MTMD02

Operational Data Assimilation Techniques

Part I: Variational techniques (Ross Bannister)

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Further reading

- Bennett A.F., 2002, Inverse Modeling of the Ocean and Atmosphere (Euler-Lagrange equations and representers - sections 1.2, 1.3).
- Daley R., 1991, Atmospheric Data Analysis (historical aspects and basic ideas - chapters 1, 13).
- Kalnay E., 2003, Atmospheric Modeling, Data Assimilation and Predictability (basic aspects of data assimilation - chapter 5).
- Lewis J.M., Lakshmivarahan S., Dhall S.K., 2006, Dynamic data assimilation: a Least Squares Approach (applications - chapters 3,4, data assimilation algorithms - chapter 19).
- Schlatter T.W., 2000, Variational Assimilation of Meteorological Observations in the Lower Atmosphere: a Tutorial on How it Works, Journal of Atmospheric and Solar-Terrestrial Physics 62, pp. 1057-1070.
- Mathematics Aide Memoir handout.

Note that page numbers on the slides and on the handouts do not always match.

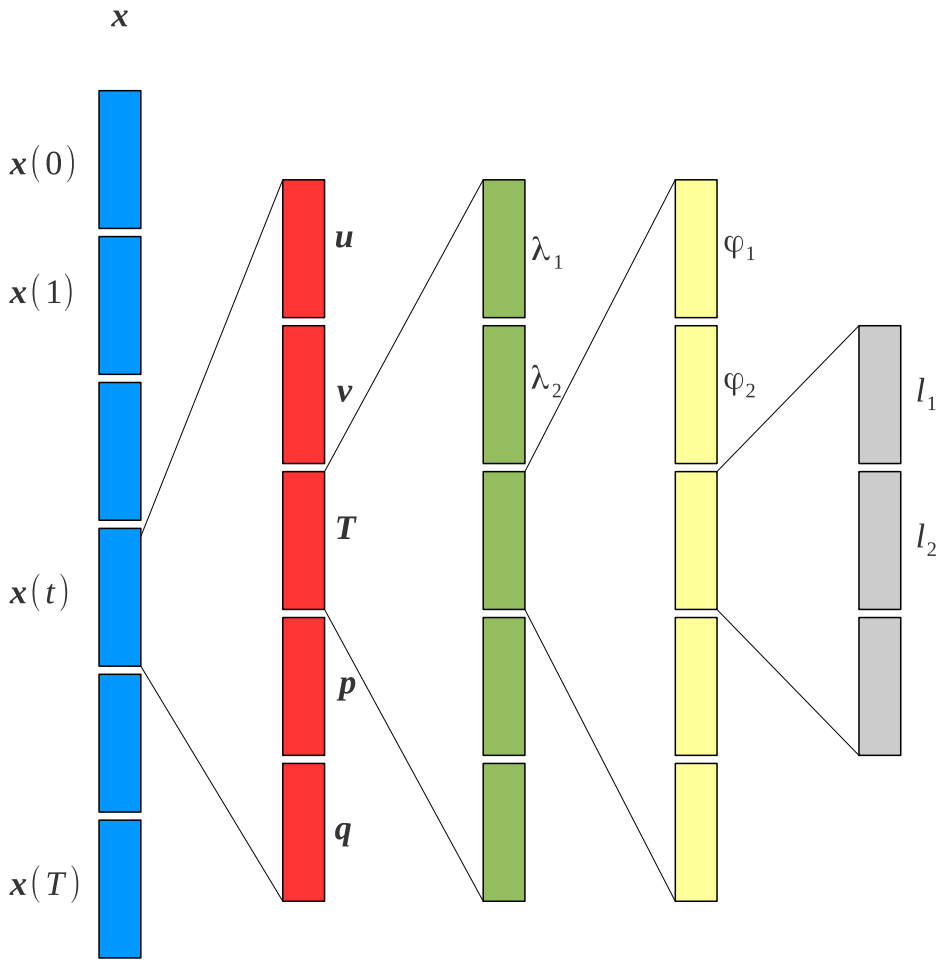
1. Introduction

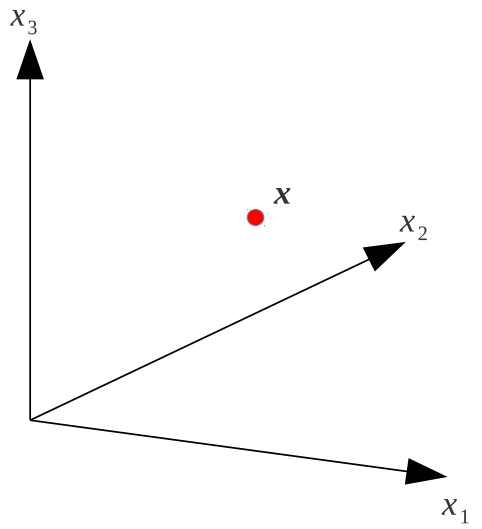
1(a) Inverse problems

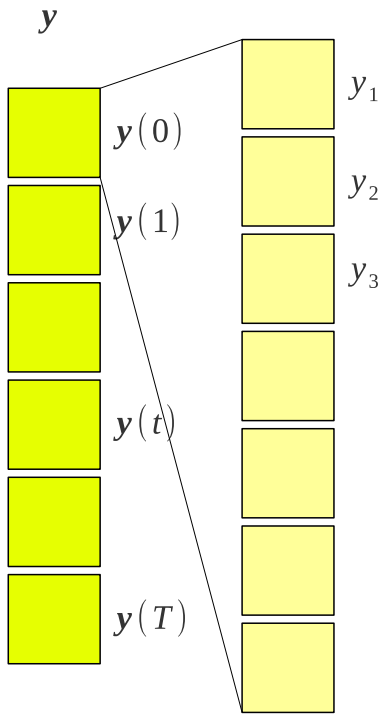
Field	Example inverse problem to be solved
Medical diagnosis	What is the 3-D structure of biological tissues from X-ray images (CAT scan)?
Seismology	Determination of subterranean properties from seismic data (e.g. porosity, hydrocarbon content)
Astrophysics	Determination of the internal structure of the Sun from surface observations
Astronomy	Orbit determination from observations
Astronautics	Landing a spacecraft safely on another planet
Parameter estimation	Determination of unknown model parameters
Atmospheric pollution	What is the source/sink field of an atmospheric pollutant?
Atmospheric retrievals	What is the vertical profile of atmospheric quantities from remotely sensed observations?
Weather forecasting	What are the initial conditions (e.g. u, v, T, p, q, cloud, SST, salinity) of an atmosphere or ocean forecast model that agrees with the latest observations?

Alternative names: data assimilation, retrievals, inverse modelling, history matching, data fusion, maximum entropy.

1(b) Notation







$\mathbf{x}_\mathrm{A}$ analysis state
$\mathbf{x}_\mathrm{B}$ background state
$\delta\mathbf{x}$ incremental state
Sometimes $\mathbf{x}$ and $\mathbf{y}$ are for only one time
$\mathbf{x}$-vectors have n elements in total
$\mathbf{y}$-vectors have p elements in total

Example use of these vectors:

$$\mathbf{x} = \mathbf{x}^\mathrm{t} + \boldsymbol{\eta}, \quad \mathbf{x}, \mathbf{x}^\mathrm{t}, \boldsymbol{\eta} \in \mathbb{R}^n \qquad \mathbf{y}(t) = \mathbf{h}_t(\mathbf{x}^\mathrm{t}(t)) + \boldsymbol{\epsilon} \quad \mathbf{y}(t), \boldsymbol{\epsilon} \in \mathbb{R}^p \quad \mathbf{h}_t : \mathbb{R}^n \to \mathbb{R}^p$$

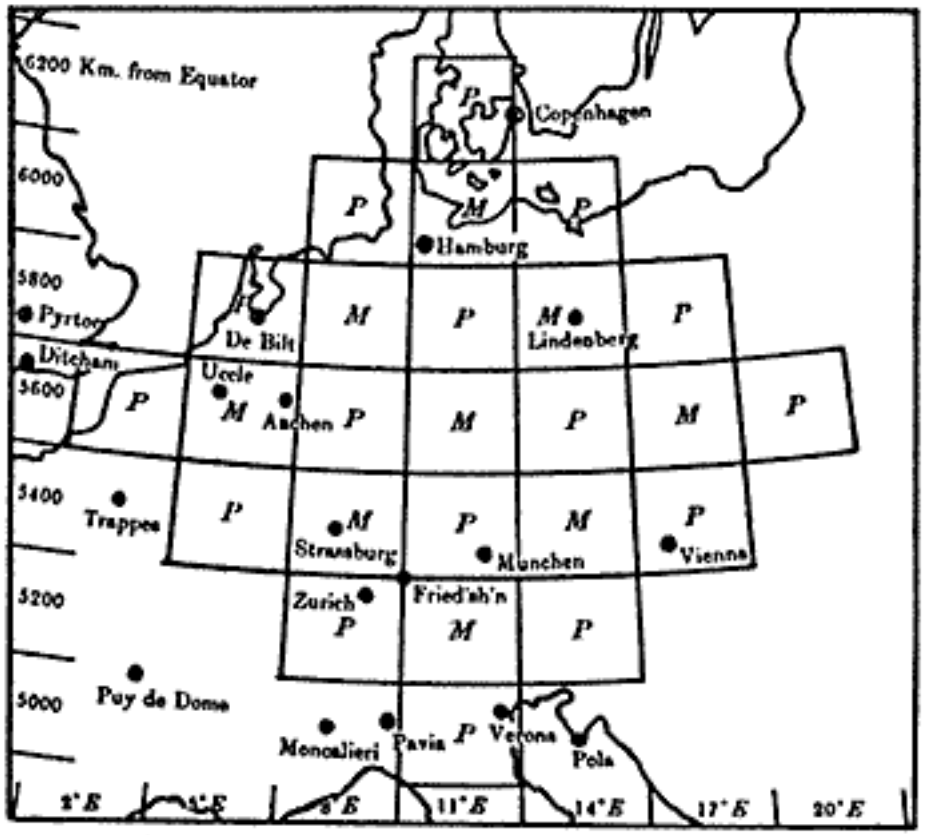
$\mathbf{y}^\mathrm{mo}(t) = \mathbf{h}_t(\mathbf{x}(t))$ will be called 'model observations'. This is the forward problem. Inverse problem tries to do opposite. Always assume that we can solve the forward problem ("what are the model observations given a model state").
EXERCISE IN MATRIX MANIPULATION - PROBLEM 1.

WHETHER $\mathbf{x}$ REFERS TO A RANGE OF TIMES OR JUST $t = 0$ DEPENDS UPON THE CONTEXT.
ALSO USE RESULTS THAT GIVE THE GRADIENT AND HESSIAN OF A COST FUNCTION - PROBLEM 2.

1(c) History of data assimilation in meteorological operations and the data assimilation cycle

Subjective 'data assimilation' 1910s, 1920s

- LF Richardson (*Weather Prediction by Numerical Process*, 1922) attempted a hind-cast (by hand!) for 20th May 1910.
- Primitive equation-based forecast model: resolution $\Delta\lambda = 3^\circ$, $\Delta\phi = 1.8^\circ$, 5 vertical levels.
- 'Data assimilation' was done for mass variables (T, p) separately from wind variables (u, v) (i.e. univariate) by interpolating observations subjectively.
- A disastrous forecast: $\Delta P/\Delta t \approx 145$ hPa /6 hours.
- Catastrophic growth rate not due to the model, but due to inadequate data assimilation – the mass and wind were out of balance.
- Bjerknes, 1911, described the analysis problem as, "The ultimate problem in Meteorology".



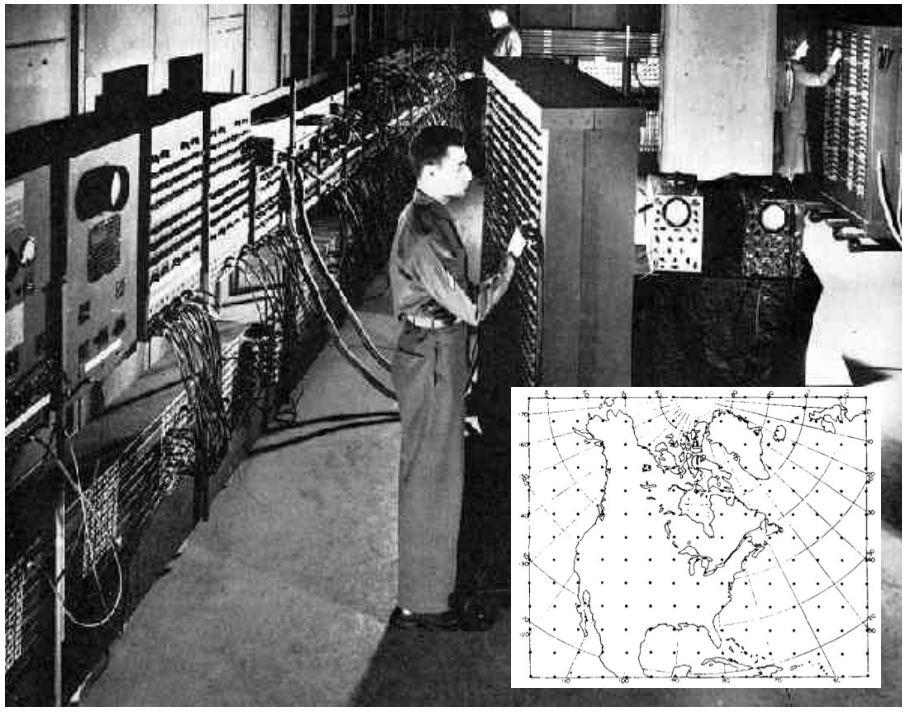
Successes in NWP, 1940s, 1950s

- Success with filtered dynamical models containing balanced motion only (e.g. barotropic vorticity equation), even with subjective analysis - Charney Fjörtoft, von Neumann, 1950.

- BVE is less accurate than the primitive equations, but is insensitive to imbalances in the initial conditions (there are no gravity waves in the BVE).

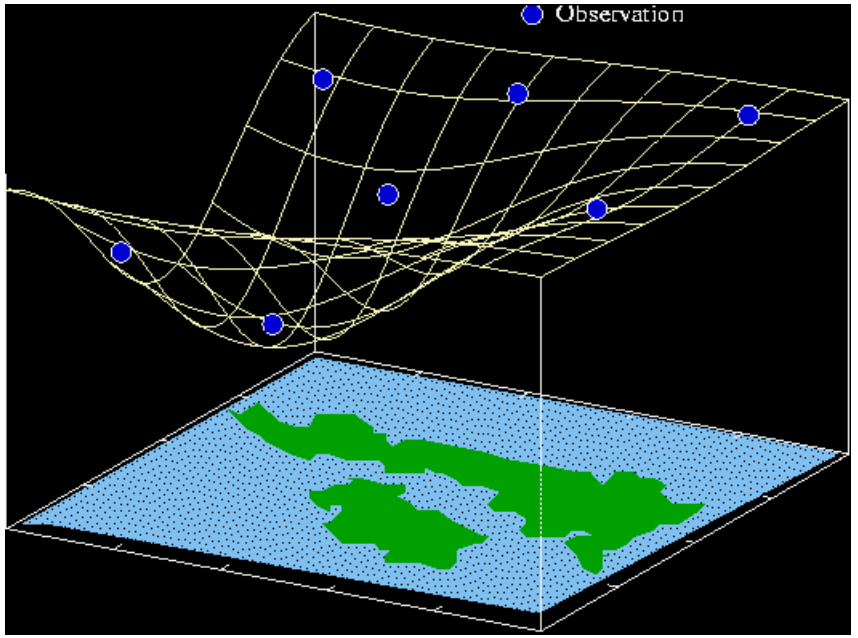
- ENIAC (Electronic Numerical Integrator and Computer) - (~0.2 ms to add two numbers, ~2.5 ms to multiply to numbers, inputs and outputs via punched cards).

