## Utility of state-space reduction in ocean and climate inverse problems

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## **Dynamics of El Niño – Southern Oscillation**





#### **December - February El Niño Conditions**





### **Global Impacts of El Niño**



# Sea Surface Height Anomaly





Altimetry principle from http://www.jason.oceanobs.com/html/alti/principe\_uk.html

## Pacific Ocean tide gauge stations network (from University of Hawaii sea level center)



# **MODIS Scanning Swath**



## **Sea Surface Temperature Anomaly**



9-15 Nov 1997







## ABSTRACT LOG M.3.4.5,

RECOMMENDED BY THE.

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#### GENERAL ORDER.

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## Number of observations in COADS



## Dec 1868: Available observations



Dec 1868

Given a choice, climatologists in general would rather use the righthand panel below than the lefthand one

### Dec 1868: Available observations



Dec 1868: Reconstruction



ec 1868

### Generic problem of the analysis of time-evolving fields



### **Carl Friedrich Gauss**



(1777 - 1855)

### Discovery of least-squares estimation method: 1795

Gauss-Markov Theorem

$$\begin{split} & \mathbf{If} \ \mathcal{T}^o = H\mathcal{T} + \varepsilon, \\ & \langle \varepsilon \rangle = 0, \quad \langle \varepsilon \varepsilon^T \rangle = R, \quad \langle \varepsilon \mathcal{T}^T \rangle = 0, \\ & \mathbf{then} \ \text{the Least Squares Estimate (LSE)} \end{split}$$

$$\hat{\mathcal{T}} = (H^T R^{-1} H)^{-1} H^T R^{-1} \mathcal{T}^o$$

minimizes

$$S[\mathcal{T}] = (H\mathcal{T} - \mathcal{T}^o)^T R^{-1} (H\mathcal{T} - \mathcal{T}^o)$$

and is the **Best<sup>1</sup> Linear Unbiased Estimate (BLUE)** with error covariance

$$P \stackrel{\text{def}}{=} \langle (\mathcal{T} - \hat{\mathcal{T}}) (\mathcal{T} - \hat{\mathcal{T}})^T \rangle = (H^T R^{-1} H)^{-1}.$$

 $\varepsilon$  is normal  $\implies \mathcal{T}$  is a Maximum Likelihood Estimate (MLE)  $\varepsilon$  and  $\mathcal{T}$  are normal  $\implies \mathcal{T}$  is the best among all (not necessarily linear) estimates.

 $^{1} \quad \|\mathcal{T} - \hat{\mathcal{T}}\|_{S}^{2} = \langle (\mathcal{T} - \hat{\mathcal{T}})^{T} S(\mathcal{T} - \hat{\mathcal{T}}) \rangle \longrightarrow \min \quad \forall S \Rightarrow \quad \text{minimal variance}$ 

## To combine various sorts of data: T=(P<sup>-1</sup>+R<sup>-1</sup>)<sup>-1</sup>(P<sup>-1</sup>M+R<sup>-1</sup>D)

Data Assimilation: Optimal Interpolation (OI), Kalman Filter (KF), Optimal Smoother (OS)

# Right on the money



#### GENERAL PROBLEM OF RECONCILING MODELS WITH DATA

$$\mathcal{T}_{n+1} = A_n \mathcal{T}_n + \varepsilon_n^{\mathrm{m}}, \quad n = 1, \dots, N-1$$
$$\mathcal{T}_n^o = H_n \mathcal{T}_n + \varepsilon_n^o, \quad n = 1, \dots, N.$$

$$\langle \varepsilon_n^o \rangle = 0, \quad \langle \varepsilon_n^o \varepsilon_n^{oT} \rangle = R_n, \quad n = 1, \dots, N \langle \varepsilon_{n_1}^o \varepsilon_{n_2}^{oT} \rangle = 0, \quad n_1 \neq n_2, \quad \langle \varepsilon_{n_1}^o \mathcal{T}_{n_2}^T \rangle = 0, \quad n_1, n_2 = 1, \dots, N, \quad \langle \varepsilon_n^m \rangle = 0, \quad \langle \varepsilon_n^m \varepsilon_n^m T \rangle = Q_n, \quad n = 1, \dots, N - 1 \langle \varepsilon_{n_1}^m \varepsilon_{n_2}^m T \rangle = 0, \quad n_1 \neq n_2, \quad \langle \varepsilon_{n_1}^m \mathcal{T}_{n_2}^T \rangle = 0, \quad n_1, n_2 = 1, \dots, N - 1 \quad \langle \varepsilon_{n_1}^o \varepsilon_{n_2}^m T \rangle = 0, \quad n_1 = 1, \dots, N, \qquad n_2 = 1, \dots, N - 1$$

#### MINIMIZATION OF THE FULL COST FUNCTION:

$$\mathbf{S}[\mathcal{T}_1, \mathcal{T}_2, \dots, \mathcal{T}_N] = \sum_{n=1}^N (H_n \mathcal{T}_n - \mathcal{T}_n^o)^T R_n^{-1} (H_n \mathcal{T}_n - \mathcal{T}_n^o) + \sum_{n=1}^{N-1} (\mathcal{T}_{n+1} - A_n \mathcal{T}_n)^T Q_n^{-1} (\mathcal{T}_{n+1} - A_n \mathcal{T}_n)$$

