

- Regularization involves *rotated predictor variables:* the orthogonal transformation looks for an "optimal" linear combination of variables.

- "Optimal" = (i) rotated predictors are nearly uncorrelated; and (ii) they are maximally correlated with the response.

- Canned packages available.

LIM extension #2

- *Motivation*: Serial correlations in the residual.

Main level, $l = 0$: $$(x^{n+1} - x^n)/\Delta t = a_{x,\,0} x^n + r_0^n$$

Level $l = 1$: $$(r_0^{n+1} - r_0^n)/\Delta t = a_{x,\,1} x^n + a_{r_0,\,1} r_0^n + r_1^n$$

… and so on …

Level L: $$r_{L-1}^{n+1} - r_{L-1}^n = \Delta t[a_{x,\,L} x^n + \ \ldots] + \Delta r_L$$

- r_L – Gaussian random deviate with appropriate variance

- If we suppress the dependence on x in levels $l = 1, 2, \ldots L$, then the model above is formally identical to an ARMA model.

Empirical Orthogonal Functions (EOFs)

- We want models that are as simple as possible, but not any simpler: use leading **empirical orthogonal functions** for data compression and capture as much as possible of the useful (predictable) variance.
- Decompose a spatio-temporal data set **D**(*t*,*s*)(*t* = 1,…,*N*; *s* = 1…,*M*) by using **principal components (PCs)** – $\mathbf{x}_i(t)$ and **empirical orthogonal functions (EOFs)** – $\mathbf{e}_i(s)$: diagonalize the *M* x *M* spatial covariance matrix **C** of the field of interest.

$$\mathbf{C} = \frac{1}{N}(\mathbf{D} - <\mathbf{D}>)^t(\mathbf{D} - <\mathbf{D}>)$$
$$\mathbf{C}\lambda_i = \lambda_i e_i, x_i = (\mathbf{D} - <\mathbf{D}>)e_i$$

- EOFs are optimal patterns to capture most of the variance.
- Assumption of robust EOFs.
- EOFs are statistical features, but may describe some dynamical (physical) mode(s).

Empirical mode reduction (EMR)–I

- *Multiple predictors*: Construct the reduced model using J leading PCs of the field(s) of interest.

- *Response variables*: one-step time differences of predictors; step = sampling interval = Δt.

- Each response variable is fitted by an *independent* multi-level model:
  The *main level* $l = 0$ is *polynomial* in the predictors;
  all the other levels are linear.

Empirical mode reduct'n (EMR) – II

- The number *L* of levels is such that each of the last-level residuals (for each channel corresponding to a given response variable) is "white" in time.

- Spatial (cross-channel) correlations of the last-level residuals are retained in subsequent regression-model simulations.

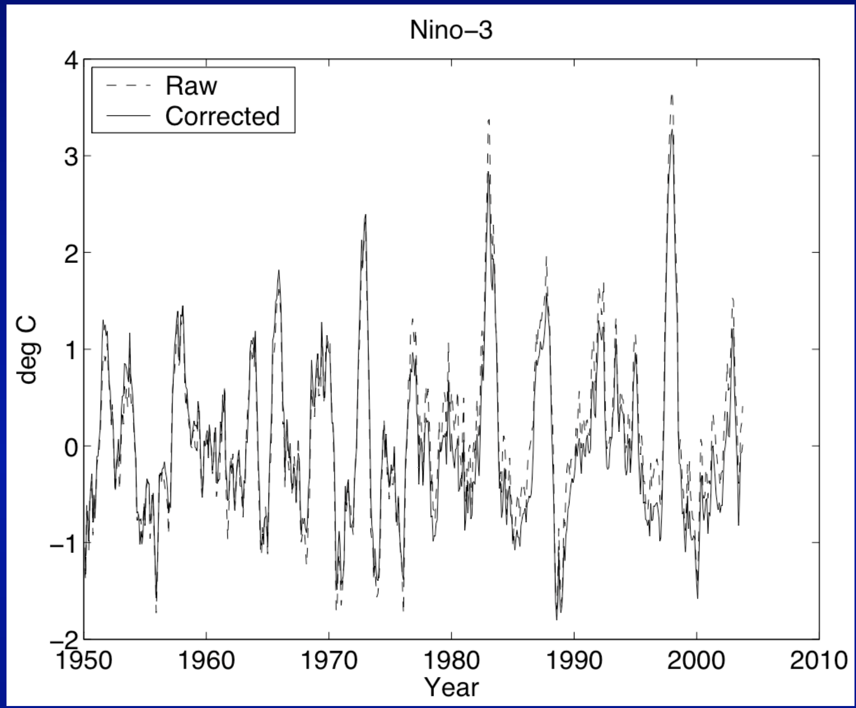
- The number *J* of PCs is chosen so as to optimize the model's performance.

- Regularization is used at the main (nonlinear) level of each channel.