- [We now use primitive equations for NWP, but with DA that inhibits imbalance.]



Beginnings of objective analysis: polynomial fitting, late 1940s

- Fit a polynomial expansion to observations.
- Made no account of observation accuracy.
- Different variables treated independently (univariate).
- Direct observations only.
- Unrealistic values in data voids.



Cressman analysis / method of successive corrections, 1950s, 1960s

- Use prior knowledge (a background state).
- Provides information in data voids.
- Prior knowledge can come from climatology or a previous forecast.
- Latter leads on to the 'data assimilation cycle'.

$$\begin{aligned} \mathbf{x}_i^0 &= \text{first guess (background)} \\ \mathbf{x}_i^{n+1} &= \mathbf{x}_i^n + \frac{\sum_{k=1}^{K_i^n} W_{ik}^n (y_k - \tilde{\mathbf{x}}_k^n)}{\sum_{k=1}^{K_i^n} (W_{ik}^n + \epsilon_k^2)} \end{aligned}$$

- $\mathbf{x}_i^n$ estimate of field at grid point i after the nth iteration.
- $\tilde{\mathbf{x}}_k^n$ field value at grid location closest to observation k.
- W_{ik}^n weight of influence of observation k on grid point i (reduces with distance).
- K_i^n number of observations within distance R^n of grid point i.
- y_k kth observation value.
- ϵ_k controls the degree of influence of the observations on the analysis (diminishing influence as $\epsilon \to \infty$).

Nudging (Newtonian relaxation), 1970s - present

- Allows the analysis to be combined with the background state smoothly.
- Relies on an intermediate analysis, $\mathbf{x}_{\text{int}}$ (e.g. from SCM).
- $\mathbf{x}_{\text{int}}$ to be introduced over a timescale τ.
- Model equations:

$$\frac{\partial \mathbf{x}}{\partial t} = \mathbf{f}(\mathbf{x}),$$

- ... are modified to:

$$\frac{\partial \mathbf{x}}{\partial t} = \mathbf{f}(\mathbf{x}) - \frac{\mathbf{x} - \mathbf{x}_{\text{int}}}{\tau}.$$

Example with a scalar (x) for a persistence model ($f(x) = 0$):

$$\begin{aligned} \frac{dx}{dt} &= -\frac{x - x_{\text{int}}}{\tau}, \\ \Rightarrow x(t) &= x_{\text{int}} + (x(0) - x_{\text{int}}) \exp -\frac{t}{\tau}. \end{aligned}$$

Optimal interpolation, 1970s / 1980s

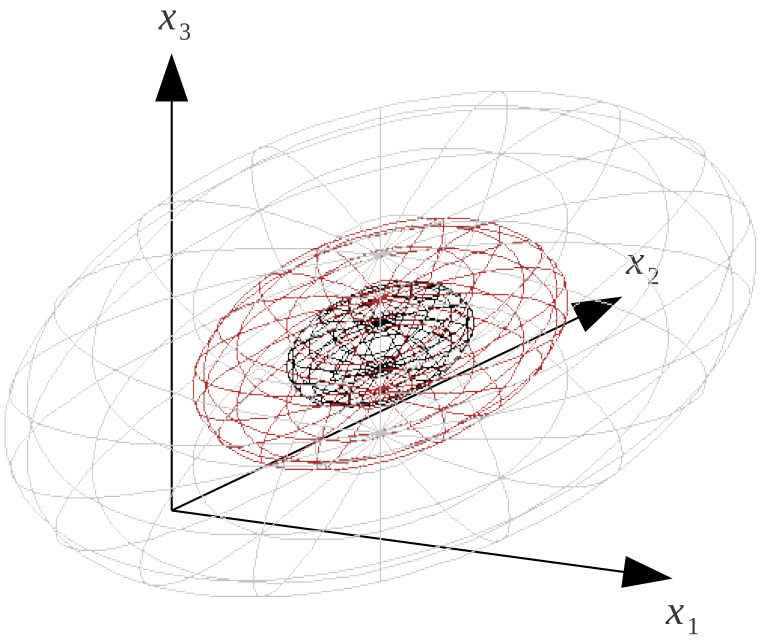
$$\mathbf{x}_\mathrm{A} = \mathbf{x}_\mathrm{B} + \mathbf{B}\mathbf{H}^\mathrm{T}(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^\mathrm{T})^{-1}(\mathbf{y} - \mathbf{h}(\mathbf{x}_\mathrm{B}))$$

- A formal way of combining observations and models.
- Intimately related to method of least squares.
- Represents uncertainties of all information.
- Too expensive to solve for the global system (solve for patches and glue together for 'global' analysis).
- Need accurate estimates of $\mathbf{B}$ and $\mathbf{R}$ matrices.

- $\mathbf{x}_\mathrm{A}$ analysis state (posterior) $\in \mathbb{R}^n$.
- $\mathbf{x}_\mathrm{B}$ background state (prior) $\in \mathbb{R}^n$.
- $\mathbf{B}$ background error covariance matrix (accounts for uncertainty in $\mathbf{x}_\mathrm{B}$) $\in \mathbb{R}^{n \times n}$.
- $\mathbf{y}$ observation vector $\in \mathbb{R}^p$.
- $\mathbf{h}$ observation operator $\mathbb{R}^n \to \mathbb{R}^p$.
- $\mathbf{H}$ Jacobian of $\mathbf{h} \in \mathbb{R}^{p \times n}$.
- $\mathbf{R}$ observation error covariance matrix (accounts for uncertainty in $\mathbf{y}$) $\in \mathbb{R}^{p \times p}$.

Variational methods (VAR), 1990s / 2000s

- Broadly speaking (in the case of 3D-VAR) a way of solving the OI equations efficiently.
- Construct a cost functional, $J[\mathbf{x}]$ as the sum of squares of deviations from data.
- Analysis is defined as the $\mathbf{x}$ that minimizes $J[\mathbf{x}]$.
- $\mathbf{B}$ is not applied as an explicit matrix, but is instead modelled (see later).
- Efficient enough for a truly global analysis.
- Still need accurate estimates of $\mathbf{B}$ and $\mathbf{R}$ matrices. $\mathbf{B}$ is usually static.
- Variants: 1D-VAR / 3D-VAR / 4D-VAR / etc. (see later).



- Example for strong constraint 4D-VAR:

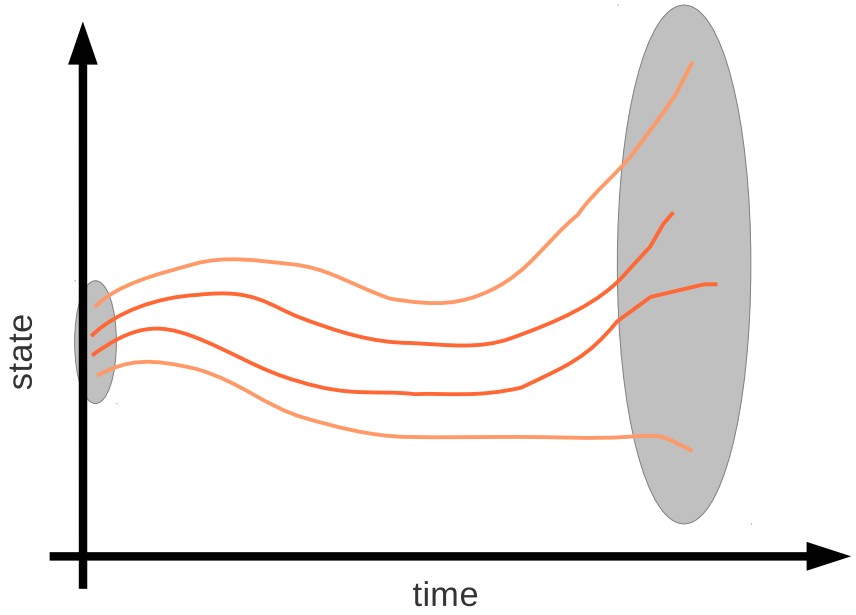
$$J(\mathbf{x}) = \frac{1}{2}\left(\mathbf{x}-\mathbf{x}_{\mathrm{B}}\right)^{\mathrm{T}}\mathbf{B}^{-1}\left(\mathbf{x}-\mathbf{x}_{\mathrm{B}}\right) + \frac{1}{2}\sum_{t=0}^{T}\left(\mathbf{y}(t)-\mathbf{h}_t[\mathcal{M}_{t\leftarrow 0}(\mathbf{x})]\right)^{\mathrm{T}}\mathbf{R}_t^{-1}\times \left(\mathbf{y}(t)-\mathbf{h}_t[\mathcal{M}_{t\leftarrow 0}(\mathbf{x})]\right),$$

where $\mathbf{x}$ is the state vector at $t=0$.

Part I of this course is mainly about variational methods.

Ensemble methods 2000s / 2010s

- The spread in an ensemble of N background forecasts has information about background uncertainty, member i $\mathbf{x}^{(i)}$.
- Flow-dependent background error covariances, $\mathbf{P}^{\mathrm{f}}$.
- Formulation starts with the OI equation ($\mathbf{B} \rightarrow \mathbf{P}^{\mathrm{f}}$), but for an ensemble of states.
- Does not need the $\mathbf{P}^{\mathrm{f}}$-matrix explicitly.
- Severe rank deficiency problems with $\mathbf{P}^{\mathrm{f}}$ due to undersampling (use, e.g., localization techniques to overcome).
- Deterministic (square-root) and non-deterministic (non-square-root) formulations exist - see part II of the course.



$$\mathbf{P}^{\mathrm{f}} \approx \mathbf{P}^{\mathrm{f}}_{(N)} = \frac{1}{N-1} \sum_{i=1}^{N} \left\langle \left(\mathbf{x}^{(i)} - \langle \mathbf{x} \rangle \right) \left(\mathbf{x}^{(i)} - \langle \mathbf{x} \rangle \right)^{\mathrm{T}} \right\rangle,$$

$$\langle \mathbf{x} \rangle \approx \frac{1}{N} \sum_{i=1}^{N} \mathbf{x}^{(i)}.$$

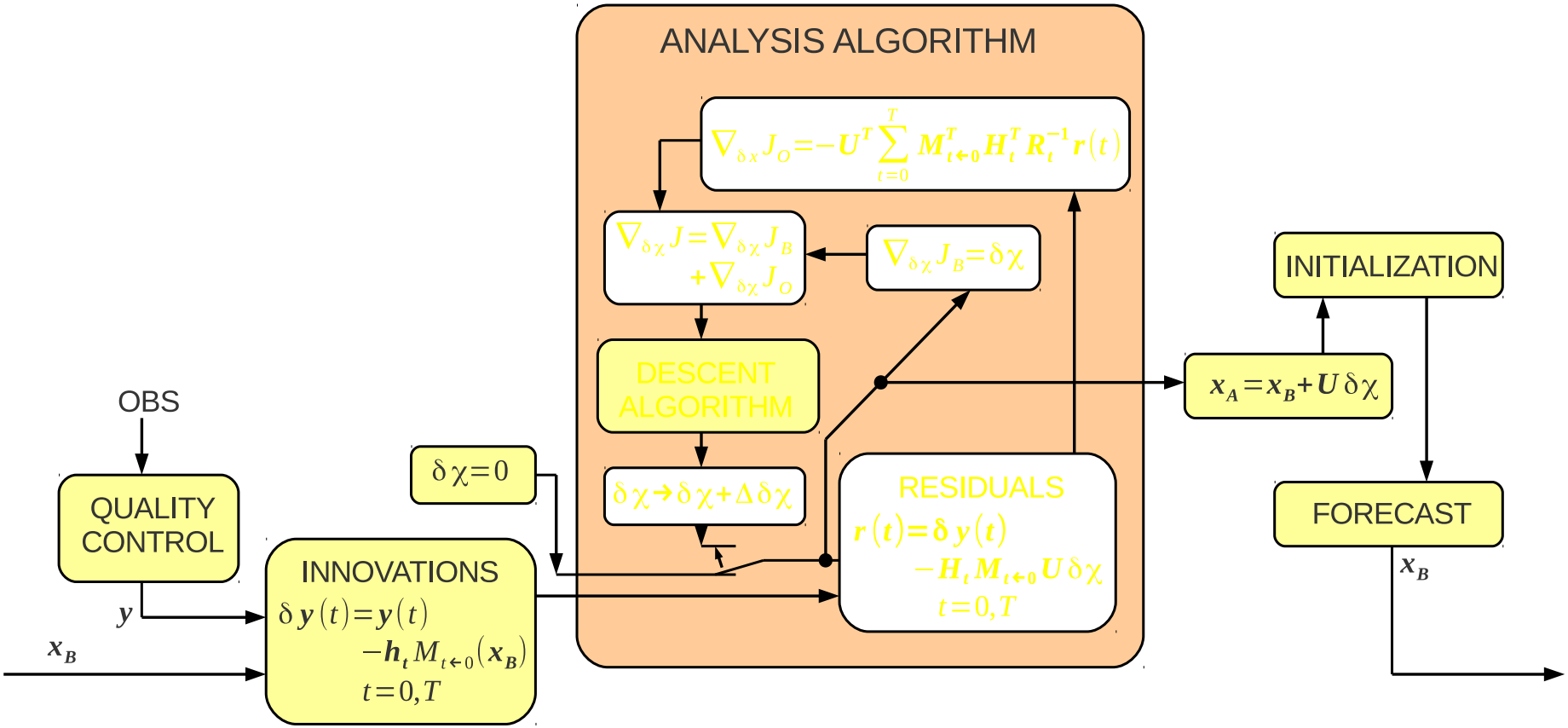
Hybrid methods 2010s

- Combine the robustness of the $\mathbf{B}$-matrix with the flow-dependence of the $\mathbf{P}^{\mathrm{f}}$-matrix.
- Most simple is the arithmetic average:

$$\mathbf{P}^{\mathrm{H}} = \alpha\mathbf{B} + (1-\alpha)\mathbf{P}^{\mathrm{f}}_{(N)}$$

- Solve a VAR-like problem but $\mathbf{B} \rightarrow \mathbf{P}^{\mathrm{H}}$.
- Still need localization methods.
- Other approaches exist too.
- Uses methods that avoid the need to hold large matrices explicitly.

