Lecture 2:
The Mechanics of 4D-Var

Outline

- The conjugate gradient algorithm
- Preconditioning
- Covariance modeling

The Conjugate Gradient Algorithm
(cgradient.h & congrad.F)

Recall the incremental cost function:

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

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

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

$$\underbrace{\left(\mathbf{D}^{-1}+\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{G}\right)\delta\mathbf{z} - \mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{d}}_{} = \mathbf{0}$$

i.e. solve $\mathbf{A}\delta\mathbf{z} = \mathbf{b}$

The Conjugate Gradient Algorithm

The ECMWF "congrad" of Fisher (1997) for inner-loop *k+1*:

$$\delta\hat{\mathbf{z}}_k = \delta\mathbf{z}_k + \tau_k \mathbf{h}_k$$ trial step

$$\hat{\mathbf{g}}_k = \partial J / \partial \delta\hat{\mathbf{z}}_k$$ TL & AD ROMS — gradient @ trial step

$$\alpha_k = -\tau_k \mathbf{h}_k^{\mathrm{T}}\mathbf{g}_k / \left(\mathbf{h}_k^{\mathrm{T}}(\hat{\mathbf{g}}_k - \mathbf{g}_k)\right)$$ optimum step

$$\delta\mathbf{z}_{k+1} = \delta\mathbf{z}_k + \alpha_k \mathbf{h}_k$$ new starting point

$$\mathbf{g}_{k+1} = \mathbf{g}_k + (\alpha_k / \tau_k)\left(\hat{\mathbf{g}}_k - \mathbf{g}_k\right)$$ gradient @new point

$$\beta_{k+1} = \mathbf{g}_{k+1}^{\mathrm{T}}\mathbf{g}_{k+1} / \mathbf{g}_k^{\mathrm{T}}\mathbf{g}_k$$

$$\mathbf{h}_{k+1} = -\mathbf{g}_{k+1} + \beta_{k+1}\mathbf{h}_k$$ new descent direction

The Lanczos Connection

The CG algorithm is equivalent to:

$$\mathbf{A}\mathbf{q}_{k+1} = \gamma_{k+1}\mathbf{q}_{k+2} + \delta_{k+1}\mathbf{q}_{k+1} + \gamma_k \mathbf{q}_k$$

"Lanczos recursion relation"

$$\mathbf{q}_k = \mathbf{g}_k / \|\mathbf{g}_k\|; \quad \delta_{k+1} = (1/\alpha_{k+1} + \beta_{k+1}/\alpha_k); \quad \gamma_k = -\beta_{k+1}^{1/2}/\alpha_k$$

Orthonormal Lanczos vectors

$$\mathbf{q}_i^{\mathrm{T}}\mathbf{q}_j = \delta_{ij}$$

$$\mathbf{A}\mathbf{V}_k = \mathbf{V}_k\mathbf{T}_k + \gamma_k \mathbf{q}_{k+1}\mathbf{e}_k^{\mathrm{T}}$$

$$\mathbf{T}_k = \begin{pmatrix} \delta_1 & \gamma_1 & & & & \\ \gamma_1 & \delta_2 & \gamma_2 & & & \\ & \ddots & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \gamma_{k-2} & \delta_{k-1} & \gamma_{k-1} \\ & & & & & \gamma_{k-1} & \delta_k \end{pmatrix}$$

The Lanczos Connection

Gain (primal form):

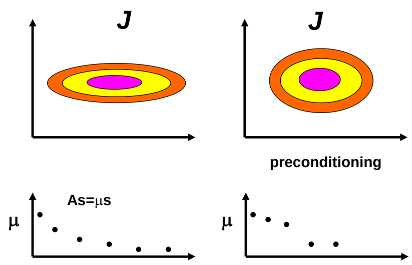
$$\mathbf{K} = (\mathbf{D}^{-1} + \mathbf{G}^T\mathbf{R}^{-1}\mathbf{G})^{-1}\mathbf{G}^T\mathbf{R}^{-1}$$

Practical gain matrix:

$$\tilde{\mathbf{K}}_k = \mathbf{V}_k\mathbf{T}_k^{-1}\mathbf{V}_k^{\mathrm{T}}\mathbf{G}^T\mathbf{R}^{-1}$$

