## **Covariance Matrices in Variational DA**

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# Lecture outline

- Reminders
- Importance of the **B**-matrix
- $\bullet \,$  Modelling  ${\bf B}$
- ullet Measuring  ${f B}$

## Example state and observation vectors





 $\mathbf{x}_A$  analysis state  $\mathbf{x}_B$  background state

Sometimes  $\mathbf{x}$  and  $\mathbf{y}$  are for only one time (3D-Var)

 ${\bf x}\text{-vectors}$  have n elements in total  ${\bf y}\text{-vectors}$  have p elements in total

#### Reminder of the variational cost function



$$\mathbf{x}_{A} = \operatorname{argmin}(\mathcal{J}[\mathbf{x}]).$$

- The covariance matrices **B** and **R** influence the analysis profoundly.
- If  $\mathcal{H}(\mathbf{x})$  is a linear or weakly non-linear function then we can write (3D-Var for simplicity):

$$\mathbf{y} - \mathcal{H}(\mathbf{x}_{\mathrm{B}} + \delta \mathbf{x}) \approx \mathbf{y} - (\mathcal{H}(\mathbf{x}_{\mathrm{B}}) + \mathbf{H}\delta \mathbf{x}),$$

and  $\mathbf{x}_A$  can be written explicitly:

$$\mathbf{x}_{A} = \mathbf{x}_{B} + \mathbf{B}\mathbf{H}^{T}\left(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{T}\right)^{-1}\left(\mathbf{y} - \boldsymbol{\mathcal{H}}(\mathbf{x}_{B})\right)$$

## Anatomy of a covariance matrix



outer product

where  $\mathbf{p}' = \mathbf{p} - \langle \mathbf{p} \rangle$ .

Multivariate background error covariance matrix (e.g. if  $\mathbf{x}$  represents pressure, zonal wind and meridional wind):

(univariate)

$$\mathbf{x} = \begin{pmatrix} \mathbf{p} \\ \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \begin{pmatrix} p_1 \\ \vdots \\ p_{n/3} \\ u_1 \\ \vdots \\ u_{n/3} \\ v_1 \\ \vdots \\ v_{n/3} \end{pmatrix}, \quad \operatorname{cov}(\mathbf{x}') = \langle \mathbf{x}' \mathbf{x}'^{\mathrm{T}} \rangle = \begin{pmatrix} \langle \mathbf{p}' \mathbf{p}'^{\mathrm{T}} \rangle & \langle \mathbf{p}' \mathbf{u}'^{\mathrm{T}} \rangle & \langle \mathbf{p}' \mathbf{v}'^{\mathrm{T}} \rangle \\ \langle \mathbf{u}' \mathbf{p}'^{\mathrm{T}} \rangle & \langle \mathbf{u}' \mathbf{u}'^{\mathrm{T}} \rangle & \langle \mathbf{u}' \mathbf{v}'^{\mathrm{T}} \rangle \\ \langle \mathbf{v}' \mathbf{p}'^{\mathrm{T}} \rangle & \langle \mathbf{v}' \mathbf{u}'^{\mathrm{T}} \rangle & \langle \mathbf{u}' \mathbf{v}'^{\mathrm{T}} \rangle \\ \langle \mathbf{v}' \mathbf{p}'^{\mathrm{T}} \rangle & \langle \mathbf{v}' \mathbf{u}'^{\mathrm{T}} \rangle & \langle \mathbf{v}' \mathbf{v}'^{\mathrm{T}} \rangle \\ \end{pmatrix}.$$
multivariate covariance sub-matrix

These covariances are symmetric matrices.

 $rac{\partial \mathbf{F}}{\partial \mathbf{x}'}$  are forecast errors,  $oldsymbol{\epsilon}_{\mathrm{B}}$ , then above is  $\mathbf{B}$ -matrix.

