Lecture 4:
4D-Var Diagnostics

Outline

- Posterior/analysis error estimates
- Consistency checks, hypothesis tests, degrees of freedom & information content
- Array modes
- Clipped analyses

Posterior Error Estimates

Posterior/Analysis Error Estimates

Posterior error covariance:

$$\mathbf{E}^{a} = \left\langle (\mathbf{z}_a - \mathbf{z}_t)(\mathbf{z}_a - \mathbf{z}_t)^{T} \right\rangle$$

$$= \left\langle (\mathbf{z}_b + \delta\mathbf{z}_a - \mathbf{z}_t)(\mathbf{z}_b + \delta\mathbf{z}_a - \mathbf{z}_t)^{T} \right\rangle$$

$$= (\mathbf{I} - \mathbf{KG})\mathbf{D}(\mathbf{I} - \mathbf{KG})^{T} + \mathbf{KRK}^{T}$$

(Caveat: $\mathbf{E}^a$ correct *only if* D and R are correct)

But for dual Lanczos vector formulation:

$$\mathbf{K} \approx \tilde{\mathbf{K}}_k = \mathbf{DG}^{T}\mathbf{R}^{-1/2}\mathbf{V}_k\mathbf{T}_k^{-1}\mathbf{V}_k^{T}\mathbf{R}^{-1/2}$$

Lanczos vectors are orthonormal, and normal to subspace neglected by $\tilde{\mathbf{K}}_k$:

$$\mathbf{E}^{a} \approx \tilde{\mathbf{E}}^{a} = (\mathbf{I} - \tilde{\mathbf{K}}\mathbf{G})\mathbf{D}$$

Posterior/Analysis Error Estimates

Approx. posterior error covariance:

$$\mathbf{E}^{a} \approx \tilde{\mathbf{E}}^{a} = (\mathbf{I} - \tilde{\mathbf{K}}\mathbf{G})\mathbf{D}$$

$$\tilde{\mathbf{E}}^{a} = \underbrace{\left(\mathbf{I} - \mathbf{DG}^{T}\mathbf{R}^{-1/2}\mathbf{V}_k\mathbf{T}_k^{T}\mathbf{V}_k^{T}\mathbf{R}^{-1/2}\mathbf{G}\right)}\mathbf{D}$$

Everything is available during inner-loops of 4D-PSAS and R4D-Var, at no extra cost

$\tilde{\mathbf{E}}^{a} \sim N_{\text{model}} \times N_{\text{model}}$ **HUGE!**

Diagonal elements – *posterior* variances

define POSTERIOR_ERROR_I

Cross-covariance information from EOFs of $\tilde{\mathbf{E}}^{a}$

define POSTERIOR_EOFS

Posterior/Analysis Error Estimates

For the primal formulation:

$$\mathbf{E}^{a} = \left(\mathbf{D}^{-1} + \mathbf{G}^{T}\mathbf{R}^{-1}\mathbf{G}\right)^{-1}$$

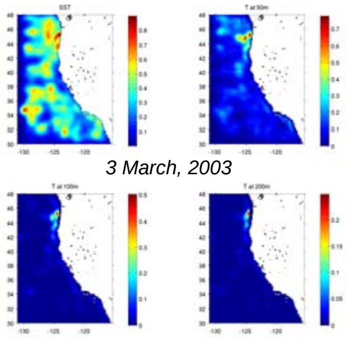
$$\mathbf{E}^{a} \approx \tilde{\mathbf{E}}^{a} = \mathbf{D}^{1/2}\mathbf{V}_k\mathbf{T}_k^{-1}\mathbf{V}_k^{T}\mathbf{D}^{1/2}$$

Straightforward but not yet implemented in ROMS I4D-Var (due to large I/O requirements)

Expected Posterior Error

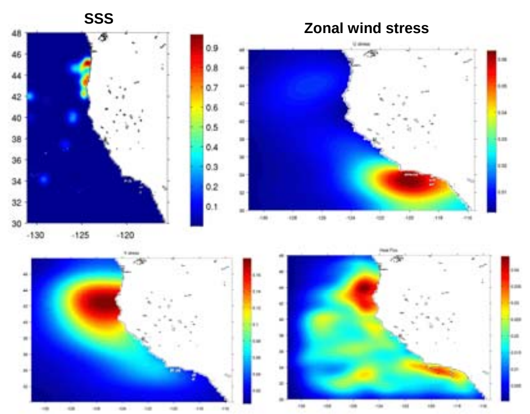
R4D-Var
1 outer-loop
100 inner-loops

3-10 March, 2003
(10km, 42 levels)

