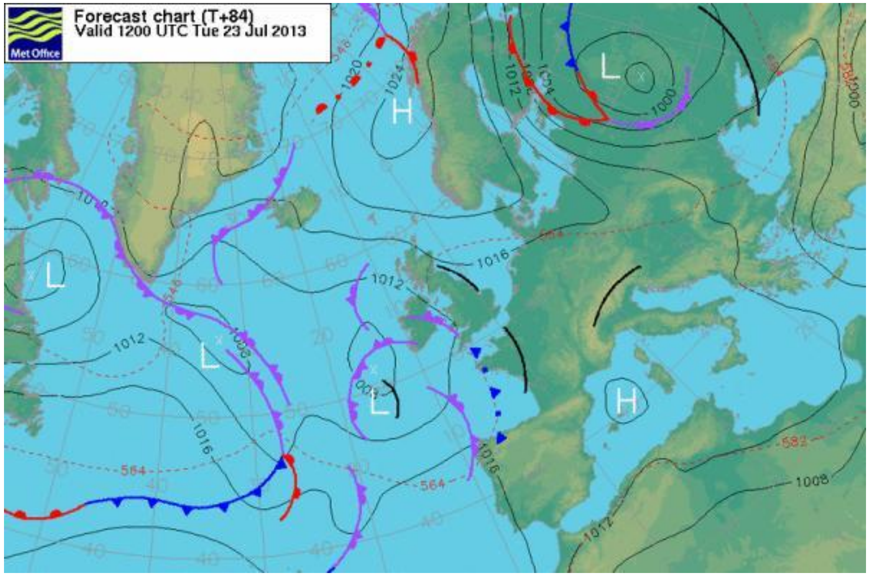
Variational Data Assimilation



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Outline

- Introduction to data assimilation
- Variational data assimilation
- Incremental 4D variational assimilation
- Ill-posedness and regularization
- Conclusions

1.
The Data Assimilation Problem

Data Assimilation

Aim:

Find the best estimate (analysis) of the expected states/parameters of a system, consistent with both observations and the system dynamics given:

- Numerical prediction model
- Observations of the system (over time)
- Background state (prior estimate)
- Estimates of error statistics

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Example - Linear System Equations

Prior: $$\mathbf{T}_b = \mathbf{T}_0 + \mathbf{e}_b$$

Model: $$\mathbf{T}_{i+1} = \mathbf{M}\,\mathbf{T}_i$$

Observations: $$\mathbf{y}_i = \mathbf{H}\mathbf{T}_i + \mathbf{e}_i$$

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Model: $$\mathbf{T}_{i+1} = \mathbf{M}\,\mathbf{T}_i$$

Observations: $$\mathbf{y}_i = \mathbf{H}\mathbf{T}_i + \mathbf{e}_i$$

where $$\mathcal{E}\{\mathbf{e}_b\} = 0 \qquad \mathcal{E}\{\mathbf{e}_b\mathbf{e}_b^T\} = \mathbf{B}$$

$$\mathcal{E}\{\mathbf{e}_i\} = 0 \qquad \mathcal{E}\{\mathbf{e}_i\mathbf{e}_i^T\} = \mathbf{R}_i$$

and errors are uncorrelated in time

Example - Data Assimilation Problem

Prior: $$\mathbf{T}_b = \mathbf{T}_0 + \mathbf{e}_b$$

Model: $$\mathbf{T}_{i+1} = \mathbf{M}\,\mathbf{T}_i$$

Observations: $$\mathbf{y}_i = \mathbf{H}\mathbf{T}_i + \mathbf{e}_i$$

Question: can we reconstruct the state of the system from this information? How accurate is the estimate?

Example - YES

Using: $$\mathbf{y}_i = \mathbf{H}\mathbf{T}_i + \mathbf{e}_i = \mathbf{H}\mathbf{M}\mathbf{T}_{i-1} + \mathbf{e}_i$$

implies:

$$\begin{array}{rcll}
\mathbf{T}_b & = & \mathbf{T}_0 & + \; \mathbf{e}_b \\
\mathbf{y}_0 & = & \mathbf{H}\mathbf{T}_0 & + \; \mathbf{e}_0 \\
\mathbf{y}_1 & = & \mathbf{H}\mathbf{M}\mathbf{T}_0 & + \; \mathbf{e}_1 \\
\mathbf{y}_2 & = & \mathbf{H}\mathbf{M}^2\mathbf{T}_0 & + \; \mathbf{e}_2 \\
\vdots & \vdots & \vdots & \vdots \quad \vdots \\
\mathbf{y}_n & = & \mathbf{H}\mathbf{M}^n\mathbf{T}_0 & + \; \mathbf{e}_n
\end{array}$$

= a set of linear equations for $\mathbf{T}_0$.