• Observation error covariance:  $\mathbf{R} = \left< \mathbf{y'} \mathbf{y'}^{\mathrm{T}} \right>$ ,  $\mathbf{y'}$  is observation error.

# Link to Gaussian PDFs



$$\mathbf{x} = \mathbf{x}_{\mathrm{B}} - \boldsymbol{\epsilon}_{\mathrm{B}},$$
  

$$\mathbf{x} \sim N(\mathbf{x}_{\mathrm{B}}, \mathbf{B}),$$
  

$$\boldsymbol{\epsilon}_{\mathrm{B}} \sim N(0, \mathbf{B}),$$
  

$$P(\boldsymbol{\epsilon}_{\mathrm{B}}) = \frac{1}{\sqrt{(2\pi)^{n} \det(\mathbf{B})}} = \exp{-\frac{1}{2}\boldsymbol{\epsilon}_{\mathrm{B}}^{\mathrm{T}} \mathbf{B}^{-1} \boldsymbol{\epsilon}_{\mathrm{B}}.$$

Importance of covariance matrices (demo with n = n, p = 1)



The analysis formula for the analysis increment is:

$$\mathbf{x} = \begin{pmatrix} T_1 \\ \vdots \\ T_i \\ \vdots \\ T_n \end{pmatrix}, \quad \mathbf{x}_{\mathrm{B}} = \begin{pmatrix} T_{\mathrm{B}1} \\ \vdots \\ T_{\mathrm{B}i} \\ \vdots \\ T_{\mathrm{B}n} \end{pmatrix}, \quad \mathbf{y} = (y), \quad \mathcal{H}(\mathbf{x}) = T_i,$$
$$\mathbf{H} = \begin{pmatrix} 0 & \cdots & 1 & \cdots & 0 \end{pmatrix},$$
$$\mathbf{H} = \begin{pmatrix} 0 & \cdots & 1 & \cdots & 0 \end{pmatrix},$$
$$\mathbf{B} = \begin{pmatrix} B_{11} & \cdots & B_{1i} & \cdots & B_{1n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ B_{i1} & \cdots & B_{ii} & \cdots & B_{in} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ B_{n1} & \cdots & B_{ni} & \cdots & B_{nn} \end{pmatrix}, \quad \mathbf{R} = \begin{pmatrix} \sigma_0^2 \end{pmatrix}.$$

$$\mathbf{x}_{A} = \mathbf{x}_{B} + \mathbf{B}\mathbf{H}^{T}\left(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{T}\right)^{-1}\left(\mathbf{y} - \boldsymbol{\mathcal{H}}(\mathbf{x}_{B})\right).$$

$$\mathbf{B}\mathbf{H}^{\mathrm{T}} = \begin{pmatrix} B_{11} & \cdots & B_{1i} & \cdots & B_{1n} \\ \vdots & \ddots & \vdots & \vdots & \vdots \\ B_{i1} & \cdots & B_{ii} & \cdots & B_{in} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ B_{n1} & \cdots & B_{ni} & \cdots & B_{nn} \end{pmatrix} \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} B_{1i} \\ \vdots \\ B_{ii} \\ \vdots \\ B_{ni} \end{pmatrix}, \qquad \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}} = \begin{pmatrix} 0 & \cdots & 1 & \cdots & 0 \end{pmatrix} \begin{pmatrix} B_{1i} \\ \vdots \\ B_{ii} \\ \vdots \\ B_{ni} \end{pmatrix} = (B_{ii}) = (\sigma_{\mathrm{B}i}^{2}),$$

$$\mathbf{x}_{\mathrm{A}} = \begin{pmatrix} T_{\mathrm{B1}} \\ \vdots \\ T_{\mathrm{Bi}} \\ \vdots \\ T_{\mathrm{Bn}} \end{pmatrix} + \begin{pmatrix} B_{1i} \\ \vdots \\ B_{ii} \\ \vdots \\ B_{ni} \end{pmatrix} \frac{1}{\sigma_{\mathrm{o}}^{2} + \sigma_{\mathrm{Bi}}^{2}} \left(y - T_{\mathrm{Bi}}\right).$$

The analysis increment is a vector  $\propto$  the *i*th column of **B** (called a structure function or covariance function).

