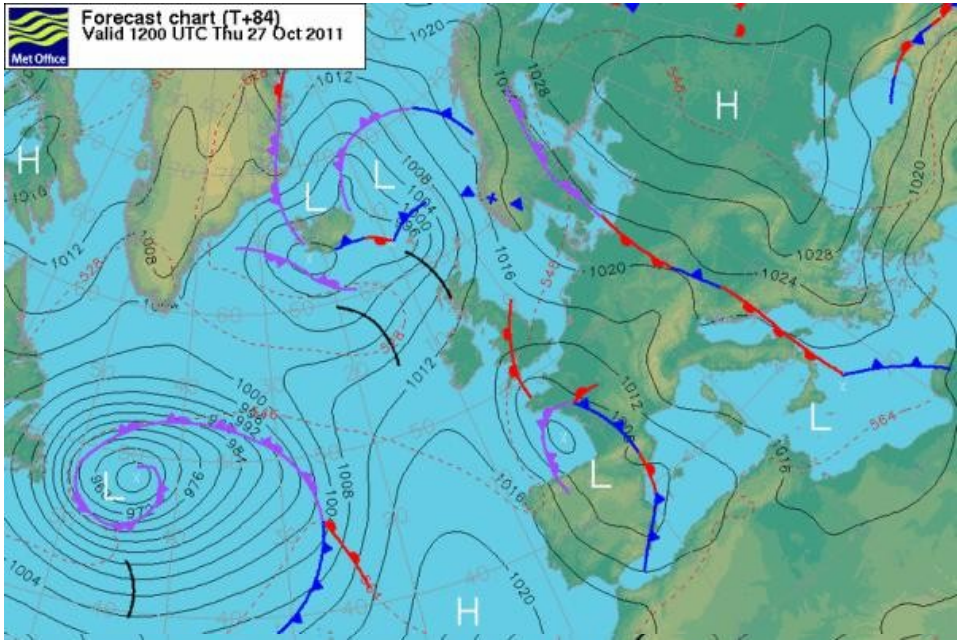
Conditioning and Preconditioning of the Optimal State Estimation Problem



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Outline

- Optimal State Estimation
- Conditioning
- Preconditioning
- Ill-posedness and Regularization
- Conclusions

1.