Example - Solution

Find the solution that minimizes the error variance and gives the weighted least square error:

$$\min_{\mathbf{T}_0} \; \mathbf{e}_b^T \mathbf{B}^{-1} \mathbf{e}_b + \sum_{0}^{n} \mathbf{e}_i^T \mathbf{R}_i^{-1} \mathbf{e}_i \quad =$$

$$\min_{\mathbf{T}_0} \; (\mathbf{T}_b - \mathbf{T}_0)^T \mathbf{B}^{-1} (\mathbf{T}_b - \mathbf{T}_0) +$$

$$+ \sum_{i=0}^{n} (\mathbf{y}_i - \mathbf{H}\mathbf{M}^i \mathbf{T}_0)^T \mathbf{R}_i^{-1} (\mathbf{y}_i - \mathbf{H}\mathbf{M}^i \mathbf{T}_0)$$

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Optimal Unbiased Estimate

$$\min_{\mathbf{T}_0} \mathcal{J} = \frac{1}{2}(\mathbf{T}_b - \mathbf{T}_0)^T \mathbf{B}^{-1}(\mathbf{T}_b - \mathbf{T}_0) +$$

$$+ \frac{1}{2}\sum_{i=0}^{n}(\mathbf{y}_i - \mathbf{H}\mathbf{T}_i)^T \mathbf{R}_i^{-1}(\mathbf{y}_i - \mathbf{H}\mathbf{T}_i)$$

subject to

$$\mathbf{T}_{i+1} = \mathbf{M}\,\mathbf{T}_i \;, \quad i = 0, 1, \ldots n-1$$

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Optimal Unbiased Estimate

$$\min_{\mathbf{T}_0} \mathcal{J} = \frac{1}{2}(\mathbf{T}_b - \mathbf{T}_0)^T \mathbf{B}^{-1} (\mathbf{T}_b - \mathbf{T}_0) +$$

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subject to

$$\mathbf{T}_{i+1} = \mathbf{M}\,\mathbf{T}_i \;, \quad i = 0, 1, \ldots n-1$$

Best Linear Unbiased Estimate

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Optimal Unbiased Estimate

$$\min_{\mathbf{T}_0} \mathcal{J} = \frac{1}{2}(\mathbf{T}_b - \mathbf{T}_0)^T \mathbf{B}^{-1} (\mathbf{T}_b - \mathbf{T}_0) +$$

$$+ \frac{1}{2} \sum_{i=0}^{n} (\mathbf{y}_i - \mathbf{H}\mathbf{T}_i)^T \mathbf{R}_i^{-1} (\mathbf{y}_i - \mathbf{H}\mathbf{T}_i)$$

subject to

$$\mathbf{T}_{i+1} = \mathbf{M}\,\mathbf{T}_i \;,\quad i = 0, 1, \ldots n-1$$

Maximum A Posteriori Likelihood

2.

Variational Data Assimilation

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Variational Data Assimilation

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Optimal Unbiased Estimate

$$\min_{\mathbf{x}_0} \mathcal{J} = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_b) + $$

$$+ \frac{1}{2}\sum_{i=0}^{n}(H[\mathbf{x}_i] - \mathbf{y}_i)^T \mathbf{R}_i^{-1}(H[\mathbf{x}_i] - \mathbf{y}_i)$$

subject to $\mathbf{x}_i = \mathcal{M}(t_i, t_0, \mathbf{x}_0)$, $i = 0, \ldots, n$

- x_b - Background state (prior estimate)
- y_i - Observations
- H_i - Observation operator
- B - Background error covariance matrix
- R_i - Observation error covariance matrix

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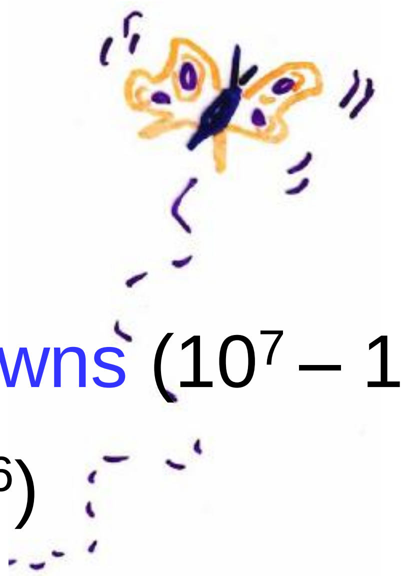
Significant Properties:



- Very large number of unknowns ($10^7 – 10^8$)
- Few observations ($10^5 – 10^6$)
- System nonlinear unstable/chaotic
- Multi-scale dynamics
- Ill-posed

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Nonlinear Least Squares Problem

$$\min J(\mathbf{x}_0) = \frac{1}{2}||\mathbf{f}(\mathbf{x}_0)||_2^2 \equiv \frac{1}{2}\mathbf{f}(\mathbf{x}_0)^T\mathbf{f}(\mathbf{x}_0)$$

with

$$\mathbf{f}(\mathbf{x}_0) = \begin{pmatrix} \mathbf{B}^{-\frac{1}{2}} & \mathbf{0} \\ \mathbf{0} & \hat{\mathbf{R}}^{-\frac{1}{2}} \end{pmatrix} \begin{pmatrix} \mathbf{x}_0 - \mathbf{x}^b \\ H_0[\mathbf{x}_0] - \mathbf{y}_0 \\ \vdots \\ H_n[\mathbf{x}_n] - \mathbf{y}_n \end{pmatrix}$$

and

$$\mathbf{x}_i = \mathcal{M}(t_i, t_0, \mathbf{x}_0)$$

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Gradient: $$\nabla J(\mathbf{x}) = \mathbf{J}^T \mathbf{f}(\mathbf{x})$$

