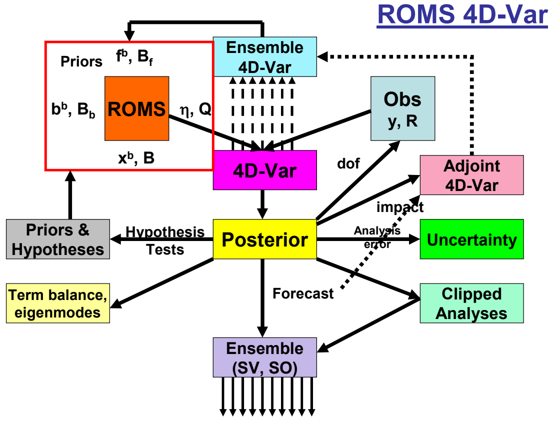
Lecture 1:
Primal 4D-Var

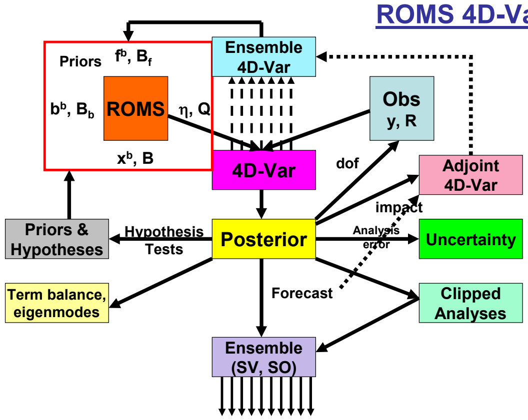
Outline

- ROMS 4D-Var overview
- 4D-Var concepts
- Primal formulation of 4D-Var
- Incremental approach used in ROMS
- The ROMS I4D-Var algorithm

ROMS 4D-Var



ROMS 4D-Var



ROMS 4D-Var Applications

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- Zhang, W.G., J.L. Wilkin, and J.C. Levin, 2010: Towards an integrated observation and modeling system in the New York Bight using variational methods, Part I. *Ocean Modelling,* Under review.
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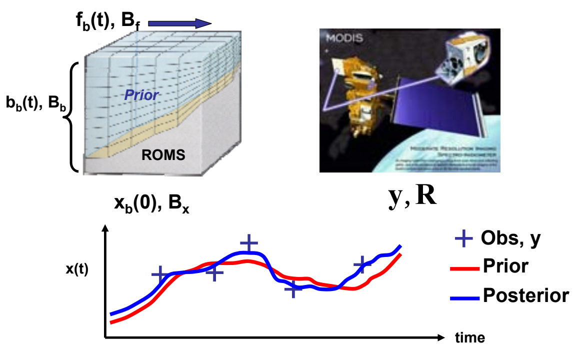
Data Assimilation



Model solutions depends on $x_b(0)$, $f_b(t)$, $b_b(t)$, $\eta(t)$

Notation & Nomenclature

$$\mathbf{x} = \begin{bmatrix} \mathbf{T} \\ \mathbf{S} \\ \boldsymbol{\zeta} \\ \mathbf{u} \\ \mathbf{v} \end{bmatrix} \quad \mathbf{z} = \begin{bmatrix} \mathbf{x}(0) \\ \mathbf{f}(t) \\ \mathbf{b}(t) \\ \boldsymbol{\eta}(t) \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ \vdots \\ y_N \end{bmatrix} \quad \mathbf{d} = \left(\mathbf{y} - H(\mathbf{x}_\mathrm{b})\right)$$

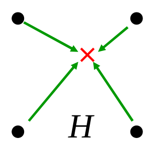
State vector

Control vector

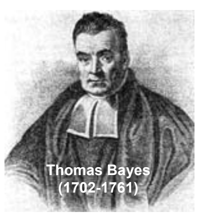
Observation vector

Prior

Innovation vector



Observation operator



Bayes Theorem

Conditional probability: (Wikle and Berliner, 2007)

$$p(\mathbf{z}\,|\,\mathbf{y}) = p(\mathbf{y}\,|\,\mathbf{z})\,p(\mathbf{z}) / p(\mathbf{y})$$