ENSO – I

Data:

- Monthly SSTs: 1950–2004, 30 S–60 N, 5x5 grid (Kaplan *et al*., 1998)



- 1976–1977 shift removed

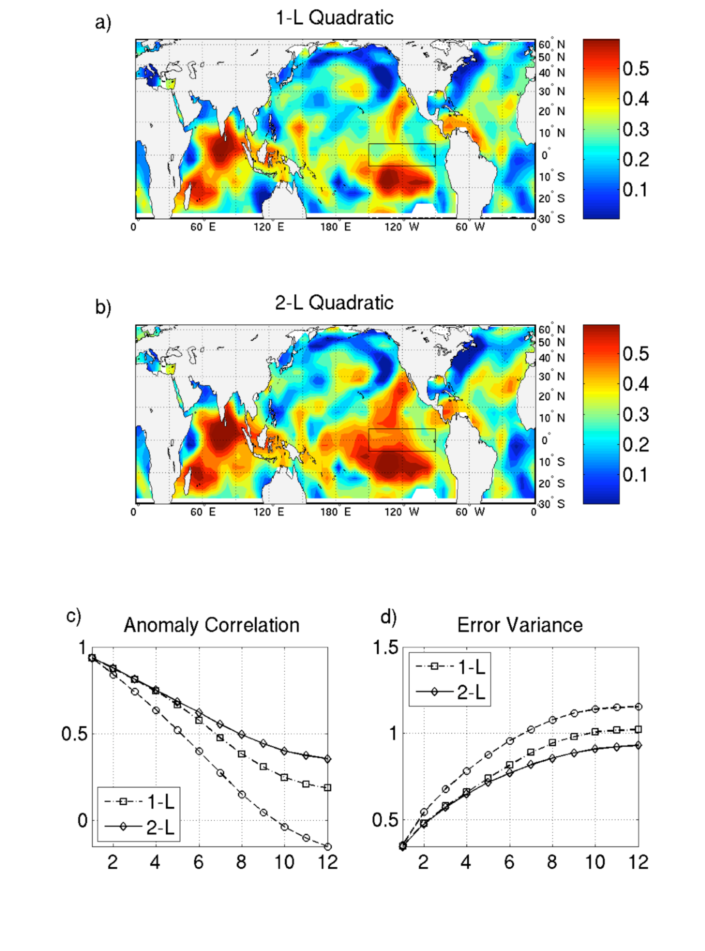
- Histogram of SST data is skewed (warm events are larger, while cold events are more frequent): Nonlinearity important?

ENSO – II

Regression model:

- *J* = 20 variables (EOFs of SST)
- *L* = 2 levels
- Seasonal variations included in the linear part of the main (quadratic) level.

The quadratic model has a slightly smaller RMS error in its extreme-event forecasts



- Competitive skill: Currently a member of a multi-model prediction scheme of the IRI, see: http://iri.columbia.edu/climate/ENSO/currentinfo/SST_table.html.

ENSO – III

ENSO development and non-normal growth of small perturbations

(Penland & Sardeshmukh, 1995; Thompson & Battisti, 2000);

Floquet analysis :

$$\dot{\mathbf{x}} = \mathbf{L}(t)\mathbf{x}$$

$$\dot{\mathbf{\Phi}} = \mathbf{L}(t)\mathbf{\Phi}, \quad \mathbf{\Phi}(0) = \mathbf{I}$$

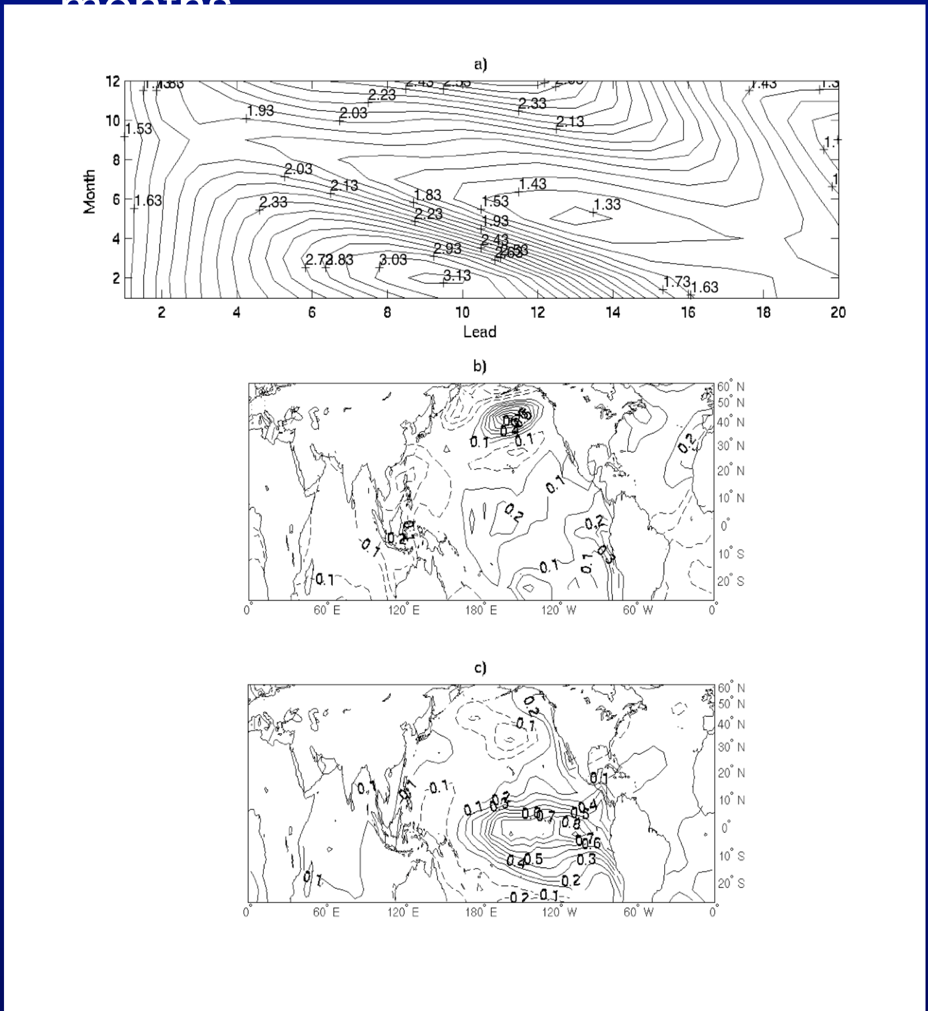
$$\mathbf{\Phi}(\tau) = \mathbf{U} \cdot \mathbf{S} \cdot \mathbf{V}^{\top}$$