Hessian: $$\nabla^2 J(\mathbf{x}) = \mathbf{J}^T \mathbf{J} + Q(\mathbf{x})$$

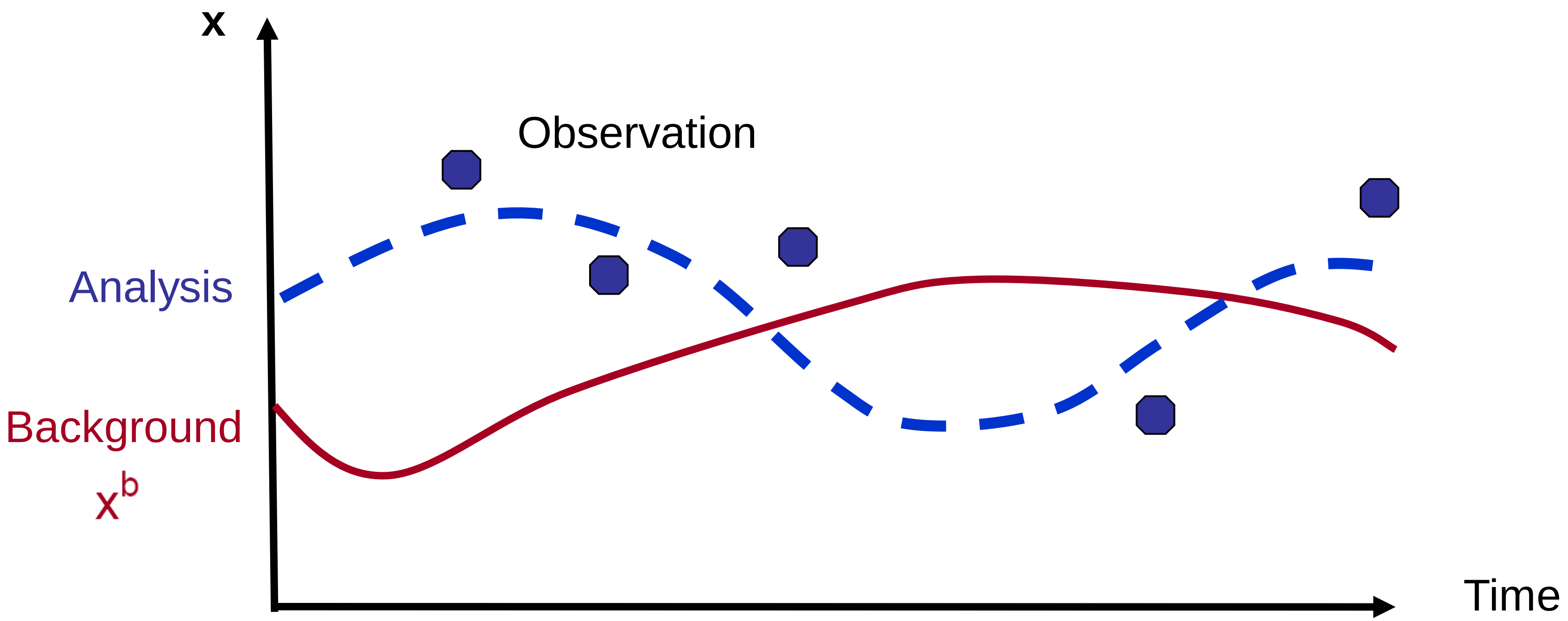
where

$$\mathbf{J} = \begin{pmatrix} \mathbf{B}^{-1/2} \\ \hat{\mathbf{R}}^{-1/2}\hat{\mathbf{H}} \end{pmatrix} \qquad \hat{\mathbf{H}} = \begin{pmatrix} \mathbf{H}_0 \\ \mathbf{H}_1 \mathbf{M}_{0,1} \\ \vdots \\ \mathbf{H}_n \mathbf{M}_{0,n} \end{pmatrix}$$

$$\mathbf{M}_{0,k} = \frac{\partial \mathcal{M}_{0,k}}{\partial \mathbf{x}}|_{\mathbf{x}_0} \qquad \mathbf{H}_k = \frac{\partial \mathcal{H}_k}{\partial \mathbf{x}}|_{\mathcal{M}_{0,k}(\mathbf{x}_0)}$$

4DVar Assimilation

Aim: Find the initial state x_0 such that the distance between the state trajectory and the observations is minimized, subject to x_0 remaining close to the prior estimate x^b



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Variational Assimilation

$$\min_{\mathbf{x}_0} \mathcal{J} = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_b) +$$

$$+ \frac{1}{2}\sum_{i=0}^{n}(H[\mathbf{x}_i] - \mathbf{y}_i)^T \mathbf{R}_i^{-1}(H[\mathbf{x}_i] - \mathbf{y}_i)$$

subject to $\mathbf{x}_{i+1} = \mathcal{M}_i(\mathbf{x}_i) \equiv \mathcal{M}(t_{i+1}, t_i, \mathbf{x}_i)$, $i = 0, \ldots, n-1$

Solve iteratively by gradient optimization methods.

Use adjoint methods to find the gradients.

3DVar if n = 0 4DVar if n $\geq$ 1

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Adjoint Model

Define the Lagrangian functional as

$$\mathrm{L} = \mathcal{J} + \sum_{t=1}^{n-1} \boldsymbol{\lambda}_{i+1}^{\mathrm{T}} (\mathbf{x}_{i+1} - \mathcal{M}_i(\mathbf{x}_i)).$$

Then the adjoint equations are

$$\boldsymbol{\lambda}_n = 0$$

$$\boldsymbol{\lambda}_i = \mathbf{M}_i^{\mathrm{T}} \boldsymbol{\lambda}_{i+1} - \mathbf{H}_i^T \mathbf{R}_i^{-1} (H_i[\mathbf{x}_i] - \mathbf{y}_i)$$

where $\mathbf{M}_i$ is the linearized dynamical model

and $\mathbf{H}_i$ is the linearized observation operator

Adjoint Model

Question - What are the adjoints?