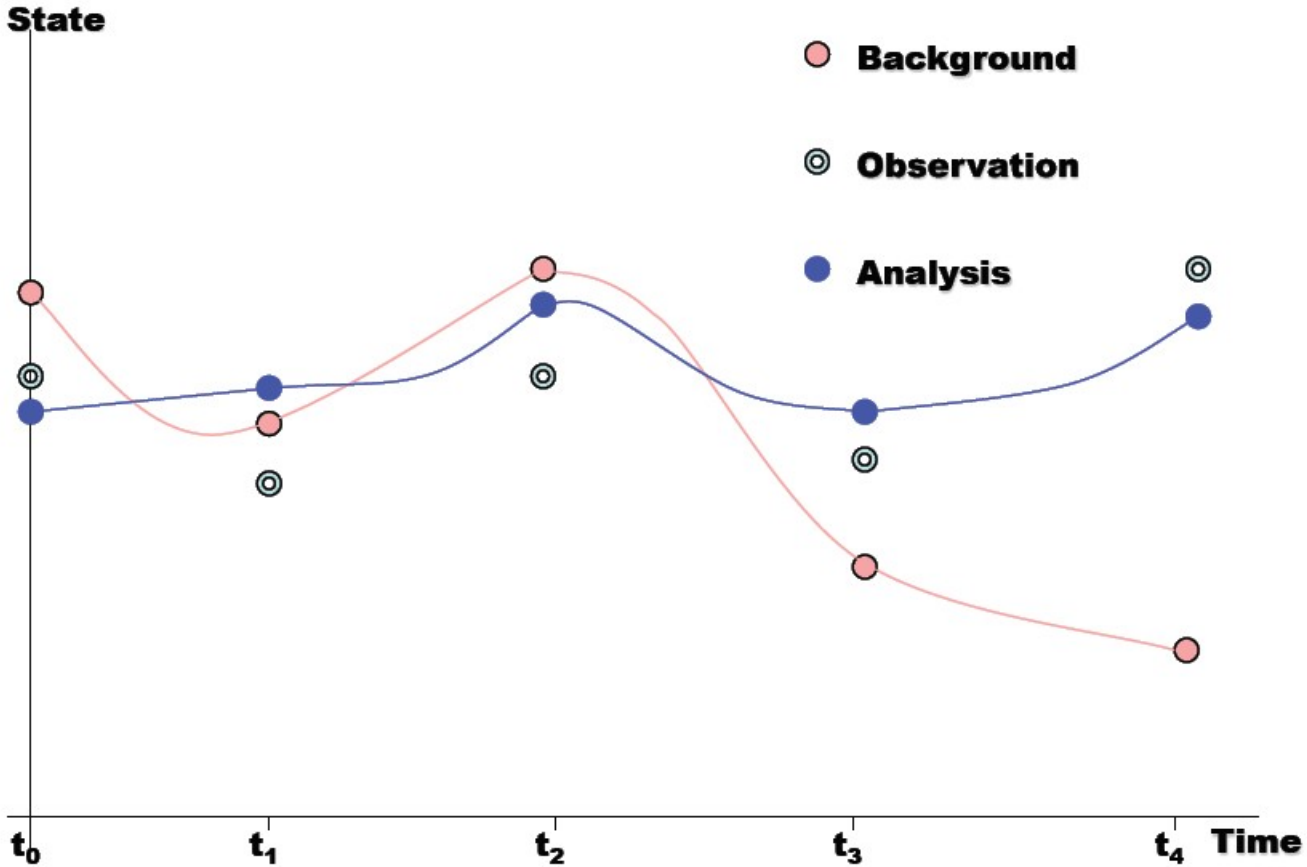
Optimal State Estimation

State Estimation / Data Assimilation

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

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

State Estimation / Data Assimilation



Optimal Bayesian Estimate

$$\min \; J(\mathbf{x}_0) = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_0^b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_0^b)$$

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

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

$\mathbf{x}_0^b$ - Background state (prior estimate)

$\mathbf{y}_i$ - Observations

$\mathcal{H}_i$ - Observation operator

$\mathbf{B}$ - Background error covariance matrix

$\mathbf{R}_i$ - Observation error covariance matrix

Significant Properties:

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

Solution of the Problem

- Solve iteratively by an approximate Gauss-Newton (incremental variational) method
- Solves a sequence of linear least-squares problems
- Use conjugate gradient/quasi-Newton iteration method to solve inner linear least-squares problem.
- Must solve in real time

Conditioning of the Problem

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

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

where

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

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

Three Questions

- What is the effect of the covariance structure on the conditioning of the Hessian
- What is the effect of preconditioning on the problem
- How does the observational system affect the conditioning of the problem

Reference: (HLN)

Haben, Lawless and Nichols, *UoR Maths Rpt 3/2009*

2.

Conditioning of the Hessian

Optimal Bayesian Estimate – 3DVar

Minimizes with respect to initial state $\mathbf{x}_0$:

$$J(\mathbf{x}_0) = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}_0^b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}_0^b) + \frac{1}{2}(\mathcal{H}(\mathbf{x}_0) - \mathbf{y})^T \mathbf{R}^{-1}(\mathcal{H}(\mathbf{x}_0) - \mathbf{y}),$$

- Hessian is:

$$\mathbf{A} = \mathbf{B}^{-1} + (\mathbf{H})^T \mathbf{R}^{-1} \mathbf{H}$$

- $\mathbf{B}$ and $\mathbf{R}$ are covariance matrices that depend on the correlation length-scales of the errors; $\mathbf{H}$ is the Jacobian of $\mathcal{H}$.

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Background Covariance Matrix

Define $\mathbf{B} = \sigma_b^2 \mathbf{C}$ on a 1D periodic domain by a Gaussian correlation structure:

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

- $r_{i,j}$ distance between points at position i and j
- L correlation lengthscale
- σ_b^2 background error variance
- Circulant