V – optimal initial vectors

U – final pattern at lead [illegible]

- *Maximum growth*:

(b) start in Feb., (c) [illegible]= 10 months



NH LFV in QG3 Model – I

The QG3 model (Marshall and Molteni, *JAS*, 1993):

- Global QG, T21, 3 levels, with topography; perpetual-winter forcing; ~1500 degrees of freedom.

- Reasonably realistic NH climate and LFV:
  (i) multiple planetary-flow regimes; and
  (ii) low-frequency oscillations
  (submonthly-to-intraseasonal).

- Extensively studied: A popular “numerical-laboratory” tool to test various ideas and techniques for NH LFV.

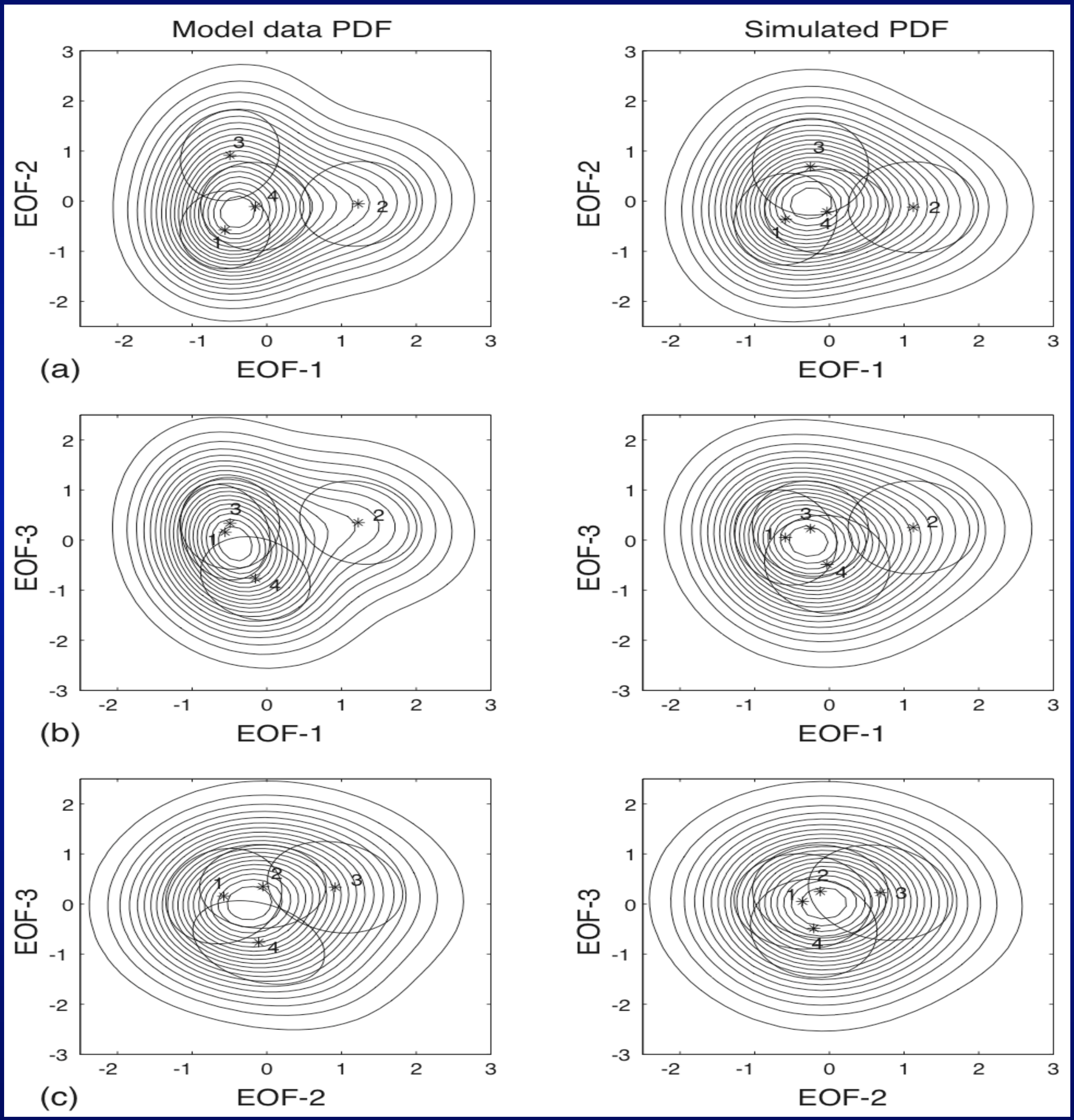
NH LFV in QG3 Model – II

Output: daily streamfunction ([illegible]) fields ([illegible] 10^5 days)

Regression model:

- 15 variables, 3 levels (L = 3), quadratic at the main level
- Variables: Leading PCs of the middle-level [illegible]
- No. of degrees of freedom = 45 (a factor of 40 less than in the QG3 model)
- Number of regression coefficients P = (15+1+15•16/2+30+45)•15 = 3165 (<< 10^5)
- Regularization via PLS applied at the main level.