$\mathbf{M}_i$ is the Jacobian $\frac{\partial \mathcal{M}_i}{\partial \mathbf{x}}$ of the linearized model operator and its adjoint is $\mathbf{M}_i^T$, known as the tangent linear model (TLM)

The adjoint variables $\boldsymbol{\lambda}_k$ measure the sensitivity of the objective function $\mathcal{J}$ to changes in the solutions $\mathbf{x}_k$ of the state equations.

Adjoint Model

The gradient of $\mathcal{J}$ with respect to the initial condition $\mathbf{x}_0$ is then given by

$$\nabla_0 J = -\boldsymbol{\lambda}_0 + \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_b)$$

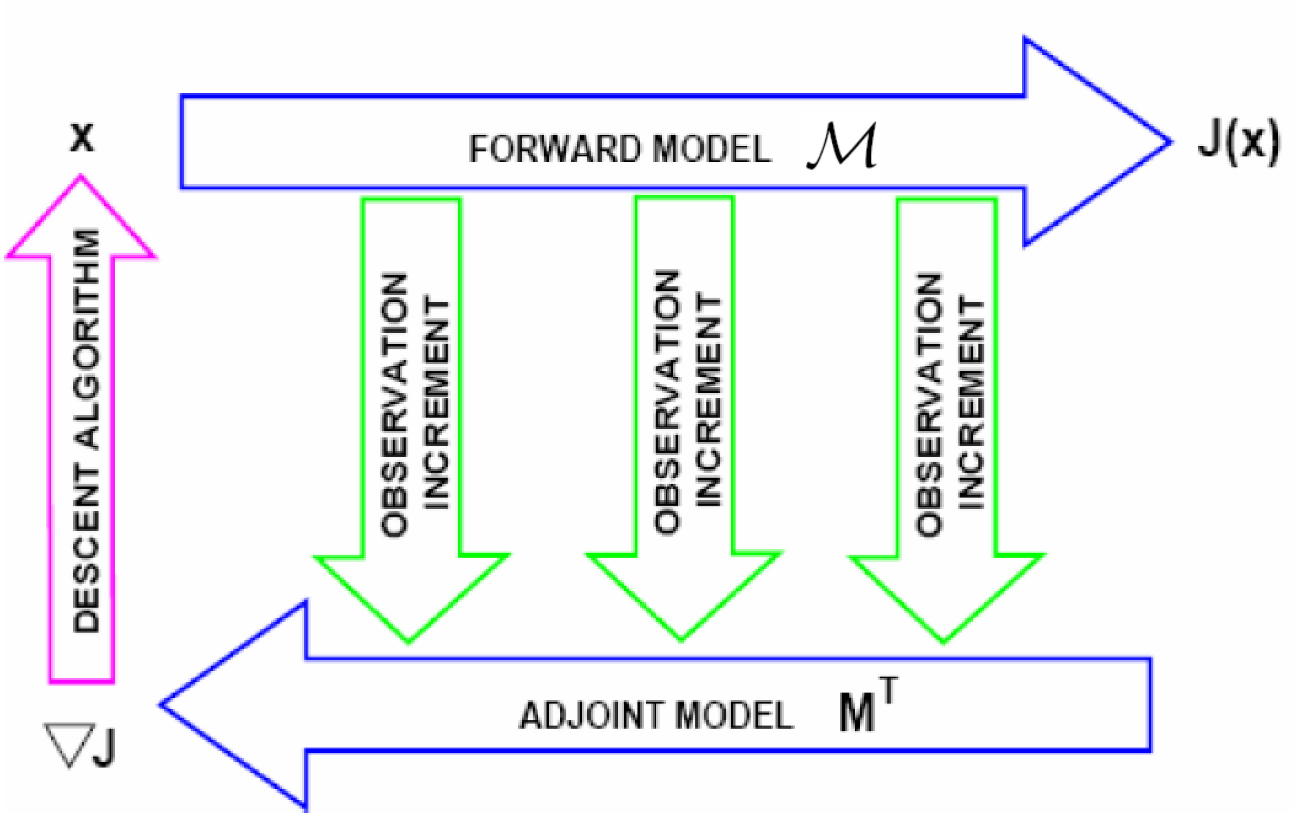
At the optimal the state and adjoint equations must both be satisfied and the gradient must equal to 0 .

Algorithm

To find the optimal:

- Estimate $\mathbf{x}_0$
- Run the nonlinear model forward; find the 'innovations' $H[\mathbf{x}_i] - \mathbf{y}_i$ and evaluate the objective function $\mathcal{J}$
- Run the adjoint model backward to find $\boldsymbol{\lambda}_0$ and evaluate the gradient $\nabla_0 J$
- Use a gradient nonlinear minimization method to find an improved estimate of $\mathbf{x}_0$
- Repeat until required accuracy is reached.