#### Structure functions for flow in the mid-latitude atmosphere



In this case the wind part of the structure function is in geostrophic balance with the pressure

# Modelling a covariance matrix

- Observation error covariance matrices (**R**):
  - Often taken to be diagonal for independent obs. Observation error variances (diagonal elements) depend on characteristics of the instrument.
  - Another contribution is representivity error which will have diagonal (and possibly off-diagonal) elements.
  - If measurements are not independent (e.g. if they are derived using some procedure) then R should not be diagonal.
- Background error covariance matrices (B):
  - Can be rarely represented explicitly ( $\mathbf{x} \in \mathbb{R}^n \ [n \sim 10^9]$ ,  $\mathbf{B} \in \mathbb{R}^{n \times n} \ [n \times n \sim 10^{18}]$ ).
  - Difficult to measure (need a large sample of (unknowable) forecast errors).
  - Can be modelled using a variety of methods:
    - \* 'Inverse Laplacians'.
    - \* Diffusion operators (used e.g. in Ocean DA).
    - \* Recursive filters
    - \* Spectral methods, wavelet methods.
    - \* Exploit physics (e.g. geophysical balance).
    - \* Control variable transforms (transform to a space where **B** is simpler e.g. diagonal).
- Model error covariance matrices (Q).

## Making variational DA work - control variable transforms (CVTs)

- Key to success of 3D/4D-Var in NWP is the **B**-matrix.
- This is modelled, e.g., via (linear) change of variables a CVT:
  - $\delta \mathbf{x} = \mathbf{U} \delta \mathbf{v}.$
  - Background errors in the  $\delta \mathbf{v}$ -representation are assumed to be mutually uncorrelated:

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m T} &pprox ~{f B}. \end{array}$$

– This problem is minimized now w.r.t.  $\delta \mathbf{v}$ :

$$\begin{aligned} \mathcal{J}[\delta \mathbf{v}] &= \frac{1}{2} \delta \mathbf{v}^{\mathrm{T}} \delta \mathbf{v} + \frac{1}{2} \left[ \mathbf{y} - \mathcal{H}(\mathbf{x}_{\mathrm{B}}) - \mathbf{H} \underbrace{\mathbf{U} \delta \mathbf{v}}_{\delta \mathbf{x}} \right]^{\mathrm{T}} \mathbf{R}^{-1} \left[ \mathbf{y} - \mathcal{H}(\mathbf{x}_{\mathrm{B}}) - \mathbf{H} \underbrace{\mathbf{U} \delta \mathbf{v}}_{\delta \mathbf{x}} \right], \\ \nabla_{\delta \mathbf{v}} \mathcal{J} &= \delta \mathbf{v} - \mathbf{U}^{\mathrm{T}} \mathbf{H}^{\mathrm{T}} \mathbf{R}^{-1} \left[ \mathbf{y} - \mathcal{H}(\mathbf{x}_{\mathrm{B}}) - \mathbf{H} \mathbf{U} \delta \mathbf{v} \right]. \end{aligned}$$

## Simple example of Control Variable Transform (CVT)

## System (two correlated variables)



• State vector ( $\langle T \rangle$  in K,  $\Delta z$  in dam):

$$\delta \mathbf{x} = \left( \begin{array}{c} \delta \left\langle T \right\rangle \\ \delta \Delta z \end{array} \right).$$

• Constraint applies (weakly applied hypsometric equation):

$$\delta \Delta z = \underbrace{L\delta \langle T \rangle}_{\text{balanced contribution}} + \underbrace{\delta \Delta z_{\text{unbal}}}_{\text{unbalanced contribution}}$$

balanced contribution

where 
$$L = \frac{R}{10q} \ln \frac{1000 \text{hPa}}{500 \text{hPa}}$$
.