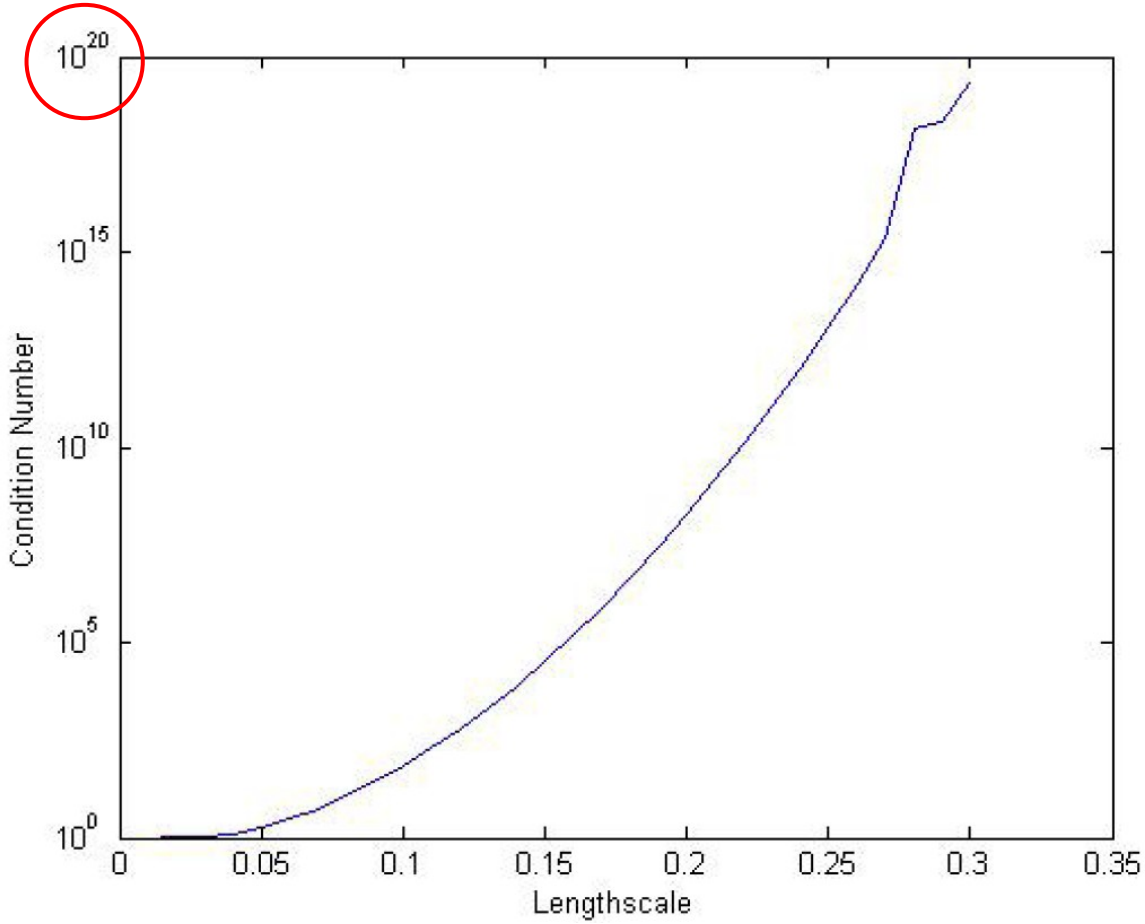
Circulant Matrices

$$\mathbf{C} = \begin{pmatrix} c_0 & c_1 & c_2 & c_3 & \cdots & c_{N-2} & c_{N-1} \\ c_{N-1} & c_0 & c_1 & c_2 & \cdots & c_{N-3} & c_{N-2} \\ c_{N-2} & c_{N-1} & c_0 & & & & \vdots \\ & & \ddots & \ddots & & & \\ \vdots & & & & \ddots & & c_2 \\ c_2 & & & & \ddots & c_0 & c_1 \\ c_1 & c_2 & \cdots & & c_{N-2} & c_{N-1} & c_0 \end{pmatrix}$$

Eigenvalues

$$\lambda_m = \sum_{k=0}^{N-1} c_k e^{-2\pi i m k/N}.$$

Condition of B - Gaussian



Condition of Hessian

$$\mathbf{A} = \mathbf{B}^{-1} + (\mathbf{H})^T \mathbf{R}^{-1} \mathbf{H}$$

- $\mathbf{B} = \sigma_b^2 \mathbf{C}$, where $\mathbf{C}$ is a correlation matrix
- Assume observations are at grid points
- Assume observation errors uncorrelated
- σ_0^2 variance observation errors
- $\mathbf{R} = \sigma_0^2 \mathbf{I}$
- $\mathbf{H}$ linear.
- $\mathbf{H}^T \mathbf{H}$ diagonal.

Condition Number of Hessian

Assume **C** has a circulant covariance structure.

Bounds on the conditioning of the Hessian are:

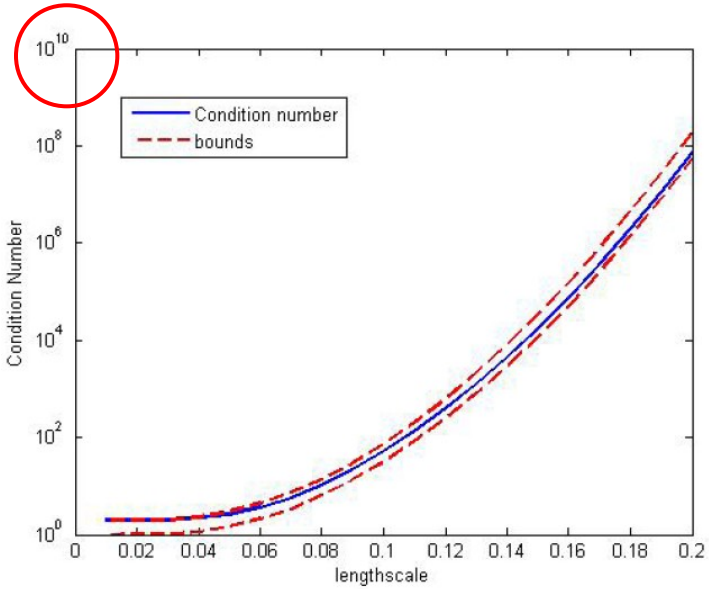
$$\alpha\kappa(\mathbf{C}) \leq \kappa(\mathbf{B}^{-1} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}) \leq \left(1 + \left(\frac{\sigma_b^2}{\sigma_o^2}\right)\lambda_{\min}(\mathbf{C})\right)\kappa(\mathbf{C})$$

