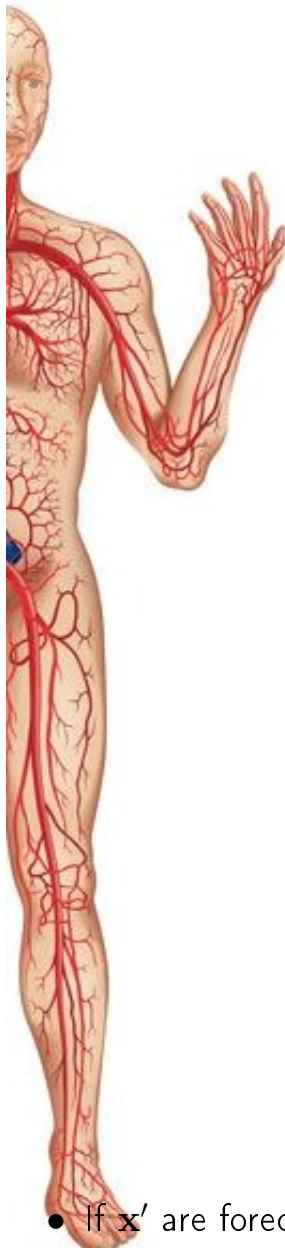


# Anatomy of a covariance matrix

Univariate background error covariance matrix (e.g. if  $\mathbf{x}$  represents a pressure field only):



$$\mathbf{x} = \mathbf{p} = \begin{pmatrix} p_1 \\ p_2 \\ \vdots \\ p_n \end{pmatrix}, \quad \text{cov}(\mathbf{p}') = \langle \mathbf{p}' \mathbf{p}'^T \rangle = \begin{pmatrix} \langle p_1'^2 \rangle & \langle p_1' p_2' \rangle & \cdots & \langle p_1' p_n' \rangle \\ \langle p_2' p_1' \rangle & \langle p_2'^2 \rangle & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ \langle p_n' p_1' \rangle & \cdots & \cdots & \langle p_n'^2 \rangle \end{pmatrix}.$$

variance (points to  $\langle p_1'^2 \rangle$ )  
outer product (points to  $\langle \mathbf{p}' \mathbf{p}'^T \rangle$ )  
covariance (univariate) (points to  $\langle p_1' p_2' \rangle$ )

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):

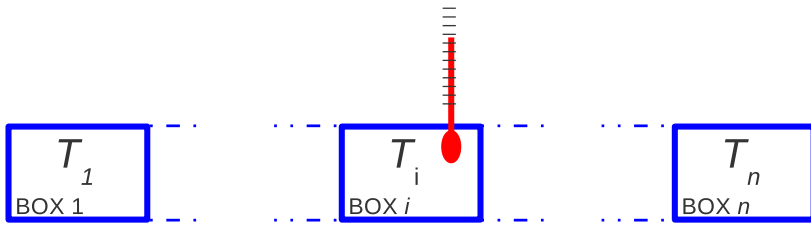
$$\mathbf{x} = \begin{pmatrix} \mathbf{p} \\ \mathbf{u} \\ \mathbf{v} \end{pmatrix} = \begin{pmatrix} p_1 \\ \vdots \\ p_{n/3} \\ u_1 \\ \vdots \\ u_{n/3} \\ v_1 \\ \vdots \\ v_{n/3} \end{pmatrix}, \quad \text{cov}(\mathbf{x}') = \langle \mathbf{x}' \mathbf{x}'^T \rangle = \begin{pmatrix} \langle \mathbf{p}'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

autocovariance sub-matrix (points to  $\langle \mathbf{p}' \mathbf{p}'^T \rangle$ )  
multivariate covariance sub-matrix (points to  $\langle \mathbf{p}' \mathbf{u}'^T \rangle$ )

These covariances are symmetric matrices.

- If  $\mathbf{x}'$  are forecast errors,  $\epsilon^b$ , then above is **B**-matrix.
- Observation error covariance:  $\mathbf{R} = \langle \mathbf{y}' \mathbf{y}'^T \rangle$ ,  $\mathbf{y}'$  is observation error.