Algorithm



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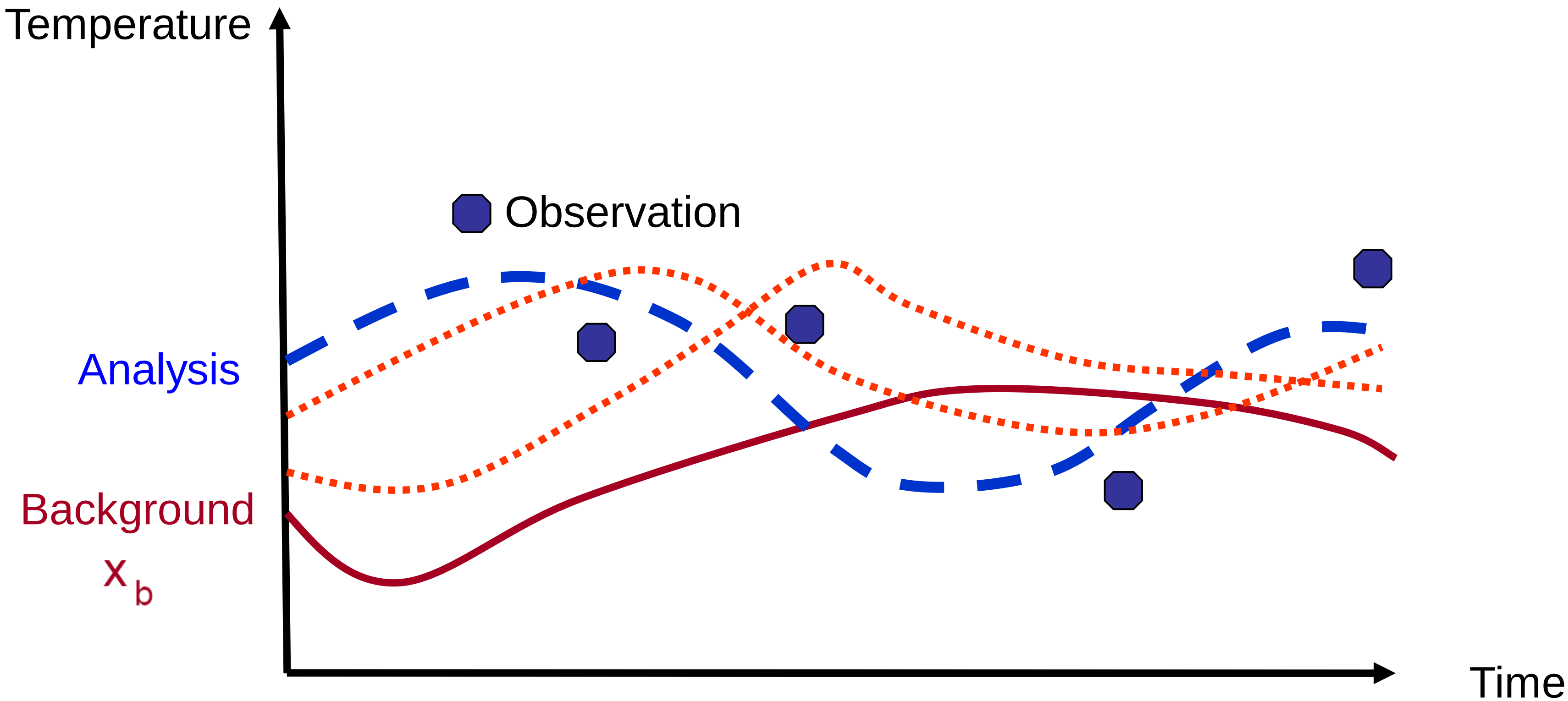
3.

Incremental 4D Variational Assimilation

Incremental 4D-Var



Solve a sequence of linear least squares problems that approximate the nonlinear problem by iteration .

Gauss-Newton

For k = 0, …K,

Solve :

$$\min_{\delta \mathbf{x}_0^{(k)}} \frac{1}{2} ||\mathbf{J}_k \delta \mathbf{x}_0^{(k)} + \mathbf{f}(\mathbf{x}_0^{(k)})||_2^2$$

subject to

$$\delta \mathbf{x}_i^{(k)} = \mathbf{M}_{0,i} \delta \mathbf{x}_0^{(k)}$$

Update:

$$\mathbf{x}_0^{(k+1)} = \mathbf{x}_0^{(k)} + \delta \mathbf{x}_0^{(k)}$$

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Algorithm

To find the optimal:

- Estimate $\mathbf{x}_0$
- Run the nonlinear model forward to find $\mathbf{x}_i$
- Estimate $\delta\mathbf{x}_0$ and run the tangent linear model (TLM) forward to find $H_k\delta\mathbf{x}_k - \mathbf{d}_k$ and evaluate the linearized objective function
- Run the adjoint model backward using forcing terms $H_k\delta\mathbf{x}_k - \mathbf{d}_k$ to find $\boldsymbol{\lambda}_0$ and evaluate the gradient of the linearized problem
- Use a gradient minimization method to find an improved estimate of $\delta\mathbf{x}_0$
- Update $\mathbf{x}_0$ by adding $\delta\mathbf{x}_0$ to old estimate and repeat

Convergence Results

- Incremental 4D-Var without is equivalent to a Gauss-Newton iteration for nonlinear problems.
- In operational implementation we usually approximate the solution procedure:
  - Truncate inner loop iterations
  - Use approximate linear system model
- Theoretical convergence results obtained by reference to Gauss-Newton method.