Posterior distribution | Data distribution ("likelihood") | Prior | Marginal

$$= c\ \exp\left(-1/2\left(\mathbf{y} - H(\mathbf{x})\right)^\mathrm{T} \mathbf{R}^{-1} \left(\mathbf{y} - H(\mathbf{x})\right)\right)$$

$$\times\ \exp\left(-1/2\left(\mathbf{z} - \mathbf{z}_\mathrm{b}\right)^\mathrm{T} \mathbf{D}^{-1} \left(\mathbf{z} - \mathbf{z}_\mathrm{b}\right)\right)$$

Maximum likelihood estimate: identify the minimum of

$$J_{NL}(\mathbf{z}) = \frac{1}{2}(\mathbf{z} - \mathbf{z}_\mathrm{b})^\mathrm{T} \mathbf{D}^{-1} (\mathbf{z} - \mathbf{z}_\mathrm{b}) + \frac{1}{2}(\mathbf{y} - H(\mathbf{x}))^\mathrm{T} \mathbf{R}^{-1} (\mathbf{y} - H(\mathbf{x}))$$

which maximizes $p(\mathbf{z}|\mathbf{y})$.

Variational Data Assimilation

Conditional Probability: $P(\mathbf{z}\,|\,\mathbf{y}) \propto \exp\left(-J_{NL}\right)$

$$J_{NL}(\mathbf{z}) = \frac{1}{2}(\mathbf{z}-\mathbf{z}_b)^T \mathbf{D}^{-1}(\mathbf{z}-\mathbf{z}_b) + \frac{1}{2}(\mathbf{y}-H(\mathbf{x}))^T \mathbf{R}^{-1}(\mathbf{y}-H(\mathbf{x}))$$

Observation error covariance

$$\mathbf{D} = \underbrace{\mathrm{diag}(\mathbf{B}_x, \mathbf{B}_b, \mathbf{B}_f, \mathbf{Q})}$$

Background error covariance

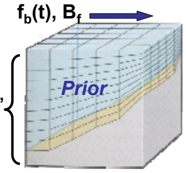
J_{NL} is called the "cost" or "penalty" function.

Problem: Find $z=z_a$ that minimizes *J (i.e. maximizes P)* using principles of variational calculus.
z_a is the "maximum likelihood" or "minimum variance" estimate.

Incremental Formulation

$f_b(t)$, B_f

$b_b(t)$, B_b



$x_b(0)$, B_x

$$\delta\mathbf{z} = (\delta\mathbf{x}^T(0), \boldsymbol{\varepsilon}_b^T(t), \boldsymbol{\varepsilon}_f^T(t), \boldsymbol{\eta}(t))^T$$

initial condition increment; boundary condition increment; forcing increment; corrections for model error

(Courtier *et al.*, 1994)

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

$$\mathbf{D} = \underbrace{\mathrm{diag}(\mathbf{B}_x, \mathbf{B}_b, \mathbf{B}_f, \mathbf{Q})}$$

Prior (background) error covariance

Tangent Linear Model sampled at obs points

Obs Error Cov.

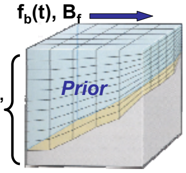
Innovation $\mathbf{d} = \mathbf{y} - H(\mathbf{x}_b)$

(H=linearized obs operator)

Incremental Formulation

$f_b(t)$, B_f

$b_b(t)$, B_b



$x_b(0)$, B_x

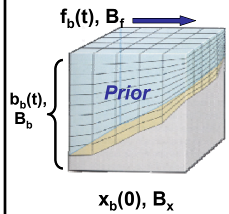
$$\delta\mathbf{z} = (\delta\mathbf{x}^T(0), \boldsymbol{\varepsilon}_b^T(t), \boldsymbol{\varepsilon}_f^T(t), \boldsymbol{\eta}(t))^T$$

initial condition increment; boundary condition increment; forcing increment; corrections for model error