where $\alpha = \left(\dfrac{1 + \frac{p}{N}\frac{\sigma_b^2}{\sigma_o^2}\lambda_{\min}(\mathbf{C})}{1 + \frac{p}{N}\frac{\sigma_b^2}{\sigma_o^2}\lambda_{\max}(\mathbf{C})}\right)$

and p = number of observations

Conditioning of Hessian

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



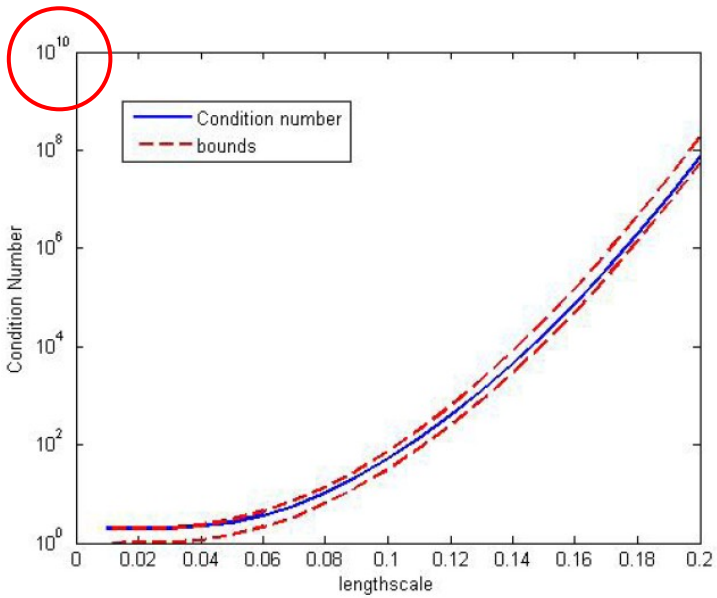
Periodic Gaussian Exponential

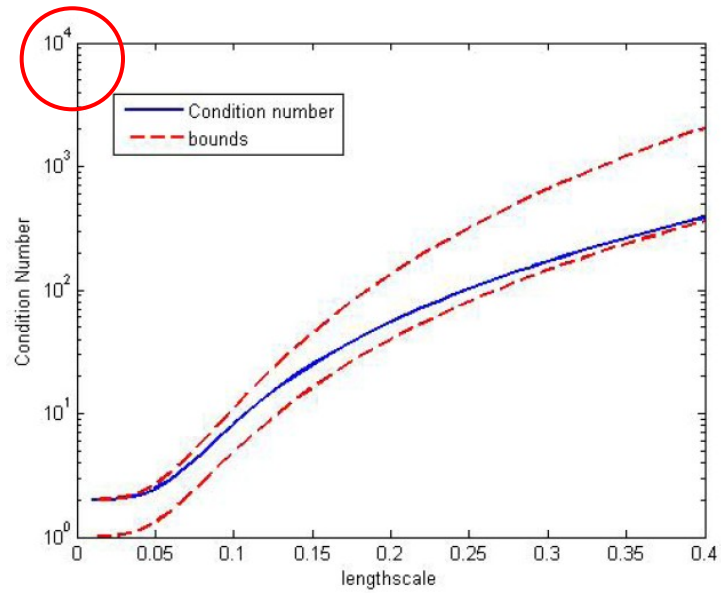
$$\mathbf{B}_{ij} = \sigma_b^2 \exp\left(\frac{-r_{i,j}^2}{2L^2}\right)$$

Blue = condition number Red = bounds

Conditioning of Hessian

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





Periodic Gaussian Exponential

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

Laplacian 2nd Derivative

$$\mathbf{B}^{-1} = \gamma^{-1}\left(\mathbf{I} + \frac{l^4}{2\Delta x^4}(\mathbf{L})^2\right)$$

Blue = condition number Red = bounds

3.

