Using reconditioning to study the impact of correlated observation errors in the Met Office 1D-Var system

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Overview

1 Motivation
   - Why do we want to include correlated observation error information?

2 Reconditioning is one solution!
   - What is reconditioning?
   - Theory of reconditioning

3 Implementation in the Met Office system
   - IASI - operational interchannel correlations
   - Impact of reconditioning on convergence
   - Impact of reconditioning on quality control procedure
Cost function for 3DVar

We want to minimise

\[ J(x) = (x - x_b)^T B^{-1} (x - x_b) + (y - h[x])^T R^{-1} (y - h[x]). \] (1)

where,

- \( B \in \mathbb{R}^{N \times N} \) background error covariance
- \( R \in \mathbb{R}^{p \times p} \) observation error covariance
- \( h : \mathbb{R}^N \rightarrow \mathbb{R}^p \) observation operator
- \( y \in \mathbb{R}^p \) vector of observations
- \( x_b \in \mathbb{R}^N \) vector representing the background

What happens to the convergence of (1) if we introduce correlated \( R \)?.
Why include correlated observation error information?

- Including correlation information allows us to take advantage of dense observation networks to get **high-resolution forecasts**.
- Using uncorrelated observation error matrices means we have to thin observations - this can result in **up to 80%** of obs being discarded!
- Neglecting correlations where they are present also **limits our skill**.
Why is it hard to include correlation information?

- For high-dimensional problems (e.g. big data) we can only estimate correlation information by sampling.
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  - Sample covariance matrices that aren’t full rank.
  - Sample matrices that are extremely ill-conditioned.
- We use $R^{-1}$ in (1) - calculating this inverse is expensive/impossible
- May have to do this online
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Reminder: If $S \in \mathbb{R}^{p \times p}$ is a symmetric and positive definite matrix with eigenvalues $\lambda_1(S) \geq \ldots \geq \lambda_p(S) > 0$ then we write the condition number

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

If $S$ is singular, we take $\kappa(S) = \infty$. 
Satellite observation errors are known to have correlated observation errors [Stewart, 2010].

**Figure**: Diagnosed correlation matrix for IASI
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**Figure:** Diagnosed correlation matrix for IASI
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Methods to diagnose covariance matrices exist but yield matrices that are highly ill-conditioned and caused problems with convergence.

[Weston et al, 2014] suggested these problems were due to very small eigenvalues and tested two methods of ‘reconditioning’.

[Tabeart et al, 2018] proved that the minimum eigenvalue of the observation error covariance matrix is important for the conditioning of the general data assimilation problem.
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**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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**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.
- We will focus on a method that is used at the Met Office for numerical weather prediction. This method works by altering the eigenvalues of the original covariance matrix $\mathbf{R}$. 
Reminder about variances and correlations

Want to also consider how variances and correlations are changed by the two methods. Let

\[ R = \Sigma C \Sigma, \] (2)

where \( C \) is the correlation matrix, and \( \Sigma \) is the diagonal matrix of standard deviations. We calculate \( C \) and \( \Sigma \) via:

\[ \Sigma(i, i) = \sqrt{R(i, i)} \] (3)

and

\[ C(i, j) = \frac{R(i, j)}{\sqrt{R(i, i)} \sqrt{R(j, j)}}. \] (4)
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 $\kappa_{\text{max}}$.

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 $\kappa(\mathbf{R}_{RR}) = \kappa_{\text{max}}$.

Setting $\delta$

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

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- Set $R_{RR} = R + \delta I$

We can prove theoretically:

- Standard deviations are increased by using this method.
- Absolute value of off-diagonal correlations decreased by this method.
Interchannel correlations for a covariance matrix of satellite observation errors

- The UK Met Office diagnosed a correlated observation error covariance matrix in 2010.
- This was extremely ill-conditioned and crashed the system when used directly.
- Use 137 channels - **Original condition number:** 27703.

We study the impact of reconditioning in the **1D-Var** procedure.

