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

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### Motivation

• Why do we want to include correlated observation error information?

### Reconditioning is one solution!

- What is reconditioning?
- Theory of reconditioning

### Implementation in the Met Office system

- IASI operational interchannel correlations
- Impact of reconditioning on convergence
- Impact of reconditioning on quality control procedure

We want to minimise

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

where,

- $\mathbf{B} \in \mathbb{R}^{N \times N}$  background error covariance
- $\mathbf{R} \in \mathbb{R}^{p \times p}$  observation error covariance
- $h: \mathbb{R}^N \to \mathbb{R}^p$  observation operator
- $\mathbf{y} \in \mathbb{R}^{p}$  vector of observations
- $\mathbf{x}_b \in \mathbb{R}^N$  vector representing the background

What happens to the convergence of (1) if we introduce correlated **R**?.

- 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.

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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 write the condition number

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

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

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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 **R**.

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

$$\mathbf{R} = \mathbf{\Sigma} \mathbf{C} \mathbf{\Sigma}, \tag{2}$$

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

$$\mathbf{\Sigma}(i,i) = \sqrt{\mathbf{R}(i,i)} \tag{3}$$

and

$$\mathbf{C}(i,j) = \frac{\mathbf{R}(i,j)}{\sqrt{\mathbf{R}(i,i)}\sqrt{\mathbf{R}(j,j)}}.$$
(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  $\kappa_{max}$ .



Figure: Illustration of recond methods: original spectrum (black), and spectrum reconditioned via  $\ensuremath{\mathsf{ME}}$  and  $\ensuremath{\mathsf{RR}}$ 

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

Setting  $\delta$ • Define  $\delta = \frac{\lambda_1(\mathbf{R}) - \lambda_p(\mathbf{R})\kappa_{max}}{\kappa_{max} - 1}$ . • Set  $\mathbf{R}_{RR} = \mathbf{R} + \delta \mathbf{I}$  Idea: Add a scalar multiple of identity to **R** to obtain reconditioned **R**<sub>RR</sub> with  $\kappa$ (**R**<sub>RR</sub>) =  $\kappa$ <sub>max</sub>.

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

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 $\mathbf{R}_{RR}$ - standard deviations



Figure: Standard deviation for each of the experiment choices

## Experimental choices of $\mathbf{R}_{RR}$ - correlations



Figure: Changes to correlation with reconditioning for the correlated experiments

## Impact of reconditioning on convergence



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:  $\triangle = \mathbf{R}_{diag}$ ,  $\circ = \mathbf{R}_{est}$ ,  $\Diamond = \mathbf{R}_{67}$ ,  $\Diamond = \mathbf{R}_{infl}$ .

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## Impact on temperature and humidity



Figure: Example retrieved profiles of temperature (a) and specific humidity (b), and differences in retrievals between  $E_{diag}$  and  $E_{67}$  for temperature (c) and specific humidity (d) for 97330 observations.

Set	No. of accepted obs	No of obs accepted by both $E_{diag}$ and $E_{exp}$
<b>R</b> <sub>diag</sub>	100686	99039
$\mathbf{R}_{est}$	100655	99175
$R_{1000}$	101002	99352
<b>R</b> <sub>500</sub>	101341	99656
<b>R</b> <sub>67</sub>	102333	100382
<b>R</b> <i>infl</i>	102859	100679

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?

	E <sub>est</sub>	$E_{1500}$	$E_{1000}$	E <sub>500</sub>	E <sub>67</sub>	Einfl
% outliers (CF)	23.9	24.0	24.2	24.6	25.3	21.4
% outliers (CTP)	22.8	22.8	23.0	22.9	21.4	18.8
% outliers (ST)	15.1	15.3	15.6	16.3	17.6	15.9
Max diff (ST (K))	21.67	21.12	21.14	22.38	21.03	26.83
Min diff (ST (K))	-33.52	-33.01	-32.14	-29.76	-23.82	-20.88

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Think about extreme outliers - defined here as mean  $\pm$  0.25  $\times$  max difference

	E <sub>est</sub>	$E_{1500}$	$E_{1000}$	$E_{500}$	E <sub>67</sub>	E <sub>infl</sub>
%   <i>CF</i>   > 0.25	4.9	4.7	4.4	3.9	3.2	7.5
%   <i>CTP</i>   > 225 <i>hPa</i>	3.3	3.3	3.3	3.3	2.7	4.4
ST  > 5K	1.6	1.5	1.5	1.4	1.4	3.6

- 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.

## References I

J. M. Tabeart, S. L. Dance, S. A. Haben, A. S. Lawless, N. K. Nichols, and J. A. Waller (2018)

The conditioning of least squares problems in variational data assimilation.

Numerical Linear Algebra with Applications http://dx.doi.org/10.1002/nla.2165



P. Weston, W. Bell and J. R. Eyre (2014)

Accounting for correlated error in the assimilation of high-resolution sounder data Q. J. R Met Soc 140, 2420 – 2429.

Niels Bormann, Massimo Bonavita, Rossana Dragani, Reima Eresmaa, Marco Matricardi, and Anthony McNally (2016)

Enhancing the impact of IASI observations through an updated observation error covariance matrix

doi: 10.1002/qj.2774

S. Rainwater, C. H. Bishop and W. F. Campbell (2015) The benefits of correlated observation errors for small scales *Q. J. R. Met. Soc.* 141, 3439–3445

### O. Ledoit and M. Wolf (2004)

A well-conditioned estimator for large-dimensional covariance matrix.

J. Multivariate Anal. 88:365-411

#### M. Tanaka and K. Nakata (2014)

Positive definite matrix approximation with condition number constraint. *Optim. Lett.* 8:939947.

#### Laura Stewart (2010)

Correlated observation errors in data assimilation

PhD thesis University of Reading