• Control vector  $(\langle \delta \mathbf{v} \delta \mathbf{v}^{\mathrm{T}} \rangle_{\mathrm{B}} = \mathbf{I})$ :

$$\delta \mathbf{v} = \left(\begin{array}{c} \delta v_{\rm bal} \\ \delta v_{\rm unbal} \end{array}\right).$$

• Scale by background error standard deviations,  $\delta \langle T \rangle =$  $\sigma_{\text{bal}}\delta v_{\text{bal}}, \ \delta \Delta z_{\text{unbal}} = \sigma_{\text{unbal}}\delta v_{\text{unbal}}$ 

$$\begin{pmatrix} \delta \langle T \rangle \\ \delta \Delta z_{\text{unbal}} \end{pmatrix} = \begin{pmatrix} \sigma_{\text{bal}} & 0 \\ 0 & \sigma_{\text{unbal}} \end{pmatrix} \begin{pmatrix} \delta v_{\text{bal}} \\ \delta v_{\text{unbal}} \end{pmatrix}.$$

• The complete CVT ( $\delta \mathbf{x} = \mathbf{U} \delta \mathbf{v}$ ):

$$\underbrace{\begin{pmatrix} \delta \langle T \rangle \\ \delta \Delta z \end{pmatrix}}_{\delta \mathbf{x}} = \underbrace{\begin{pmatrix} 1 & 0 \\ L & 1 \end{pmatrix} \begin{pmatrix} \sigma_{\text{bal}} & 0 \\ 0 & \sigma_{\text{unbal}} \end{pmatrix}}_{\mathbf{U}} \underbrace{\begin{pmatrix} \delta v_{\text{bal}} \\ \delta v_{\text{unbal}} \end{pmatrix}}_{\delta \mathbf{v}}$$

• Implied covariances  $(\mathbf{B} = \mathbf{U}\mathbf{U}^{\mathrm{T}})$ :

$$\mathbf{B} = \begin{pmatrix} \sigma_{\rm bal}^2 & \sigma_{\rm bal}^2 L \\ \sigma_{\rm bal}^2 L & \sigma_{\rm bal}^2 L^2 + \sigma_{\rm unbal}^2 \end{pmatrix}.$$

• Observation of  $\langle T \rangle$  then gives information about  $\Delta z$  (and vice-versa) in a physically consistent way.

## Methods to estimate B

#### Reminder

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}, \quad \mathbf{B} = \left\langle (\mathbf{x}_{B} - \mathbf{x}_{t}) (\mathbf{x}_{B} - \mathbf{x}_{t})^{T} \right\rangle_{B}, \\ = \left( \begin{array}{ccc} \left\langle (x_{B1} - x_{t1})^{2} \right\rangle_{B} & \left\langle (x_{B1} - x_{t1}) (x_{B2} - x_{t2}) \right\rangle_{B} & \cdots & \left\langle (x_{B1} - x_{t1}) (x_{Bn} - x_{tn}) \right\rangle_{B} \\ \left\langle (x_{B2} - x_{t2}) (x_{B1} - x_{t1}) \right\rangle_{B} & \left\langle (x_{B2} - x_{t2})^{2} \right\rangle_{B} & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ \left\langle (x_{Bn} - x_{tn}) (x_{B1} - x_{t1}) \right\rangle_{B} & \cdots & \left\langle (x_{Bn} - x_{tn})^{2} \right\rangle_{B} \end{array} \right)$$

 $\langle \bullet \rangle_{\mathrm{B}} \colon$  average over population of possible backgrounds.

#### Problem

 $\mathbf{x}_t$  is unknowable so need a proxy for forecast error  $\mathbf{x}_B - \mathbf{x}_t$ .