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

The minimum of *J* is identified iteratively by searching for *∂J/∂δz=0*

Incremental Formulation



$$\delta\mathbf{z} = (\delta\mathbf{x}^T(0), \boldsymbol{\varepsilon}_b^T(t), \boldsymbol{\varepsilon}_f^T(t), \boldsymbol{\eta}(t))^T$$

initial condition increment; boundary condition increment; forcing increment; corrections for model error

$$\mathbf{z} = \mathbf{z}_b + \delta\mathbf{z}$$

Assumptions:

(i) $\delta\mathbf{z} \ll \mathbf{z}_b$

(ii) $\mathbf{x}(t)=\mathbf{x}_b(t)+\delta\mathbf{x}(t)$

(iii) $\delta\mathbf{x}(t) \simeq \mathbf{M}\delta\mathbf{z}$

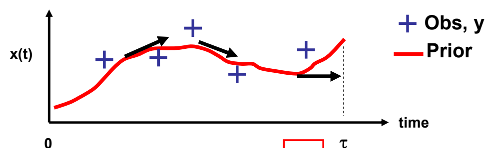
(iv) $\mathbf{H} * \delta\mathbf{x}(t) \simeq \mathbf{H} * \mathbf{M}\delta\mathbf{z} = \mathbf{G}\delta\mathbf{z}$

$\mathbf{M}$ = Tangent Linear Model

$\mathbf{H}$ = Tangent Linear H

The Tangent Linear Model

(TLROMS)



Prior is solution of model: $\mathbf{x}_b(t_i) = \mathcal{M}(\mathbf{x}_b(t_{i-1}), \mathbf{f}_b(t_i), \mathbf{b}_b(t_i))$

Nonlinear model

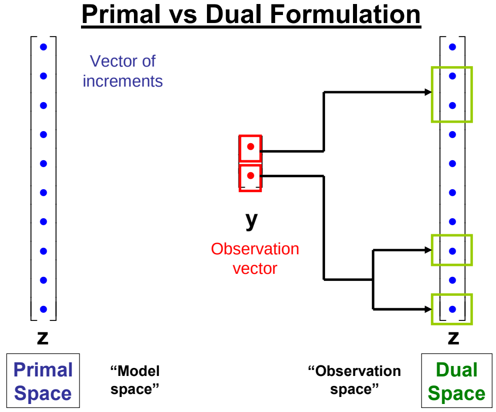
Increment: $\delta\mathbf{x}(t) \ll \mathbf{x}_b(t);\ \ \delta\mathbf{f}(t) \ll \mathbf{f}_b(t)$; etc

$$\mathbf{x}(t_i) = \mathcal{M}(\mathbf{x}_b(t_{i-1}) + \delta\mathbf{x}(t_{i-1}), \cdots)$$

$$\simeq \mathcal{M}(\mathbf{x}_b(t_{i-1}), \cdots) + \mathbf{M}_{\mathbf{x}_b}\delta\mathbf{z}$$

Tangent linear model

Primal vs Dual Formulation



The Solution

Analysis: $\mathbf{z_a} = \mathbf{z_b} + \mathbf{Kd}$

Gain matrix (dual form):

$$\mathbf{K} = \mathbf{DG}^{\mathrm{T}}(\mathbf{GDG}^{\mathrm{T}} + \mathbf{R})^{-1}$$

Gain matrix (primal form):

$$\mathbf{K} = (\mathbf{D}^{-1} + \mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{G})^{-1}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}$$

Two Spaces

Gain (dual):

$$\mathbf{K} = \mathbf{DG}^{\mathrm{T}}\underbrace{(\mathbf{GDG}^{\mathrm{T}} + \mathbf{R})}_{N_{\mathrm{obs}} \times N_{\mathrm{obs}}}{}^{-1}$$

Gain (primal):

$$\mathbf{K} = \underbrace{(\mathbf{D}^{-1} + \mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{G})}_{N_{\mathrm{model}} \times N_{\mathrm{model}}}{}^{-1}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}$$

$N_{\mathrm{obs}} \ll N_{\mathrm{model}}$

Two Spaces

G maps from model space
to observation space

$\mathbf{G}^{\mathrm{T}}$ maps from observation space
to model space

Iterative Solution of Primal Formulation

(define IS4DVAR, is4dvar_ocean.h)