Ref: Gratton, Lawless and Nichols, SIAM J on Optimization, 2007

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Analysis

The analysis $\mathbf{x}_a$ is the optimal solution to the assimilation problem and $\mathbf{x}_a = \mathbf{x}_0 + \mathbf{e}_a$. The uncertainty is given by

$$\mathcal{E}\{\mathbf{e}_a\mathbf{e}_a^T\} \equiv \mathbf{A} = (\mathbf{B}^{-1} + \hat{\mathbf{H}}^T\hat{\mathbf{R}}^{-1}\hat{\mathbf{H}})^{-1}$$

where

$$\hat{\mathbf{H}} = \begin{pmatrix} \mathbf{H}_0 \\ \mathbf{H}_1\mathbf{M}_0 \\ \mathbf{H}_2\mathbf{M}_1\mathbf{M}_0 \\ \vdots \\ \mathbf{H}_n\mathbf{M}_{n-1}\ldots\mathbf{M}_0 \end{pmatrix} \qquad \hat{\mathbf{R}} = \begin{pmatrix} \mathbf{R}_0 & 0 & 0 & \cdots & 0 \\ 0 & \mathbf{R}_1 & 0 & \cdots & 0 \\ 0 & 0 & \mathbf{R}_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \mathbf{R}_n \end{pmatrix}$$

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Ill-posedness and Regularization of the Problem

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Conditioning of the Problem

Accuracy/rate of convergence depend on the condition number = $\lambda_{max} / \lambda_{min}$ of the Hessian:

$$\mathbf{J}^T\mathbf{J} = \mathbf{B}^{-1} + \hat{\mathbf{H}}^T\hat{\mathbf{R}}^{-1}\hat{\mathbf{H}}$$

where

$$\hat{\mathbf{H}} = \begin{pmatrix} \mathbf{H}_0 \\ \mathbf{H}_1\mathbf{M}_{0,1} \\ \vdots \\ \mathbf{H}_n\mathbf{M}_{0,n} \end{pmatrix} \qquad \hat{\mathbf{R}} = \begin{pmatrix} \mathbf{R}_0 & 0 & \cdots & 0 \\ 0 & \mathbf{R}_1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \mathbf{R}_n \end{pmatrix}$$

$$\mathbf{M}_{0,k} = \frac{\partial \mathcal{M}_{0,k}}{\partial \mathbf{x}}\Big|_{\mathbf{x}_0} \qquad \mathbf{H}_k = \frac{\partial \mathcal{H}_k}{\partial \mathbf{x}}\Big|_{\mathcal{M}_{0,k}(\mathbf{x}_0)}$$

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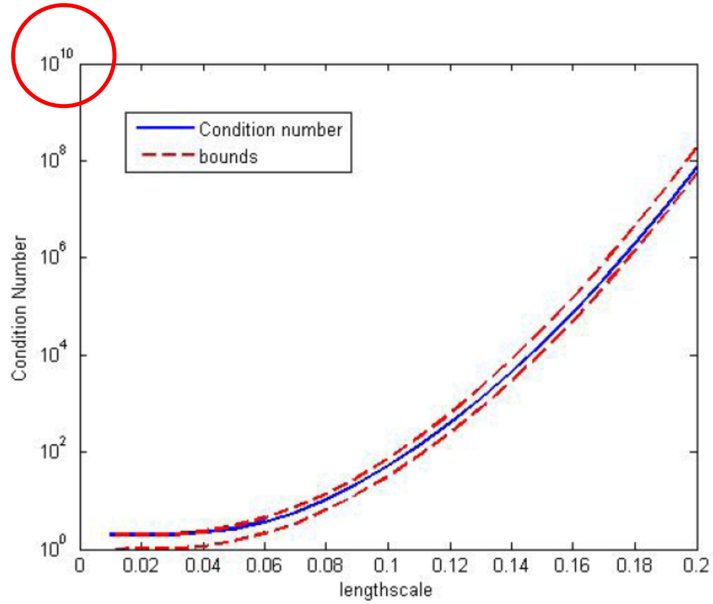
Conditioning of Hessian

Condition Number of $(B^{-1} + HR^{-1}H^T)$ vs Correlation Length Scale



Periodic Gaussian Exponential

$$\mathbf{B}_{ij} = \sigma_b^2 \exp\left(\frac{-r_{i,j}^2}{2L^2}\right)$$

Blue = condition number Red = bounds

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Preconditioning the Hessian

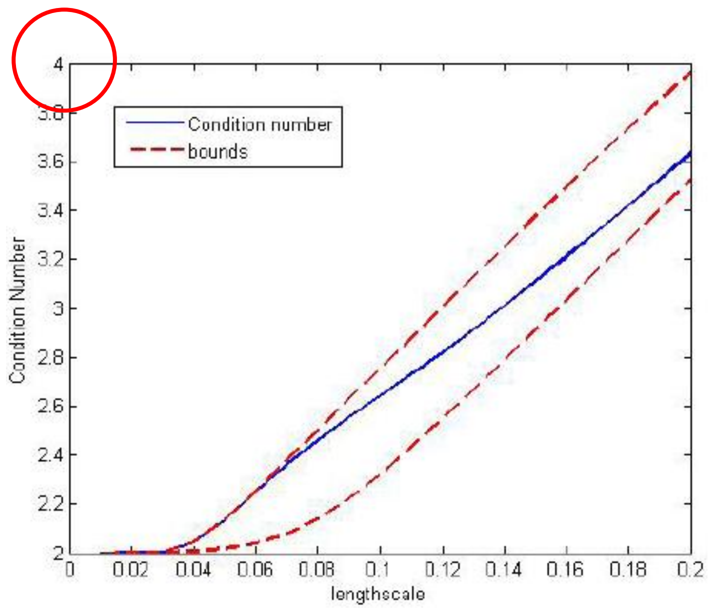
To improve conditioning transform to new variable :

