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**: f^b, B_f, b^b, B_b, x^b, B
- **Priors**: f^b, B_f
- **Ensemble 4D-Var**: η, Q
- **4D-Var**: x^b, B
- **Observation**: y, R
- **Adjoint 4D-Var**: dof
- **Impact**: 4D-Var
- **Term balance, eigenmodes**: Priors & Hypotheses
- **Hypothesis Tests**: Posterior
- **Uncertainty**: Analysis error
- **Forecast**: Clipped Analyses
ROMS 4D-Var

Priors: \( f^b, B_f \)

ROMS: \( b^b, B_b \)

\( x^b, B \)

\( \eta, Q \)

Ensemble 4D-Var

Obs: \( y, R \)

Hypothesis Tests

Posterior

Forecast

Uncertainty

Analysis error

Clipped Analyses

Term balance, eigenmodes

Priors & Hypotheses

Ensemble (SV, SO)

4D-Var

Adjoint 4D-Var

Impact

dof

Impact Term balance, eigenmodes

Analysis error
ROMS 4D-Var Applications

Data Assimilation

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

ROMS

Prior

$y, R$

Prior

Posterior

Obs, $y$

$\mathbf{f}_b(t), \mathbf{B}_f$

$b_b(t), \mathbf{B}_b$

$x_b(0), \mathbf{B}_x$
Notation & Nomenclature

\[
x = \begin{bmatrix} T \\ S \\ \zeta \\ u \\ v \end{bmatrix} \quad z = \begin{bmatrix} x(0) \\ f(t) \\ b(t) \\ \eta(t) \end{bmatrix} \quad y = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} \quad d = (y - H(x_b))
\]

State vector  Control vector  Observation vector

Prior

Innovation vector

Observation operator
Thomas Bayes (1702-1761)
Bayes Theorem

Conditional probability:

\[
p(z \mid y) = \frac{p(y \mid z)p(z)}{p(y)}
\]

Posterior distribution  Data distribution  Prior  Marginal

("likelihood")

\[
= c \exp\left(-\frac{1}{2} (y - H(x))^T R^{-1} (y - H(x))\right) \\
\times \exp\left(-\frac{1}{2} (z - z_b)^T D^{-1} (z - z_b)\right)
\]

Maximum likelihood estimate: identify the minimum of

\[
J_{NL}(z) = \frac{1}{2} (z - z_b)^T D^{-1} (z - z_b) + \frac{1}{2} (y - H(x))^T R^{-1} (y - H(x))
\]

which maximizes \(p(z \mid y)\).

(Wikle and Berliner, 2007)
**Variational Data Assimilation**

**Conditional Probability:** \( P(z \mid y) \propto \exp(-J_{NL}) \)

\[
J_{NL}(z) = \frac{1}{2} (z - z_b)^T D^{-1} (z - z_b) + \frac{1}{2} (y - H(x))^T R^{-1} (y - H(x))
\]

\( D = \text{diag}(B_x, B_b, B_f, Q) \)

\( J_{NL} \) is called the “cost” or “penalty” function.

**Observation error covariance**

**Background error covariance**

**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

\[ \delta z = (\delta x^T(0), \varepsilon_b^T(t), \varepsilon_f^T(t), \eta(t))^T \]

- Initial condition increment
- Boundary condition increment
- Forcing increment
- Corrections for model error

(Courtier et al., 1994)

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

- Tangent Linear Model
- Linearized obs operator
- Sampled at obs points
- Error Cov.
- Innovation
- (H=linearized obs operator)

Prior (background) error covariance

Prior, \( b_b(t), B_b \)

\( f_b(t), B_f \)
Incremental Formulation

\[ \delta z = \left( \delta x^T(0), \varepsilon_b^T(t), \varepsilon_f^T(t), \eta(t) \right)^T \]

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

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

The minimum of \( J \) is identified iteratively by searching for \( \partial J / \partial \delta z = 0 \)
**Incremental Formulation**

\[ \delta z = (\delta x^T (0), \varepsilon_b^T (t), \varepsilon_f^T (t), \eta(t))^T \]

- **Assumptions:**
  1. \( \delta z \ll z_b \)
  2. \( x(t) = x_b(t) + \delta x(t) \)
  3. \( \delta x(t) \approx M \delta z \)
  4. \( H \star \delta x(t) \approx H \star M \delta z = G \delta z \)

**Prior**

\[ (x_b(0), B_x) \]

\[ (f_b(t), B_f) \]

- **Initial condition increment**
- **Boundary condition increment**
- **Forcing increment**
- **Corrections for model error**

\[ Z = Z_b + \delta z \]
The Tangent Linear Model (TLROMS)

Prior is solution of model: \( x_b(t_i) = M(x_b(t_{i-1}), f_b(t_i), b_b(t_i)) \)

Increment: \( \delta x(t) \ll x_b(t); \quad \delta f(t) \ll f_b(t); \) etc

\[
\begin{align*}
x(t_i) &= M(x_b(t_{i-1}) + \delta x(t_{i-1}), \cdots) \\
&\approx M(x_b(t_{i-1}), \cdots) + M_{x_t} \delta z 
\end{align*}
\]