The data assimilation cycle



1(d) The scale/challenges of the operational problem

- The atmosphere is large ~ 5 billion km^3.
- All forecasts are wrong (even if models were perfect - chaos) and all observations are imperfect.
- n is very large, e.g. $n_\lambda \approx 1000$, $n_\phi \approx 800$, $n_l \approx 70$, $n_{\mathrm{param}} = 6$, $\therefore n \sim n_\lambda \times n_\phi \times n_l \times n_{\mathrm{param}} \sim \mathcal{O}(350 \times 10^6)$.
- Do not have the computer power to deal with matrices $\mathbf{B}$, $\mathbf{P}^{\mathrm{f}}$, etc. $\mathcal{O}(n \times n) \sim \mathcal{O}(10^{17})$.
- Do not have enough information to completely determine $\mathbf{B}$, $\mathbf{P}^{\mathrm{f}}$, etc.
- Huge numbers of diverse observations from all over the world and from satellites, $p \sim \mathcal{O}(10^6)$.
- Many observations are indirect, and they are sparse in some places (especially over oceans and in upper parts of the atmosphere).
- A sensible analysis must be found even if observations are unavailable.
- Some observations have problems (e.g. instrument biases).
- Model and observation operators may be non-linear ($\boldsymbol{\mathcal{M}}$, $\mathbf{h}$).
- For VAR methods, need linearizations ($\mathbf{M}$, $\mathbf{H}$), and their adjoints ($\mathbf{M}^{\mathrm{T}}$, $\mathbf{H}^{\mathrm{T}}$), and we usually don't know these operators as explicit matrices.
- Model and observation operators are imperfect ("model error") and the model state cannot represent flow on all scales ("representivity error").
- The conditioning of the minimization problem can be very bad leading to inefficiencies and inaccuracies in determining the solution (see later).

2. Variational techniques

2(a) The Euler-Lagrange equations

This section teaches us formally about the variational solution of an inverse problem, backward (or adjoint) variables and the strong and weak constraint formulations. The method of representers, used to solve the Euler-Lagrange equations, is introduced.

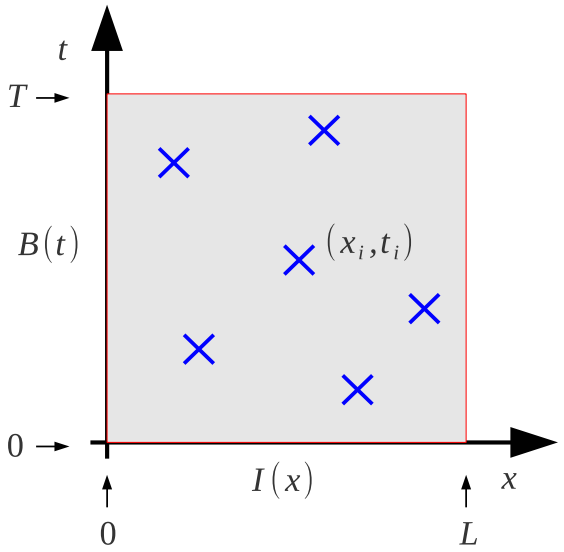
Statement of problem

What is the optimal state, $\phi(x,t)$ of the 1-D system whose dynamics are governed by

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} - F = e, \tag{1}$$

which lies close to some given observations, some initial conditions and some boundary conditions?The symbols have the following meanings:

- ϕ unknown tracer concentration,
- u known, but constant advection speed,
- F known source field, which may vary in time and space
- e unknown model error, which may vary in time and space.



The (imperfectly known) information we have about the system is (see Fig.):

- $\phi(x,0) \approx I(x)$ imperfectly known initial conditions (i.c.s), $0 \leq x \leq L$,
- $\phi(0,t) \approx B(t)$ imperfectly known boundary conditions (b.c.s), $0 \leq t \leq T$, and
- y_m imperfect observation of the system (a direct observation of $\phi(x_m,t_m)$), $1 \leq m \leq p$.

The error standard deviations of all the data are specified as:

- $W_{\rm ic}^{-1/2}$ a-priori i.c. error standard deviation,
- $W_{\rm bc}^{-1/2}$ a-priori b.c. error standard deviation,
- $W_{\rm ob}^{-1/2}$ observation error standard deviation, and
- $W_{\rm e}^{-1/2}$ model error error standard deviation.

The a-priori state $\phi_{\rm B}(x,t)$ satisfies the known bits of the problem (the specified i.c.s and b.c.s, and (1) with $e=0$):

$$\frac{\partial \phi_{\rm B}}{\partial t} + u\frac{\partial \phi_{\rm B}}{\partial x} - F = 0, \qquad \phi_{\rm B}(x,0) = I(x), \qquad \phi_{\rm B}(0,t) = B(t). \tag{2}$$

Strong vs weak constraint formulations of the problem

- **Strong constraint**: impose the known parts of the system equations exactly (i.e. we assume that $e = 0$, even though in reality $e \neq 0$). We still allow for imperfections in the other pieces of information though (i.c.s, b.c.s and obs.).
  - Construct a cost function measuring the departure between an arbitrary field ϕ, and the i.c.s, b.c.s and obs.
  - Impose (1) ($e = 0$) as a constraint using the method of Lagrange multipliers.
  - Minimum of the cost function leads to strong constraint Euler-Lagrange equations.
- **Weak constraint**: impose the system equations approximately (i.e. allow for the fact that $e \neq 0$). Also allow for imperfections in the other pieces of information (i.c.s, b.c.s and obs).
  - Construct a cost function measuring the departure between ϕ and the i.c.s, b.c.s, obs. and the system equation.
  - Minimum of the cost function leads to weak constraint Euler-Lagrange equations.
  - Can control the degree to which the system equations are satisfied with a parameter, W_e.
  - Is equivalent to the strong constraint formulation when $W_e \to \infty$.

The weak constraint formulation is the most general, so we look only at that.

The weak constraint formulation

The weak constraint formulation imposes the known parts of the system equations approximately (that is we acknowledge that there is unknown model error). In order to find the optimal solution to the problem in this formulation, construct a functional $J[\phi]$ which measures the total departure between $\phi$and each of the i.c.s, the b.c.s, the obs., and the known parts of the system equations:

$$\begin{aligned} J[\phi] \;=\; & W_{\rm ic} \int_{x=0}^{L} dx \{\phi(x,0) - I(x)\}^2 + W_{\rm bc} \int_{t=0}^{T} dt \{\phi(0,t) - B(t)\}^2 + \\ & W_{\rm ob} \sum_{i=1}^{p} \{\phi(x_i,t_i) - y_i\}^2 + W_{\rm e} \int_{x=0}^{L} dx \int_{t=0}^{T} dt \left\{ \frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} - F \right\}^2 . \end{aligned} \tag{3}$$

We ask the question: what $\phi(x,t)$ makes $J[\phi]$ stationary?

Variations of J Construct variations of J about some reference field $\hat{\phi}$, i.e. $J[\hat{\phi}+\delta\phi] = J[\hat{\phi}] + \delta J|_{\hat{\phi}}$, where:

$$\begin{aligned}
\delta J|_{\hat{\phi}} &= \int_{x=0}^{L} dx \int_{t=0}^{T} dt \, \frac{\partial J}{\partial \phi}|_{\hat{\phi}} \delta\phi + O(\delta\phi^2), \\
&= 2W_{\mathrm{ic}} \int_{x=0}^{L} dx \{\hat{\phi}(x,0) - I(x)\}\delta\phi(x,0) + 2W_{\mathrm{bc}} \int_{t=0}^{T} dt \{\hat{\phi}(0,t) - B(t)\}\delta\phi(0,t) + \\
&\quad 2W_{\mathrm{ob}} \sum_{i=1}^{p} \{\hat{\phi}(x_i,t_i) - y_i\}\delta\phi(x_i,t_i) + \\
(*) \qquad &\quad 2W_{\mathrm{e}} \int_{x=0}^{L} dx \int_{t=0}^{T} dt \left\{ \frac{\partial\hat{\phi}}{\partial t} + u\frac{\partial\hat{\phi}}{\partial x} - F \right\} \left\{ \frac{\partial\delta\phi}{\partial t} + u\frac{\partial\delta\phi}{\partial x} \right\} + O(\delta\phi^2). \qquad (4)
\end{aligned}$$

$$\text{Define:} \qquad \hat{\mu}(x,t) = W_{\mathrm{e}} \left(\frac{\partial\hat{\phi}}{\partial t} + u\frac{\partial\hat{\phi}}{\partial x} - F \right). \qquad (5)$$

$$(*) \text{ in (4) is then:} \qquad 2\int_{x=0}^{L} dx \int_{t=0}^{T} dt \, \hat{\mu} \left\{ \frac{\partial\delta\phi}{\partial t} + u\frac{\partial\delta\phi}{\partial x} \right\}.$$

Changing form We would like to have terms to do with $\delta\phi$ at different positions and times. The line marked (*) in (4) is not in the required form as it involves *derivatives* of $\delta\phi$ in space and time. Use the integration by parts formula to rewrite (*). In generic form the integration by parts formula is:

$$\int_a^b v\frac{du}{dx}dx = [uv]_a^b - \int_a^b u\frac{dv}{dx}dx. \qquad (6)$$

Using this to rewrite the first term in (*):

$$\begin{aligned}\int_{t=0}^{T} dt\, \hat{\mu}\frac{\partial \delta\phi}{\partial t} &= [\delta\phi(x,t)\hat{\mu}(x,t)]_0^T - \int_{t=0}^{T} dt\, \delta\phi\frac{\partial \hat{\mu}}{\partial t}, \\ &= \delta\phi(x,T)\hat{\mu}(x,T) - \delta\phi(x,0)\hat{\mu}(x,0) - \int_{t=0}^{T} dt\, \delta\phi\frac{\partial \hat{\mu}}{\partial t}, \end{aligned} \tag{7}$$

and the second term in (*):

$$\begin{aligned}\int_{x=0}^{L} dx\, \hat{\mu}u\frac{\partial \delta\phi}{\partial x} &= u[\delta\phi(x,t)\hat{\mu}(x,t)]_0^L - \int_{x=0}^{L} dx\, u\delta\phi\frac{\partial \hat{\mu}}{\partial x}, \\ &= u\delta\phi(L,t)\hat{\mu}(L,t) - u\delta\phi(0,t)\hat{\mu}(0,t) - \int_{x=0}^{L} dx\, u\delta\phi\frac{\partial \hat{\mu}}{\partial x}. \end{aligned} \tag{8}$$

Note also for the observation term:

$$\{\hat{\phi}(x_i,t_i) - y_i\}\delta\phi(x_i,t_i) = \int_{x=0}^{L} dx \int_{t=0}^{T} dt\, \{\hat{\phi}(x_i,t_i) - y_i\}\delta\phi(x,t)\delta(x-x_i)\delta(t-t_i). \tag{9}$$

These make (4) into:

$$\begin{aligned}
\delta J|_{\hat{\phi}} \;=\; & 2W_{\mathrm{ic}} \int_{x=0}^{L} dx \Big\{\hat{\phi}(x,0) - I(x)\Big\}\delta\phi(x,0) + 2W_{\mathrm{bc}} \int_{t=0}^{T} dt \Big\{\hat{\phi}(0,t) - B(t)\Big\}\delta\phi(0,t) + \\
& 2W_{\mathrm{ob}} \int_{x=0}^{L} dx \int_{t=0}^{T} dt \sum_{i=1}^{p} \Big\{\hat{\phi}(x_i,t_i) - y_i\Big\}\,\delta(x-x_i)\delta(t-t_i)\delta\phi(x,t) + \\
& 2\Bigg\{ \int_{x=0}^{L} dx\, \hat{\mu}(x,T)\delta\phi(x,T) - \int_{x=0}^{L} dx\, \hat{\mu}(x,0)\delta\phi(x,0) - \int_{x=0}^{L} dx \int_{t=0}^{T} dt\, \frac{\partial\hat{\mu}}{\partial t}\delta\phi(x,t) + \\
& \int_{t=0}^{T} dt\, u\hat{\mu}(L,t)\delta\phi(L,t) - \int_{t=0}^{T} dt\, u\hat{\mu}(0,t)\delta\phi(0,t) - \int_{t=0}^{T} dt \int_{x=0}^{L} dx\, u\frac{\partial\hat{\mu}}{\partial x}\delta\phi(x,t) \Bigg\} + O(\delta\phi^2). \qquad (10)
\end{aligned}$$

The Euler-Lagrange equations for the weak constraint formulation Setting the linear part of (10) to zero, using the model equation (1), and definition (21) gives Euler-Lagrange equations for the weak constraint:

$$\begin{aligned}
\frac{\partial\hat{\phi}}{\partial t} + u\frac{\partial\hat{\phi}}{\partial x} - F &= W_{\mathrm{e}}^{-1}\hat{\mu}, && (11)\\
W_{\mathrm{ic}}\{\hat{\phi}(x,0) - I(x)\} - \hat{\mu}(x,0) &= 0, && (12)\\
W_{\mathrm{bc}}\{\hat{\phi}(0,t) - B(t)\} - u\hat{\mu}(0,t) &= 0, && (13)\\
W_{\mathrm{ob}} \sum_{i=1}^{p} \{\hat{\phi}(x_i,t_i) - y_i\}\delta(x-x_i)\delta(t-t_i) - \left(\frac{\partial\hat{\mu}}{\partial t} + u\frac{\partial\hat{\mu}}{\partial x}\right) &= 0, && (14)\\
\hat{\mu}(x,T) &= 0, && (15)\\
\hat{\mu}(L,t) &= 0. && (16)
\end{aligned}$$

(11) is known as the forward equation, and (12)/(13) are its initial/boundary conditions. (14) is known as the backward equation, and (15)/(16) are its conditions. Note that the strong constraint is a limit of the weak constraint when $W_{\mathrm{e}}^{-1} \to 0$. The

solution to these Euler-Lagrange equations for $\hat{\phi}$ solves the original problem that we posed in Section 1 (with the acknowledgement of an imperfect model). The next section outlines how these equations can be solved using the method of representers.

Solving the weak-constraint Euler-Lagrange equations using the method of representers

The forward equation (11) is solved for $\hat{\phi}(x,t)$ 'upwards and to the right' (since the conditions for $\hat{\phi}$ are given for $x = 0$ and $t = 0$, see Fig.), and the backward equation (14) is solved for $\hat{\mu}(x,t)$ 'downwards and to the left' (since the conditions for $\hat{\phi}$ are given for $x = L$ and $t = T$, see Fig.).

Problem: In order to solve (11) for $\hat{\phi}(x,t)$, $\hat{\mu}(x,t)$ is needed, but in order to solve (14) for $\hat{\mu}(x,t)$, $\hat{\phi}(x,t)$ is needed! The set of Euler-Lagrange equations must be all solved together.

The way that we will solve the Euler-Lagrange equations is by the method of representers. In this method we define a set of forward and backward 'representer functions' which will solve a set of modified equations which we shall propose. We then form the solution of the full Euler-Lagrange equations as a special linear combination of the representer functions.

Recipe for the solution using the method of representers

1. Solve the background problem (2) for $\phi_{\mathrm{B}}(x,t)$. This is an exercise in solving partial differential equations (PDEs) analytically or numerically.

