A comparison of the model error and state formulations of weak-constraint 4D-Var

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Outline

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Four-dimensional variational assimilation (4D-Var)

The 4D-Var data assimilation problem can be expressed as the minimization of

$$\mathcal{J}[x_0] = \frac{1}{2}(x_0 - x^b)^{\mathrm{T}} B^{-1}(x_0 - x^b) + \frac{1}{2}\sum_{i=0}^{N}(\mathcal{H}_i[x_i] - y_i)^{\mathrm{T}} R_i^{-1}(\mathcal{H}_i[x_i] - y_i)$$

subject to the dynamical system

$$x_{i+1} = \mathcal{M}_i(x_i)$$

where

x^b	A priori (background) estimate
y_i	Observation
B	Background error covariance matrix
R_i	Observation error covariance matrix
$\mathcal{H}_i$	Observation operator

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Weak-constraint 4D-Var

We consider the model as a weak constraint

$$x_{i+1} = \mathcal{M}_i(x_i) + \eta_i, \qquad \eta_i \sim \mathcal{N}(0, Q_i)$$

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State formulation

$$\begin{aligned} &\mathcal{J}(x_0, x_1, \ldots, x_N) \\ = \quad &\mathcal{J}_b + \mathcal{J}_o + \frac{1}{2}\sum_{i=0}^{N-1}(x_{i+1} - \mathcal{M}_i(x_i))^T Q_i^{-1}(x_{i+1} - \mathcal{M}_i(x_i)) \end{aligned}$$

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Error formulation

$$\mathcal{J}(x_0, \eta_0, \ldots, \eta_{N-1}) = \mathcal{J}_b + \mathcal{J}_o + \frac{1}{2}\sum_{i=0}^{N-1} \eta_i^T Q_i^{-1} \eta_i$$

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Condition number

The inner loop is solved using a gradient minimization method. The expected accuracy of the numerical solution and the speed of convergence are both determined by the condition number of the Hessian.

Condition number

$$\kappa(\mathbf{A}) = ||\mathbf{A}||||\mathbf{A}^{-1}||$$

In the matrix 2-norm, for a symm. pos. def. matrix $\mathbf{A}$, we have

$$\kappa(\mathbf{A}) = \lambda_{\text{max}}(\mathbf{A})/\lambda_{\text{min}}(\mathbf{A})$$

In 4D-Var the condition number of the Hessian matrix determines convergence properties.

Notation

Define

$$
\begin{aligned}
\mathbf{D} &= diag\{B, Q_1, \ldots, Q_n\} \\
\mathbf{R} &= diag\{R_1, \ldots, R_n\} \\
\mathbf{H} &= diag\{H_1, \ldots, H_n\}
\end{aligned}
$$

$$
\mathbf{L} = \begin{pmatrix} I & 0 & 0 & \cdots & 0 \\ -M_1 & I & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 - M_n & I \end{pmatrix}
$$

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Hessian - Error formulation

$$\mathbf{S}_p = \mathbf{D}^{-1} + \mathbf{L}^{-T}\mathbf{H}^{T}\mathbf{R}^{-1}\mathbf{H}\mathbf{L}^{-1}$$

$$\mathbf{S}_p = \begin{pmatrix} B_0^{-1} & & & \\ & Q_1^{-1} & & \\ & & \ddots & \\ & & & Q_n^{-1} \end{pmatrix} +$$

$$\begin{pmatrix} H_0^T & (H_1M_1)^T & (H_2M_2M_1)^T & \dots & (H_nM_n\dots M_1)^T \\ & H_1^T & (H_2M_2)^T & \dots & (H_nM_n\dots M_2)^T \\ & & H_2^T & \ddots & \vdots \\ & & & \ddots & (H_nM_n)^T \\ & & & & H_n^T \end{pmatrix} \mathbf{R}^{-1} \begin{pmatrix} H_0 & & & & \\ H_1M_1 & H_1 & & & \\ H_2M_2M_1 & H_2M_2 & H_2 & & \\ \vdots & & \ddots & \ddots & \\ H_nM_n\dots M_1 & \dots & & H_nM_n & H_n \end{pmatrix}$$