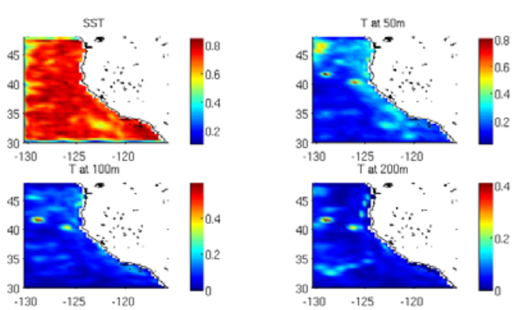


σ_b = prior error std
σ_a = posterior error std

$$(\sigma_b - \sigma_a)/\sigma_b$$



Cautionary Note about E^a Estimates



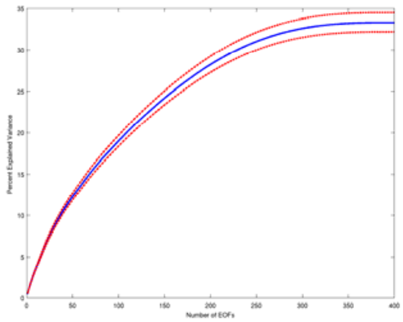
800 Lanczos vectors vs 100 Lanczos vectors (30 km)

$$(\sigma_{800}^2 - \sigma_{100}^2)/\sigma_{100}^2$$

EOF spectrum is quite "flat"

Expected Posterior Error EOFs

Flat spectrum - perhaps due to preconditioning which clusters eigenvalues of ($R^{1/2}GDG^TR^{1/2}$+I) around 1.



Consistency checks, hypothesis tests, degrees of freedom & information content

Consistency Checks in Obs Space

Statistics of the innovation vectors following Desroziers et al (2005):

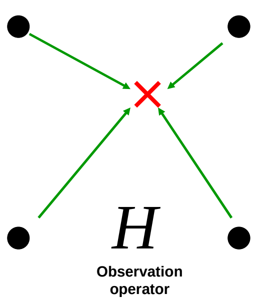
$$\mathbf{d} = (\mathbf{y} - H(\mathbf{x_b}))$$

$$\mathbf{d_a^o} = (\mathbf{y} - H(\mathbf{x_a}))$$

$$\mathbf{d_b^a} = (H(\mathbf{x_a}) - H(\mathbf{x_b}))$$

$$\tilde{\sigma}_b^2 = (\mathbf{d_b^a})^{\mathrm{T}}\mathbf{d} / p$$

$$\tilde{\sigma}_o^2 = (\mathbf{d_a^o})^{\mathrm{T}}\mathbf{d} / p$$



Compare $\tilde{\sigma}_o$ with σ_o & $\tilde{\sigma}_b$ with σ_b

Consistency Checks in Obs Space

Statistics of the innovation vectors following Desroziers et al (2005):

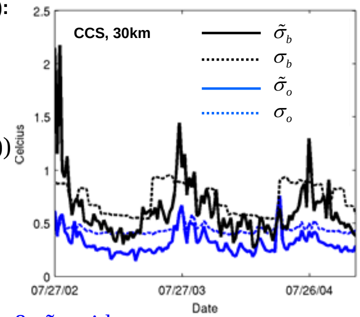
$$\mathbf{d} = (\mathbf{y} - H(\mathbf{x}_\mathrm{b}))$$

$$\mathbf{d}_\mathrm{a}^\mathrm{o} = (\mathbf{y} - H(\mathbf{x}_\mathrm{a}))$$

$$\mathbf{d}_\mathrm{b}^\mathrm{a} = (H(\mathbf{x}_\mathrm{a}) - H(\mathbf{x}_\mathrm{b}))$$

$$\tilde{\sigma}_b^2 = (\mathbf{d}_\mathrm{b}^\mathrm{a})^\mathrm{T}\mathbf{d}/p$$

$$\tilde{\sigma}_o^2 = (\mathbf{d}_\mathrm{a}^\mathrm{o})^\mathrm{T}\mathbf{d}/p$$



Compare $\tilde{\sigma}_o$ with σ_o & $\tilde{\sigma}_b$ with σ_b

Hypothesis Tests &Degrees of Freedom

Recall that the optimal increments minimize:

$$J = \underbrace{\frac{1}{2}\delta\mathbf{z}^T\mathbf{D}^{-1}\delta\mathbf{z}}_{J_b} + \underbrace{\frac{1}{2}\left(\mathbf{G}\delta\mathbf{z} - \mathbf{d}\right)^T\mathbf{R}^{-1}\left(\mathbf{G}\delta\mathbf{z} - \mathbf{d}\right)}_{J_o}$$