2. Define the p forward representer functions and the p backward representer functions (one each per observation) as:

$$\left.\begin{array}{ll} \text{Forward representer function} & r_i(x,t) \\ \text{Backward representer function} & \alpha_i(x,t) \end{array}\right\} 1 \leq i \leq p.$$

The modified equations that these representers satisfy are based on the Euler-Lagrange equations, but have $\hat{\phi} \to r_i$, $\hat{\mu} \to \alpha_i$, $F = 0$, $I(x) = 0$, $B(t) = 0$ and replace the observations with a single impulse at the position and time of the ith

observation ($W_{\rm ob}\sum_{i=1}^{p}\{\hat{\phi}(x_i,t_i)-y_i\}\delta(x-x_i)\delta(t-t_i)\rightarrow\delta(x-x_i)\delta(t-t_i)$).

$$\frac{\partial r_i}{\partial t}+u\frac{\partial r_i}{\partial x} = W_{\rm e}^{-1}\alpha_i, \tag{17}$$

$$W_{\rm ic}r_i(x,0)-\alpha_i(x,0) = 0, \tag{18}$$

$$W_{\rm bc}r_i(0,t)-u\alpha_i(0,t) = 0, \tag{19}$$

$$\delta(x-x_i)\delta(t-t_i)-\left(\frac{\partial\alpha_i}{\partial t}+u\frac{\partial\alpha_i}{\partial x}\right) = 0, \tag{20}$$

$$\alpha_i(x,T) = 0, \tag{21}$$

$$\alpha_i(L,t) = 0. \tag{22}$$

3. Start with the backward representers. Solve (20), (21) and (22) for each i 'downwards and to the left' (again an exercise in solving PDEs). This gives the p backward representers, $\alpha_i(x,t)$. In the modified equations, the backward representers do not depend upon the forward representers, $r_i(x,t)$.

4. Now find the forward representers. Solve (17), (18) and (19) for each i 'upwards and to the right' (again an exercise in solving PDEs). This gives the p forward representers, $r_i(x,t)$, which can be found because the α_i are now known.

5. Look for a solution of $\hat{\phi}(x,t)$ (the field that we are really interested in) that is a linear combination of the forward representer functions:

$$\hat{\phi}(x,t)=\phi_{\rm B}(x,t)+\sum_{i=1}^{p}\beta_i r_i(x,t), \tag{23}$$

where the β_i are the coefficients which are determined by insisting that $\hat{\phi}(x,t)$ satisfies the Euler-Lagrange equations.

6. To make (23) satisfy the Euler-Lagrange equations, act with $\partial/\partial t + u\partial/\partial x$ on (23), then use (11), (2) and (17):

$$\begin{aligned}
\frac{\partial \hat{\phi}}{\partial t} + u\frac{\partial \hat{\phi}}{\partial x} &= \frac{\partial \phi_{\mathrm{B}}}{\partial t} + u\frac{\partial \phi_{\mathrm{B}}}{\partial x} + \sum_{i=1}^{p} \beta_i \left(\frac{\partial r_i}{\partial t} + u\frac{\partial r_i}{\partial x} \right), \\
\Rightarrow F + W_{\mathrm{e}}^{-1}\hat{\mu} &= F + \sum_{i=1}^{p} \beta_i W_{\mathrm{e}}^{-1} \alpha_i, \\
\Rightarrow \hat{\mu}(x,t) &= \sum_{i=1}^{p} \beta_i \alpha_i(x,t). \qquad (24)
\end{aligned}$$

7. Substitute (24) into (14), then use (23) and (20):

$$\begin{aligned}
W_{\mathrm{ob}} \sum_{i=1}^{p} \{\hat{\phi}(x_i,t_i) - y_i\} \delta(x-x_i)\delta(t-t_i) &= \sum_{i=1}^{p} \beta_i \left(\frac{\partial \alpha_i}{\partial t} + u\frac{\partial \alpha_i}{\partial x} \right), \\
\Rightarrow W_{\mathrm{ob}} \sum_{i=1}^{p} \{\phi_{\mathrm{B}}(x_i,t_i) + & \\
\sum_{j=1}^{p} \beta_j r_j(x_i,t_i) - y_i\} \delta(x-x_i)\delta(t-t_i) &= \sum_{i=1}^{p} \beta_i \delta(x-x_i)\delta(t-t_i). \qquad (25)
\end{aligned}$$

8. Equate coefficients of impulses in (25):

$$\begin{aligned}
W_{\mathrm{ob}} \left\{ \phi_{\mathrm{B}}(x_i,t_i) + \sum_{j=1}^{p} \beta_j r_j(x_i,t_i) - y_i \right\} &= \beta_i, \\
\Rightarrow W_{\mathrm{ob}} \left\{ \phi_{\mathrm{B}}(x_i,t_i) - y_i \right\} + \sum_{j=1}^{p} \left\{ W_{\mathrm{ob}} r_j(x_i,t_i) - \delta_{ij} \right\} \beta_j &= 0, \qquad (26)
\end{aligned}$$

where δ_{ij} is the Kronecker delta-function. This is the equation that we have to solve for the β_i coefficients. Once these are known, the solution can be built using (23).

Finding the coefficients Equation (26) is the remaining equation to solve. We will use some linear algebra (vectors and matrices) to do this. This is a standard procedure in a wide range of numerical analysis problems. Let the vectors $\mathbf{y} \in \mathbb{R}^p$, $\boldsymbol{\beta} \in \mathbb{R}^p$ and $\boldsymbol{\phi}_{\mathrm{B}}^{\mathrm{ob}} \in \mathbb{R}^p$ (bold symbols) represent the following collections of information:

$$\mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_p \end{pmatrix}, \qquad \boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_p \end{pmatrix}, \qquad \boldsymbol{\phi}_{\mathrm{B}}^{\mathrm{ob}} = \begin{pmatrix} \phi_{\mathrm{B}}(x_1, t_1) \\ \phi_{\mathrm{B}}(x_2, t_2) \\ \vdots \\ \phi_{\mathrm{B}}(x_p, t_p) \end{pmatrix}.$$

These represent (respectively) the observations, the (as yet) unknown coefficients that we are trying to find and the background values at the observation positions and times. The equations represented by (26) $(1 \leq i \leq p)$ may be written in linear algebraic form:

$$W_{\mathrm{ob}} \left(\boldsymbol{\phi}_{\mathrm{B}}^{\mathrm{ob}} - \mathbf{y} \right) + \left(W_{\mathrm{ob}} \mathbf{P} - \mathbf{I} \right) \boldsymbol{\beta} = 0,$$

where $\mathbf{P} \in \mathbb{R}^{p \times p}$ is

$$\mathbf{P} = \begin{pmatrix} r_1(x_1, t_1) & r_2(x_1, t_1) & \cdots & r_p(x_1, t_1) \\ r_1(x_2, t_2) & r_2(x_2, t_2) & \cdots & r_p(x_2, t_2) \\ \vdots & \vdots & \ddots & \vdots \\ r_1(x_p, t_p) & r_2(x_p, t_p) & \cdots & r_p(x_p, t_p) \end{pmatrix},$$

and $\mathbf{I} \in \mathbb{R}^{p \times p}$ is the identity matrix. All of these vectors and matrices are known except for $\boldsymbol{\beta}$. Providing that the matrix $W_{\mathrm{ob}} \mathbf{P} - \mathbf{I}$ is full rank, then the solution is found to be

$$\boldsymbol{\beta} = W_{\mathrm{ob}} \left(W_{\mathrm{ob}} \mathbf{P} - \mathbf{I} \right)^{-1} \left(\mathbf{y} - \boldsymbol{\phi}_{\mathrm{B}}^{\mathrm{ob}} \right).$$

PROBLEM 3 ON METHOD OF REPRESENTERS.

2(b) Error covariance matrices

In the Euler-Lagrange equations, we used, e.g., $W_{\mathrm{ic}}^{-1/2}$ and $W_{\mathrm{ob}}^{-1/2}$. These are the standard deviations of the errors in the initial conditions, $I(x)$, and the observations, y_i, respectively. Increasing (decreasing) the value of $W_{\mathrm{ic}}^{-1/2}$ will decrease (increase) the weight that the information that $I(x)$ holds in the inverse problem (similarly for $W_{\mathrm{ob}}^{-1/2}$ and the information in y_i).

If we represent $I(x)$, y_i and $\phi(x,t)$ as the vectors $\mathbf{x}_\mathrm{B}$, $\mathbf{x}$ and $\mathbf{y}$ (respectively), then the initial condition and observation terms in (3) take the form of inner products:

$$W_\mathrm{ic} \int_{x=0}^{L} dx\{\phi(x,0) - I(x)\}^2 \;\rightarrow\; (\mathbf{x}(0) - \mathbf{x}_\mathrm{B})^\mathrm{T} \mathbf{P}^{\mathrm{f}-1} (\mathbf{x}(0) - \mathbf{x}_\mathrm{B}),$$

$$W_\mathrm{ob} \sum_{i=1}^{p} \{\phi(x_i,t_i) - y_i\}^2 \;\rightarrow\; (\mathbf{h}(\mathbf{x}) - \mathbf{y})^\mathrm{T} \mathbf{R}^{-1} (\mathbf{h}(\mathbf{x}) - \mathbf{y}),$$

where $\mathbf{h}(\mathbf{x})$ in this case returns a vector of model observations at each observation's position and time and

$$\mathbf{P}^\mathrm{f} = \begin{pmatrix} \sigma_\mathrm{B}^2 & 0 & \cdots & 0 \\ 0 & \sigma_\mathrm{B}^2 & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \vdots & \cdots & \sigma_\mathrm{B}^2 \end{pmatrix}, \; \sigma_\mathrm{B} = W_\mathrm{ic}^{-1/2}; \qquad \mathbf{R} = \begin{pmatrix} \sigma_\mathrm{O}^2 & 0 & \cdots & 0 \\ 0 & \sigma_\mathrm{O}^2 & \cdots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \vdots & \cdots & \sigma_\mathrm{O}^2 \end{pmatrix}, \; \sigma_\mathrm{O} = W_\mathrm{ob}^{-1/2}.$$

(PROBLEM 4 TO SHOW THAT THESE FORMS ARE EQUIVALENT.) (In the case of the initial conditions we have moved from the continuous to a discrete system.)

In this case the initial condition uncertainty is homogeneous (σ_B does not change with position or time) and initial condition errors at different locations are not correlated ($\mathbf{P}^\mathrm{f}$ is diagonal), and observation uncertainty is constant (σ_O does not change with observation) and observation errors are not correlated ($\mathbf{R}$ is diagonal). The former situation in particular is not at all realistic (from now on $\mathbf{P}^\mathrm{f}$ will be assumed not to be diagonal), but the roles of the error covariance matrices still have the effect of weighting the information that it represents the error covariances of (large value in error covariance matrix $\rightarrow$ smaller weight of the information in the data assimilation).

2(c) Cost functions and simplifications for operational assimilation

The Euler-Lagrange approach to solving the inverse problem is tricky to apply to complicated models. In operational systems, a cost function is formulated and then minimized using descent algorithms. Here we consider some standard forms of cost functions, starting from the most general and progressively getting simpler (and hence easier and cheaper to deal with).

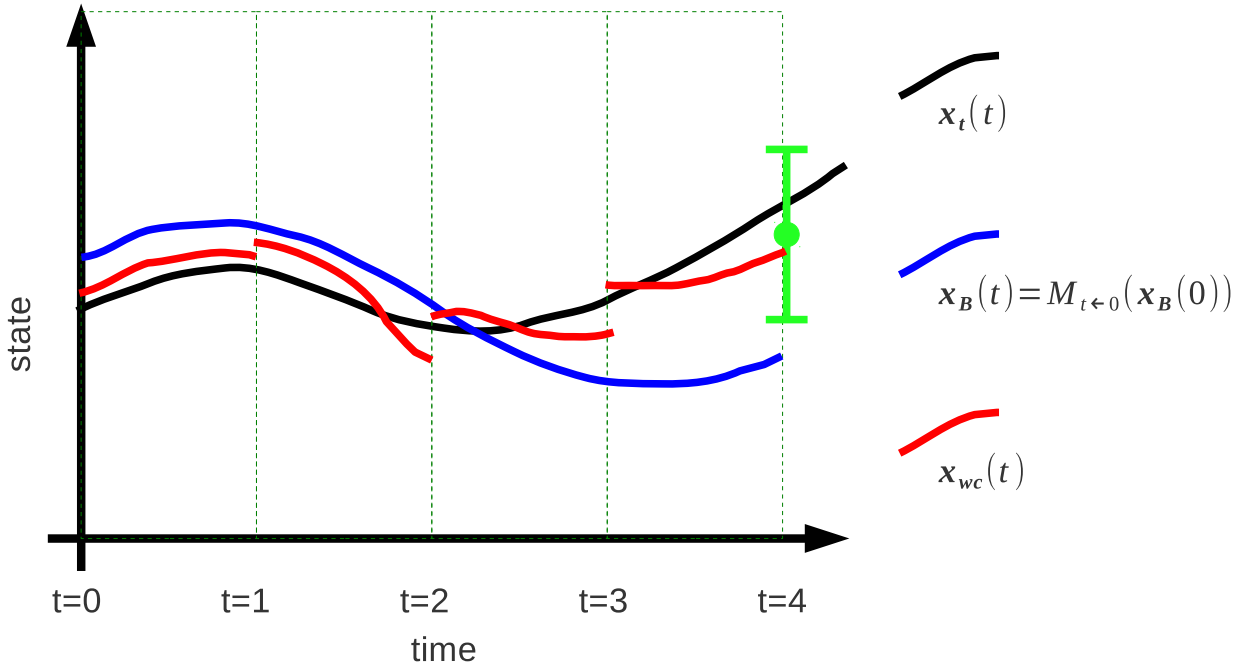
Weak constraint 4D-VAR

The form of the cost function that is as general as we will consider accounts for as many sources of error as possible (background error, observation error, model error). This is WC 4D-VAR: (WRITE THIS ON THE BOARD AS WELL AS SHOWING ON THE SCREEN - FOR COMPARISON WITH SC 4D-VAR.)

$$
\begin{aligned}
J_{\mathrm{wc}}[\mathbf{x}] \;=\; & \frac{1}{2}\left[\mathbf{x}(0)-\mathbf{x}_{\mathrm{B}}(0)\right]^{\mathrm{T}}\mathbf{P}^{\mathrm{f}-1}\left[\mathbf{x}(0)-\mathbf{x}_{\mathrm{B}}(0)\right]+ \\
& \frac{1}{2}\sum_{t=0}^{T}\left[\mathbf{y}(t)-\mathbf{h}_t\left(\mathbf{x}(t)\right)\right]^{\mathrm{T}}\mathbf{R}_t^{-1}\left[\mathbf{y}(t)-\mathbf{h}_t\left(\mathbf{x}(t)\right)\right]+ \\
& \frac{1}{2}\sum_{t=1}^{T}\sum_{t'=1}^{T}\left[\mathbf{x}(t)-\boldsymbol{\mathcal{M}}_{t\leftarrow t-1}\left(\mathbf{x}(t-1)\right)\right]^{\mathrm{T}}\left(\mathbf{Q}^{-1}\right)_{tt'}\left[\mathbf{x}(t')-\boldsymbol{\mathcal{M}}_{t'\leftarrow t'-1}\left(\mathbf{x}(t'-1)\right)\right].
\end{aligned}
$$

Here $\mathbf{x}$ is called the control variable and is the 4D state vector:

$$
\boldsymbol{x}=\begin{pmatrix}\boldsymbol{x}(0)\\ \boldsymbol{x}(1)\\ \vdots\\ \boldsymbol{x}(T)\end{pmatrix}
$$



The first term penalizes misfit to the background state at $t = 0$ under the $\mathbf{P}^{\mathrm{f}}$ norm.