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Hessian - State formulation

$$\mathbf{S}_x = \mathbf{L}^T\mathbf{D}^{-1}\mathbf{L} + \mathbf{H}^T\mathbf{R}^{-1}\mathbf{H}$$

$$\mathbf{S}_x = \begin{pmatrix} B_0^{-1}+M_1^TQ_1^{-1}M_1 & -M_1^TQ_1^{-1} & & & \\ -Q_1^{-1}M_1 & Q_1^{-1}+M_2^TQ_2^{-1}M_2 & -M_2^TQ_2^{-1} & & \\ & -Q_2^{-1}M_2 & \ddots & & \\ & & & -M_{n-1}^TQ_{n-1}^{-1} & \\ & & -Q_{n-1}^{-1}M_{n-1} & Q_{n-1}^{-1}+M_n^TQ_n^{-1}M_n & -M_n^TQ_n^{-1} \\ & & & -Q_n^{-1}M_n & Q_n^{-1} \end{pmatrix}$$

$$+ \begin{pmatrix} H_0^TR_0^{-1}H_0 & & & \\ & H_1^TR_1^{-1}H_1 & & \\ & & \ddots & \\ & & & H_n^TR_n^{-1}H_n \end{pmatrix}$$

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Aims

- How does the condition number of the Hessian change with different input parameters?
- How does this affect convergence of the minimisation?

Note: Theoretical bounds on the condition number have been obtained. Here we just illustrate the effects with numerical results.

Previous results

Previously we have shown for the strong constraint case (preconditioned by $B^{1/2}$) that the bounds on the condition number will increase as

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Previously we have shown for the strong constraint case (preconditioned by $B^{1/2}$) that the bounds on the condition number will increase as

- the observations become more accurate;
- the observations spacing decreases;
- the background becomes less accurate;
- the background error correlation lengthscales increase.

(Haben *et al.* (2014) *Tellus*, Haben *et al.* (2014) *Comput. Fluids*)

Numerical model

We consider results in the context of a simple system, the 1D advection equation with periodic boundary conditions:

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0$$

with

$$u(x,0) = be^{-\frac{(x-c)^2}{2d^2}}.$$

The model is discretized using an upwind numerical scheme with $N = 50$ grid points, $a = -1$.

Assimilation scheme

- Background error covariance matrix $B = \sigma_b^2 C_{SOAR}$, with $\sigma_b = 0.1, L(C) = 2\Delta x$.
- Model error covariance matrix $Q_i = \sigma_q^2 C_{LAP}$, with $\sigma_q = 0.05, L(C) = \Delta x,$.
- Observation error covariance matrix $R_i = \sigma_o^2 I$, with $\sigma_o = 0.05$.
- Observations every 2 grid points and every 5 time steps in 50 time step window.
- $\Delta x = 0.01, \Delta t = 0.02$.

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Effect of observation accuracy

- Large observation error variance

Matrix	Condition Number	No. of iterations
$\mathbf{S}_p$	834	87
$\mathbf{S}_x$	1.11×10^5	2821
$\mathbf{D}$	838	-

- Small observation error variance

Matrix	Condition Number	No. of iterations
$\mathbf{S}_p$	2.71×10^6	191
$\mathbf{S}_x$	1.84×10^5	176
$\mathbf{D}$	838	-

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Effect of observation accuracy

Condition number as σ_q/σ_o varies:

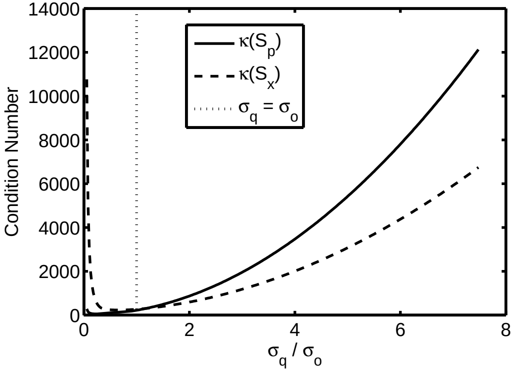

Figure : $\kappa(\mathbf{S}_p)$ (solid line) and $\kappa(\mathbf{S}_x)$ (dashed line) as a function of ratio σ_q/σ_o. Condition number minimum point at $\sigma_q = \sigma_o$ (dotted line).