Theoretical min: $J_\mathrm{min} = N_\mathrm{obs}/2$

No. of dof in obs $\longrightarrow (J_b)_\mathrm{min} = \mathrm{Tr}(\mathbf{KG})/2$

No. of dof in *prior* $\longrightarrow (J_o)_\mathrm{min} = \left(N_\mathrm{obs} - \mathrm{Tr}(\mathbf{KG})\right)/2$

"dof" – degrees of freedom

(Bennett et al, 1993; Cardinali et al, 2004; Desroziers et al., 2009)

Degrees of Freedom & Information Content

Degrees of freedom in the obs:

$$(J_b)_\mathrm{min} = \mathrm{Tr}(\mathbf{KG})/2$$

But for $m = N_{obs}$**:**

$$\mathbf{K} = \mathbf{D}\mathbf{G}^\mathrm{T}\mathbf{R}^{-1/2}\mathbf{V}_m\mathbf{T}_m^{-1}\mathbf{V}_m^\mathrm{T}\mathbf{R}^{-1/2}$$

So:

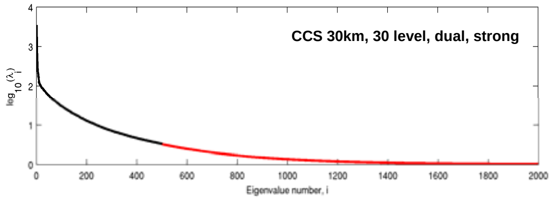
$$(J_b)_\mathrm{min} = \frac{1}{2}(N_{obs} - \mathrm{Tr}(\mathbf{T}_m^{-1}))$$

$$= \frac{1}{2}\left(N_{obs} - \sum_{i=1}^{N_{obs}} \boxed{\lambda_i^{-1}}\right)$$

Eigenvalues of $\mathbf{T}_m^{-1}$

Degrees of Freedom & Information Content

(LhessianEV=T, s4dvar.in)

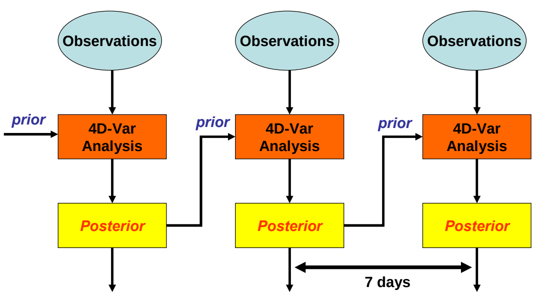


Computed directly during R4D-Var

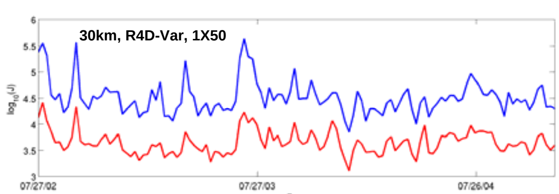
Computed from a curve fit

$$\log_{10}(\lambda_i) = ae^{-bi},\ a = 1.684,\ b = 2.7\times10^{-3}$$

Sequential 4D-Var with 30km CCS ROMS



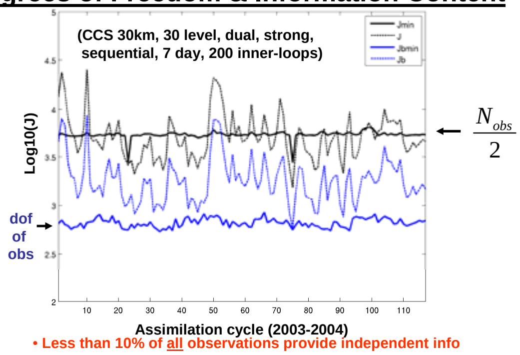
Sequential 4D-Var CCS ROMS



J initial

J final

Degrees of Freedom & Information Content



- Less than 10% of <u>all</u> observations provide independent info
- LOTS OF REDUNDANCY!
- $J_b > (J_b)_{min}$ and indicates over fitting to the obs
- $J \neq J_{min}$ and indicates that *prior* hypotheses are incorrect

Array Modes

The eigenvalues λ_i of T_m are also the eigenvalues of $(\mathbf{R}^{1/2}\mathbf{G}\mathbf{D}\mathbf{G}^T\mathbf{R}^{1/2}+\mathbf{I})$, the preconditioned "stabilized representer matrix."