Tangent linear model

Obs, y

Prior

Nonlinear model

\( x(t) \)

0

time

 Prior
Primal vs Dual Formulation

Vector of increments

Z

Primal Space

“Model space”

y

Observation vector

Z

“Observation space”

Dual Space
The Solution

Analysis: \[ Z_a = Z_b + Kd \]

Gain matrix (dual form):
\[ K = DG^T (GDG^T + R)^{-1} \]

Gain matrix (primal form):
\[ K = (D^{-1} + G^T R^{-1} G)^{-1} G^T R^{-1} \]
Two Spaces

Gain (dual):

\[ K = DG^T (GDG^T + R)^{-1} \]

Gain (primal):

\[ K = (D^{-1} + G^T R^{-1} G)^{-1} G^T R^{-1} \]

\[ N_{\text{obs}} \times N_{\text{obs}} \]

\[ N_{\text{model}} \times N_{\text{model}} \]

\[ N_{\text{obs}} \ll N_{\text{model}} \]
**Two Spaces**

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

$\mathbf{G}^T$ maps from observation space to model space
Iterative Solution of Primal Formulation

(defined IS4DVAR, is4dvar_ocean.h)

Recall the incremental cost function:

\[
J = \frac{1}{2} \delta z^T D^{-1} \delta z + \frac{1}{2} (G \delta z - d)^T R^{-1} (G \delta z - d)
\]

\[J_b\]
\[J_o\]

At the minimum of \(J\) we have \(\partial J / \partial \delta z = 0\)

\[
\partial J / \partial \delta z = D^{-1} \delta z + G^T R^{-1} (G \delta z - d)
\]

Given \(J\) and \(\partial J / \partial \delta z\), we can identify the \(\delta z\) that minimizes \(J\)
Matrix-less Operations

There are no matrix multiplications!

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

Zonal shear flow
Matrix-less Operations

There are no matrix multiplications!

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

Tangent Linear Model

Zonal shear flow
Matrix-less Operations

There are no matrix multiplications!

\[ G^T R^{-1} (G\delta z - d) \]

Tangent Linear Model

Zonal shear flow
Matrix-less Operations

There are no matrix multiplications!

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

Consider a single Observation

Zonal shear flow
Matrix-less Operations

There are no matrix multiplications!

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

Consider a single Observation

Zonal shear flow
There are no matrix multiplications!

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

Inverse Obs Error Covariance

Zonal shear flow
Matrix-less Operations

There are no matrix multiplications!

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

Inverse Obs Error Covariance

Zonal shear flow
Matrix-less Operations

There are no matrix multiplications!

\[ G^T R^{-1} (G \delta z - d) \]

Adjoint Model

Zonal shear flow
Matrix-less Operations

There are no matrix multiplications!

\[ \mathbf{G}^T \mathbf{R}^{-1} (\mathbf{G} \delta \mathbf{z} - \mathbf{d}) \]

Adjoint Model

Green’s Function

Zonal shear flow
Primal 4D-Var Algorithm (I4D-Var)

Choose $\delta z$

Run TLROMS

$R^{-1}$

Run ADROMS

Conjugate Gradient Algorithm

$\delta z$

$G\delta z, \ (G\delta z - d), \ J$

$R^{-1} (G\delta z - d)$

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

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

$x_b(t), \ d$

$NLROMS, z_b$

$NLROMS, z_a$

$x_a(t)$
Choose $\delta z$

Run TLROMS

$R^{-1}$

Run ADROMS

Conjugate Gradient Algorithm

Outer-loop

NLROMS, $z_b$

Inner-loop

Primal 4D-Var Algorithm (I4D-Var)

NLROMS, $z_a$
Conjugate Gradient (CG) Methods

Contours of $J$
An Example: ROMS CCS

COAMPS forcing \[ f_b(t), B_f \]

ECCO open boundary conditions \[ b_b(t), B_b \]

Previous assimilation cycle \[ x_b(0), B_x \]

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

ARGO

TOPP Elephant Seals

Ingleby and Huddleston (2007)

Data from Dan Costa

Argo
4D-Var Configuration

• Case studies for a representative case 3-10 March, 2003.
• 1 outer-loop, 100 inner-loops
• 7 day assimilation window
• Prior \( \mathbf{D} \): \( x \) \( L_h = 50 \) km, \( L_v = 30 \) m, \( \sigma \) from clim
  \( f \) \( L_T = 300 \) km, \( L_Q = 100 \) km, \( \sigma \) from COAMPS
  \( b \) \( L_h = 100 \) km, \( L_v = 30 \) m, \( \sigma \) from clim
• Super observations formed
• Obs error \( \mathbf{R} \) (diagonal):
  SSH 2 cm
  SST 0.4 C
  hydrographic 0.1 C, 0.01 psu
4D-Var Performance

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