Useful for diagnostic applications (Lecture 5)
(The Lanczos vectors are in ADJname)

Preconditioning



Preconditioning seeks to cluster the eigenvalues of A via a transformation of variable

Preconditioning

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

$$\left(\mathbf{D}^{-1} + \mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{G}\right)\delta\mathbf{z} - \mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{d} = \mathbf{0}$$

i.e. solve $\mathbf{A}\delta\mathbf{z} = \mathbf{b}$

Minimize:

$$J = \frac{1}{2}\delta\mathbf{z}^{\mathrm{T}}\mathbf{A}\delta\mathbf{z} - \delta\mathbf{z}^{\mathrm{T}}\mathbf{b} + c$$

Introduce a new variable: $\mathbf{v} = \mathbf{A}^{1/2}\delta\mathbf{z}$

$$J = \frac{1}{2}\mathbf{v}^{\mathrm{T}}\mathbf{v} - \mathbf{v}^{\mathrm{T}}\mathbf{A}^{-\mathrm{T}/2}\mathbf{b} + c$$

At the minimum: $\partial J/\partial\mathbf{v} = \mathbf{v} - \mathbf{A}^{-\mathrm{T}/2}\mathbf{b} = \mathbf{0}$

Preconditioning

Recall the incremental cost function:

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

Introduce a new variable: $\mathbf{v} = \mathbf{D}^{-1/2}\delta\mathbf{z}$

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

$$= \frac{1}{2}\mathbf{v}^{T}\left(\mathbf{I} + \mathbf{D}^{1/2}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{G}\mathbf{D}^{1/2}\right)\mathbf{v} - \mathbf{v}^{T}\mathbf{D}^{1/2}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{d} + \frac{1}{2}\mathbf{d}^{T}\mathbf{R}^{-1}\mathbf{d}$$

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

$$\left(\mathbf{I} + \mathbf{D}^{1/2}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{G}\mathbf{D}^{1/2}\right)\mathbf{v} - \mathbf{D}^{1/2}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{d} = \mathbf{0}$$

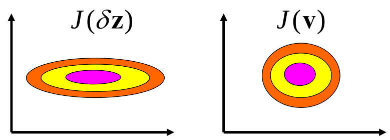
i.e. solve $\tilde{\mathbf{A}}\mathbf{v} = \tilde{\mathbf{b}}$ then $\delta\mathbf{z} = \mathbf{D}^{1/2}\mathbf{v}$

Preconditioning

Solve $\tilde{\mathbf{A}}\mathbf{v} = \tilde{\mathbf{b}}$

$$\tilde{\mathbf{A}} = \underbrace{\left(\mathbf{I} + \mathbf{D}^{1/2}\mathbf{G}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{G}\mathbf{D}^{1/2}\right)}$$

Has eigenvalues clustered around 1



The Conjugate Gradient Algorithm

cgradient.h in v-space to minimize $J(\mathbf{v})$

$\hat{\mathbf{v}}_k = \mathbf{v}_k + \tau_k \mathbf{h}_k$	trial step
$\hat{\mathbf{g}}_k = \mathbf{D}^{\mathrm{T}/2}\,\partial J / \partial\delta\hat{\mathbf{z}}_k$	gradient @ trial step
$\alpha_k = -\tau_k \mathbf{h}_k^{\mathrm{T}}\mathbf{g}_k / \left(\mathbf{h}_k^{\mathrm{T}}(\hat{\mathbf{g}}_k - \mathbf{g}_{\mathbf{k}})\right)$	optimum step
$\mathbf{v}_{k+1} = \mathbf{v}_k + \alpha_k \mathbf{h}_k$	new starting point
$\mathbf{g}_{k+1} = \mathbf{g}_k + (\alpha_k / \tau_k)\left(\hat{\mathbf{g}}_k - \mathbf{g}_k\right)$	gradient @new point
$\beta_{k+1} = \mathbf{g}_{k+1}^{\mathrm{T}}\mathbf{g}_{k+1} / \mathbf{g}_k^{\mathrm{T}}\mathbf{g}_k$	
$\mathbf{h}_{k+1} = -\mathbf{g}_{k+1} + \beta_{k+1}\mathbf{h}_k$	new descent direction
$\delta\mathbf{z}_{k+1} = \mathbf{D}^{1/2}\mathbf{v}_{k+1}$	project into state-space

