Improving the conditioning of estimated covariance matrices

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Motivation

- Including correlated observation error allows us to maximise the information content of observations.
- But diagnosed correlated covariance matrices have caused problems with convergence of the data assimilation minimisation procedure.
- Need to treat diagnosed matrices (symmetry, positive definiteness).

What is reconditioning?

- *Methods which can be applied to matrices to reduce their condition number, while retaining underlying matrix structure.*
- Examples of methods:
    - Thresholding
    - Tapering
    - General regularisation methods.

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Reminder: If $\mathbf{S} \in \mathbb{R}^{p \times p}$ *is a symmetric and positive definite matrix with eigenvalues* $\lambda_1(\mathbf{S}) \geq \ldots \geq \lambda_p(\mathbf{S}) > 0$ *then we can write the condition number in the* L_2 *norm as*

$$\kappa(\mathbf{S}) = \frac{\lambda_1(\mathbf{S})}{\lambda_p(\mathbf{S})}.$$

If $\mathbf{S}$ *is singular, we take* $\kappa(\mathbf{S}) = \infty$.

The ridge regression (RR) and minimum eigenvalue (ME) methods

Both methods improve the condition number of a covariance matrix by altering their eigenvalues to yield a reconditioned matrix with a user-defined condition number κ_{max}.

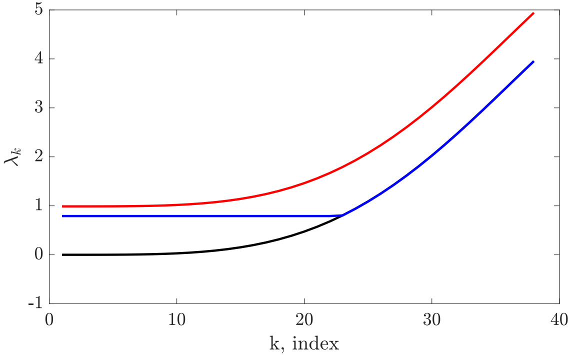

Figure: Illustration of recond methods: original spectrum (black), and spectrum reconditioned via ME and RR

Ridge regression method

Idea: Add a scalar multiple of identity to $\mathbf{R}$ *to obtain reconditioned* $\mathbf{R}_{RR}$ *with* $\kappa(\mathbf{R}_{RR}) = \kappa_{max}$.

Setting δ

- *Define* $\delta = \frac{\lambda_1(\mathbf{R}) - \lambda_p(\mathbf{R})\kappa_{max}}{\kappa_{max} - 1}$.
- *Set* $\mathbf{R}_{RR} = \mathbf{R} + \delta \mathbf{I}$

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- Similar to Steinian linear shrinkage [Ledoit and Wolf, 2004]
- Used at the Met Office [Weston et al, 2014].

Theory of the ridge regression method

Effect of RR on standard deviations:

$$\mathbf{\Sigma}_{RR} = (\mathbf{\Sigma}^2 + \delta \mathbf{I}_p)^{1/2}. \quad (1)$$

i.e. variances are increased by the reconditioning constant, δ.

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Effect of RR on correlations:

$$\text{For } i \neq j, |\mathbf{C}_{RR}(i,j)| < |\mathbf{C}(i,j)| \tag{2}$$

i.e. the magnitude of all off-diagonal correlations is strictly decreased.

Minimum eigenvalue method

Idea: Fix a threshold, T, below which all eigenvalues of the reconditioned matrix, $\mathbf{R}_{ME}$, are set equal to T to yield $\kappa(\mathbf{R}_{ME}) = \kappa_{max}$.

Setting T:

- *Set $\lambda_1(\mathbf{R}_{ME}) = \lambda_1(\mathbf{R})$*
- *Define $T = \lambda_1(\mathbf{R})/\kappa_{max}$.*
- *Set the remaining eigenvalues of $\mathbf{R}_{ME}$ via*

$$\lambda_k(\mathbf{R}_{ME}) = \begin{cases} \lambda_k(\mathbf{R}) & \text{if } \lambda_k(\mathbf{R}) > T \\ T & \text{if } \lambda_k(\mathbf{R}) \leq T \end{cases}. \tag{3}$$

- *We define $\mathbf{\Gamma}(k,k) = max\{T - \lambda_i, 0\}$.*

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A variant of this method is used at the European Centre for Medium-Range Weather Forecasts (ECMWF) [Bormann et al, 2016].

Theory of the minimum eigenvalue method

Effect of ME on standard deviations:

$$\boldsymbol{\Sigma}_{ME}(i,i) = \left(\boldsymbol{\Sigma}(i,i)^2 + \sum_{k=1}^{p} \mathbf{V}_R(i,k)^2 \boldsymbol{\Gamma}(k,k)\right)^{1/2} \tag{4}$$

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This can be bounded by

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Effect of ME on correlations:

It is not evident how correlation entries are altered in general.
This is due to the fact that the spectrum of **R** is not altered uniformly by this method.