## Popular approaches

#### Method Description and references

"Canadian quick" method	${f x}_{ m B}-{f x}_{ m t}\sim \left({f x}_{ m B}(t+T)-{f x}_{ m B}(T) ight)/\sqrt{2}.$ Take population from one long time run. Polavarapu et al. (2005)
Analysis of innovations $\mathbf{d} = \mathbf{y} - \mathbf{H}\mathbf{x}_{\mathrm{B}}$	Choose a pair of direct and independent obs separated by r: $\begin{split} & [y(r) - x_{\rm B}(r)] \left[ y(r + \Delta r) - x_{\rm B}(r + \Delta r) \right] = \\ & [\{y(r) - x_{\rm t}(r)\} - \{x_{\rm B}(r) - x_{\rm t}(r)\}] \left[ \{y(r + \Delta r) - x_{\rm t}(r + \Delta r)\} - \{x_{\rm B}(r + \Delta r) - x_{\rm t}(r + \Delta r)\} \right] \\ & \langle [\epsilon^{y}(r) - \epsilon^{x_{\rm B}}(r)] \left[ \epsilon^{y}(r + \Delta r) - \epsilon^{x_{\rm B}}(r + \Delta r) \right] \rangle = \langle \epsilon^{y}(r)\epsilon^{y}(r + \Delta r) \rangle + \langle \epsilon^{x_{\rm B}}(r)\epsilon^{x_{\rm B}}(r + \Delta r) \rangle , \end{split}$ (above assumes obs and bg errors are uncorrelated). Take population from many pairs with same $\Delta r$ . Furthermore if $\Delta r > 0$ : $\langle \epsilon^{y}(r)\epsilon^{y}(r + \Delta r) \rangle = 0$ . Rutherford (1972), Hollingsworth and Lönnberg (1986), Järvinen (2001)
NMC method	Choose pairs of lagged forecasts valid at the same time, e.g.: $\mathbf{x}_{\rm B} - \mathbf{x}_{\rm t} \sim (\mathbf{x}_{\rm B}^{48}(t) - \mathbf{x}_{\rm B}^{24}(t)) / \sqrt{2}$ . Take population from difference at many times. Parrish and Derber (1992), Berre et al. (2006)

Ensemble method If you have an ensemble that is correctly spread:  $\mathbf{x}_{\mathrm{B}} - \mathbf{x}_{\mathrm{t}} \sim \mathbf{x}_{\mathrm{B}}^{(i)} - \langle \mathbf{x}_{\mathrm{B}} \rangle \text{ or } \mathbf{x}_{\mathrm{B}} - \mathbf{x}_{\mathrm{t}} \sim \left( \mathbf{x}_{\mathrm{B}}^{(i)} - \mathbf{x}_{\mathrm{B}}^{(j)} \right) / \sqrt{2}.$ Take population from ensemble members and over many times. Houtekamer et al. (1996), Buehner (2005), Bonavita et al. (2015)

## Summary

- Covariance matrices appear in many DA methods (especially variational DA).
  - A covariance matrix describes the shape of a Gaussian distribution.
  - $\mathbf{B}$  and  $\mathbf{R}$  appear in variational cost function (and  $\mathbf{Q}$  in weak constraint formulations).
- Covariance matrices are important.
  - E.g. B specifies how precise  $\mathbf{x}_B$  is, and how to give smooth analysis increments between positions in space and between different variables.
- $\mathbf{B}$  is too large to be known (and there is too little information to know it anyway!)
  - ${f B}$  needs to be modelled based on reasonable ideas.
  - The method of "control variable transforms" is a leading method.
  - Minimize  ${\cal J}$  in "control variable space" (easy) which is related to model space via the control variable transform.
- $\bullet\,$  It is impossible to measure  ${\bf B}$  exactly.
  - Use a proxy method.