The Lanczos Connection

Gain (primal form):

$$\mathbf{K} = \mathbf{D}^{1/2}(\mathbf{I} + \mathbf{D}^{\mathrm{T}/2}\mathbf{G}^{T}\mathbf{R}^{-1}\mathbf{G}\mathbf{D}^{1/2})^{-1}\mathbf{D}^{\mathrm{T}/2}\mathbf{G}^{T}\mathbf{R}^{-1}$$

Practical gain matrix:

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

Useful for diagnostic applications (Lecture 5)
(The Lanczos vectors are in ADJname)

Covariance Modeling

Recall the incremental cost function:

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

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

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

where $\mathbf{D} = \mathrm{diag}(\mathbf{B_x}, \mathbf{B_b}, \mathbf{B_f}, \mathbf{Q})$

Covariance Modeling

$\mathbf{B_x}$ = initial condition *prior* (or background) error covariance matrix
$\mathbf{B_f}$ = surface forcing *prior* error covariance matrix
$\mathbf{B_b}$ = open boundary condition *prior* error covariance matrix
Q = *prior* model error covariance matrix

Each covariance matrix is factorized according to:

$$\mathbf{B} = \mathbf{K_b}\boldsymbol{\Sigma}\mathbf{C}\boldsymbol{\Sigma}^{\mathrm{T}}\mathbf{K_b^{\mathrm{T}}}$$

C = univariate correlation matrix
Σ = diagonal matrix of error standard deviations
$\mathbf{K_b}$ = multivariate balance operator

Correlation Models

C is further factorized as:

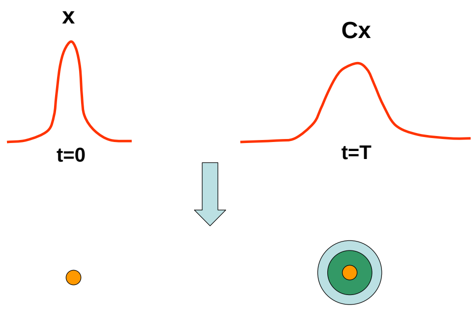
$$\mathbf{C} = \boldsymbol{\Lambda}\mathbf{L_v^{1/2}}\mathbf{L_h^{1/2}}\mathbf{W}^{-1}\mathbf{L_h^{T/2}}\mathbf{L_v^{T/2}}\boldsymbol{\Lambda}^{\mathrm{T}}$$

W = diagonal matrix of grid box volumes
$\mathbf{L_h}$ = horizontal correlation function model
$\mathbf{L_v}$ = vertical correlation function model
Λ = matrix of normalization coefficients

$\mathbf{L_h}$ and $\mathbf{L_v}$ are based on solutions of 2D and 1D pseudo diffusion equations respectively:

$$\partial\eta/\partial t - \kappa_h\nabla^2\eta = 0 \qquad \partial\eta/\partial t - \kappa_v\,\partial^2\eta/\partial z^2 = 0$$

Correlation Models



Correlation length, *L*: $L^2 \approx 2\kappa T$

Covariance Modeling

$$\mathbf{C} = \mathbf{\Lambda} \mathbf{L}_{\mathbf{v}}^{1/2} \mathbf{L}_{\mathbf{h}}^{1/2} \mathbf{W}^{-1} \mathbf{L}_{\mathbf{h}}^{T/2} \mathbf{L}_{\mathbf{v}}^{T/2} \mathbf{\Lambda}^{T}$$

Λ ensures that the range of **C** is ±1.