Recall the incremental cost function:

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

At the minimum of J we have $\partial J/\partial\delta\mathbf{z}=\mathbf{0}$

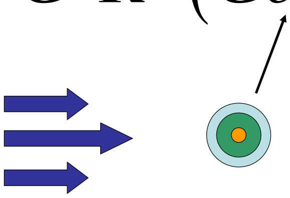
$$\partial J/\partial\delta\mathbf{z} = \mathbf{D}^{-1}\delta\mathbf{z}+\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\left(\mathbf{G}\delta\mathbf{z}-\mathbf{d}\right)$$

Given J and $\partial J/\partial\delta\mathbf{z}$, we can identify the $\delta\mathbf{z}$ that minimizes J

Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\left(\mathbf{G}\delta\mathbf{z}-\mathbf{d}\right)$$



Zonal shear flow

Matrix-less Operations

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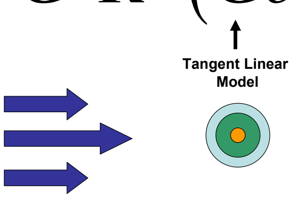


Zonal shear flow

Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{G}^{T}\mathbf{R}^{-1}\left(\mathbf{G}\delta\mathbf{z}-\mathbf{d}\right)$$

↑ Tangent Linear Model

Zonal shear flow

Matrix-less Operations

There are no matrix multiplications!

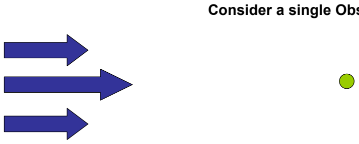
$$\mathbf{G}^{T}\mathbf{R}^{-1}\left(\underbrace{\mathbf{G}\delta\mathbf{z}-\mathbf{d}}_{\text{Consider a single Observation}}\right)$$

Zonal shear flow

Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{G}^{T}\mathbf{R}^{-1}\left(\underbrace{\mathbf{G}\delta\mathbf{z}-\mathbf{d}}_{\text{Consider a single Observation}}\right)$$



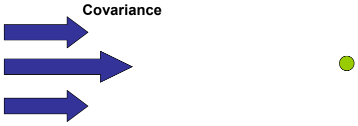
Zonal shear flow

Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{G}^{T}\mathbf{R}^{-1}\left(\mathbf{G}\delta\mathbf{z}-\mathbf{d}\right)$$

↑ Inverse Obs Error Covariance



Zonal shear flow

Matrix-less Operations

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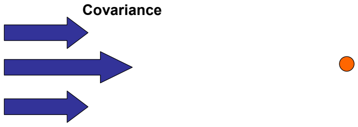


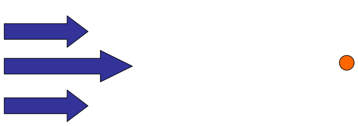
Zonal shear flow

Matrix-less Operations

There are no matrix multiplications!

$$\mathbf{G}^{T}\mathbf{R}^{-1}\left(\mathbf{G}\delta\mathbf{z}-\mathbf{d}\right)$$

↑ Adjoint Model

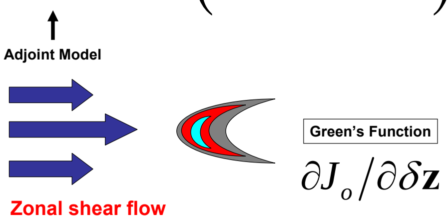


Zonal shear flow

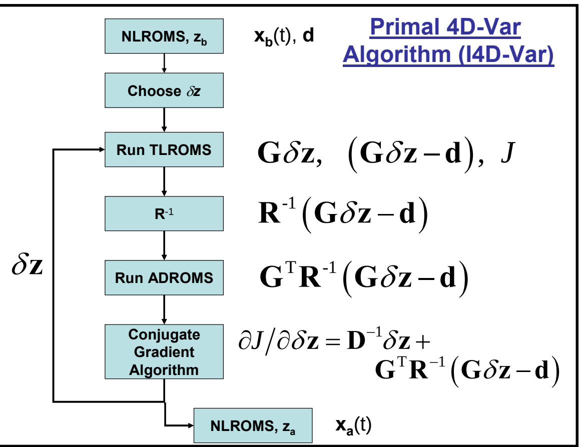
Matrix-less Operations

There are no matrix multiplications!