Comparison of both methods

- Both methods increase (or maintain) standard deviations

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- Both methods increase (or maintain) standard deviations
- We can show that $T - \lambda_p(\mathbf{R}) < \delta$ which yields:

$$\mathbf{\Sigma}_{ME}(i,i) \leq \left(\mathbf{\Sigma}(i,i)^2 + T - \lambda_p(\mathbf{R})\right)^{1/2} < (\mathbf{\Sigma}(i,i)^2 + \delta)^{1/2} = \mathbf{\Sigma}_{RR}(i,i)$$

- Therefore RR increases standard deviations more than ME

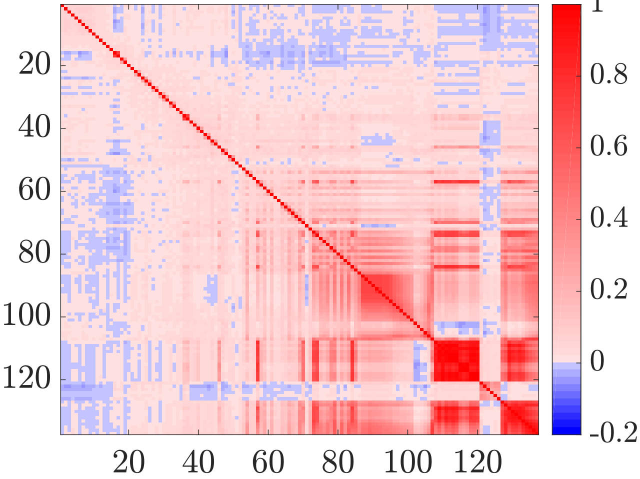
IASI matrix - framework

Interchannel correlations for a covariance matrix of satellite observation errors

- The UK Met Office diagnosed a correlated observation error covariance matrix in 2011.
- This was extremely ill-conditioned and crashed the system when used directly.
- Recondition 137 channels.

Original condition number: 27703.

Diagnosed IASI correlation matrix



IASI - change to standard deviations

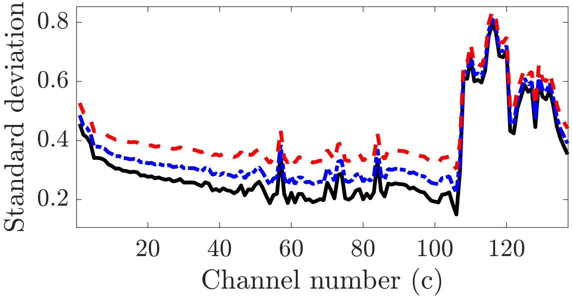


Figure: Standard deviations $\mathbf{\Sigma}$ (solid), $\mathbf{\Sigma}_{RR}$ and $\mathbf{\Sigma}_{ME}$ for $\kappa_{max} = 100$. Recall $\kappa(\mathbf{R}) = 27703.45$ for the original IASI matrix.

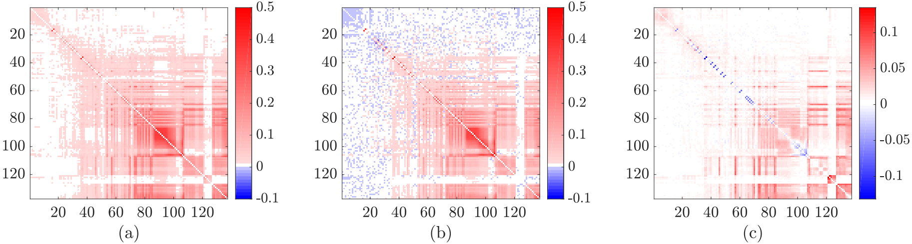


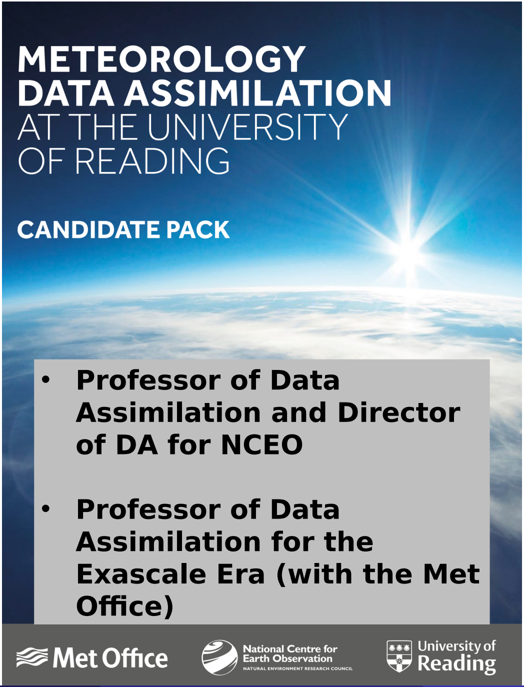
Figure: Difference in correlations (a) $(\mathbf{C} - \mathbf{C}_{RR}) \circ sign(\mathbf{C})$, (b) $(\mathbf{C} - \mathbf{C}_{ME}) \circ sign(\mathbf{C})$, and (c) $(\mathbf{C}_{ME} - \mathbf{C}_{RR}) \circ sign(\mathbf{C})$. The colorscale is the same for (a) and (b) but different for (c).