The second term penalizes misfit to the observations at each time under the $\mathbf{R}_t$ norm.

The third term penalizes misfit to the solution of the numerical model at each pair of times under the $\mathbf{Q}_{tt'}$ norm. Given the state vector at neighbouring times, $\mathbf{x}(t)$ and $\mathbf{x}(t-1)$, we want $\mathbf{x}(t)$ to be close to $\boldsymbol{\mathcal{M}}_{t\leftarrow t-1}\left(\mathbf{x}(t-1)\right)$.

Weak constraint 4D-VAR gives a 4D solution that is close to the a-priori, close to the observations and close to a model trajectory. It does not need to follow a model trajectory exactly.

For the Fig.

- If the background were used as a forecast then the forecast would not agree well with the observation.
- In this example the observation is a direct observation of the state (the curves between each time level are just for effect).
- The weak constraint analysis is in terms of the state at each time.
- Want to minimize the deviation between $\mathbf{x}(0)$ and $\mathbf{x}_{\mathrm{B}}(0)$, between $\mathbf{x}(4)$ and the observation, and minimize the jumps at each time in $\mathbf{x}(t)$.

Even though we have considered this a general cost function, we have still made some assumptions:

- Assume that the errors in the quantities (a-priori, observations, numerical model) are random (e.g. unbiased), and obey Gaussian statistics.
- Assume that the error covariance matrices $\mathbf{P}^{\mathrm{f}}$, $\mathbf{R}_t$ and $\mathbf{Q}_{tt'}$ correctly describe the error covariances.
- Assume that the observation operator $\mathbf{h}_t$ is perfect.
- Assume that all observations are instantaneous, i.e. have the form $\mathbf{h}_t\left(\mathbf{x}(t)\right)$ and not $\mathbf{h}_t\left(\mathbf{x}(t), \mathbf{x}(t-1), \mathbf{x}(t-2), \ldots\right)$. An example of the latter kind of operator is for rainfall accumulation.
- Assume that the observation errors are uncorrelated in time.

Simplification 1: Assume model errors are uncorrelated in time (white noise)

$$(\mathbf{Q}^{-1})_{tt'} \rightarrow \delta_{tt'}(\mathbf{Q}^{-1})_{tt}.$$

Simplification 2: Static forecast error covariance matrix

$$\mathbf{P}^{\mathrm{f}} \rightarrow \mathbf{B}$$

- $\mathbf{P}^{\mathrm{f}}$: this matrix changes with the flow (e.g. recognizes areas that are forecast well and those that are forecast badly). This matrix is almost impossible to determine well.
- $\mathbf{B}$: this matrix is static (doesn't change from one time window to the next). It contains information on the climatological average error covariances of forecasts. This matrix is still difficult to determine, but is possible to approximate.

This is pragmatic choice - the information that would be present in $\mathbf{P}^{\mathrm{f}}$ is extremely important, but is not technologically possible to deal with currently. $\mathbf{Q}$ is also a very difficult matrix to deal with (hence simplification 3).

Simplification 3: Assume that the numerical model is perfect (strong constraint 4D-VAR)

If we assume that the model is perfect (or at least good enough over the time window), then we only need to determine the initial conditions. The control vector is now the 3D state at the start of the time window:

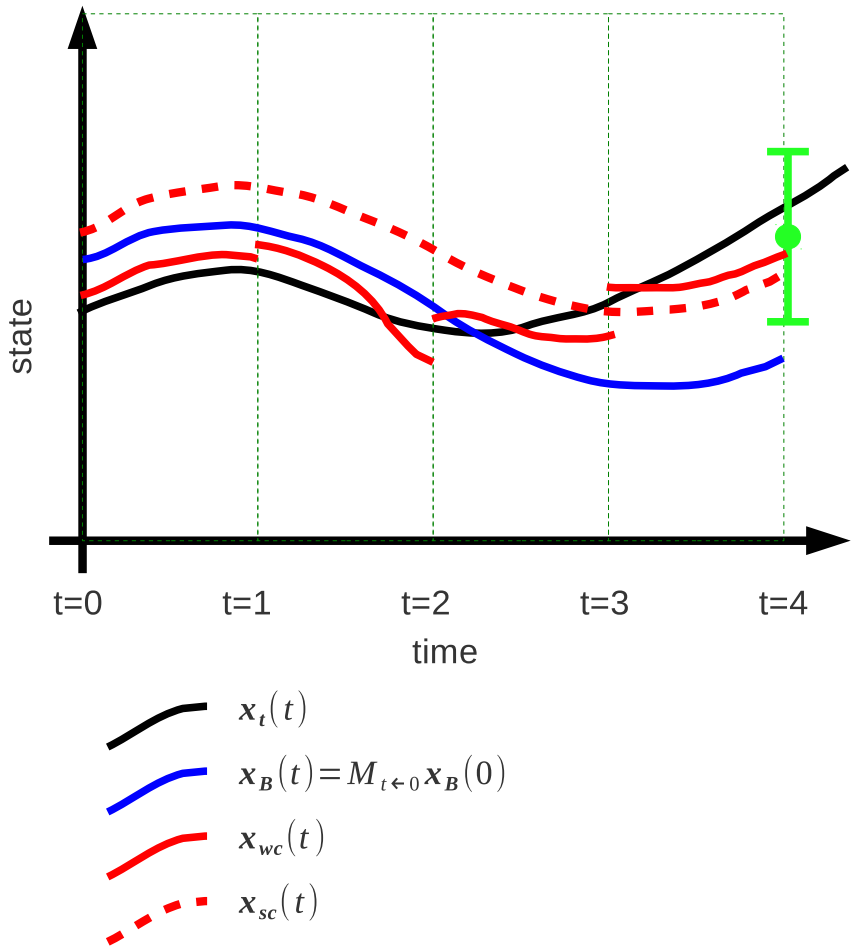
$$\mathbf{x} = \mathbf{x}(0),$$

and the state at later times is found from the numerical model:

$$\mathbf{x}(t) = \boldsymbol{\mathcal{M}}_{t\leftarrow 0}(\mathbf{x}).$$

The SC 4D-VAR cost function now has just background and observation terms:

$$\begin{aligned} J_{\mathrm{sc}}[\mathbf{x}] &= \frac{1}{2}(\mathbf{x}-\mathbf{x}_{\mathrm{B}})^{\mathrm{T}}\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}_{\mathrm{B}}) + \\ &\quad \frac{1}{2}\sum_{t=0}^{T}\left[\mathbf{y}(t)-\mathbf{h}_t\left(\boldsymbol{\mathcal{M}}_{t\leftarrow 0}(\mathbf{x})\right)\right]^{\mathrm{T}}\mathbf{R}_t^{-1}\times \\ &\quad\qquad \left[\mathbf{y}(t)-\mathbf{h}_t\left(\boldsymbol{\mathcal{M}}_{t\leftarrow 0}(\mathbf{x})\right)\right], \\ \boldsymbol{\mathcal{M}}_{t\leftarrow 0}(\mathbf{x}) &= \begin{cases} \boldsymbol{\mathcal{M}}_{t\leftarrow t-1}\left(\cdots \boldsymbol{\mathcal{M}}_{2\leftarrow 1}\left(\boldsymbol{\mathcal{M}}_{1\leftarrow 0}(\mathbf{x})\right)\right) & t>0 \\ \mathbf{I} & t=0 \end{cases}. \end{aligned}$$



This is equivalent to making $\mathbf{Q}_{tt} \to 0$ in the weak constraint cost function.

The strong constraint is useful when model errors introduced over the time window are negligible compared to other errors. For use with global-scale weather models, SC 4D-VAR has $T = 12$ hours typically, for use with mesoscale weather models, SC 4D-VAR has $T = 6$ hours, for use with convective-scale weather models, SC 4D-VAR has $T = 3$ hours.

Potential problems with the SC 4D-VAR formulation

- The real world is not a model trajectory.
- The SC 4D-VAR may have to make a less realistic analysis at $t = 0$ (than for WC 4D-VAR at $t = 0$) to be close to an observation at a later time. This is an example of aliasing (where one error can project onto another - in this case the (inevitable, but neglected) model error can be (wrongly) interpreted as background error.

Simplification 4: Incremental data assimilation

In the previous formulations, the operators $\mathbf{h}_t$ and $\boldsymbol{\mathcal{M}}$ can be non-linear functions. This means that the cost function is no longer a quadratic function of the control variable, $\mathbf{x}$. Algorithms that minimize functions in multi-dimensions are almost always designed for quadratic functions. A solution is to linearize the operators and the deal with increments to the control variable, which are assumed to behave linearly.

Define (for time t) a full state $\mathbf{x}(t)$, a reference state $\mathbf{x}_k^{\rm ref}(t)$, and an increment $\delta\mathbf{x}(t)$:

$$\mathbf{x}(t) = \mathbf{x}_k^{\rm ref}(t) + \delta\mathbf{x}(t).$$

Linearizing the forecast model:

$$\begin{aligned}
\mathbf{x}(t) &= \boldsymbol{\mathcal{M}}_{t\leftarrow t-1}(\mathbf{x}(t-1)),\\
\mathbf{x}_k^{\rm ref}(t) + \delta\mathbf{x}(t) &= \boldsymbol{\mathcal{M}}_{t\leftarrow t-1}\left(\mathbf{x}_k^{\rm ref}(t-1) + \delta\mathbf{x}(t-1)\right),\\
&\simeq \boldsymbol{\mathcal{M}}_{t\leftarrow t-1}\left(\mathbf{x}_k^{\rm ref}(t-1)\right) + \mathbf{M}_{t\leftarrow t-1}\delta\mathbf{x}(t-1),\\
\delta\mathbf{x}(t) &= \mathbf{M}_{t\leftarrow t-1}\delta\mathbf{x}(t-1),
\end{aligned}$$

where the reference state

$$\begin{aligned}
\mathbf{x}_k^{\rm ref}(t) &\equiv \boldsymbol{\mathcal{M}}_{t\leftarrow t-1}\left(\mathbf{x}_k^{\rm ref}(t-1)\right),\\
\text{and } \mathbf{M}_{t\leftarrow t-1} &\equiv \left.\frac{\partial\boldsymbol{\mathcal{M}}_{t\leftarrow t-1}\left(\mathbf{x}(t-1)\right)}{\partial\mathbf{x}(t-1)}\right|_{\mathbf{x}_k^{\rm ref}} \in \mathbb{R}^{n\times n},
\end{aligned}$$

with matrix elements

$$\{\mathbf{M}_{t\leftarrow t-1}\}_{ij} = \left.\frac{\partial\left\{\boldsymbol{\mathcal{M}}_{t\leftarrow t-1}\left(\mathbf{x}(t-1)\right)\right\}_i}{\partial\left\{\mathbf{x}(t-1)\right\}_j}\right|_{\mathbf{x}_k^{\rm ref}}.$$

Linearizing the observation operator:

$$\begin{aligned}
\mathbf{y}^{\rm mo}(t) &= \mathbf{h}_t(\mathbf{x}(t)),\\
&= \mathbf{h}_t\left(\mathbf{x}_k^{\rm ref}(t) + \delta\mathbf{x}(t)\right),\\
&\simeq \mathbf{h}_t\left(\mathbf{x}_k^{\rm ref}(t)\right) + \mathbf{H}_t\delta\mathbf{x}(t),\\
&\simeq \mathbf{y}_{{\rm ref},k}^{\rm mo}(t) + \mathbf{H}_t\delta\mathbf{x}(t),\\
\delta\mathbf{y}^{\rm mo}(t) &= \mathbf{H}_t\delta\mathbf{x}(t),
\end{aligned}$$

where $\delta\mathbf{y}^{\rm mo}(t) \equiv \mathbf{y}^{\rm mo}(t) - \mathbf{y}_{{\rm ref},k}^{\rm mo}(t)$,

$$\text{and } \mathbf{H}_t \equiv \left.\frac{\partial\mathbf{h}_t(\mathbf{x}(t))}{\partial\mathbf{x}(t)}\right|_{\mathbf{x}_k^{\rm ref}} \in \mathbb{R}^{p\times n},$$

with matrix elements

$$\{\mathbf{H}_t\}_{ij} = \left.\frac{\partial\left\{\mathbf{h}_t(\mathbf{x}(t))\right\}_i}{\partial\left\{\mathbf{x}(t)\right\}_j}\right|_{\mathbf{x}_k^{\rm ref}}.$$

(PROBLEM 5 FOR AN EXAMPLE OF LINEARIZING A NON-LINEAR OPERATOR.)

By writing the background as a perturbation with respect to the reference state, $\mathbf{x}_{\rm B}(t) \equiv \mathbf{x}_k^{\rm ref}(t) + \delta\mathbf{x}_{\rm B}(t)$, and defining $\delta\mathbf{y}(t) \equiv \mathbf{y}(t) - \mathbf{h}_t\left(\boldsymbol{\mathcal{M}}_{t\leftarrow 0}(\mathbf{x}_k^{\rm ref})\right)$, the strong constraint cost function becomes:

$$J_{\rm 4Dinc}[\delta\mathbf{x}] = \frac{1}{2}(\delta\mathbf{x}-\delta\mathbf{x}_{\rm B})^{\rm T}\mathbf{B}^{-1}(\delta\mathbf{x}-\delta\mathbf{x}_{\rm B}) + \frac{1}{2}\sum_{t=0}^{T}\left[\delta\mathbf{y}(t)-\mathbf{H}_t\mathbf{M}_{t\leftarrow 0}\delta\mathbf{x}\right]^{\rm T}\mathbf{R}_t^{-1}\left[\delta\mathbf{y}(t)-\mathbf{H}_t\mathbf{M}_{t\leftarrow 0}\delta\mathbf{x}\right].$$

- The control variable is $\delta\mathbf{x}=\delta\mathbf{x}(0)$ in this incremental formulation.
- Later we will call $\delta\mathbf{y}(t)-\mathbf{H}_t\mathbf{M}_{t\leftarrow 0}\delta\mathbf{x}$ the residual vector, $\mathbf{r}(t)$.
- $J_{\rm 4Dinc}[\delta\mathbf{x}]$ is exactly quadratic in $\delta\mathbf{x}$ and so is easier to minimize than $J_{\rm 4D}[\delta\mathbf{x}]$.
- If the value of $\delta\mathbf{x}$ that minimizes this is $\delta\mathbf{x}_{\rm A}$ ('inner loop'), then the analysis is

$$\mathbf{x}_{\rm A}=\mathbf{x}_k^{\rm ref}+\delta\mathbf{x}_{\rm A}.$$

- Set $\mathbf{x}_{k+1}^{\rm ref}(t)=\mathbf{x}_{\rm A}$ and repeat ('outer loop').