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



$$\mathbf{x} = \begin{pmatrix} T_1 \\ \vdots \\ T_i \\ \vdots \\ T_n \end{pmatrix}, \quad \mathbf{x}^b = \begin{pmatrix} T_1^b \\ \vdots \\ T_i^b \\ \vdots \\ T_n^b \end{pmatrix}, \quad \mathbf{y} = (y), \quad \mathcal{H}(\mathbf{x}) = T_i,$$

The analysis formula for the analysis increment is:

$$\mathbf{H} = (0 \ \cdots \ 1 \ \cdots \ 0),$$

$$\mathbf{B} = \begin{pmatrix} B_{11} & \cdots & B_{1i} & \cdots & B_{1n} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ B_{i1} & \cdots & B_{ii} & \cdots & B_{in} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ B_{n1} & \cdots & B_{ni} & \cdots & B_{nn} \end{pmatrix}, \quad \mathbf{R} = (\sigma_o^2).$$

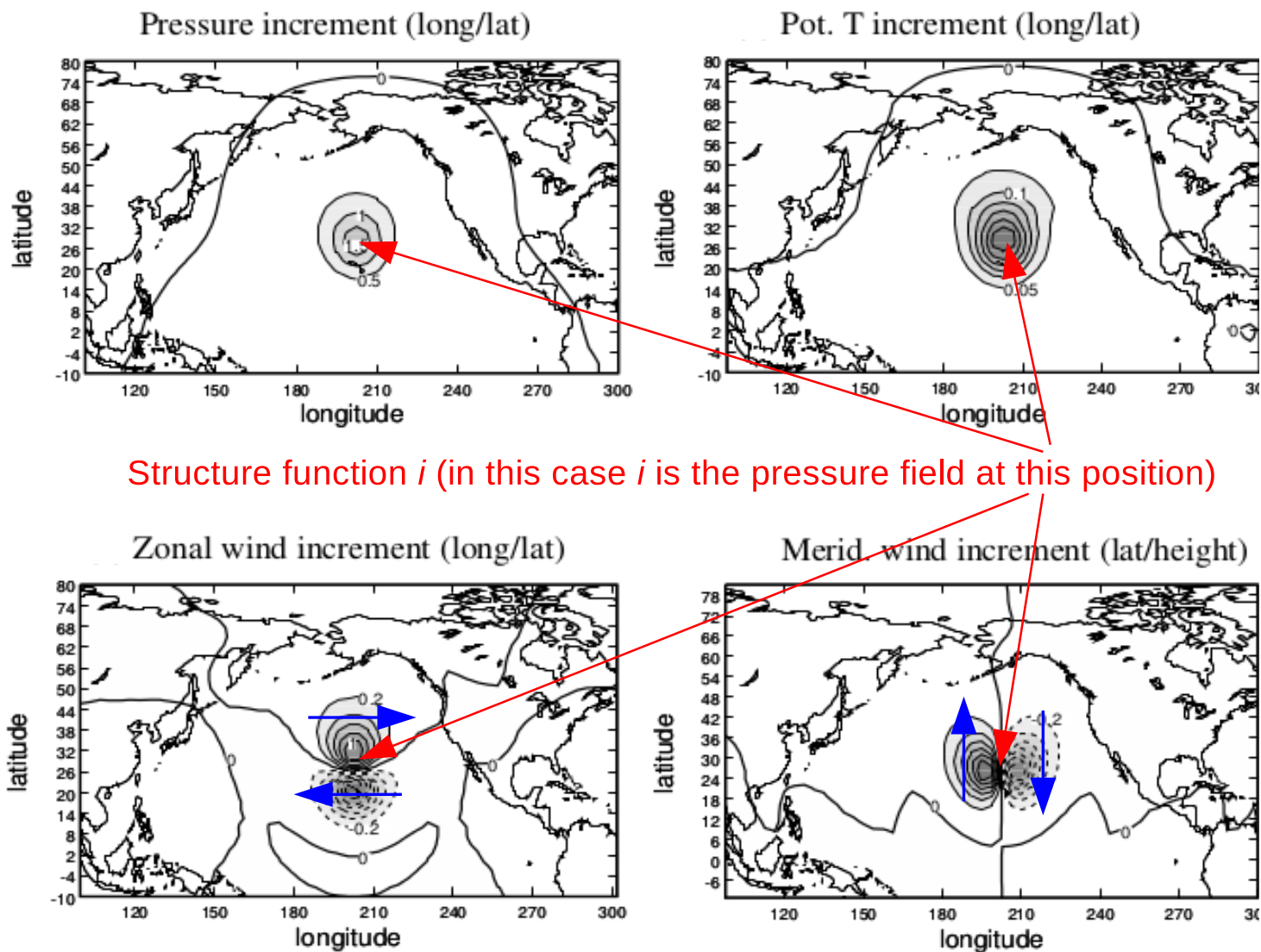
$$\mathbf{x}^a = \mathbf{x}^b + \mathbf{B}\mathbf{H}^T (\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^T)^{-1} (y - \mathcal{H}(\mathbf{x}^b)).$$

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

$$\mathbf{x}^a = \begin{pmatrix} T_1^b \\ \vdots \\ T_i^b \\ \vdots \\ T_n^b \end{pmatrix} + \begin{pmatrix} B_{1i} \\ \vdots \\ B_{ii} \\ \vdots \\ B_{ni} \end{pmatrix} \frac{1}{\sigma_o^2 + \sigma_{Bi}^2} (y - T_i^b).$$