NH LFV in QG3 Model – III



- Our EMR is based on 15 EOFs of the QG3 model and has *L* = 3 regression levels, *i.e.,* a total of 45 predictors (*).

- The EMR approximates the QG3 model's major statistical features (PDFs, spectra, regimes, transition matrices, etc.) strikingly well.

NH LFV in QG3 Model – II

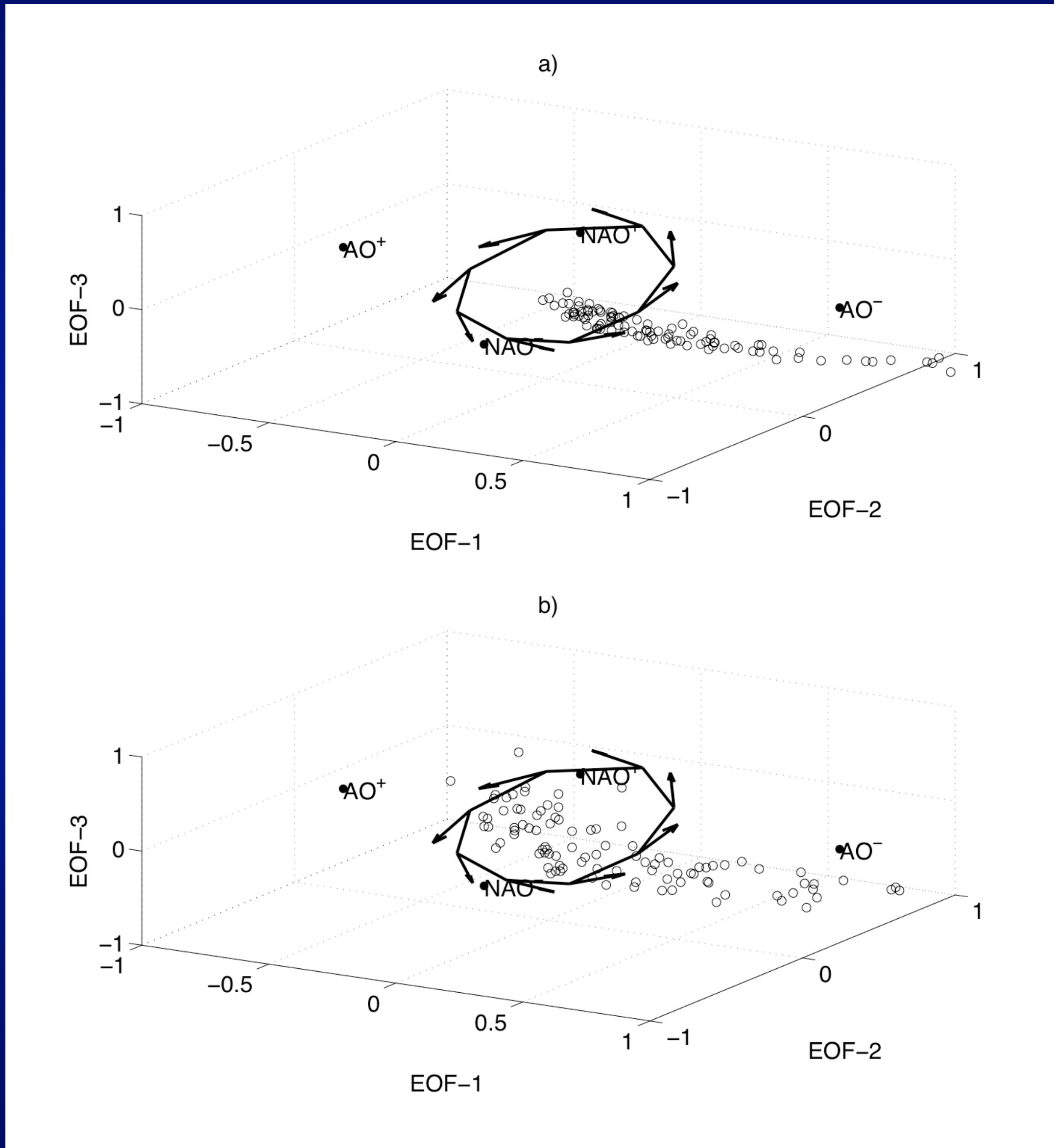
Quasi-stationary states
of the EMR model's
deterministic component
explain dynamics!

Tendency threshold
a) = 10^{-6}; and
b) = 10^{-5}.