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Effect of assimilation window length - Error formulation

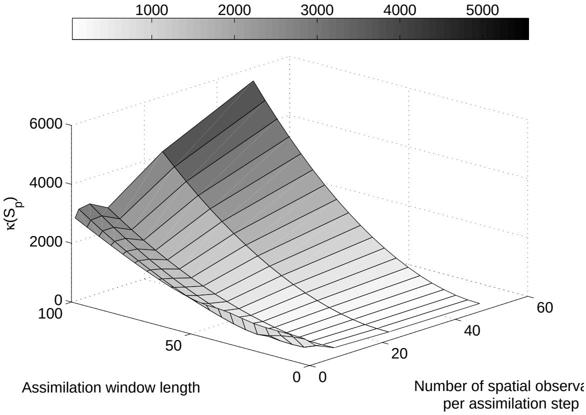

Figure : $\kappa(\mathbf{S}_p)$ as a function of assimilation window length, n, and number of spatial observations, q.

Effect of assimilation window length - State formulation

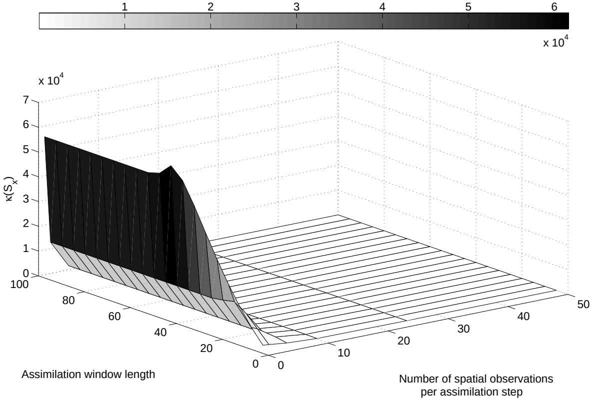

Figure : $\kappa(\mathbf{S}_x)$ as a function of assimilation window length, n, and number of spatial observations, q.

Reduction of model error variance

We now set $\sigma_b/\sigma_q = 200$.

Matrix	Condition Number	No. of iterations
$\mathbf{S}_p$	8.53×10^6	635
$\mathbf{S}_x$	1.00×10^8	1756
$\mathbf{D}$	8.53×10^6	-

Change in model error variance - Condition numbers

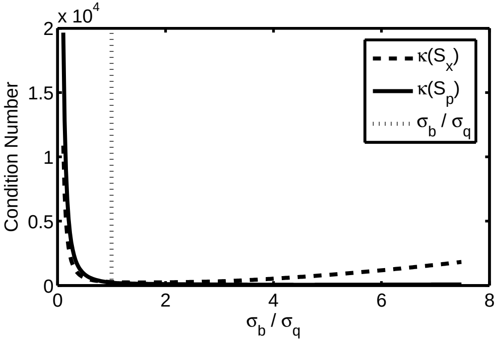

Figure : $\kappa(\mathbf{S}_p)$ (solid line) and $\kappa(\mathbf{S}_x)$ (dashed line) as a function of ratio σ_b/σ_q. Condition number minimum point at $\sigma_b = \sigma_q$ (dotted line).

Correlation length-scales

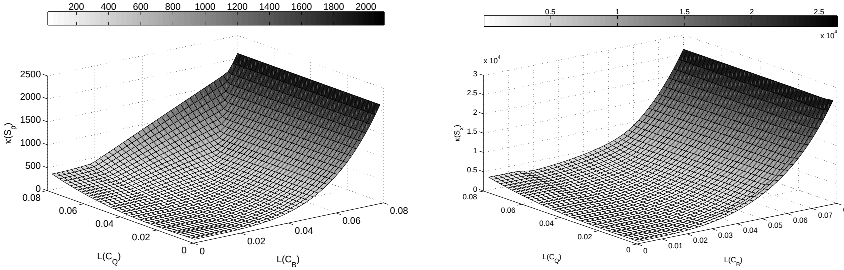

Figure : Condition number of $\kappa(\mathbf{S}_p)$ (left) and $\kappa(\mathbf{S}_x)$ (right) as a function of $L(C_B)$ and $L(C_Q)$.

Conclusions

- The two different formulations of the WC problem have Hessians with different structures.

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- The condition number of both Hessians is sensitive to input parameters, with the state formulation generally being more sensitive.
- Sensitivities backed up by theory (not shown).

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In particular we find the following sensitivities:

- For increasing observation accuracy the error formulation is more sensitive, while for small observation accuracy the state formulation is badly conditioned.

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- The error formulation is more sensitive to an increase in window length.
- The state formulation is more sensitive to having fewer observations.
- For larger model error the state formulation becomes more ill conditioned than the error formulation.
- The state formulation is more sensitive to changes in the condition number of $\mathbf{D}$.

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- Saddle-point formulation.