OPTIMAL SMOOTHER (OS) and KALMAN FILTER (KF) "Sweep up" – KF:

$$\hat{\mathcal{T}}_{n}^{a} = \hat{\mathcal{T}}_{n}^{f} + K_{n} \left( \hat{\mathcal{T}}_{n}^{o} - H_{n} \hat{\mathcal{T}}_{n}^{f} \right), \\ \hat{\mathcal{T}}_{n}^{f} = A_{n} \hat{\mathcal{T}}_{n-1}^{a}, \\ K_{n} = P_{n}^{f} H_{n}^{T} \left( H_{n} P_{n}^{f} H_{n}^{T} + R_{n} \right)^{-1} \\ P_{n}^{a} = (I_{M} - K_{n} H_{n}) P_{n}^{f} \\ P_{n}^{f} = A_{n-1} P_{n-1}^{a} A_{n-1}^{T} + Q_{n-1}, \qquad n = 2, 3, \dots, N$$

"Sweep down" – OS:

$$\hat{\mathcal{T}}_n^s = \hat{\mathcal{T}}_n^a + G_n \left( \hat{\mathcal{T}}_{n+1}^s - A_n \hat{\mathcal{T}}_n^a \right), \qquad G_n = P_n^a A_n^T (P_{n+1}^f)^{-1}, P_n^s = P_n^a + G_n \left( P_{n+1}^s - P_{n+1}^f \right) G_n^T, \qquad n = N - 1, \dots, 2, 1$$

## **Example of Optimal Interpolation**

 $T = T_B + e_B$   $HT = T_0 + e_0$   $< e_B > = < e_0 > = < e_B e_0^T > = 0$   $< e_B e_B^T > = C - Hard to know in detaill$  $< e_0 e_0^T > = R$ 

Solution minimizes the cost function  $S[T] = (HT - T_o)^T R^{-1} (HT - T_o) + (T - T_B)^T C^{-1} (T - T_B)$ 

 $T = (H^{T}R^{-1}H + C^{-1})^{-1}(H^{T}R^{-1}T_{o} + C^{-1}T_{B})$ 

Projection of OI solution on eigenvectors of C (EOFs) C=EDET

T = Ea

For simplicity: H=I, R=rI,  $T:=T-T_B$ Then  $a=D(D+R)^{-1}E^TT_o$ 

 $D(D+R)^{-1} = \operatorname{diag}[d_i/(d_i+r)]$ 

In many applications (for spectrally red signals) diagonal elements of this matrix decrease from ~1 to ~0. In effect, the solution is constrained to the subspace spanned by the patterns with d<sub>i</sub>>>r.





Eigenvalue spectrum for global SST: 1951–1991 Same in log–log coordinates

## EOFs of SST (#1.2.3.15.80.120)

### EOF 1 14%



2 0

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### EOF 15 1%

EOF 120 0.02%

### EOF 80 0.1%

## 3 corollaries:

 The first is good: the tail (strongly dampened) modes can be filtered from the solution, i.e. the solution can be effectively approximated by a linear combination of a few leading (only slightly dampened) modes



Reduced space optimal analysis

Successive corrections; Kriging

### SPACE REDUCTION

$$C = E\Lambda E^T + E'\Lambda' E'^T$$
$$\mathcal{T}_n = E\alpha_n + \varepsilon_n^r, \quad n = 1, \dots, N$$

## ESTIMATION PROBLEM IN THE REDUCED SPACE $\mathcal{T}_n^o = H_n E \alpha_n + (H_n \varepsilon_n^r + \varepsilon_n^o) \stackrel{\text{def}}{=} \mathcal{H}_n \alpha_n + \check{\varepsilon}_n^o, \quad n = 1, \dots, N,$

$$\alpha_{n+1} = \mathcal{A}_n \alpha_n + E^T \varepsilon_n^{\mathrm{m}} \stackrel{\mathrm{def}}{=} \mathcal{A}_n \alpha_n + \check{\varepsilon}_n^{\mathrm{m}}, \quad n = 1, \dots, N-1.$$

$$\mathcal{Q}_n = \langle \check{\varepsilon}_n^{\mathrm{m}} \check{\varepsilon}_n^{\mathrm{m}\,T} \rangle = E^T \langle \varepsilon_n^{\mathrm{m}} \varepsilon_n^{\mathrm{m}\,T} \rangle E = E^T Q_n E$$

$$\mathcal{R}_n = \langle \check{\varepsilon}_n^o \check{\varepsilon}_n^{o T} \rangle = \langle (H_n \varepsilon_n^r + \varepsilon_n^o) (H_n \varepsilon_n^r + \varepsilon_n^o)^T \rangle = \\ \langle \varepsilon_n^o \varepsilon_n^{o T} \rangle + H_n \langle \varepsilon_n^r \varepsilon_n^{r T} \rangle H_n^T \stackrel{\text{def}}{=} R_n + H_n Q^r H_n^T \stackrel{\text{def}}{=} R_n + R'_n.$$