Suppose that **x** is divided into a balanced and unbalanced contribution: $\mathbf{x}=\mathbf{x}_b+\mathbf{x}_u$

Examples of balance: geostrophy, hydrostatic

$$(\mathbf{B}_{\mathbf{x}})_{\mathbf{u}} = \mathbf{\Sigma} \mathbf{C} \mathbf{\Sigma}^{T}$$

$$\mathbf{B}_{\mathbf{x}} = \mathbf{K}_{\mathbf{b}} (\mathbf{B}_{\mathbf{x}})_{\mathbf{u}} \mathbf{K}_{\mathbf{b}}^{T}$$

The Balance Operator

(define BALANCE_OPERATOR)

Following Weaver et al (2005):

$$\delta\mathbf{x} = \begin{bmatrix} \delta\mathbf{T} \\ \delta\mathbf{S} \\ \delta\zeta \\ \delta\mathbf{u} \\ \delta\mathbf{v} \end{bmatrix} \qquad \delta\hat{\mathbf{x}} = \begin{bmatrix} \delta\mathbf{T} \\ \delta\mathbf{S}_{\mathbf{u}} \\ \delta\zeta_{\mathbf{u}} \\ \delta\mathbf{u}_{\mathbf{u}} \\ \delta\mathbf{v}_{\mathbf{u}} \end{bmatrix}$$

Total state vector increments

Unbalanced state vector increments (except for δT)

$$(\mathbf{B}_{\mathbf{x}})_{\mathbf{u}} = \left\langle \delta\hat{\mathbf{x}} \delta\hat{\mathbf{x}}^{T} \right\rangle$$

$$\delta\mathbf{x} = \mathbf{K}_{\mathbf{b}} \delta\hat{\mathbf{x}}$$

$$\begin{aligned} \mathbf{B}_{\mathbf{x}} &= \left\langle \delta\mathbf{x} \delta\mathbf{x}^{T} \right\rangle \\ &= \mathbf{K}_{\mathbf{b}} \left\langle \delta\hat{\mathbf{x}} \delta\hat{\mathbf{x}}^{T} \right\rangle \mathbf{K}_{\mathbf{b}}^{T} \\ &= \mathbf{K}_{\mathbf{b}} (\mathbf{B}_{\mathbf{u}})_{\mathbf{x}} \mathbf{K}_{\mathbf{b}}^{T} \end{aligned}$$

The Balance Operator

$$\delta\mathbf{S} = \mathbf{K}_{ST}\delta\mathbf{T} + \delta\mathbf{S}_{\mathbf{u}}$$ *T-S* relation

$$\delta\varsigma = \mathbf{K}_{\varsigma\rho}\delta\rho + \delta\varsigma_{\mathbf{u}}$$ Level of no motion or elliptic eqn

$$\delta\mathbf{u} = \mathbf{K}_{up}\delta\mathbf{p} + \delta\mathbf{u}_{\mathbf{u}}$$ Geostrophic balance

$$\delta\mathbf{v} = \mathbf{K}_{vp}\delta\mathbf{p} + \delta\mathbf{v}_{\mathbf{u}}$$ Geostrophic balance

$$\delta\rho = \mathbf{K}_{\rho T}\delta\mathbf{T} + \mathbf{K}_{\rho S}\delta\mathbf{S}$$ Linear equation of state

$$\delta\mathbf{p} = \mathbf{K}_{p\rho}\delta\rho + \mathbf{K}_{p\varsigma}\delta\varsigma$$ Hydrostatic balance

The Balance Operator

$$\delta\mathbf{x} = \mathbf{K}_{\mathbf{b}}\delta\hat{\mathbf{x}}$$

$$\mathbf{K}_{\mathbf{b}} = \begin{pmatrix} \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{K}_{ST} & \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{K}_{\varsigma T} & \mathbf{K}_{\varsigma S} & \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{K}_{uT} & \mathbf{K}_{uS} & \mathbf{K}_{u\varsigma} & \mathbf{I} & \mathbf{0} \\ \mathbf{K}_{vT} & \mathbf{K}_{vS} & \mathbf{K}_{v\varsigma} & \mathbf{0} & \mathbf{I} \end{pmatrix}$$

The Balance Operator

$\mathbf{K}_{ST}$ from *prior* (background) *T-S* relationship

$$\delta S_b = \gamma \left.\frac{\partial S}{\partial z}\right|_S \left.\frac{\partial z}{\partial T}\right|_T \delta T$$

$$\gamma = \left.\begin{matrix} 0 \\ 1 \end{matrix}\right\} \text{depending on mixed layer}$$