- $\mathbf{z} = \mathrm{B}^{1/2} \ (\mathbf{x}_0 - \mathbf{x}_0^{\mathbf{b}})$
- Uncorrelated variables
- Equivalent to preconditioning by
- Hessian of transformed problem is

$$\mathbf{I} + \mathbf{B}^{1/2}\hat{\mathbf{H}}^T\hat{\mathbf{R}}^{-1}\hat{\mathbf{H}}\mathbf{B}^{1/2}$$

Preconditioned Hessian

Condition Number of Preconditioned Hessian vs Correlation Length Scale



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Convergence Rates of CG in 4D – using SOAR Correlation Matrix

	Iterations	
Lengthscale	Unprecond	Precond
0.01	8	8
0.1	54	11
0.2	187	12
0.3	361	12

Haben et al, 2011

Theory - Conditioning of Hessian

Bounds on the conditioning of the preconditioned Hessian are:

$$1+\frac{1}{p(n+1)}\frac{\sigma_b^2}{\sigma_o^2}\sum_{i,j=1}^{p(n+1)}(\hat{\mathbf{H}}\mathbf{C}\hat{\mathbf{H}}^T)_{i,j} \leq \kappa(\mathbf{A}_p) \leq 1+\frac{\sigma_b^2}{\sigma_o^2}||\hat{\mathbf{H}}\mathbf{C}\hat{\mathbf{H}}^T||_\infty$$

where

- $\mathbf{B} = \sigma_b{}^2\,\mathbf{C}$, **C** is correlation matrix
- $\mathbf{R}_k = \sigma_0^2\mathbf{I}$ for $k = 0, \ldots, n$

Ref: Haben et al, Tellus, 2011

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Regularized Problem

Let $\mathbf{B} = \sigma_b^2 \mathbf{C}_B \qquad \hat{\mathbf{R}} = \sigma_o{}^2 \mathbf{I} \qquad \mu^2 = \frac{\sigma_o^2}{\sigma_b^2}$

Then the preconditioned optimal state estimation problem may be written in the form of a classical Tikhonov regularized problem:

$$\hat{J} = \mu^2 ||\mathbf{z}||_2^2 + ||\hat{\mathbf{H}}\mathbf{C}_B^{1/2}\mathbf{z} - \hat{\mathbf{d}}||_2^2$$

$$\hat{\mathbf{H}} = \begin{pmatrix} \mathbf{H}_0 \\ \mathbf{H}_1 \mathbf{M}_{0,1} \\ \vdots \\ \mathbf{H}_n \mathbf{M}_{0,n} \end{pmatrix} \qquad \hat{\mathbf{d}} = \begin{pmatrix} \mathbf{y}_0 - \mathcal{H}_0(\mathbf{x}_0^b) \\ \mathbf{y}_1 - \mathcal{H}_1(\mathbf{x}_1^b) \\ \vdots \\ \mathbf{y}_n - \mathcal{H}_n(\mathbf{x}_n^b) \end{pmatrix}$$

Information Content

Rewrite the 4D solution as:

$$\mathbf{z} = \sum_i \frac{\lambda_i^2}{\mu^2 + \lambda_i^2} \frac{\mathbf{u}_i^T \hat{\mathbf{d}}}{\lambda_i} \mathbf{v}_i$$

where $\mu^2 = \frac{\sigma_o^2}{\sigma_b^2}$ and λ_i, $\mathbf{v}_i$, $\mathbf{u}_i$ are

the singular values and right and left singular vectors of $\hat{\mathbf{H}}\mathbf{C}_B^{1/2} = \mathbf{U}\mathbf{\Lambda}\mathbf{V}^T$.