Ongoing work

- Focused on improving conditioning and the relationship between condition number and convergence of a conjugate gradient type minimisation.
- But by reconditioning we are altering the problem we are solving!
- Studying impact of reconditioning on an operational system - 1D-Var QC procedure used at the Met Office.
- Focussed on RR - run experiments comparing uncorrelated $\mathbf{R}$ with different values of δ.
- Increasing δ improves convergence - better than current operational choice of $\mathbf{R}$!
- But difficult to assess impacts on retrieved variables:
  Differences between retrieved values mostly small for ctrl - expt
  But some very large differences which are hard to explain

Conclusions and ongoing work

- Developed new theory showing how two reconditioning methods alter covariance matrices theoretically.
- The ridge regression method increases standard deviations more than the minimum eigenvalue method.
- The ridge regression method moves all correlations closer to zero, whereas the minimum eigenvalue method can increase correlations.
- The ridge regression method changes most correlation entries by a larger amount than the minimum eigenvalue method in numerical testing.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Met Office
National Centre for Earth Observation
NATURAL ENVIRONMENT RESEARCH COUNCIL
University of Reading

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PhD thesis University of Reading

SOAR matrix - simple framework

Spatial correlations for a simple numerical experiment

- Use a second-order auto-regressive function to construct a circulant correlation matrix - i.e. a matrix fully defined by its first row.
- We fix the standard deviations to be constant for all variables.
- In this framework we have update the standard deviations for the minimum eigenvalue method via:

$$\mathbf{\Sigma}_{ME}(i,i) = \left(\mathbf{\Sigma}(i,i)^2 + \frac{1}{p}\sum_{k=1}^{p} \mathbf{\Gamma}(k,k) \right)^{1/2}. \tag{6}$$

Original condition number: 81121.

SOAR matrix - results

Table: Change to standard deviations of the SOAR matrix.

κ_{max}	σ	σ_{RR}	% change RR	σ_{ME}	% change ME
1000	2.23606	2.26471	+1.28%	2.25439	+0.82%
500	2.23606	2.29340	+2.56%	2.27599	+1.79%
100	2.23606	2.51306	+12.39%	2.45737	+9.90%

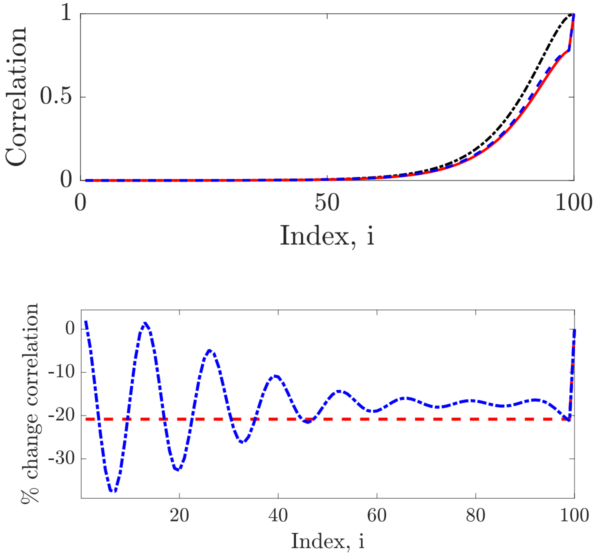
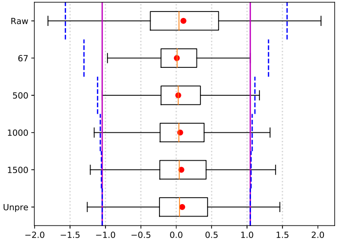
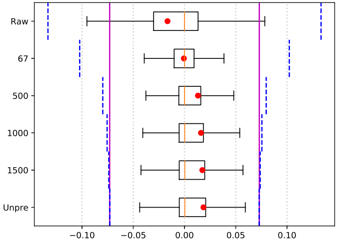


Figure: Changes to correlations between the 100th row of the original SOAR matrix and the reconditioned matrices (for $\kappa_{max} = 100$). (a) $\mathbf{C}$ (black), $\mathbf{C}_{RR}$, $\mathbf{C}_{ME}$ (b) $100 \times \frac{\mathbf{C}-\mathbf{C}_{RR}}{\mathbf{C}}$ and $100 \times \frac{\mathbf{C}-\mathbf{C}_{ME}}{\mathbf{C}}$.

Changes to retrievals in 1D-Var





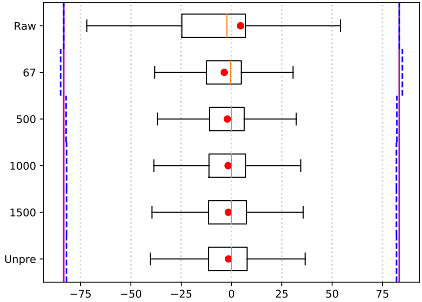


Figure: (a) Skin temperature, (b) cloud fraction, (c) cloud top pressure