Preconditioning of the Hessian

Control Variable Transform

To improve conditioning transform to new variable :

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

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

Preconditioned Hessian

Bounds on the conditioning of the preconditioned Hessian are:

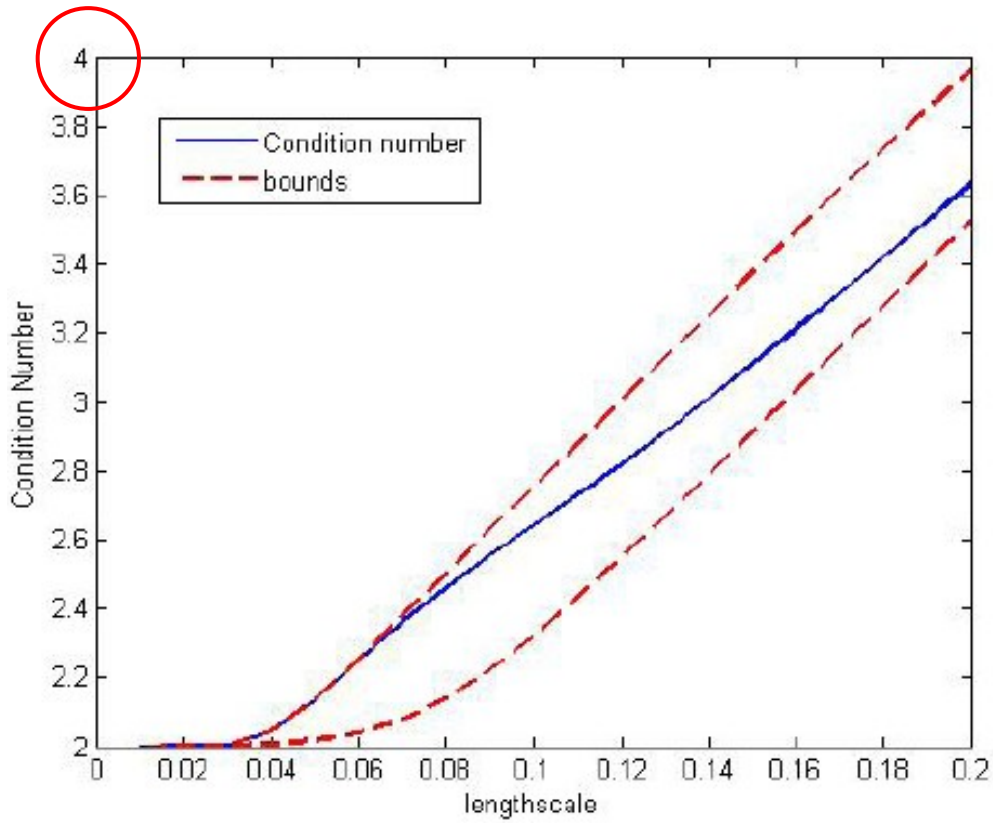
$$1 + \frac{\sigma_b^2}{\sigma_o^2}\gamma \leq \kappa(\mathbf{I} + \sigma_o^{-2}(\mathbf{B}^{1/2}\mathbf{H}^T\mathbf{H}\mathbf{B}^{1/2})) \leq 1 + \frac{\sigma_b^2}{\sigma_o^2}\nu_0$$

where

$$\nu_0 = \| \mathbf{HCH^T} \|_\infty \ , \quad \gamma = \frac{1}{p}\sum_{i,j\in J} c_{i,j} \ .$$

ν_0 changes slowly as a function of length scale.

Preconditioned Hessian - Gaussian



Preconditioned (blue)
Bounds (red)