Ref: Johnson et al, QJ RMetS, 2005

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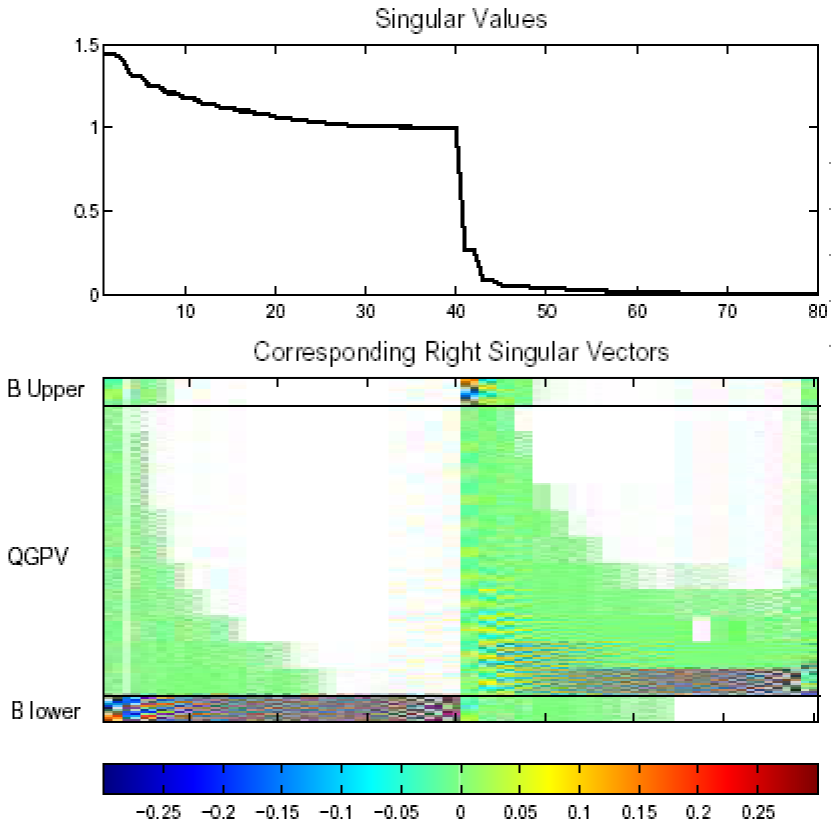
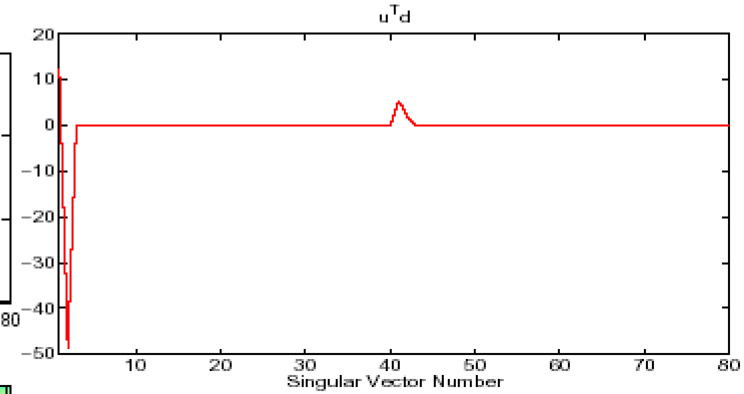
SVD





2 pairs of RSVs contribute towards the analysis increment. The second pair lie in the near-null space.

Ref: Johnson et al, QJ RMetS, 2005

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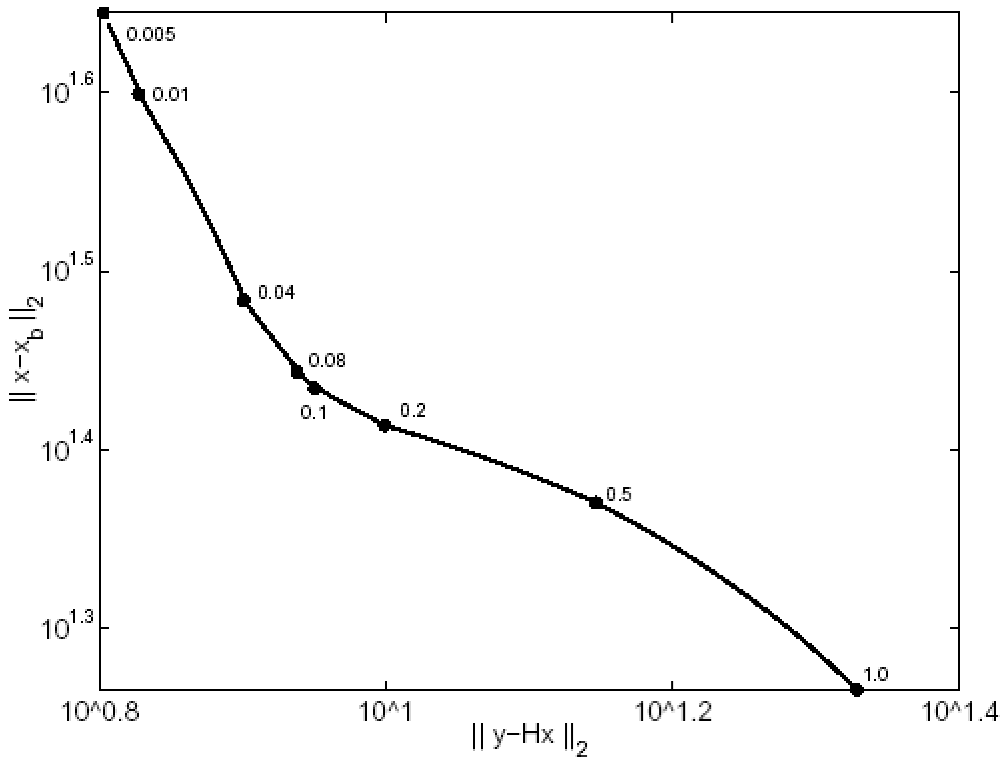
L - Curve



Compute the values of $\|\mathbf{x}-\mathbf{x}_b\|_2^2$ and $\|\mathbf{y}-\mathbf{H}\mathbf{x}\|_2^2$ at the minimum, for different values of μ. The optimal value of μ should be at the corner of the L.

Conclusions

- 4DVar is able to use a time sequence of observations to reconstruct the state in unobserved regions.
- Reconstructed regions are sensitive to noise and the required information is filtered by the background state.
- More information can be extracted from the observations and reconstruction can be improved by preconditioning the system and using a good choice of the regularization parameter.

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New Research

- Allowing for errors in the model as well as in the prior and observations - provides a weak constraint optimization problem.

- Investigating the use of different forms of regularization in the formulation of the problem.

- Analyzing stability of the 'cycled' 4DVar problem where the assimilation scheme is evolved as a dynamical system over a sequence of time windows.

- Combining 4DVar with Ensemble Filters

Many challenges left!

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