## Further reading - selected books and papers

- Barlow, R.J., Statistics A guide to the use of statistical methods in the physical sciences, John Wiley and Sons (1989). This is an elementary, readable book on statistics for the scientist (e.g. it derives the Gaussian distribution from first principles). It also covers the least squares problem.
- Rodgers C.D., Inverse Methods for Atmospheric Sounding: Theory and Practice, World Scientific Publishing (2000). This is a very readable book. Even though it focuses on satellite retrieval theory (mathematically a similar problem to data assimilation), this is a good book for virtually everything that you need to know about covariances. It also contains a summary of basic data assimilation methods and has a useful appendix on linear algebra.
- Lewis J.M., Lakshmivarahan S., Dhall S., Dynamic Data Assimilation: A Least Squares Approach, Cambridge University Press (2006). This huge book covers a lot of material with a lot of repetition. It has some good introductory chapters and some useful results if you know where to look. (Unfortunately there are LOADS of typos.)
- Kalnay E., Atmospheric Modeling, Data Assimilation and Predictability, Cambridge University Press (2002). A large section of this book covers data assimilation, and there is also a lot of basic material for the budding dynamic modeller. The data assimilation part is introductory, but covers most key ideas. It will leave you wanting to know more!
- Schlatter T.W., Variational assimilation of meteorological observations in the lower atmosphere: a tutorial on how it works, J. Atmos. and Solar-Terr. Phys. 62 pp.1057-1070 (2000). It is worth getting hold of this paper as it is an excellent description of variational data assimilation (relevant to lectures later in the course).
- Bannister R.N., A review of forecast error covariance statistics in atmospheric variational data assimilation. I: Characteristics and measurements of forecast error covariances., Q.J. Roy. Met. Soc. 134, 1951-1970 (2008) and Bannister R.N., A review of forecast error covariance statistics in atmospheric variational data assimilation. II: Modelling the forecast error covariance statistics., Q.J. Roy. Met. Soc. 134, 1971-1996 (2008). What can I say blatant self publicity! A source of information about background error covariances and how they can be modelled.
- Polavarapu S., Ren S., Rochon Y., Sankey D., Ek N., Koshyk J., Tarasick D., Data assimilation with the Canadian middle atmosphere model. Atmos.-Ocean 43: 77-100 (2005). "Canadian quick" method.
- Rutherford I.D. 1972. Data assimilation by statistical interpolation of forecast error fields. J. Atmos. Sci. 29: 809–815. Original reference to the analysis of innovations method.
- Hollingsworth A., Lönnberg P., The statistical structure of short-range forecast errors as determined from radiosonde data. Part I: The wind field. Tellus 38A: 111–136 (1986). The most famous work on the analysis of innovations method.
- Järvinen H., Temporal evolution of innovation and residual statistics in the ECMWF variational data assimilation systems. Tellus 53A: 333–347 (2001). More recent work on the analysis of innovations method.
- Parrish D.F., Derber J.C., The National Meteorological Center's spectral statistical interpolation analysis system. Mon. Wea. Rev. 120 1747–1763 (1992). Original reference for the NMC method.
- Berre L., Stefanescu S.E., Pereira M.B., The representation of the analysis effect in three error simulation techniques. Tellus 58A 196–209 (2006). In-depth analysis of the NMC method.
- Houtekamer P.L., Lefaivre L., Derome J., Ritchie H., Mitchell H.L., A system simulation approach to ensemble prediction. Mon. Wea. Rev. 124, 1225–1242 (1996). Explains the ideas behind the generation of an ensemble.
- Buehner M., Ensemble derived stationary and flow dependent background error covariances: Evaluation in a quasi-operational NWP setting. Q.J.R. Meteorol. Soc. 131, 1013–1043 (2005). Example background error covariances derived from an ensemble.
- Bonavita M., Holm E., Isaksen L., Fisher M., The evolution of the ECMWF hybrid data assimilation system, Q.J.R. Meteor. Soc. (2015). Latest paper documenting the ensemble-based calibration of the ECMWF B-matrix.