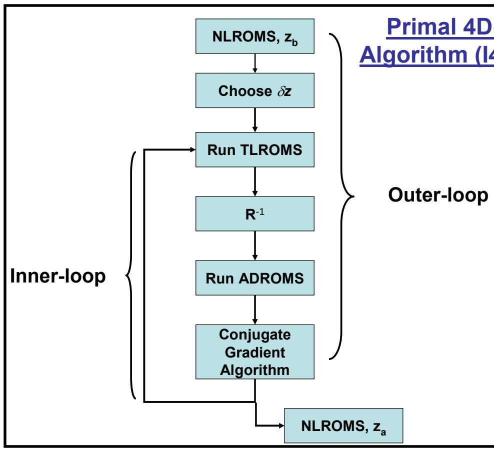
$$\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\left(\mathbf{G}\delta\mathbf{z}-\mathbf{d}\right)$$



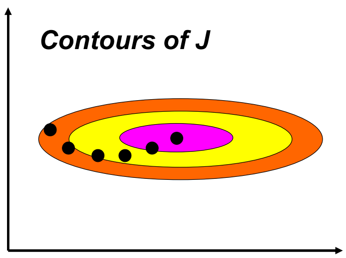
Primal 4D-Var Algorithm (I4D-Var)



Primal 4D-Var Algorithm (I4D-Var)



Conjugate Gradient (CG) Methods



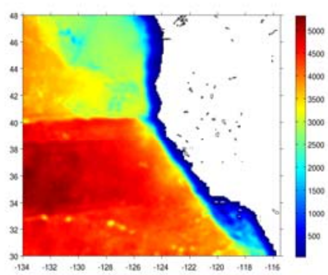
An Example: ROMS CCS

COAMPS forcing $f_b(t)$, B_f

ECCO open boundary conditions $b_b(t)$, B_b

$x_b(0)$, B_x

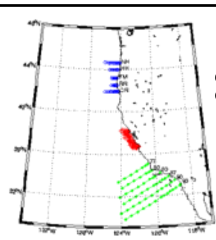
Previous assimilation cycle



30km, 10 km & 3 km grids, 30- 42 levels

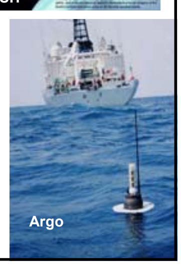
Veneziani et al (2009)
Broquet et al (2009)
Moore et al (2010)

Observations (y)



CalCOFI & GLOBEC

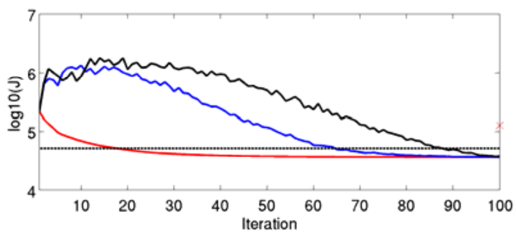
Ingleby and Huddleston (2007)



4D-Var Configuration

- Case studies for a representative case 3-10 March, 2003.
- 1 outer-loop, 100 inner-loops
- 7 day assimilation window
- *Prior* **D**: **x** L_h=50 km, L_v=30m, σ from clim
  f L_τ=300km, L_Q=100km, σ from COAMPS
  b L_h=100 km, L_v=30m, σ from clim
- Super observations formed
- Obs error **R** (diagonal):
  SSH 2 cm
  SST 0.4 C
  hydrographic 0.1 C, 0.01psu

4D-Var Performance



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

- **Primal, strong**
- **Dual, strong**
- **Dual, weak**
- **Jmin**

Summary

- Strong constraint incremental 4D-Var, primal formulation:
  define IS4DVAR
  Drivers/is4dvar_ocean.h
- Matrix-less iterations to identify cost function minimum using TLROMS and ADROMS

References

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