Condition number as a function of length scale

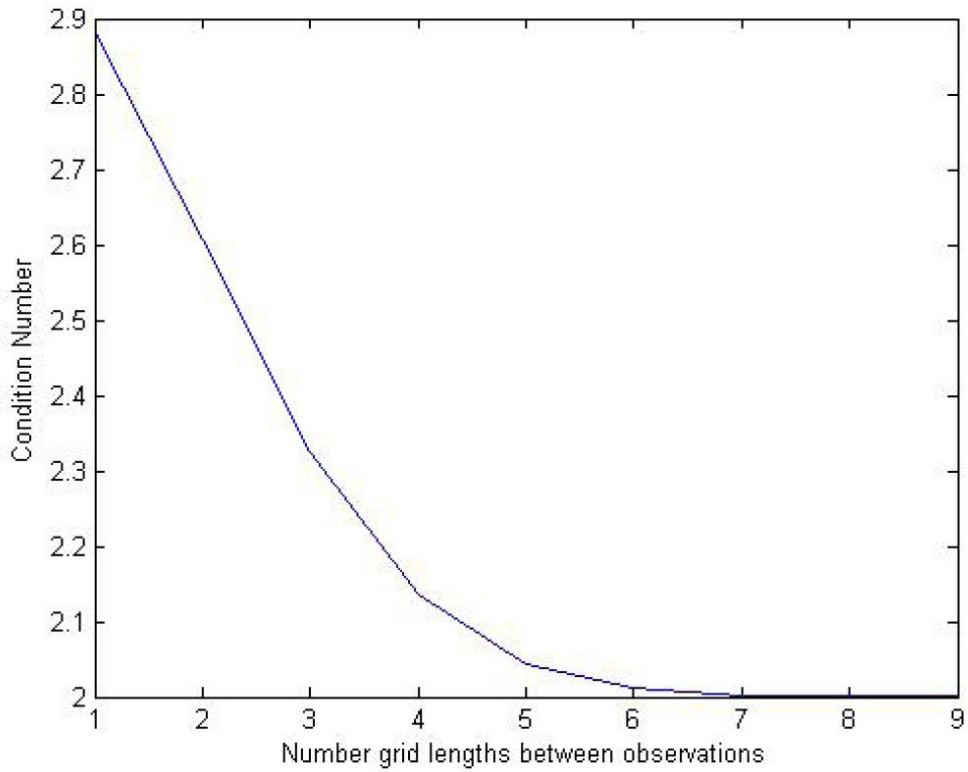
Preconditioned Hessian - Gaussian

Assume two observations at k^{th} and m^{th} grid points

$$\kappa(\mathbf{I} + \sigma_o^{-2}(\mathbf{B}^{1/2}\mathbf{H}^T\mathbf{H}\mathbf{B}^{1/2})) = 1 + \frac{\sigma_b^2}{\sigma_o^2} + \frac{\sigma_b^2}{\sigma_o^2}\,|c_{k,m}|$$

Condition number decreases as the separation of the observations increases

Preconditioned Hessian - Gaussian



Condition number as a function of observation spacing

Extension to 4DVar

Convergence depends on condition number of

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

where

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

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

Preconditioned 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

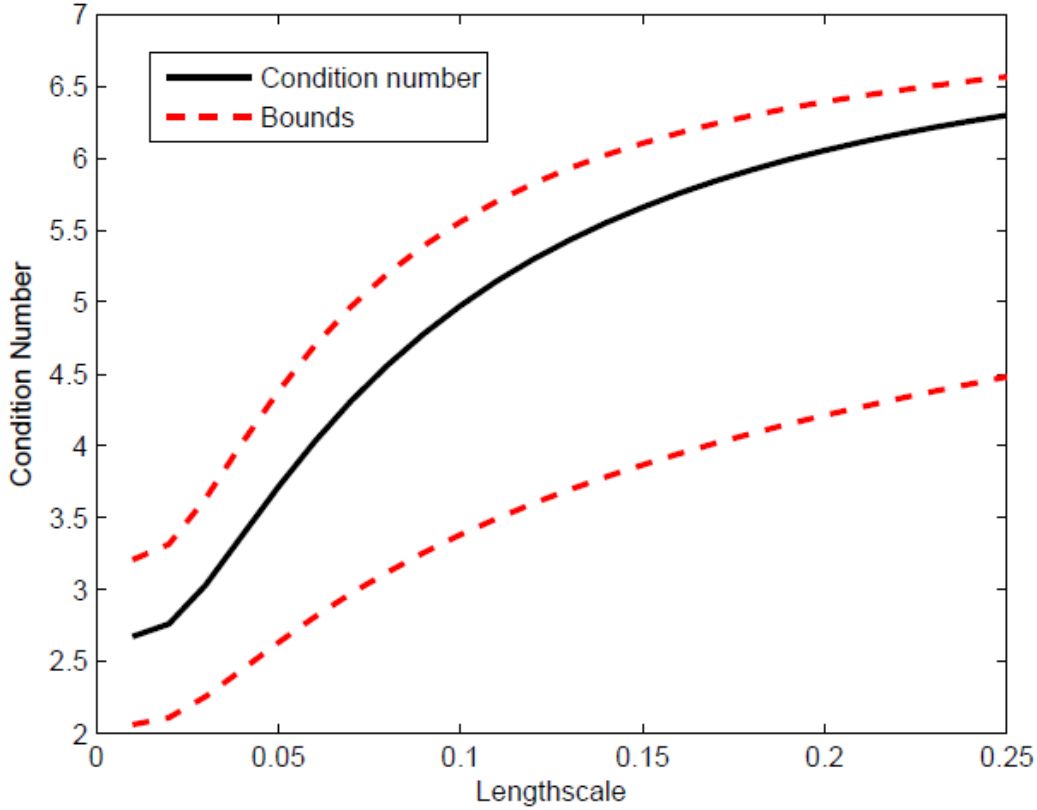
- $\mathbf{B} = \sigma_b^2 \mathbf{C}$, $\mathbf{C}$ is correlation matrix
- $\mathbf{R}_k = \sigma_0^2 \mathbf{I}$ for $k = 0, \ldots, n$
- Advection model discretized using upwind scheme