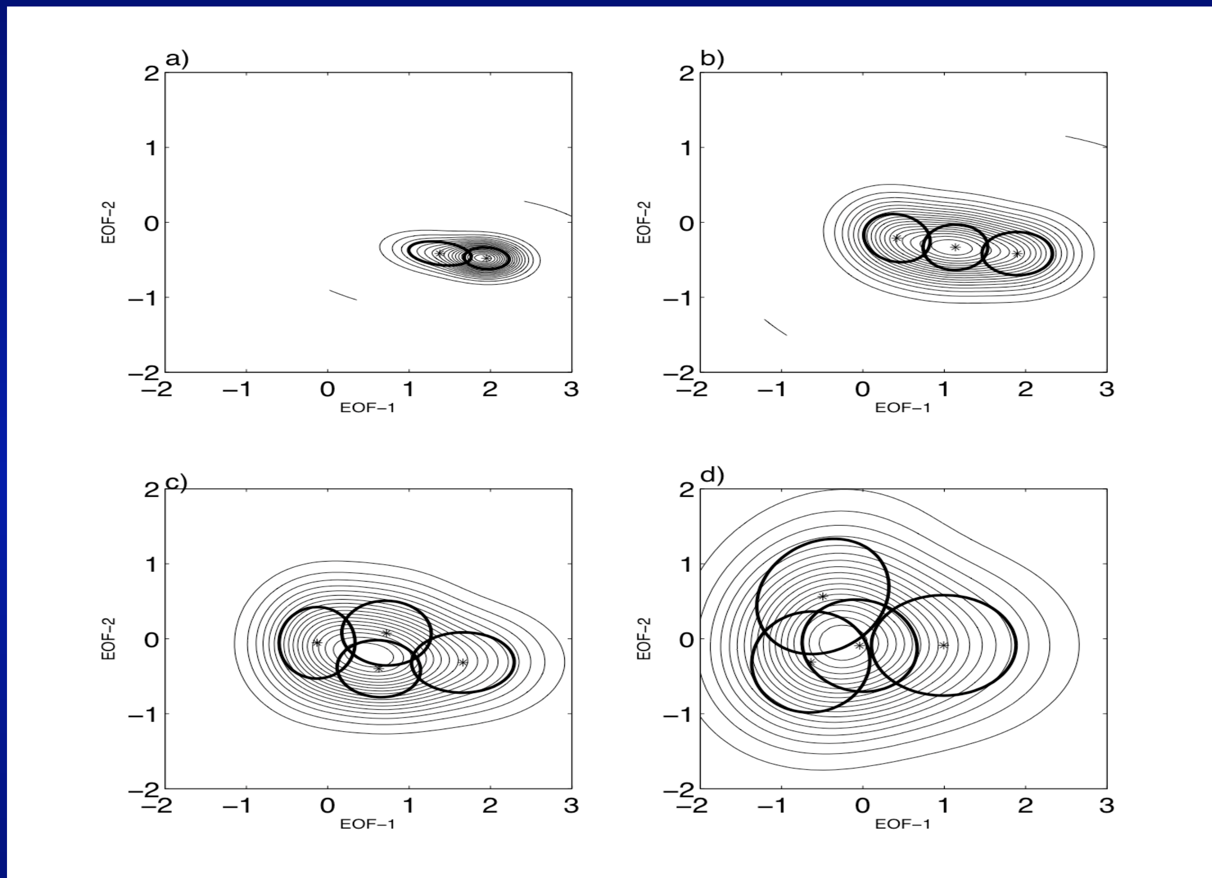
•The 37-day mode is associated, in the reduced model with the least-damped linear eigenmode.

•AO⁻ is the model's unique steady state.

• Regimes AO⁺, NAO⁻ and NAO⁺ are associated with anomalous slow-down of the 37-day oscillation's trajectory nonlinear mechanism.



NH LFV in QG3 Model – III



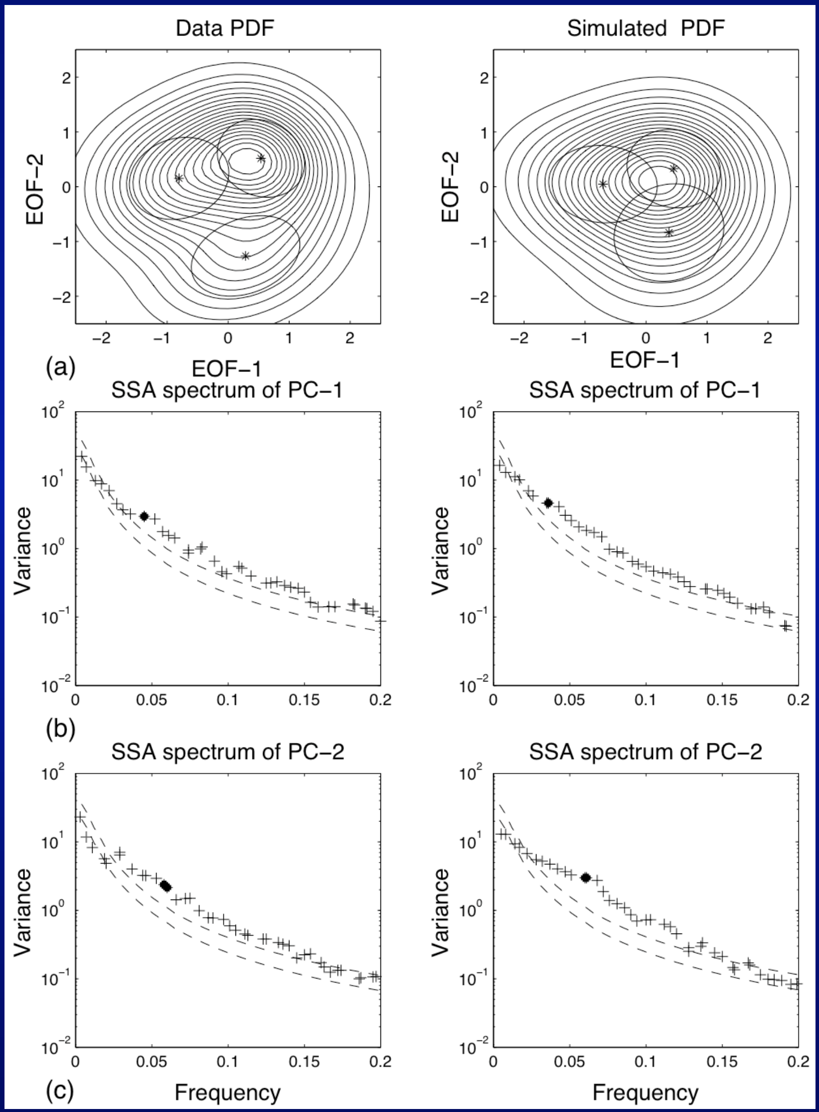
•The additive noise interacts with the nonlinear dynamics to yield the full EMR's (and QG3's) phase-space PDF.