The Balance Operator

$$\mathbf{K_b} = \begin{pmatrix} \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{K}_{ST} & \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \boxed{\mathbf{K}_{\varsigma T}} & \boxed{\mathbf{K}_{\varsigma S}} & \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{K}_{uT} & \mathbf{K}_{uS} & \mathbf{K}_{u\varsigma} & \mathbf{I} & \mathbf{0} \\ \mathbf{K}_{vT} & \mathbf{K}_{vS} & \mathbf{K}_{v\varsigma} & \mathbf{0} & \mathbf{I} \end{pmatrix}$$

The Balance Operator

$$\left.\begin{aligned} \mathbf{K}_{\varsigma T} &= \mathbf{K}_{\varsigma\rho}\left(\mathbf{K}_{\rho T} + \mathbf{K}_{\rho S}\mathbf{K}_{ST}\right) \\ \mathbf{K}_{\varsigma S} &= \mathbf{K}_{\varsigma\rho}\mathbf{K}_{\rho S} \end{aligned}\right\} \delta\rho = \rho_0\left(-\alpha\delta T + \beta\delta S\right)$$

Either:

(i) $\delta\varsigma_b = -\int_{z_r}^{0} \delta\rho / \rho_0 dz$ (level of no motion z_r)

(ii) $\nabla(h\nabla\delta\varsigma_b) = -\nabla\int_{-h}^{0}\int_{z}^{0}\delta\rho/\rho_0 dz' dz + \ldots$

(define ZETA_ELLIPTIC)

The Balance Operator

$$\mathbf{K_b} = \begin{pmatrix} \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{K}_{ST} & \mathbf{I} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{K}_{\varsigma T} & \mathbf{K}_{\varsigma S} & \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \boxed{\mathbf{K}_{uT}} & \boxed{\mathbf{K}_{uS}} & \boxed{\mathbf{K}_{u\varsigma}} & \mathbf{I} & \mathbf{0} \\ \mathbf{K}_{vT} & \mathbf{K}_{vS} & \mathbf{K}_{v\varsigma} & \mathbf{0} & \mathbf{I} \end{pmatrix}$$

The Balance Operator

$$
\begin{aligned}
\mathbf{K}_{uT} &= \mathbf{K}_{up}\left(\mathbf{K}_{p\rho} + \mathbf{K}_{p\varsigma}\mathbf{K}_{\varsigma\rho}\right)\left(\mathbf{K}_{\rho T} + \mathbf{K}_{\rho S}\mathbf{K}_{ST}\right) \\
\mathbf{K}_{uS} &= \mathbf{K}_{up}\left(\mathbf{K}_{p\rho} + \mathbf{K}_{p\varsigma}\mathbf{K}_{\varsigma\rho}\right)\mathbf{K}_{\rho S} \\
\mathbf{K}_{u\varsigma} &= \mathbf{K}_{up}\mathbf{K}_{p\varsigma}
\end{aligned}
$$