Simplification 5: 3D-VAR, with the first guess at the appropriate time (3D-FGAT)

This is the same cost function as for SC 4D-VAR, but with $\mathbf{M}_{t\leftarrow 0}\rightarrow\mathbf{I}$:

$$J_{\rm 3DFGAT}[\delta\mathbf{x}] = \frac{1}{2}(\delta\mathbf{x}-\delta\mathbf{x}_{\rm B})^{\rm T}\mathbf{B}^{-1}(\delta\mathbf{x}-\delta\mathbf{x}_{\rm B}) + \frac{1}{2}\sum_{t=0}^{T}\left[\delta\mathbf{y}(t)-\mathbf{H}_t\delta\mathbf{x}\right]^{\rm T}\mathbf{R}_t^{-1}\left[\delta\mathbf{y}(t)-\mathbf{H}_t\delta\mathbf{x}\right],$$

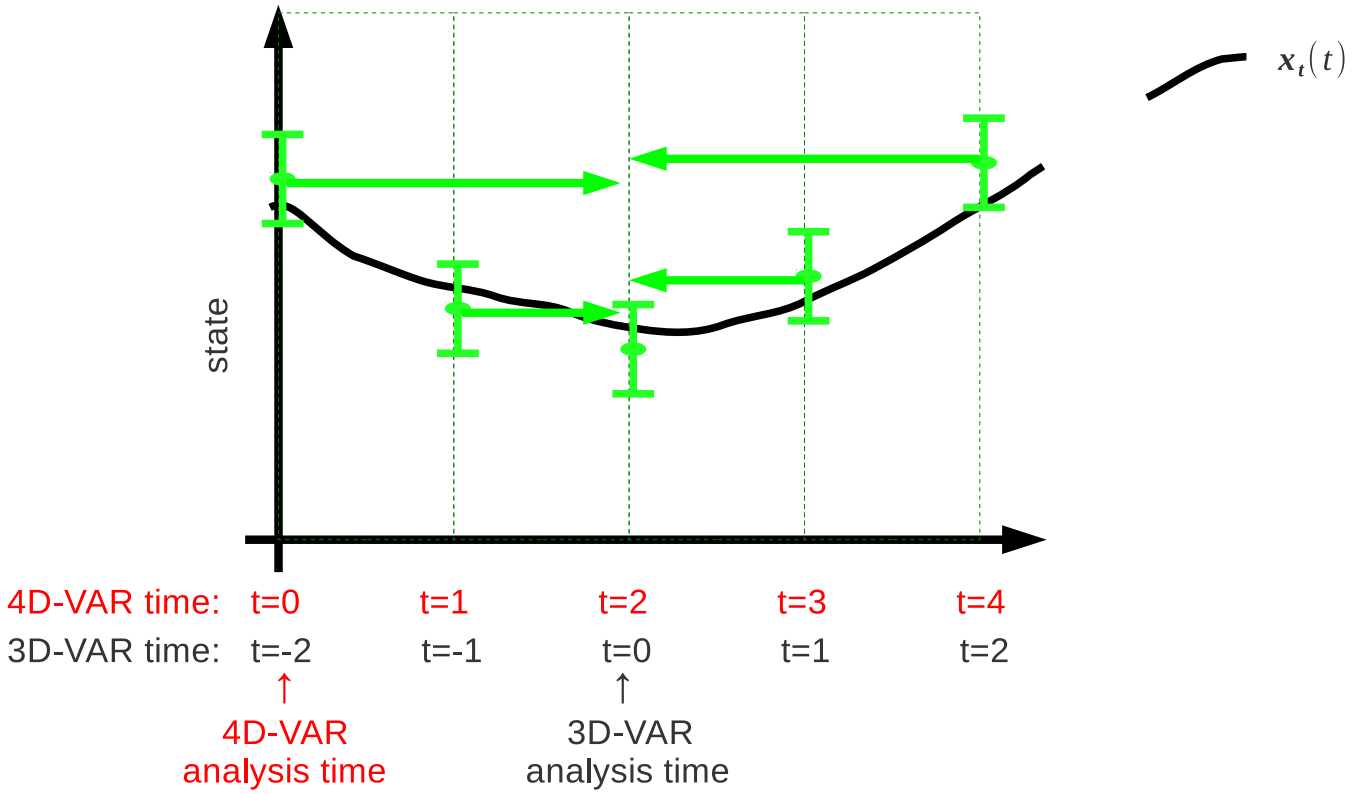
where, recall

$$\delta\mathbf{y}(t)\equiv\mathbf{y}(t)-\mathbf{h}_t\left(\boldsymbol{\mathcal{M}}_{t\leftarrow 0}(\mathbf{x}_k^{\rm ref})\right).$$

In 3D-FGAT, the non-linear nature of the model and observation operators are accounted for for the reference state, but linear corrections do not include the linear model $\mathbf{M}_{t\leftarrow 0}$.

Simplification 6: 3D-VAR

In 3D-VAR there is no time evolution accounted for at all. Now $\delta\mathbf{y} \equiv \mathbf{y} - \mathbf{h}\left(\mathbf{x}_k^{\text{ref}}\right)$, where observations spread throughout the time window lose their time label and are considered to be at one time. In order for the errors introduced by the 3D-VAR approximation to be as small as possible, observations should be as close as possible in time to the analysis time. The 'zero of time' used in 3D-VAR is shifted with respect to that of 4D-VAR.



Potential problems in going from 4D-VAR to 3D-VAR

- The real world is not static.
- Significant errors are introduced if the difference in the model observations $\mathbf{h}\left(\mathbf{x}_k^{\text{ref}}\right)$ and $\mathbf{h}_t\left(\boldsymbol{\mathcal{M}}_{t\leftarrow 0}(\mathbf{x}_k^{\text{ref}})\right)$ are significant compared to the observation errors.

2(d) Optimal interpolation and physical space analysis systems

Optimal interpolation

If the observation operator is linear ($\mathbf{h}(\mathbf{x}) = \mathbf{H}\mathbf{x}$), and the reference state is taken as the background, $\mathbf{x}^{\mathrm{ref}} = \mathbf{x}_{\mathrm{B}}$ then the state that minimizes the 3D-VAR cost function is given by the optimal interpolation (OI) or best linear unbiased estimator (BLUE) formula:

$$\mathbf{x}_{\mathrm{A}} = \mathbf{x}_{\mathrm{B}} + \mathbf{B}\mathbf{H}^{\mathrm{T}}(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}})^{-1}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}},$$

where $\mathbf{d}_{\mathrm{b}}^{\mathrm{o}} = \mathbf{y} - \mathbf{h}(\mathbf{x}_{\mathrm{B}})$ is called the innovation vector. Using this explicit form for the analysis is less efficient than running a 3D-VAR procedure, but it is useful for two reasons:

1. As it is equivalent to VAR (for linear $\mathbf{h}$), it is a useful formula for understanding the way that VAR works.
2. It has a very similar form to the analysis step in the Kalman Filter, and is a starting point for derivations of the ensemble Kalman Filter equations.

Note that the OI formula can be written in a way that is equivalent to 4D-VAR too.

Physical space analysis system

A physical space analysis system is a variational method that is equivalent to evaluating the OI equation/running 3D-VAR, but is more efficient when $p \ll n$. Instead of minimizing a cost function with respect to the n-dimensional 3D-VAR control vector $\mathbf{x}$ (or $\delta\mathbf{x}$ in the incremental formulation), PSAS minimizes an alternative cost function with respect to a new p-dimensional control vector that we shall call $\mathbf{w}$. Start with the OI formula:

1. Calculate the innovation, $\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}$.
2. Calculate $\mathbf{w}^* = (\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}})^{-1}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}$ (see below for how to do this efficiently).
3. Act with $\mathbf{B}\mathbf{H}^{\mathrm{T}}$ and add to $\mathbf{x}_{\mathrm{B}}$

$$\mathbf{x}_{\mathrm{A}} = \mathbf{x}_{\mathrm{B}} + \mathbf{B}\mathbf{H}^{\mathrm{T}}\mathbf{w}^*.$$

A difficult part is in step 2 as it requires the inverse of a $p \times p$ matrix (even though $p \ll n$, p can still be large). This matrix inversion can be avoided by solving the following new variational problem with respect to $\mathbf{w}$:

$$J[\mathbf{w}] = \frac{1}{2}\mathbf{w}^{\mathrm{T}}(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}})\mathbf{w} - \mathbf{w}^{\mathrm{T}}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}.$$

The minimum of this cost function is the special value of $\mathbf{w} = \mathbf{w}^*$ as in step 2.

3. A-priori information and the B-matrix

3(a) The null space of the observation operator and the importance of a-priori information

Recall that the state vector and the observations are related via the observation operator (forward problem):

$$\begin{aligned} \mathbf{y} &= \mathbf{h}(\mathbf{x}^{\mathrm{t}}) + \boldsymbol{\epsilon}, \\ &= \mathbf{H}\mathbf{x}^{\mathrm{t}} + \boldsymbol{\epsilon} \qquad \text{if the obs. operator is linear,} \end{aligned}$$

$$\mathbf{y}, \boldsymbol{\epsilon} \in \mathbb{R}^p \quad \mathbf{h}, \mathbf{H} : \mathbb{R}^n \to \mathbb{R}^p,$$

and assume (unbiased) Gaussian statistics:

$$\langle \boldsymbol{\epsilon} \rangle = 0, \qquad \left\langle \boldsymbol{\epsilon}\boldsymbol{\epsilon}^{\mathrm{T}} \right\rangle = \mathbf{R}.$$

The PDF for $\boldsymbol{\epsilon}$ given $\mathbf{x}$ is the truth is the Gaussian:

$$\begin{aligned} P_\epsilon(\boldsymbol{\epsilon}|\mathbf{x}) &= \frac{1}{(2\pi)^{p/2}|\mathbf{R}|^{1/2}} \exp -\frac{1}{2}\boldsymbol{\epsilon}^{\mathrm{T}}\mathbf{R}^{-1}\boldsymbol{\epsilon} \\ &= C \exp -\frac{1}{2}\left(\mathbf{y} - \mathbf{H}\mathbf{x}\right)^{\mathrm{T}} \mathbf{R}^{-1} \left(\mathbf{y} - \mathbf{H}\mathbf{x}\right) = P_{\mathbf{y}}(\mathbf{y}|\mathbf{x}), \\ C &= \frac{1}{(2\pi)^{p/2}|\mathbf{R}|^{1/2}}. \end{aligned}$$

In the inverse problem, we treat $\mathbf{x}$ as the variable instead of ϵ or $\mathbf{y}$ and define the likelihood function, $L(\mathbf{x}|\mathbf{y}) = P_{\mathbf{y}}(\mathbf{y}|\mathbf{x})$. Note that the cost function is defined as $J_{\mathrm{O}}(\mathbf{x}) = -\ln L(\mathbf{x}|\mathbf{y})$. The *maximum likelihood* solution is equivalent to the *minimum variance* solution given by:

$$\mathbf{x}_{\mathrm{ML/MV}} = \left(\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\right)^{-1}\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{y}.$$

(PROBLEMS 6 & 7 TO FIND THE FOLLOWING RESULT BY USING EACH METHOD) If $p < n$ (or, more strictly, if $\mathrm{rank}(\mathbf{H}) < n$) then the inverse problem of estimating $\mathbf{x}$ from $\mathbf{y}$ is ill-posed. How can we show this? Do an eigenvalue decomposition of the operator that is inverted, $\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}$:

$$\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^{\mathrm{T}},$$

$\mathbf{V}$ is the orthogonal matrix of eigenvectors, $\mathbf{V}^{\mathrm{T}}\mathbf{V} = \mathbf{I}$, and Λ is the diagonal matrix of eigenvalues. The rank of $\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}$ is the number of non-zero eigenvalues. Inverting both sides and using the orthogonal property of $\mathbf{V}$ ($\mathbf{V}^{\mathrm{T}} = \mathbf{V}^{-1}$):

$$\left(\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\right)^{-1} = \mathbf{V}\mathbf{\Lambda}^{-1}\mathbf{V}^{\mathrm{T}}.$$

Say the rank of $\mathbf{V}\mathbf{\Lambda}\mathbf{V}^{\mathrm{T}}$ is $q(< n)$, then

$$\mathbf{\Lambda} = \begin{pmatrix} \lambda_1 & & & & & & \\ & \lambda_2 & & & & & \\ & & \ddots & & & & \\ & & & \lambda_q & & & \\ & & & & 0 & & \\ & & & & & 0 & \\ & & & & & & \ddots \end{pmatrix}, \qquad \mathbf{\Lambda}^{-1} = \begin{pmatrix} \lambda_1^{-1} & & & & & & \\ & \lambda_2^{-1} & & & & & \\ & & \ddots & & & & \\ & & & \lambda_q^{-1} & & & \\ & & & & \infty & & \\ & & & & & \infty & \\ & & & & & & \ddots \end{pmatrix}.$$

The solution has a meaning only within the subspace (space of eigenvectors) defined by the non-zero eigenvalues. The space spanned by the eigenvectors with zero eigenvalue is called the *null space*. This is how the rank deficiency issue manifests itself in the data assimilation problem. In real problems, usually $p < n$ and so this is an issue in operational data assimilation.

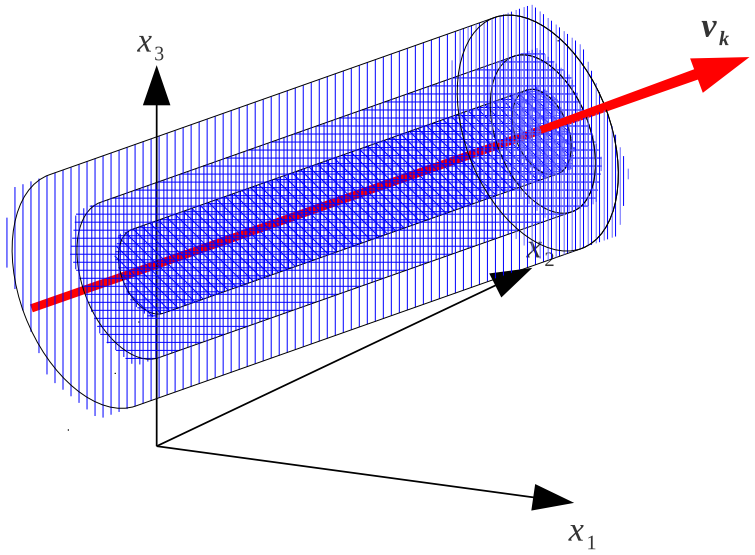
The MAP/MV analysis is not unique when there is a null space. Let $\mathbf{x}^{(1)}$ be one solution of the inverse problem. Let us take the Taylor expansion of $J_{\mathrm{O}}(\mathbf{x})$:

$$\begin{aligned} J_{\mathrm{O}}(\mathbf{x}^{(1)} + \delta\mathbf{x}) &= J_{\mathrm{O}}(\mathbf{x}^{(1)}) + \frac{\partial J_{\mathrm{O}}}{\partial \mathbf{x}}\delta\mathbf{x} + \frac{1}{2}\delta\mathbf{x}^{\mathrm{T}}\frac{\partial^2 J_{\mathrm{O}}}{\partial \mathbf{x}^2}\delta\mathbf{x}, \\ &= J_{\mathrm{O}}(\mathbf{x}^{(1)}) + 0 + \frac{1}{2}\delta\mathbf{x}^{\mathrm{T}}\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\delta\mathbf{x}. \end{aligned}$$

(At the minimum of J_{O}, the gradient $\partial J_{\mathrm{O}}/\partial\mathbf{x} = 0$. The Hessian $\partial^2 J_{\mathrm{O}}/\partial\mathbf{x}^2 = \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}$.) $\delta\mathbf{x}$ represents a departure from $\mathbf{x}^{(1)}$. Let this be in the direction $\mathbf{v}_k$, which is the kth eigenvector of $\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}$, where $k > q$ (i.e. is within the null space so $\lambda_k = 0$). Then

$$J_{\mathrm{O}}(\mathbf{x}^{(1)} + \alpha\mathbf{v}_k) = J_{\mathrm{O}}(\mathbf{x}^{(1)}) + 0 + \frac{\alpha^2}{2}\mathbf{v}_k^{\mathrm{T}}\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\mathbf{v}_k = J_{\mathrm{O}}(\mathbf{x}^{(1)}) + 0 + 0,$$

i.e. the state $\mathbf{x}^{(1)} + \alpha\mathbf{v}_k$ has exactly the same cost (and likelihood) as $\mathbf{x}^{(1)}$ (is equally likely).