Consider the eigenpairs: $(\lambda_i, \hat{\mathbf{w}}_i)$

Following Bennett (1985):

$$\delta\mathbf{x}_a(t) = \mathcal{R}(t)\mathbf{R}^{-1/2}\mathbf{W}\mathbf{\Lambda}^{-1}\mathbf{W}^T\mathbf{R}^{-1/2}\mathbf{d}$$

$$= \sum_{i=1}^{N_{obs}} \lambda_i^{-1}\left(\hat{\mathbf{w}}_i^T\mathbf{R}^{-1/2}\mathbf{d}\right)\mathbf{\Psi}_i(t)$$

Analysis state-vector increment

$$\mathbf{\Psi}_i(t) = \sum_{j=1}^{N_{obs}} w'_{ji}\mathbf{r}_j(t)$$

"array modes"

$$\mathbf{w}'_i = (w'_{ji}) = \mathbf{R}^{-1/2}\hat{\mathbf{w}}_i$$

Array Modes

State-vector analysis increment:

$$\delta\mathbf{x}_a(t) = \sum_{i=1}^{N_{obs}} \boxed{\lambda_i^{-1}}\left(\hat{\mathbf{w}}_i^T\mathbf{R}^{-1/2}\mathbf{d}\right)\mathbf{\Psi}_i(t)$$

Largest eigenvalue λ_1 associated with Ψ_1(t), nominally contributes least to analysis increment.

Thus Ψ_1(t) represents the most stable component of $\delta\mathbf{x}_a$ with respect to changes in **d**.

Array modes can be readily computed after dual 4D-Var:

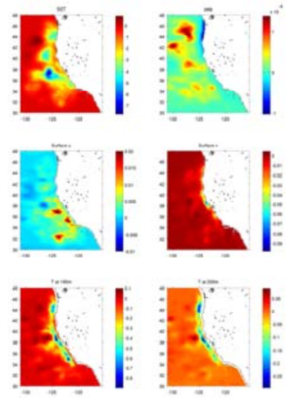
$$\mathbf{\Psi}_j(t) = \mathcal{M}_b(t,t_0)\mathbf{D}\mathbf{G}^T\mathbf{R}^{-1/2}\hat{\mathbf{w}}_j$$

(define ARRAY_MODES)

Example:

CCS, 10km
R4D-Var
3-7 March, 2003

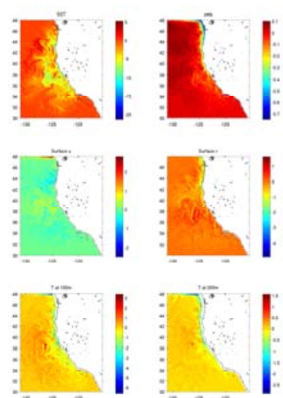
Ψ_1 3 March



Example:

CCS, 10km
R4D-Var
3-7 March, 2003

Ψ_1 7 March

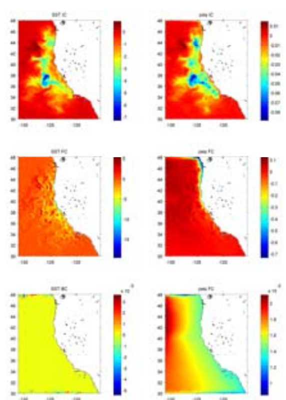


Example:

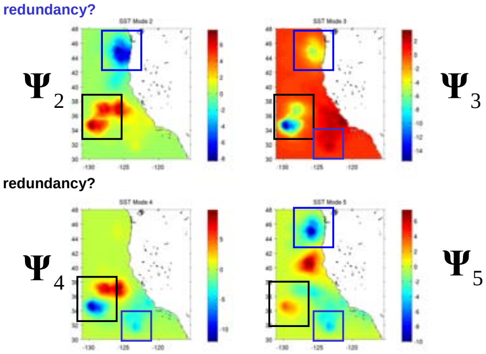
CCS, 10km
R4D-Var
3-7 March, 2003

Ψ_1 3 March

Control vector contributions



Array Mode SST: 3 March



Clipped Analyses

Following Bennett (1985)

$$\delta \mathbf{x}_{\mathbf{a}}(t) = \sum_{i=1}^{M} \lambda_i^{-1} \left(\hat{\mathbf{w}}_i^{\mathrm{T}} \mathbf{R}^{-1/2} \mathbf{d} \right) \boldsymbol{\Psi}_i(t)$$

Truncate ("clip") the summation, discarding array modes Ψ_i for $i>M$

M is based on a criteria that reflects information content (*i.e.* $\lambda_i<\alpha\lambda_1$ for $i>M$).