$\mathbf{K}_{p\rho}$ hydrostatic balance

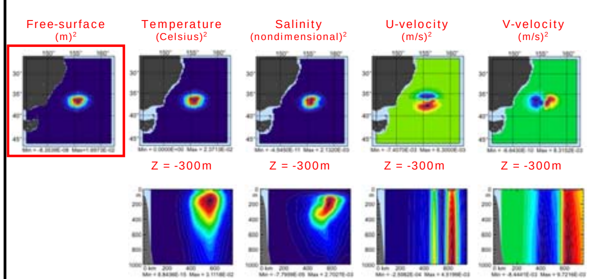
$\mathbf{K}_{up}$ geostrophic balance

$\mathbf{K}_{p\varsigma}$ free-surface contribution to *p*

The Balance Operator

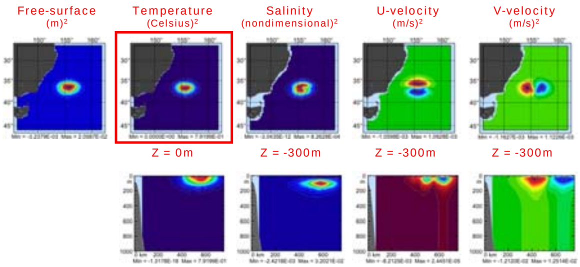
$$
\mathbf{B}_{\mathbf{x}} = \mathbf{K}_{\mathbf{b}}\left(\mathbf{B}_{\mathbf{x}}\right)_{\mathbf{u}}\mathbf{K}_{\mathbf{b}}^{\mathrm{T}} = \begin{pmatrix}
\mathbf{B}_{TT} & \mathbf{B}_{ST}^{T} & \mathbf{B}_{\varsigma T}^{T} & \mathbf{B}_{uT}^{T} & \mathbf{B}_{vT}^{T} \\
\mathbf{B}_{ST} & \mathbf{B}_{SS} & \mathbf{B}_{\varsigma S}^{T} & \mathbf{B}_{uS}^{T} & \mathbf{B}_{vS}^{T} \\
\mathbf{B}_{\varsigma T} & \mathbf{B}_{\varsigma S} & \mathbf{B}_{\varsigma\varsigma} & \mathbf{B}_{u\varsigma}^{T} & \mathbf{B}_{v\varsigma}^{T} \\
\mathbf{B}_{uT} & \mathbf{B}_{uS} & \mathbf{B}_{u\varsigma} & \mathbf{B}_{uu} & \mathbf{B}_{vu}^{T} \\
\mathbf{B}_{vT} & \mathbf{B}_{vS} & \mathbf{B}_{v\varsigma} & \mathbf{B}_{vu} & \mathbf{B}_{vv}
\end{pmatrix}
$$

IS4DVAR Balanced Operator Covariances: EAC



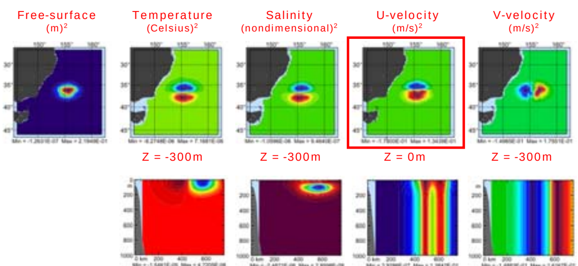
The cross-covariances are computed from a single sea surface height observation using multivariate physical balance relationships.

IS4DVAR Balanced Operator Covariances: EAC



The cross-covariances are computed from a single temperature observation at the surface using multivariate physical balance relationships.

IS4DVAR Balanced Operator Covariances: EAC



The cross-covariances are computed from a single U-velocity observation at the surface using multivariate physical balance relationships.

Initial condition *prior:*

$$\mathbf{B}_x = \mathbf{K}_b \mathbf{\Sigma}_x \mathbf{C}_x \mathbf{\Sigma}_x^T \mathbf{K}_b^T$$

Surface forcing *prior:*

$$\mathbf{B}_f = \mathbf{\Sigma}_f \mathbf{C}_f \mathbf{\Sigma}_f^T$$ No balance

Open boundary condition *prior:*

$$\mathbf{B}_b = \mathbf{\Sigma}_b \mathbf{C}_b \mathbf{\Sigma}_b^T$$ No balance

Model error *prior:*

$$\mathbf{Q} = \mathbf{K}_b \mathbf{\Sigma}_q \mathbf{C}_q \mathbf{\Sigma}_q^T \mathbf{K}_b^T$$

Preconditioning Again

General form of the *prior* error covariance matrix:

$$\mathbf{D} = \mathbf{K_b}\mathbf{\Sigma}\mathbf{C}\mathbf{\Sigma}^{\mathrm{T}}\mathbf{K_b}^{\mathrm{T}}$$