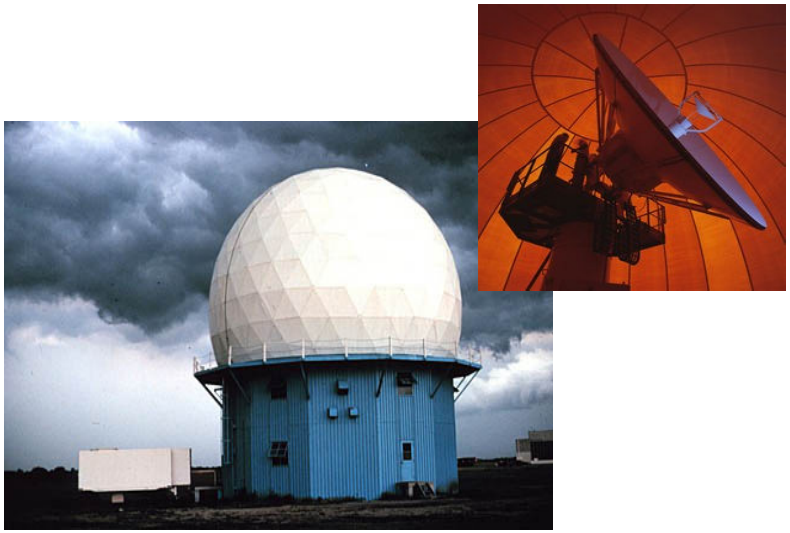
Physical example of an observation operator and null space

Let

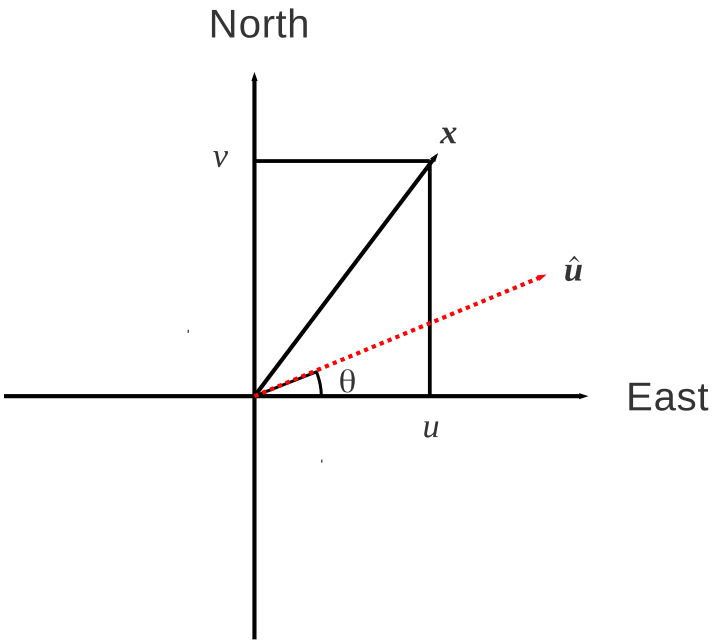
$$\mathbf{x} = \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} \text{uniform zonal wind } {}^{-}_{+} \\ \text{uniform meridional wind } {}^{+}_{-} \end{pmatrix},$$

$$\mathbf{y} = \text{measurement of wind component in a direction } \theta \text{ from E},$$

$$\sigma^2_{\mathbf{y}} = \text{Error variance of measurement.}$$



This measurement is given e.g. by a Doppler radar instrument.



$\hat{\mathbf{u}}$ is the unit vector in the line of sight of the radar beam,

$$\hat{\mathbf{u}} = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}.$$

The model observation is therefore the projection of the wind, $\mathbf{x}$ along $\hat{\mathbf{u}}$:

$$\mathbf{H} = \begin{pmatrix} \cos\theta & \sin\theta \end{pmatrix}, \qquad \mathbf{R} = \sigma_{\mathbf{y}}^2,$$

$$\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H} = \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \sigma_{\mathbf{y}}^{-2} \begin{pmatrix} \cos\theta & \sin\theta \end{pmatrix} = \sigma_{\mathbf{y}}^{-2} \begin{pmatrix} \cos^2\theta & \cos\theta\sin\theta \\ \cos\theta\sin\theta & \sin^2\theta \end{pmatrix}.$$

The eigenvalue and eigenvector matrices of this are:

$$\mathbf{\Lambda} = \begin{pmatrix} \sigma_{\mathbf{y}}^{-2} & 0 \\ 0 & 0 \end{pmatrix}, \qquad \mathbf{V} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}.$$

The first eigenvalue This eigenvalue, $\lambda_1 = \sigma_{\mathbf{y}}^{-2}$ and eigenvector $\mathbf{v}_1 = \begin{pmatrix} \cos\theta & \sin\theta \end{pmatrix}^{\mathrm{T}}$. This is the direction being observed.

The second eigenvalue This eigenvalue, $\lambda_2 = 0$ and eigenvector $\mathbf{v}_2 = \begin{pmatrix} -\sin\theta & \cos\theta \end{pmatrix}^{\mathrm{T}}$. This is the null space of the observing system. It is perpendicular to the direction being observed. Replacing $\mathbf{x} \rightarrow \mathbf{x} + \alpha\mathbf{v}_2$ does not affect $\mathbf{Hx}$. (PROBLEM 8 IS ANOTHER EXAMPLE OF A FORWARD MODEL)

A-priori information The use of a-priori information eliminates the null space. Instead of dealing with $L(\mathbf{x}|\mathbf{y})$, we define $P_{\mathbf{x}}(\mathbf{x}|\mathbf{y})$ and deal with that. $P_{\mathbf{x}}(\mathbf{x}|\mathbf{y})$ (the posterior distribution) is found via Bayes' theorem:

$$P_{\mathbf{x}}(\mathbf{x}|\mathbf{y}) = \frac{P_{\mathbf{x}}(\mathbf{x})P_{\mathbf{y}}(\mathbf{y}|\mathbf{x})}{P_{\mathbf{y}}(\mathbf{y})}.$$

(Again the cost function is defined as $-\ln P_{\mathbf{x}}(\mathbf{x}|\mathbf{y})$. Assuming that $P_{\mathbf{x}}(\mathbf{x})$ (the prior distribution) obeys Gaussian statistics (mean $\mathbf{x}_{\mathrm{B}}$ and covariance $\mathbf{P}^{\mathrm{f}}$) this has a maximum at $\mathbf{x} = \mathbf{x}_{\mathrm{A}}$:

$$\begin{aligned}
\mathbf{x}_{\mathrm{A}} &= \mathbf{x}_{\mathrm{B}} + \mathbf{P}^{\mathrm{f}}\mathbf{H}^{\mathrm{T}}\left(\mathbf{R} + \mathbf{H}\mathbf{P}^{\mathrm{f}}\mathbf{H}^{\mathrm{T}}\right)^{-1}(\mathbf{y} - \mathbf{h}(\mathbf{x}_{\mathrm{B}})), \\
&= \mathbf{x}_{\mathrm{B}} + \left(\mathbf{P}^{\mathrm{f}-1} + \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\right)^{-1}\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{y} - \mathbf{h}(\mathbf{x}_{\mathrm{B}})),
\end{aligned}$$

by the Shermann-Morrison-Woodbury formula. The important matrix is now $\mathbf{P}^{\mathrm{f}-1} + \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}$ instead of $\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}$. A-priori information fills data voids, and it also regularizes the problem in the way described here (like Tikhonov regularization).

3(b) The role of the background error covariance matrix

We saw in Sec. 2(b) that error covariance matrices weight the information according to the uncertainty of the data via the variances, σ^2_{B}. Covariance matrices also have a non-local effect due to correlations between errors at different positions and different variables (PROBLEM 9 EXPLORES THE RELATIONSHIP BETWEEN COVARIANCE AND CORRELATION). Background error covariances are special because the background state fills the model space. Here are some other effects of the background error covariance matrix.

- $\mathbf{P}^{\mathrm{f}}$ allows the analysis increments to be smooth and balanced.

$$\begin{aligned}
\delta\mathbf{x}_{\mathrm{A}} &= \mathbf{P}^{\mathrm{f}}\mathbf{H}^{\mathrm{T}}\left(\mathbf{R} + \mathbf{H}\mathbf{P}^{\mathrm{f}}\mathbf{H}^{\mathrm{T}}\right)^{-1}(\mathbf{y} - \mathbf{h}(\mathbf{x}_{\mathrm{B}})), \\
&= \mathbf{P}^{\mathrm{f}}\mathbf{v}, \qquad \text{where } \mathbf{v} = \mathbf{H}^{\mathrm{T}}\left(\mathbf{R} + \mathbf{H}\mathbf{P}^{\mathrm{f}}\mathbf{H}^{\mathrm{T}}\right)^{-1}(\mathbf{y} - \mathbf{h}(\mathbf{x}_{\mathrm{B}})), \\
&= \sum_{i=1}^{n} \mathbf{p}_i v_i.
\end{aligned}$$

  Here $\mathbf{p}_i$ is the ith column of $\mathbf{P}^{\mathrm{f}}$ and v_i is the ith component of $\mathbf{v}$ (SEE PROBLEM 10 TO SHOW THIS). The $\mathbf{p}_i$ can be interpreted as states (i.e. fields) and are called structure functions. This says that the analysis is a linear combination

of structure functions. Structure functions tend to be smooth and (if they are realistic) close to a state of balance (see Sec. 3d). THIS IS THE PATTERN OF THE ANALYSIS INCREMENT AFTER ASSIMILATION OF A SINGLE PRESSURE OBSERVATION. THE EFFECT OF THE PRESSURE OBSERVATION IS NON-LOCAL AND MULTIVARIATE. SEE PROBLEM 11.

- The analysis increments lie in the space spanned by $\mathbf{P}^{\mathrm{f}}$.
  The spaced spanned by $\mathbf{P}^{\mathrm{f}}$ is the space occupied by the sample of error states used to define $\mathbf{P}^{\mathrm{f}}$:

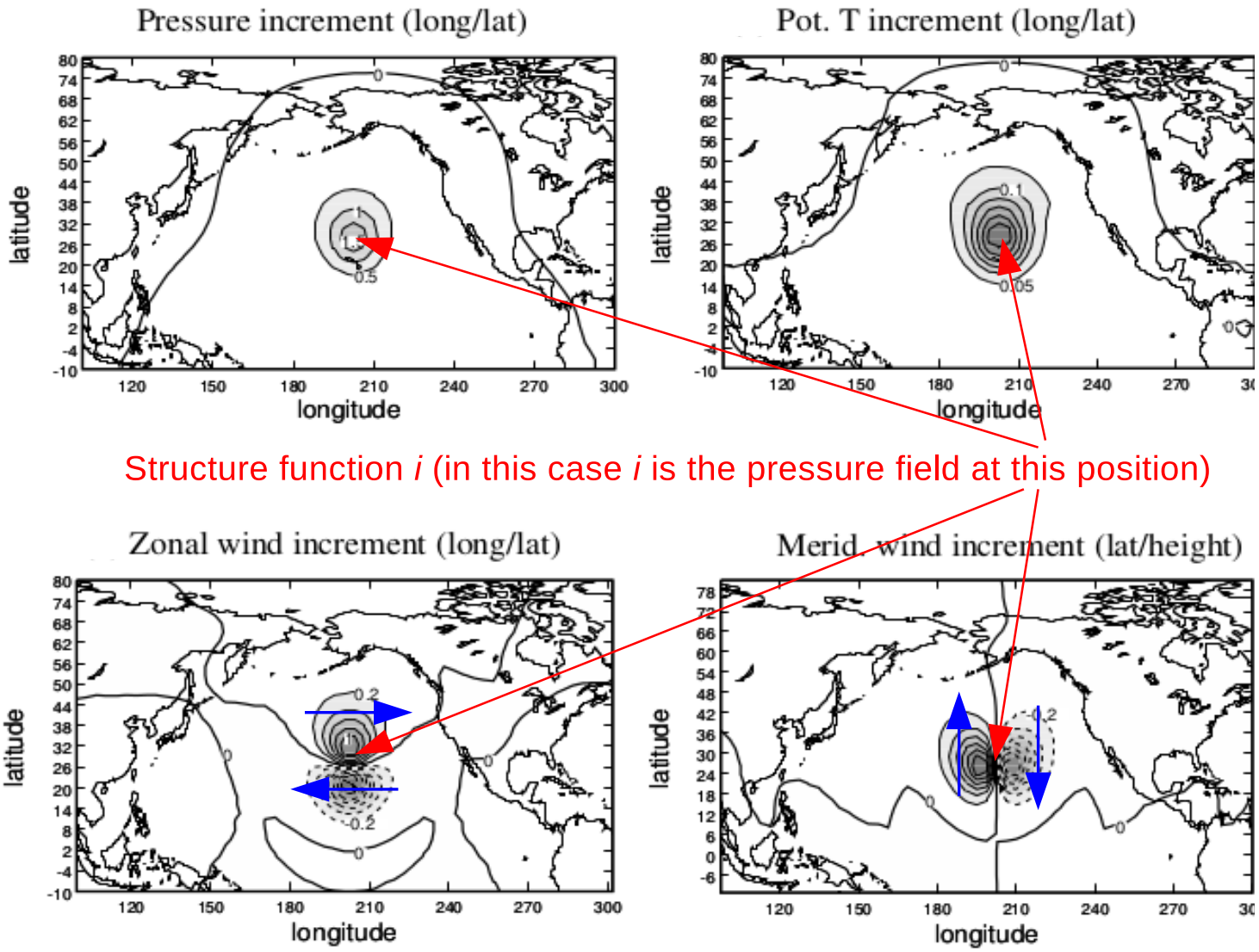
$$
\begin{aligned}
\mathbf{P}^{\mathrm{f}} &= \left\langle (\mathbf{x}_{\mathrm{B}} - \mathbf{x}^{\mathrm{t}})(\mathbf{x}_{\mathrm{B}} - \mathbf{x}^{\mathrm{t}})^{\mathrm{T}} \right\rangle, \\
&= \left\langle \boldsymbol{\eta}_{\mathrm{B}} \boldsymbol{\eta}_{\mathrm{B}}^{\mathrm{T}} \right\rangle, \\
\approx \mathbf{P}^{\mathrm{f}}_{(N)} &= \frac{1}{N-1} \sum_{i=1}^{N} \boldsymbol{\eta}_{\mathrm{B}}^{(i)} \boldsymbol{\eta}_{\mathrm{B}}^{(i)\mathrm{T}}, \quad \text{where } \boldsymbol{\eta}_{\mathrm{B}}^{(i)} \text{ is the } i\text{th error sample}, \\
&= \frac{1}{N-1} \mathbf{X}\mathbf{X}^{\mathrm{T}}, \quad \text{where } \mathbf{X} \in \mathbb{R}^{n \times N} \text{ and the } i\text{th column of } \mathbf{X} \text{ is } \boldsymbol{\eta}_{\mathrm{B}}^{(i)}, \ (*) \\
\therefore \delta\mathbf{x}_{\mathrm{A}} &= \mathbf{P}^{\mathrm{f}}_{(N)} \mathbf{v}, \\
&= \frac{1}{N-1} \sum_{i=1}^{N} \boldsymbol{\eta}_{\mathrm{B}}^{(i)} \boldsymbol{\eta}_{\mathrm{B}}^{(i)\mathrm{T}} \mathbf{v} = \frac{1}{N-1} \sum_{i=1}^{N} \left(\boldsymbol{\eta}_{\mathrm{B}}^{(i)\mathrm{T}} \mathbf{v} \right) \boldsymbol{\eta}_{\mathrm{B}}^{(i)},
\end{aligned}
$$

  which is a linear combination of the sample states used to determine $\mathbf{P}^{\mathrm{f}}$. Thus the analysis increments cannot lie outside of the sample space (this is especially a problem with the ensemble Kalman filter). This highlights the need for a good quality and large sample set (ideally $N \gtrsim n$, although not practical). (*) THIS NOTATION IS INTRODUCED HERE AS IT WILL BE USEFUL LATER - SEE PROBLEM 12 TO SHOW THIS.