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

# Structure functions for flow in the mid-latitude atmosphere



Structure function  $i$  (in this case  $i$  is the pressure field at this position)

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

# Modelling covariance matrices

- **Observation error covariance matrices ( $\mathbf{R}$ ):**
  - Describes errors in the observing system (e.g. the instrument), errors in the observation operator, and representativity error.
  - Often taken to be diagonal for independent obs.
  - If obs. errors are not independent, then there are off-diagonal elements.  
If measurements are not independent (e.g. if they are derived using some procedure) then  $\mathbf{R}$  should not be diagonal.
- **Background error covariance matrices ( $\mathbf{B}$ ):**
  - Describes errors in the background state (forecast from previous analysis).
  - Depends on the analysis errors of the previous assimilation, and on forecast model error.
  - 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  $\mathbf{B}$  is simpler - e.g. diagonal).
- **Model error covariance matrices ( $\mathbf{Q}$ ):**
  - Describes errors in the forecast model used within 4D-Var.
  - Often completely neglected operationally.

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

- Key to success of 3D/4D-Var in NWP is the  $\mathbf{B}$ -matrix. Incremental 3dVar cost fn:

$$\mathcal{J}[\delta\mathbf{x}] = \delta\mathbf{x}^T \mathbf{B}^{-1} \delta\mathbf{x} + [\mathbf{y} - \mathcal{H}(\mathbf{x}^b) - \mathbf{H}\delta\mathbf{x}]^T \mathbf{R}^{-1} [\mathbf{y} - \mathcal{H}(\mathbf{x}^b) - \mathbf{H}\delta\mathbf{x}]$$

$$\mathbf{x} = \mathbf{x}^b + \delta\mathbf{x}$$

- $\mathbf{B}$  can be 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:

$$\begin{aligned} \langle \boldsymbol{\epsilon}^b \boldsymbol{\epsilon}^{bT} \rangle_{\mathbf{B}} &\approx \mathbf{B}, \\ \langle \delta\mathbf{v} \delta\mathbf{v}^T \rangle_{\mathbf{B}} &= \mathbf{I}, \\ \langle [\mathbf{U}^{-1} \boldsymbol{\epsilon}^b] [\mathbf{U}^{-1} \boldsymbol{\epsilon}^b]^T \rangle_{\mathbf{B}} &\approx \mathbf{I}, \\ \therefore \mathbf{U}\mathbf{U}^T &\approx \mathbf{B}. \end{aligned}$$

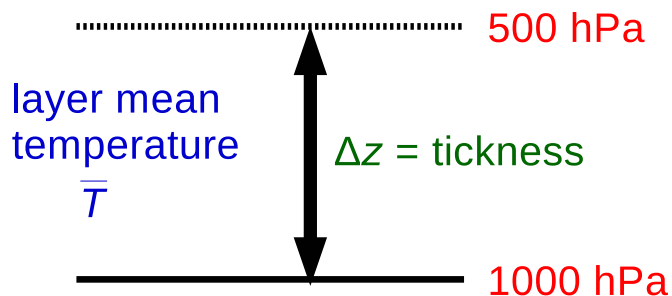
- This problem is minimized now w.r.t.  $\delta\mathbf{v}$ :

$$\mathcal{J}[\delta\mathbf{v}] = \frac{1}{2} \delta\mathbf{v}^T \delta\mathbf{v} + \frac{1}{2} \left[ \mathbf{y} - \mathcal{H}(\mathbf{x}^b) - \underbrace{\mathbf{H}\mathbf{U}\delta\mathbf{v}}_{\delta\mathbf{x}} \right]^T \mathbf{R}^{-1} \left[ \mathbf{y} - \mathcal{H}(\mathbf{x}^b) - \underbrace{\mathbf{H}\mathbf{U}\delta\mathbf{v}}_{\delta\mathbf{x}} \right],$$

$$\nabla_{\delta\mathbf{v}} \mathcal{J} = \delta\mathbf{v} - \mathbf{U}^T \mathbf{H}^T \mathbf{R}^{-1} [\mathbf{y} - \mathcal{H}(\mathbf{x}^b) - \mathbf{H}\mathbf{U}\delta\mathbf{v}].$$

# Simple example of Control Variable Transform (CVT)

System (two correlated variables)



- State vector ( $\bar{T}$  in K,  $\Delta z$  in dam):

$$\delta \mathbf{x} = \begin{pmatrix} \delta \bar{T} \\ \delta \Delta z \end{pmatrix}.$$

- Constraint applies (weakly applied hypsometric equation):

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

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

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

$$\delta \mathbf{v} = \begin{pmatrix} \delta v_{\text{bal}} \\ \delta v_{\text{unbal}} \end{pmatrix}.$$

- Scale by background error standard deviations,  $\delta \bar{T} = \sigma_{\text{bal}} \delta v_{\text{bal}}$ ,  $\delta \Delta z_{\text{unbal}} = \sigma_{\text{unbal}} \delta v_{\text{unbal}}$ :

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

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

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

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

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

- Observation of  $\bar{T}$  then gives information about  $\Delta z$  (and vice-versa) in a physically consistent way.