Introduce a new variable:

$$\mathbf{v} = \mathbf{U}^{-1}\delta\mathbf{z}$$

where

$$\mathbf{D} = \mathbf{U}\mathbf{U}^{\mathrm{T}}$$

$$\mathbf{U} = \mathbf{K_b}\mathbf{\Sigma}\mathbf{C}^{1/2}$$

The Conjugate Gradient Algorithm

cgradient.h in v-space to minimize $J(\mathbf{v})$

$$\hat{\mathbf{v}}_k = \mathbf{v}_k + \tau_k \mathbf{h}_k$$ trial step

$$\hat{\mathbf{g}}_k = \mathbf{C}^{\mathrm{T}/2}\mathbf{\Sigma}^{\mathrm{T}}\mathbf{K_b}^{\mathrm{T}}\,\partial J/\partial\delta\hat{\mathbf{z}}_k$$ gradient @ trial step

$$\alpha_k = -\tau_k \mathbf{h}_k^{\mathrm{T}}\mathbf{g}_k / \left(\mathbf{h}_k^{\mathrm{T}}(\hat{\mathbf{g}}_k - \mathbf{g_k})\right)$$ optimum step

$$\mathbf{v}_{k+1} = \mathbf{v}_k + \alpha_k \mathbf{h}_k$$ new starting point

$$\mathbf{g}_{k+1} = \mathbf{g}_k + (\alpha_k/\tau_k)\left(\hat{\mathbf{g}}_k - \mathbf{g}_k\right)$$ gradient @new point

$$\beta_{k+1} = \mathbf{g}_{k+1}^{\mathrm{T}}\mathbf{g}_{k+1} / \mathbf{g}_k^{\mathrm{T}}\mathbf{g}_k$$

$$\mathbf{h}_{k+1} = -\mathbf{g}_{k+1} + \beta_{k+1}\mathbf{h}_k$$ new descent direction

$$\delta\mathbf{z}_{k+1} = \mathbf{K_b}\mathbf{\Sigma}\mathbf{C}^{1/2}\mathbf{v}_{k+1}$$ project into state-space

The Lanczos Connection

Gain (primal form):

$$\mathbf{K} = \mathbf{K_b}\mathbf{\Sigma}\mathbf{C}^{1/2}(\mathbf{I} + \mathbf{D}^{\mathrm{T}/2}\mathbf{G}^{T}\mathbf{R}^{-1}\mathbf{G}\mathbf{D}^{1/2})^{-1}\mathbf{C}^{\mathrm{T}/2}\mathbf{\Sigma}^{\mathrm{T}}\mathbf{K_b}^{\mathrm{T}}\mathbf{G}^{T}\mathbf{R}^{-1}$$

Practical gain matrix:

$$\tilde{\mathbf{K}}_k = \mathbf{K_b}\mathbf{\Sigma}\mathbf{C}^{1/2}\mathbf{V}_k\mathbf{T}_k^{-1}\mathbf{V}_k^{\mathrm{T}}\mathbf{C}^{\mathrm{T}/2}\mathbf{\Sigma}^{\mathrm{T}}\mathbf{K_b}^{\mathrm{T}}\mathbf{G}^{T}\mathbf{R}^{-1}$$

Useful for diagnostic applications (Lecture 5)
(The Lanczos vectors are in ADJname)

Issues, Things to do, & Coming Soon

- Relax horizontal homogeneity and isotropy of L_x and L_y correlation lengths.
- Include temporal correlations (there is some implicit time corr. already in $\delta\mathbf{f}(t)$, $\delta\mathbf{b}(t)$, & $\eta(t)$).
- Elliptic solver for free-surface balance:
  - cannot handle islands at the moment
  - add additional boundary condition option
- Cannot assimilate obs right at the open boundary.
- Div and curl of $\delta\tau$ are not constrained.
- No restart option for 4D-Var.

Summary

- Lanczos formulation of CG: cgradient.h
- Lanczos vectors saved in ADJname
- Covariance models using diffusion operators:
  define VCONVOLUTION
  define IMPLICIT_VCONV, etc
- Multivariate balance operator:

$\mathbf{K_b}$ - tl_balance.F
$\mathbf{K_b^T}$ - ad_balance.F
$\mathbf{\Sigma}$ - tl_variability.F
$\mathbf{\Sigma^T}$ - ad_variability.F
$\mathbf{C}^{1/2}$ - tl_convolution.F
$\mathbf{C}^{T/2}$ - ad_convolution.F

References

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