Panels (a)–(d): noise amplitude [illegible] = 0.2, 0.4, 0.6, 1.0.

NH LFV – Observed Heights

- 44 years of daily 700-mb-height winter data

- 12-variable, 2-level model works OK, but dynamical operator has unstable directions: "sanity checks" required.



Mean phase space tendencies

• 2-D mean tendencies $<(dx_j, dx_k)>=F(x_j, x_k)$ in a given plane of the EOF pair *(j, k)* have been used to identify distinctive signatures of nonlinear processes in both the intermediate QG3 model (Selten and Branstator, 2004; Franzke et al. 2007) and more detailed GCMs (Branstator and Berner, 2005).

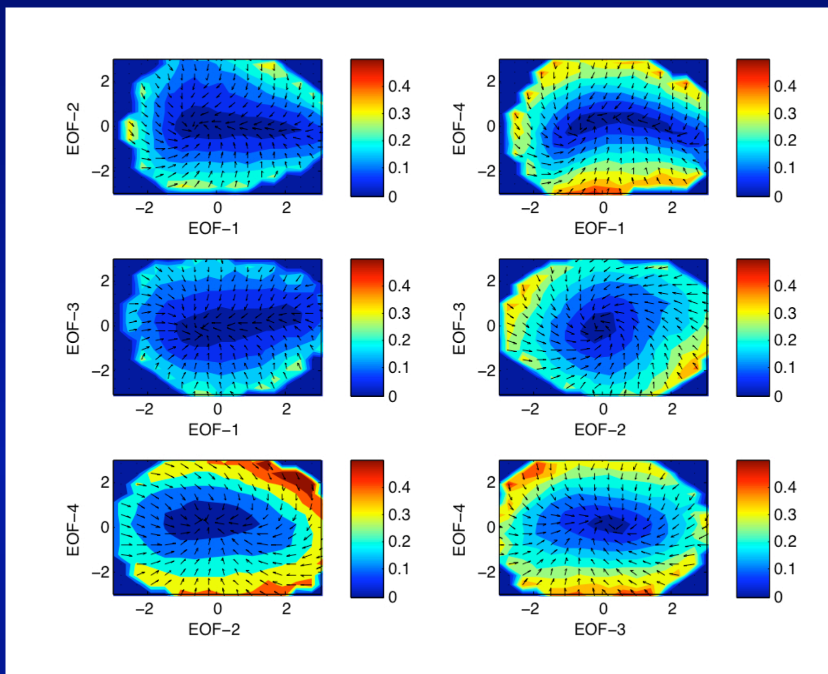
• Relative contributions of ”resolved” and ”unresolved” modes (EOFs) that may lead to observed deviations from Gaussianity; it has been argued that contribution of ”unresolved” modes is important.

•We can estimate mean tendencies from the output of QG3 and EMR simulations.

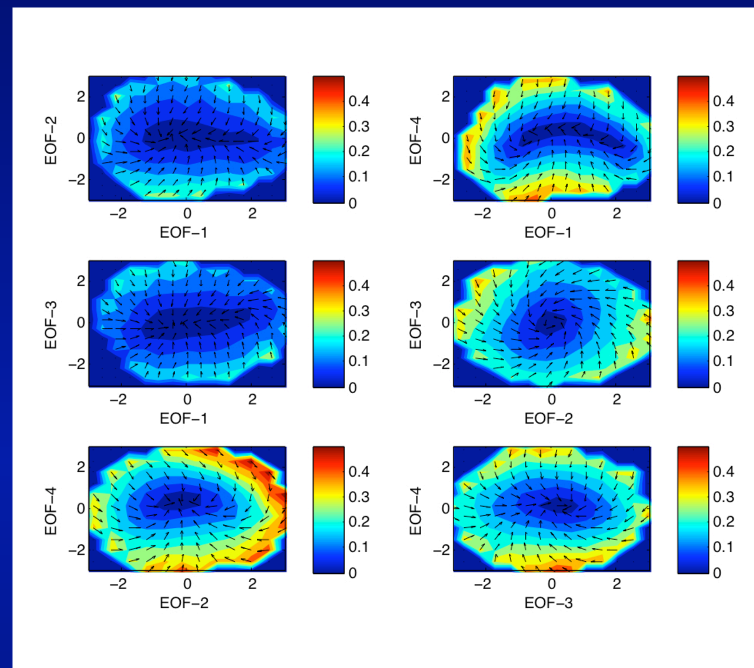
• Explicit quadratic form of $F(x_j, x_k)$ from EMR allows to study nonlinear contributions of ”resolved” and ”unresolved” modes.