4D Background Correlation Matrix

$$\begin{pmatrix} \mathbf{B} & \mathbf{B}\mathbf{M}_1^T & \mathbf{B}\mathbf{M}_2^T & \cdots & \mathbf{B}\mathbf{M}_n^T \\ \mathbf{M}_1\mathbf{B} & \mathbf{M}_1\mathbf{B}\mathbf{M}_1^T & \mathbf{M}_1\mathbf{B}\mathbf{M}_2^T & \cdots & \mathbf{M}_1\mathbf{B}\mathbf{M}_n^T \\ \mathbf{M}_2\mathbf{B} & \mathbf{M}_2\mathbf{B}\mathbf{M}_1^T & \mathbf{M}_2\mathbf{B}\mathbf{M}_2^T & & \mathbf{M}_2\mathbf{B}\mathbf{M}_n^T \\ & & \ddots & \ddots & \\ \vdots & & & \ddots & \\ & & & \ddots & \\ \mathbf{M}_n\mathbf{B} & \mathbf{M}_n\mathbf{B}\mathbf{M}_1^T & \mathbf{M}_n\mathbf{B}\mathbf{M}_2^T & & \mathbf{M}_n\mathbf{B}\mathbf{M}_n^T \end{pmatrix}.$$

Each block describes a covariance matrix between the background errors at different times.

Condition of Preconditioned 4DVar – using SOAR Correlation Matrix



Convergence Rates of CG in 4DVar – 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

4.

Regularization

Preconditioned Hessian – 4DVar

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

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

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

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

Information Content

Rewrite the 4D Var solution as:

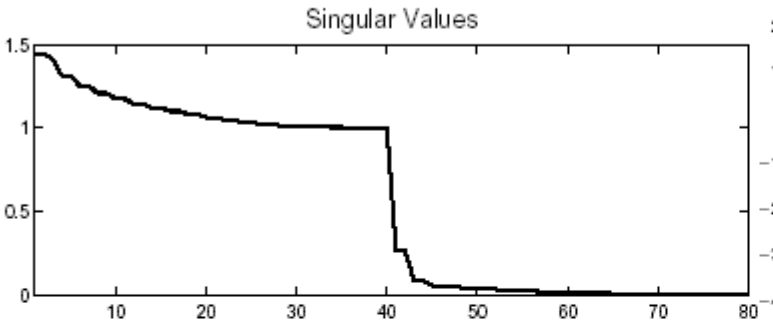
$$\mathbf{z} = \sum_i \frac{\lambda_i^2}{\mu^2 + \lambda_i^2} \frac{\mathbf{u}_i^T \hat{\mathbf{d}}}{\lambda_i} \mathbf{v}_i$$

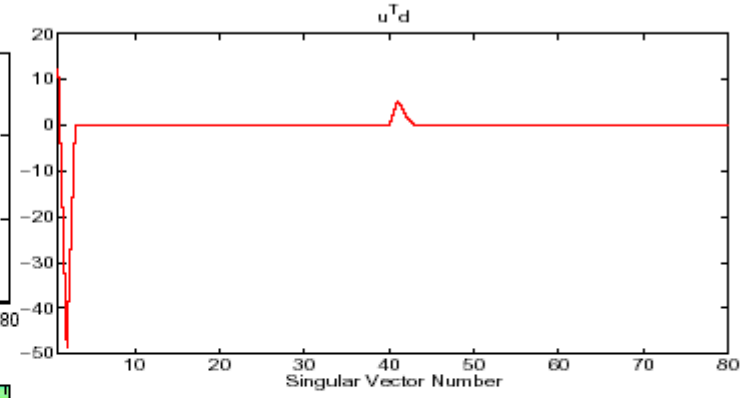
where $\mu^2 = \frac{\sigma_o^2}{\sigma_b^2}$ and λ_i, $\mathbf{v}_i$, $\mathbf{u}_i$ are