- Run prior to every 4D-Var/forecast cycle.
- Assimilates each observation individually
- Used as quality control (reject ob if it doesn’t converge in 10 iterations)
- Also used to fix values for variables that aren’t assimilated in 4D-Var procedure.
Diagnosed IASI correlation matrix
Experimental choices of $R_{RR}$ - standard deviations

Figure: Standard deviation for each of the experiment choices
Experimental choices of $R_{RR}$ - correlations

Figure: Changes to correlation with reconditioning for the correlated experiments
Figure: Number of iterations required to reach convergence of the 1D-Var minimization as a fraction of the total number of observations common to all choices of R. Symbols correspond to: △ = $R_{diag}$, ○ = $R_{est}$, ♦ = $R_{67}$, ◆ = $R_{infl}$. 
Impact on temperature and humidity

Figure: Example retrieved profiles of temperature (a) and specific humidity (b), and differences in retrievals between $E_{\text{diag}}$ and $E_{67}$ for temperature (c) and specific humidity (d) for 97330 observations.
Impact of reconditioning on quality control procedure

<table>
<thead>
<tr>
<th>Set</th>
<th>No. of accepted obs</th>
<th>No of obs accepted by both $E_{diag}$ and $E_{exp}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_{diag}$</td>
<td>100686</td>
<td>99039</td>
</tr>
<tr>
<td>$R_{est}$</td>
<td>100655</td>
<td>99175</td>
</tr>
<tr>
<td>$R_{1000}$</td>
<td>101002</td>
<td>99352</td>
</tr>
<tr>
<td>$R_{500}$</td>
<td>101341</td>
<td>99656</td>
</tr>
<tr>
<td>$R_{67}$</td>
<td>102333</td>
<td>100382</td>
</tr>
<tr>
<td>$R_{infl}$</td>
<td>102859</td>
<td>100679</td>
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**Table:** Change to number of accepted observations with reconditioning
Impact of reconditioning on variables not in 4D-Var state vector

**Figure:** Change to estimates for skin temperature (left), cloud fraction (centre) and cloud top pressure (right) with reconditioning.
What about the outliers?

<table>
<thead>
<tr>
<th></th>
<th>$E_{est}$</th>
<th>$E_{1500}$</th>
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<td>23.9</td>
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<td>24.6</td>
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<td>21.4</td>
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<tr>
<td>% outliers (ST)</td>
<td>15.1</td>
<td>15.3</td>
<td>15.6</td>
<td>16.3</td>
<td>17.6</td>
<td>15.9</td>
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<tr>
<td>Min diff (ST (K))</td>
<td>-33.52</td>
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Think about **extreme outliers** - defined here as mean ± 0.25 × max difference

| % $|CF| > 0.25 $ | $E_{est}$ | $E_{1500}$ | $E_{1000}$ | $E_{500}$ | $E_{67}$ | $E_{infl}$ |
|----------------|----------|------------|------------|----------|---------|-----------|
|                 | 4.9      | 4.7        | 4.4        | 3.9      | 3.2     | 7.5       |

| % $|CTP| > 225hPa $ | $E_{est}$ | $E_{1500}$ | $E_{1000}$ | $E_{500}$ | $E_{67}$ | $E_{infl}$ |
|----------------|----------|------------|------------|----------|---------|-----------|
|                 | 3.3      | 3.3        | 3.3        | 3.3      | 2.7     | 4.4       |

| % $|ST| > 5K $ | $E_{est}$ | $E_{1500}$ | $E_{1000}$ | $E_{500}$ | $E_{67}$ | $E_{infl}$ |
|----------------|----------|------------|------------|----------|---------|-----------|
|                 | 1.6      | 1.5        | 1.5        | 1.4      | 1.4     | 3.6       |
Conclusions

- Including correlated observation error in data assimilation methods is important for high-resolution forecasts and to make the best use of observation information.
- Convergence problems can be mitigated by using reconditioning methods.
- Tests in the Met Office 1D-Var system show that:
  - the ridge regression method improves convergence.
  - the quality control process is altered.
- Future work is needed to understand why some retrieved values change by a large amount.
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