# Methods to estimate $\mathbf{B}$

## Reminder

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}, \quad \mathbf{B} = \left\langle (\mathbf{x}^b - \mathbf{x}^t) (\mathbf{x}^b - \mathbf{x}^t)^T \right\rangle_{\mathbf{B}},$$

$$= \begin{pmatrix} \langle (x_1^b - x_1^t)^2 \rangle_{\mathbf{B}} & \langle (x_1^b - x_1^t)(x_2^b - x_2^t) \rangle_{\mathbf{B}} & \cdots & \langle (x_1^b - x_1^t)(x_n^b - x_n^t) \rangle_{\mathbf{B}} \\ \langle (x_2^b - x_2^t)(x_1^b - x_1^t) \rangle_{\mathbf{B}} & \langle (x_2^b - x_2^t)^2 \rangle_{\mathbf{B}} & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ \langle (x_n^b - x_n^t)(x_1^b - x_1^t) \rangle_{\mathbf{B}} & \cdots & \cdots & \langle (x_n^b - x_n^t)^2 \rangle_{\mathbf{B}} \end{pmatrix}.$$

$\langle \bullet \rangle_{\mathbf{B}}$ : 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	$\mathbf{x}^b - \mathbf{x}^t \sim (\mathbf{x}^b(t + T) - \mathbf{x}^b(T)) / \sqrt{2}$ . Take population from one long time run. <a href="#">Polavarapu et al. (2005)</a>
Analysis of innovations $\mathbf{d} = \mathbf{y} - \mathbf{H}\mathbf{x}^B$	Choose a pair of direct and independent obs separated by $r$ : $[y(r) - x^b(r)] [y(r + \Delta r) - x^b(r + \Delta r)] =$ $[\{y(r) - x^t(r)\} - \{x^b(r) - x^t(r)\}] [\{y(r + \Delta r) - x^t(r + \Delta r)\} - \{x^b(r + \Delta r) - x^t(r + \Delta r)\}]$ $\left\langle [\epsilon^y(r) - \epsilon^{x^b}(r)] [\epsilon^y(r + \Delta r) - \epsilon^{x^b}(r + \Delta r)] \right\rangle = \langle \epsilon^y(r) \epsilon^y(r + \Delta r) \rangle + \langle \epsilon^{x^b}(r) \epsilon^{x^b}(r + \Delta r) \rangle,$ (above assumes obs and bg errors are uncorrelated). Take population from many pairs with same $\Delta r$ . Furthermore suppose that $\Delta r > 0$ : $\langle \epsilon^y(r) \epsilon^y(r + \Delta r) \rangle = 0$ . <a href="#">Rutherford (1972)</a> , <a href="#">Hollingsworth and Lönnberg (1986)</a> , <a href="#">Järvinen (2001)</a>
NMC method	Choose pairs of lagged forecasts valid at the same time, e.g.: $\mathbf{x}^b - \mathbf{x}^t \sim (\mathbf{x}_{48}^b(t) - \mathbf{x}_{24}^b(t)) / \sqrt{2}$ . Take population from difference at many times. <a href="#">Parrish and Derber (1992)</a> , <a href="#">Berre et al. (2006)</a>
Ensemble method	If you have an ensemble that is correctly spread: $\mathbf{x}^b - \mathbf{x}^t \sim \mathbf{x}_{(i)}^b - \langle \mathbf{x}^b \rangle$ or $\mathbf{x}^b - \mathbf{x}^t \sim (\mathbf{x}_{(i)}^b - \mathbf{x}_{(j)}^b) / \sqrt{2}$ . Take population from ensemble members and over many times. <a href="#">Houtekamer et al. (1996)</a> , <a href="#">Buehner (2005)</a> , <a href="#">Bonavita et al. (2015)</a>



# 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.  $\mathbf{B}$  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!)
  - $\mathbf{B}$  needs to be modelled based on reasonable ideas.
  - The method of “control variable transforms” is a leading method.
  - Minimize  $\mathcal{J}$  in “control variable space” (easy) which is related to model space via the control variable transform.
- It is impossible to measure  $\mathbf{B}$  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., Lakshminarayanan 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., Ștefănescu 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., Lefaiivre 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.*