Mean phase-space tendencies

QG3 tendencies



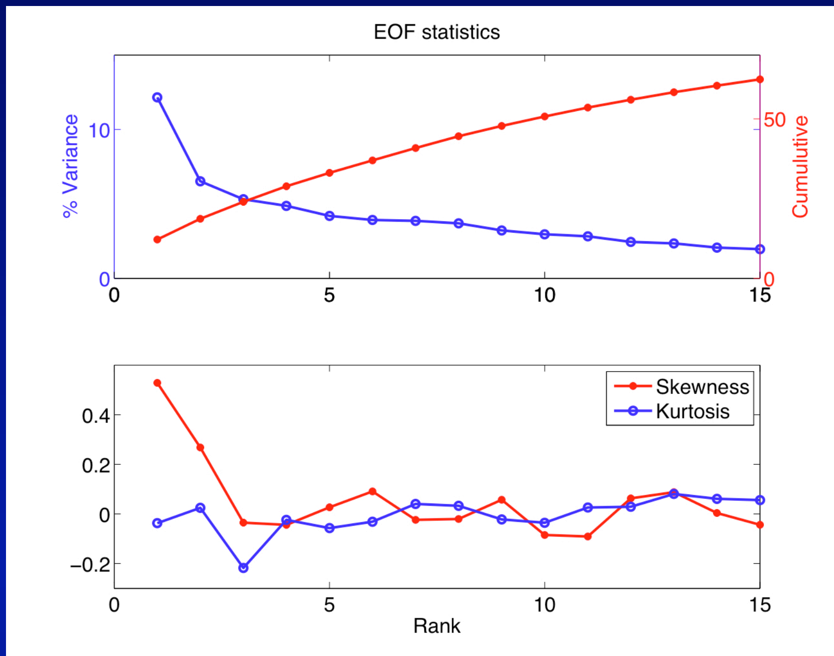
EMR tendencies

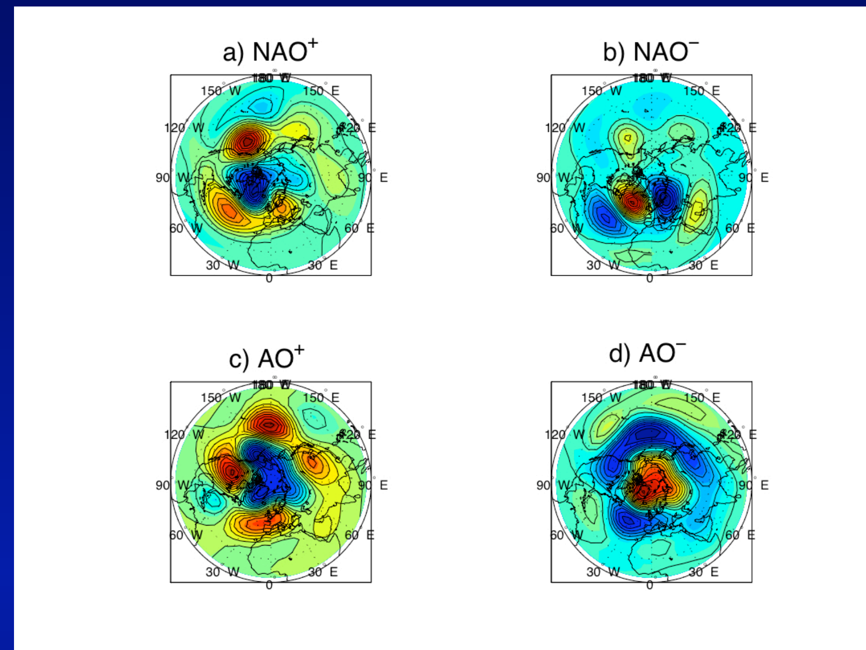


•Linear features for EOF pairs (1-3), (2-3) only: antisymmetric for reflections through the origin; constant speed along ellipsoids (Branstator and Berner, 2005).

- Very good agreement between EMR and QG3!

“Resolved” vs. “Unresolved”?





- It depends on assumptions about ”signal” and ”noise”. We consider EOFs x_i *($i \leq 4$) as ”resolved” because:*

- these EOFs have the most pronounced deviations from the Gaussianity in terms of skewness and kurtosis.

- they determine the most interesting dynamical aspects of LFV; linear (intraseasonal oscillations) as well as nonlinear (regimes) (Kondrashov et al. 2004, 2006).

EMR Tendencies budget

$$\Delta x_i^{(n)} = (N_{ijk} x_j^{(n)} x_k^{(n)} + L_{ij} x_j^{(n)} + F_i)\Delta t + r_i^{(n)} \Delta t$$