α chosen so Ψ_i have scales < model resolution for $i>M$

Clipping using Indirect Representer Algorithm

Clipped analyses can be computed AFTER running R4D-Var or 4D-PSAS by exploiting the indirect representer algorithm according to:

$$\delta \mathbf{x}_{\mathbf{a}}(t) = \mathcal{M}_{\mathbf{b}}(t,t_0)\mathbf{D}\mathbf{G}^{\mathrm{T}} \sum_{i=1}^{M} \lambda_i^{-1} \left(\hat{\mathbf{w}}_i^{\mathrm{T}} \mathbf{R}^{-1/2} \mathbf{d} \right) \hat{\mathbf{w}}_i$$

where $\mathcal{M}_{\mathbf{b}}(t,t_0)$ is TLROMS linearized about the *prior*/background.

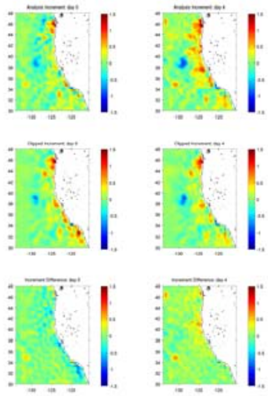
(Moore et al, 2010b)

<u>Example</u>:
CCS, 30km
R4D-Var
3-7 March, 2003
1 outer-loop
800 inner-loops

Clipped using
"1% rule" of
Bennett & McIntosh
(1985)

Discard Ψ_i for which

$$\lambda_i < 0.01\lambda_1$$
$$M = 255$$



<u>Issues, Things to do, & Coming Soon</u>

- *Posterior* error estimates available for 4D-PSAS & R4D-Var
  - available soon for I4D-Var
- *Posterior* error estimates are likely <u>over estimates</u> due to span of observation or model space by Lanczos vectors
- $(4D\text{-Var})^T$ provides more reliable estimates (Lecture 5)

Summary

- Posterior error estimates available via the utility afforded by the Lanczos algorithm.
- Posterior errors tend to be overestimates since $m \ll N_{obs}$
- Consistency checks and hypothesis tests are useful indicators of validity of *prior* hypotheses and info content.
- Array modes provide info about possible data redundancy.
- Clipping can remove unphysical features from analyses.

References

- Bennett, A.F., 1985: Array design by inverse methods. *Prog. Oceanog.*, **15**, 129-156.
- Bennett, A.F. and P.C. McIntosh, 1982: Open ocean modelling as an inverse problem: tidal theory. *J. Phys. Oceanogr.*, **12**, 1004-1018.
- Bennett, A.F., L. Leslie, C. Hagelberg and P. Powers, 1993: Tropical cyclone prediction using a barotropic model initialized by a generalized inverse method. *Mon. Wea. Rev.*, **121**, 1714-1729.
- Cardinali, C., S. Pezzulli and E. Andersson, 2004: Influence-matrix diagnostic of a data assimilation system. *Q. J. R. Meteorol. Soc.*, **130**, 2767-2786.
- Desroziers, G., L. Berre, B. Chapnik and P. Poli, 2005: Diagnosis of observation, background and analysis-error statistics in observation space. *Q. J. R. Meteorol. Soc.*, **131**, 3385-3396.
- Desroziers, G., L. Berre, V. Chabot and B. Chapnik, 2009: A posteriori diagnostics in an ensemble of perturbed analyses. *Mon. Wea. Rev.*, **137**, 3420-3436.

References

- Moore, A.M., H.G. Arango, G. Broquet, B.S. Powell, J. Zavala-Garay and A.T. Weaver, 2010a: The Regional Ocean Modeling System (ROMS) 4-dimensional data assimilation systems: Part I – System overview. *Ocean Modelling*, Submitted.
- Moore, A.M., H.G. Arango, G. Broquet, C.. Edwards, M. Veneziani, B.S. Powell, D. Foley, J. Doyle, D. Costa and P. Robinson, 2010b: The Regional Ocean Modeling System (ROMS) 4-dimensional data assimilation systems: Part II – Performance and application to the California Current System. *Ocean Modelling*, Submitted.