### **REDUCED SPACE OPTIMAL ANALYSIS** Cost function:

$$\mathcal{S}[\alpha_1, \alpha_2, \dots, \alpha_N] = \sum_{n=1}^N (\mathcal{H}\alpha_n - \mathcal{T}_n^o)^T \mathcal{R}_n^{-1} (\mathcal{H}\alpha_n - \mathcal{T}_n^o) + \sum_{n=1}^{N-1} (\alpha_{n+1} - \mathcal{A}_n \alpha_n)^T \mathcal{Q}_n^{-1} (\alpha_{n+1} - \mathcal{A}_n \alpha_n).$$

### KF:

$$\begin{aligned} \alpha_n^a &= \alpha_n^f + \mathcal{K}_n \left( \mathcal{T}_n^o - \mathcal{H}_n \alpha_n^f \right), \\ \alpha_n^f &= \mathcal{A}_n \alpha_{n-1}^a, \\ \mathcal{K}_n &= \left( \mathcal{H}_n^T \mathcal{R}_n^{-1} \mathcal{H}_n + \mathcal{P}_n^{f-1} \right)^{-1} \mathcal{H}_n^T \mathcal{R}_n^{-1} \\ \mathcal{P}_n^a &= (I_L - \mathcal{K}_n \mathcal{H}_n) \mathcal{P}_n^f \\ \mathcal{P}_n^f &= \mathcal{A}_{n-1} \mathcal{P}_{n-1}^a \mathcal{A}_{n-1}^T + \mathcal{Q}_{n-1}, \qquad n = 2, 3, \dots, N \end{aligned}$$

### OS:

$$\alpha_n^s = \alpha_n^a + G_n \left( \alpha_{n+1}^s - \mathcal{A}_n \alpha_n^a \right), G_n = \mathcal{P}_n^a \mathcal{A}_n^T (\mathcal{P}_{n+1}^f)^{-1}, \mathcal{P}_n^s = \mathcal{P}_n^a + G_n \left( \mathcal{P}_{n+1}^s - \mathcal{P}_{n+1}^f \right) G_n^T, \qquad n = N-1, \dots, 2, 1$$



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### El Niño of 1877-1878 in analyzed anomalies







RSA\_COADS\_uwnd OI uwnda T=Nov 1877 point mean:  $0.0229419\pm1.4972$  range [-4.8119 to 5.9475] Reduced space (80 EOFs) analysis of COADS uwnd data



#### SLP, mb: Sep 1877-Jan 1878



#### Meridional wind, m/s: Nov 1877



RSA\_COADS\_vwnd OI vwnda T=Nov 1877 point mean: 0.20265 ± 0.96678 range [-3.1376 to 4.5608]





| 1 | 1 10 |    | 1 | 1000 |   |   |
|---|------|----|---|------|---|---|
| 5 | -4   | -2 | 0 | 2    | 4 | 6 |

Cane, M.A., **A. Kaplan**, R.N. Miller, B. Tang, E.C. Hackert, and A.J.Busalacchi, 1996: Mapping tropical Pacific sea level: data assimilation via a reduced state space Kalman filter. *J. Geophys. Res.*, **101**, 22599--22617. Reverdin, G., **A. Kaplan**, and M. Cane, 1996: Sea level from temperature profiles in the tropical Pacific Ocean 1975--1992. *J. Geophys. Res.*, **101**, 18105-18119.

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Evans, M.N. and A. Kaplan, 2004: The Pacific sector Hadley and Walker Circulations in historical marine wind analyses, in *The Hadley Circulation: Present, Past and Future*. H.F.Diaz and R.S. Bradley (Eds.), Kluwer Academic Publishers, Netherland, 239-258.



# 3 corollaries: $\begin{bmatrix} of D(D+R)^{-1} = cliag[d/(d_i+r)] & factor \end{bmatrix}$

The first is good: the solution can be effectively approximated by a linear combination of a few leading modes.
The second is bad: the solution always has less variance than the true field. In fact, C=<TT<sup>T</sup>>+P

# 3 corollaries: $\begin{bmatrix} of D(D+R)^{-1} = diag[ d/(d_i+r) ] & factor \end{bmatrix}$

- The first is good: the solution can be approximated by a few leading modes.
- The second is bad: the solution always has less variance than the true field.
- The third is ugly: the solution is always redder than the truth (because of predominant dampening of tail modes).
   Again, it helps to remember that

 $C = < TT^T > + F$ 



## Take home points

- Spagetti-western properties of least-squares estimates of spectrally red signals: (good) can be approximated by a few modes, (bad) have less variance than the true signal, and (ugly) redder than the true signal.
- These properties can be used for making analyses of sparse climate data cheaper and less ambiguous in their setup.
- Since the effect of these properties is stronger for poor data, and the data quality generally improves with time, use of least-squares analyses at face value, as if they were the truth, poses a threat of misinterpretation.
- A possible way out (however expensive): use of ensembles drawn from the posterior distributions rather than a single ensemble mean.