For a given x_i $(i \leq 4)$, we split nonlinear interaction $x_j x_k$ as "resolved" (set Ω of (j,k); j,k ≤4):

$$T_R = N_{ijk} x_j, x_k - R_i,$$

$$R_i = < N_{ijk} x_j, x_k >$$

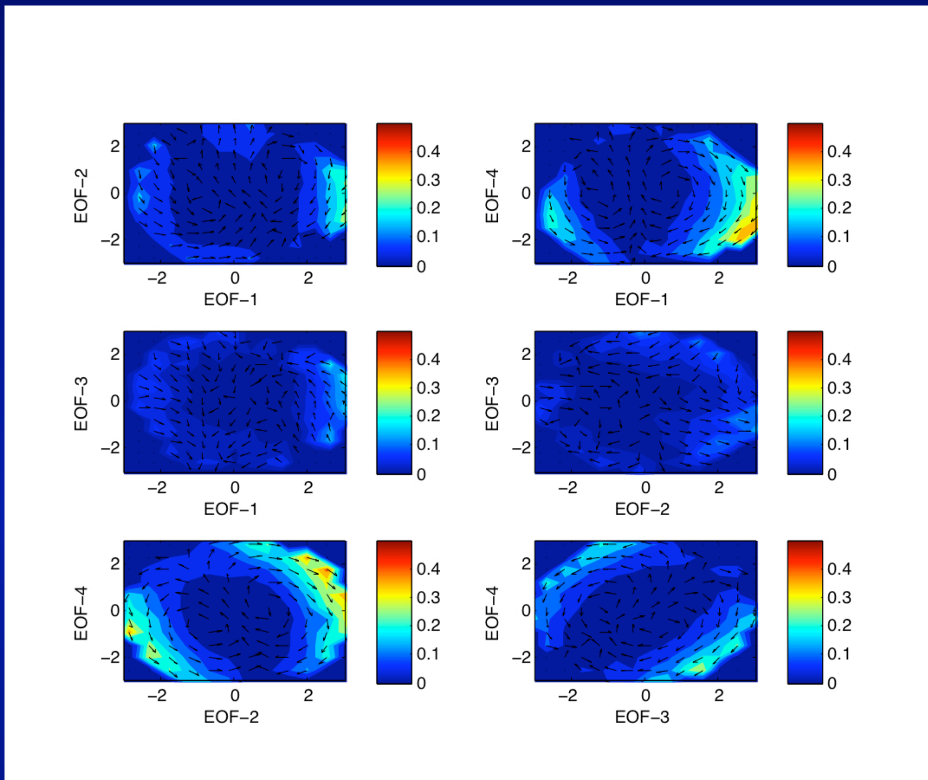
and "unresolved" for $(j,k) \notin \Omega$:

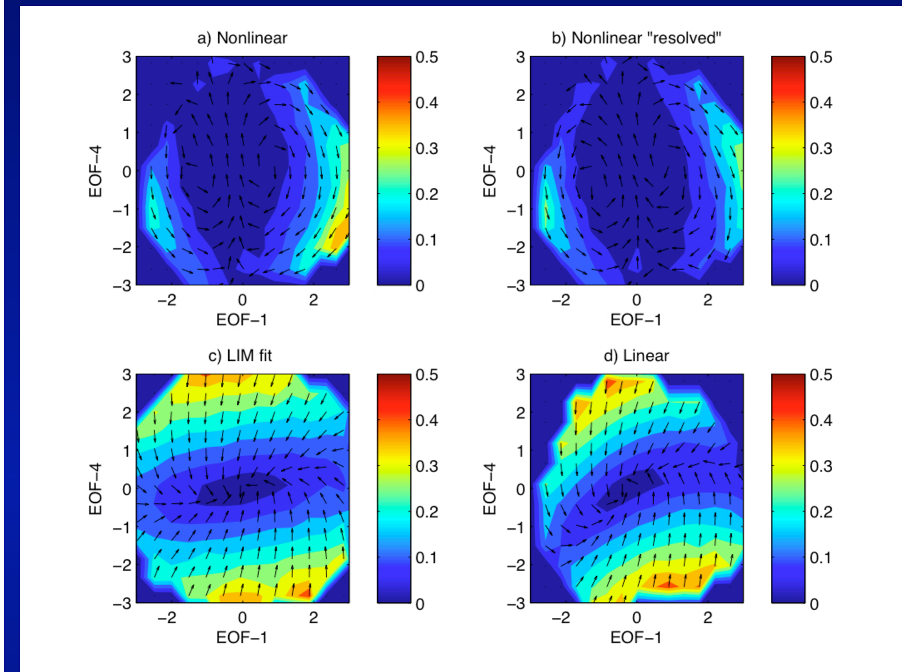
$$T_U = N_{ijk} x_j, x_k + R_i + F_i$$

Since F_i ensures $< dx_i > = 0$: $F_i = - < N_{ijk} x_j, x_k > \;\forall\; j,k$

we have $<T_R> = 0$, $<T_U> = 0$, *and* $<T_R + T_U> = 0$!

EMR Nonlinear Tendencies





- Pronounced nonlinear double swirls for EOF pairs (1-2), (1-4), (2-4) and (3-4).

- The nonlinear ”double-swirl” feature is mostly due to the ”resolved” nonlinear interactions, while the effects of the ”unresolved” modes are small!!

Concluding Remarks – I

- The generalized least-squares approach is well suited to derive nonlinear, reduced models (EMR models) of geophysical data sets; regularization techniques such as PCR and PLS are important ingredients to make it work.

- Easy add-ons, such as seasonal cycle (for ENSO, etc.).

- The dynamic analysis of EMR models provides conceptual insight into the mechanisms of the observed statistics.

Concluding Remarks – II

Possible pitfalls:

- The EMR models are maps: need to have an idea about (time & space) scales in the system and sample accordingly.
- Our EMRs are parametric: functional form is pre-specified, but it can be optimized within a given class of models.
- Choice of predictors is subjective, to some extent, but their number can be optimized.
- Quadratic invariants are not preserved (or guaranteed) – spurious nonlinear instabilities may arise.

References

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