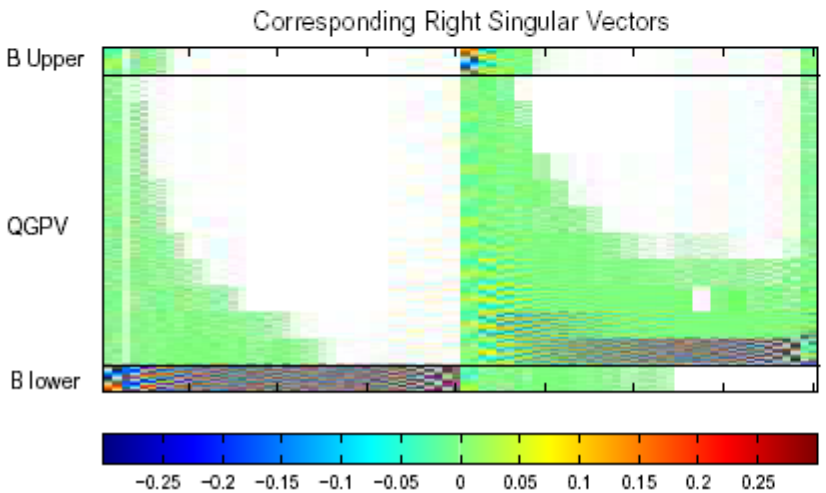
the singular values and right and left singular vectors of $\hat{\mathbf{H}}\mathbf{C}_B^{1/2} = \mathbf{U}\mathbf{\Lambda}\mathbf{V}^T$.

Johnson et al, 2005a,b

SVD







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

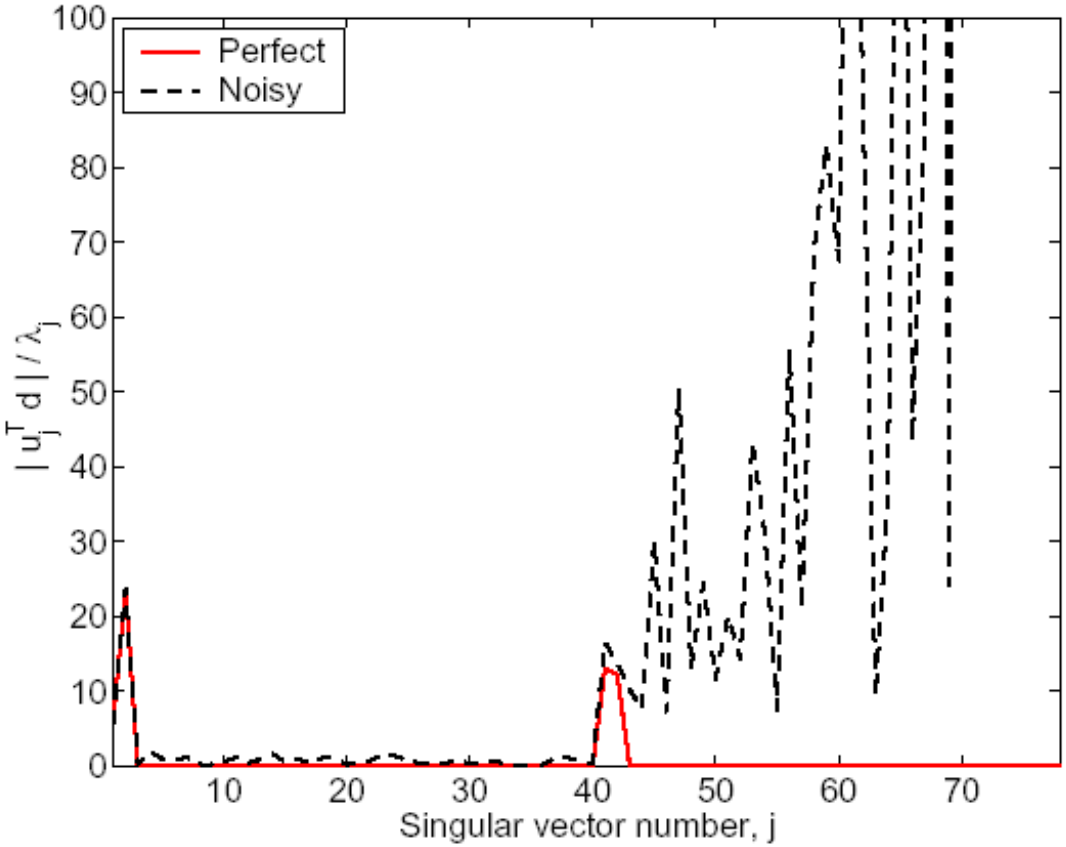
Johnson et al, 2005a,b

Effect of Observational Noise

Values of

$$\left| \frac{\mathbf{u}_j^T \hat{\mathbf{d}}}{\lambda_j} \right|$$

for perfect and noisy observations.



Johnson et al, 2005a,b

5.

Conclusions

Conclusions

- The condition number of the Hessian is sensitive to lengthscale
- Preconditioning with $\mathbf{B}^{1/2}$ generally reduces the condition number and improves the convergence rates
- The condition number of the Hessian increases as the observations become more accurate and as their separation decreases.

References

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Future

Many more challenges left!