In practical situations, the background error covariance matrix is too large to invert, or even to store, so we need to have efficient ways of modelling its effect. Some notes:

- We normally deal with a static version of the background error covariance matrix, i.e. $\mathbf{P}^{\mathrm{f}} \rightarrow \mathbf{B}$.
- There are spatial aspects of the background error covariance matrix (how does background error at one position correlate to background error at another position?).

- There are multivariate aspects of the background error covariance matrix (how does background error in one variable correlate to background error in another?).
- We can see both of these aspects in the last Fig.



3(c) Spatial aspects (inverse Laplacians, diffusion operators)

Inverse Laplacians

Consider the following form of a $\mathbf{B}$-matrix for a single field (univariate):

$$\begin{aligned} \mathbf{B} &= \sigma_{\mathrm{B}}^2\gamma\left(1+\frac{l^4}{2}(\nabla^2)^2\right)^{-1}, \\ \therefore \mathbf{B}^{-1} &= \sigma_{\mathrm{B}}^{-2}\gamma^{-1}\left(1+\frac{l^4}{2}(\nabla^2)^2\right), \end{aligned}$$

(where l is the (chosen) correlation length-scale and γ is a scalar to ensure that $\mathbf{B}$ has the right magnitude). To help understand this covariance model, what is the result of acting with $\mathbf{B}$ on an arbitrary function $f(x)$ in 1-D?

$$\text{Let } g(x) = \mathbf{B}\{f(x)\} = \sigma_{\mathrm{B}}^2\gamma\left(1+\frac{l^4}{2}\frac{d^4}{dx^4}\right)^{-1} f(x).$$

This can be easily solved in Fourier space:

$$f(x) = \frac{1}{\sqrt{2\pi}}\int dk\ \bar{f}(k)e^{ikx} \qquad g(x) = \frac{1}{\sqrt{2\pi}}\int dk\ \bar{g}(k)e^{ikx},$$

$$\begin{aligned} f(x) &= \sigma_{\mathrm{B}}^{-2}\gamma^{-1}\left(1+\frac{l^4}{2}\frac{d^4}{dx^4}\right) g(x), \\ \int dk\ \bar{f}(k)e^{ikx} &= \sigma_{\mathrm{B}}^{-2}\gamma^{-1}\left(1+\frac{l^4}{2}\frac{d^4}{dx^4}\right)\int dk\ \bar{g}(k)e^{ikx}, \\ &= \int dk\ \sigma_{\mathrm{B}}^{-2}\gamma^{-1}\left(1+\frac{l^4k^4}{2}\right)e^{ikx}\bar{g}(k). \end{aligned}$$

Multiply each side by $e^{-ik'x}$, integrate over x, and use orthogonality of complex exponentials:

$$\begin{aligned} \bar{f}(k) &= \bar{g}(k)\sigma_{\mathrm{B}}^{-2}\gamma^{-1}\left(1+\frac{l^4k^4}{2}\right), \\ \text{or } \bar{g}(k) &= \sigma_{\mathrm{B}}^2\gamma\left(1+\frac{l^4k^4}{2}\right)^{-1}\bar{f}(k). \end{aligned}$$

The Fourier transformed equations are easy to invert because the derivatives disappear in Fourier space. Inverse Fourier transform this to get the result in x-space:

$$\begin{aligned} g(x) &= \text{I.F.T.}\left\{\sigma_{\mathrm{B}}^2\gamma\left(1+\frac{l^4k^4}{2}\right)^{-1}\bar{f}(k)\right\}, \\ &= \text{I.F.T.}\left\{\bar{c}(k)\bar{f}(k)\right\}, \\ &= \frac{1}{2\pi}\int dx'\ c(x-x')f(x'), \end{aligned}$$

by the convolution theorem of Fourier transforms. $c(x)$ is the inverse Fourier transform of $\sigma_{\mathrm{B}}^2\gamma/(1+l^4k^4/2)$. [$\gamma$ would be chosen such that $c(0) = 2\pi\sigma_{\mathrm{B}}^2$.]

Note: Doing a convolution is the continuous space analogue of acting with a covariance matrix which has all rows the same but shifted (i.e. homogeneous structure functions - a symmetric Toepliz matrix). The convolution in discrete space is:

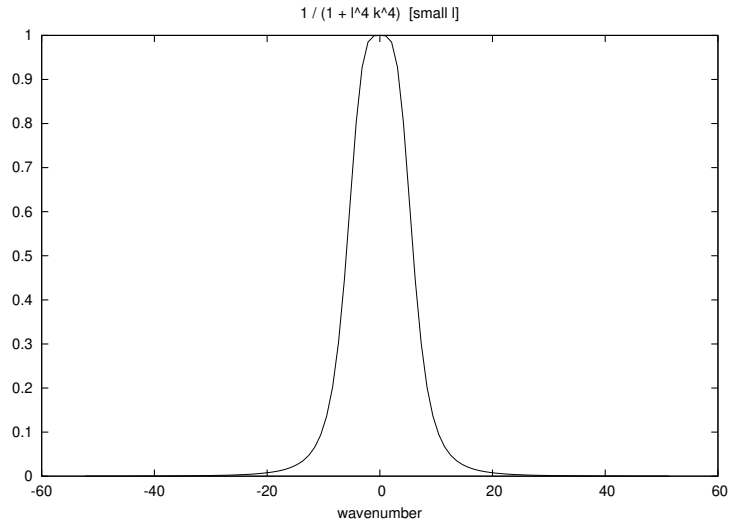
$$
\begin{aligned}
g_i &= \sum_j C_{ij} f_j, \text{ where } C_{ij} = c_{|i-j|}, \\
\mathbf{g} &= \mathbf{C}\mathbf{f}, \\
\begin{pmatrix} g_1 \\ g_2 \\ g_3 \\ g_4 \\ \vdots \\ g_n \end{pmatrix} &= \begin{pmatrix} c_0 & c_1 & c_2 & c_3 & \cdots & c_{n-1} \\ c_1 & c_0 & c_1 & c_2 & \cdots & c_{n-2} \\ c_2 & c_1 & c_0 & c_1 & \cdots & c_{n-3} \\ c_3 & c_2 & c_1 & c_0 & \cdots & c_{n-4} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ c_{n-1} & c_{n-2} & c_{n-3} & c_{n-4} & \cdots & c_0 \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ \vdots \\ f_n \end{pmatrix}.
\end{aligned}
$$

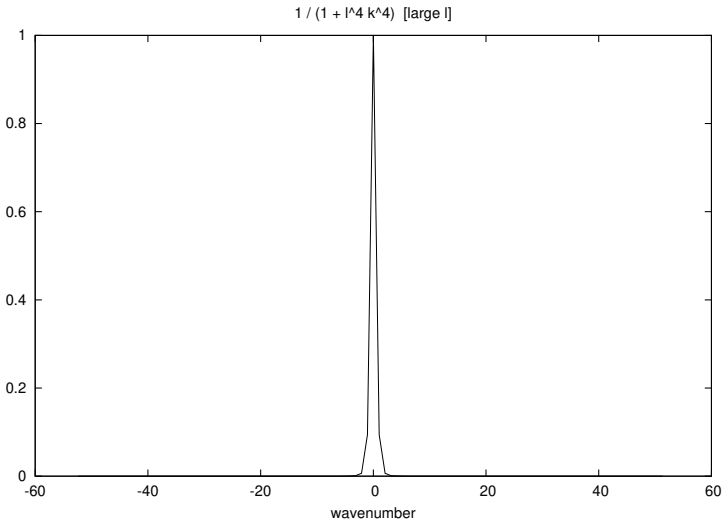
Summary of inverse Laplacians: The differential operator $\mathbf{B}^{-1} = \sigma_{\mathrm{B}}^{-2}\gamma^{-1}\left(1 + l^4(\nabla^2)^2/2\right)$ (as it appears in the cost function) can be relatively easily evaluated. The structure functions (rows or columns of $\mathbf{B}$) implied by this covariance model are revealed by doing a Fourier analysis and are found to be equal to the inverse Fourier transform of $\sigma_{\mathrm{B}}^2\gamma(1 + l^4k^4/2)^{-1}$. The Fig. shows this function in spectral and real spaces for when l is small and l is large. In practice the value of l is chosen to be realistic for the assimilation variable in question.

SMALL LENGTHSCALE

LARGE LENGTHSCALE

SPECTRAL SPACE

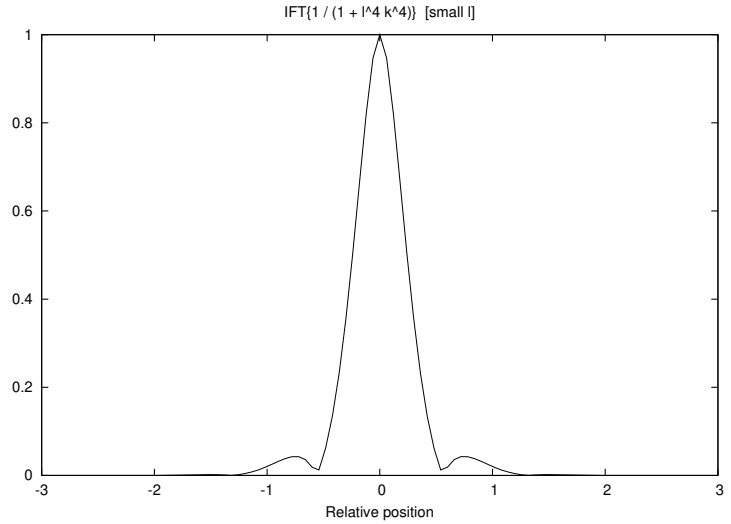


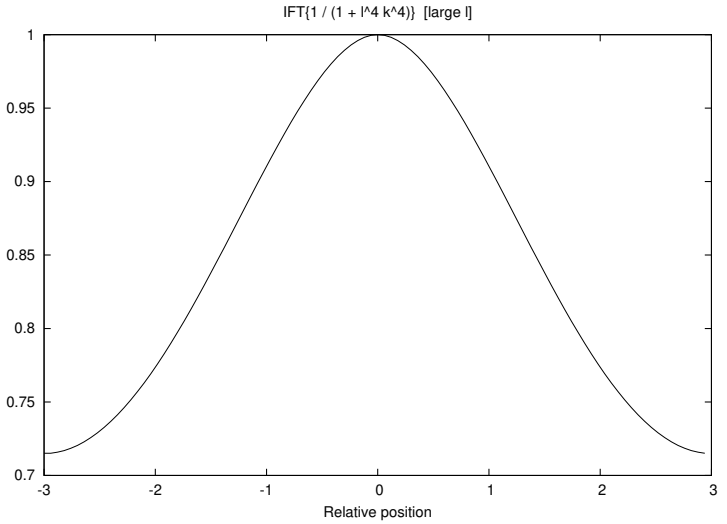


Filter away very large wavenumbers only
(keep all but smallest scales)

Filter away all except very small wavenumbers
(keep large−scales)

REAL SPACE





Diffusion operators

Consider the following diffusion equation for integration from $t = 0$ to T:

$$\frac{\partial g(x,t)}{\partial t} - \kappa \frac{\partial^2 g(x,t)}{\partial x^2} = 0,$$

κ : diffusion co-efficient, initial condition $g(x,0) = f(x)$.

The diffusion equation can be integrated analytically in Fourier space. For wavenumber k:

$$\frac{\partial \bar{g}(k,t)}{\partial t} + \kappa k^2 \bar{g}(k,t), \qquad \bar{g}(k,0) = \bar{f}(k).$$

Integrate from $t = 0$ to T:

$$\begin{aligned} \int_{t=0}^{T} d \ln \bar{g}(k,t) + \kappa k^2 \int_{t=0}^{T} dt &= 0, \\ \ln \bar{g}(k,T) - \ln \bar{g}(k,0) + \kappa k^2 T &= 0, \\ \bar{g}(k,T) = \bar{f}(k) \exp(-\kappa k^2 T). & \end{aligned}$$

To find the solution in real space, inverse Fourier transform the above. The right hand side is a product of functions in Fourier space, so use the convolution theorem again:

$$g(x,T) = \frac{1}{2\pi} \int dx' \, f(x') \, c(x - x').$$

$c(x)$ is here the inverse Fourier transform of $\exp(-\kappa k^2 T)$, which is $\sqrt{\pi/\kappa T} \exp(-x^2/4\kappa T)$ (a Gaussian function with length-scale $\sqrt{2\kappa T}$). The solution is thus:

$$g(x,T) = \frac{1}{\sqrt{4\pi\kappa T}} \int dx' \, f(x') \exp(-(x - x')^2/4\kappa T).$$

Note the correspondence between the convolution and action with a homogeneous covariance matrix (as in the previous section on inverse Laplacians), which means that the structure functions have the form:

$$\frac{1}{\sqrt{4\pi\kappa T}} \exp(-(x - x')^2/4\kappa T).$$

Summary of diffusion operators: Integrating the diffusion equation from initial condition $f(x)$ at $t = 0$ to time T is equivalent to acting with a covariance operator ($\mathbf{B}$) on $f(x)$ which has structure functions - e.g. when the the standard deviation field, σ, is constant - equal to $\sigma^2/\sqrt{4\pi\kappa T} \exp(-x^2/4\kappa T)$. The inverse B-matrix that appears in the cost function can be dealt with by integrating the diffusion equation backwards in time.

Summary: If we are willing to assume a particular spatial structure of the covariances then we can use various methods to simulate the effect of the background error covariance matrix without the need to store an explicit matrix. There are other methods in addition to those mentioned, e.g. recursive filters.

3(d) Multivariate aspects and balance

We have already seen an example of a multivariate aspect of the background error covariance matrix (see Fig. of the structure functions). How can we model this without resort to an explicit matrix?

The horizontal momentum equations are as follows:

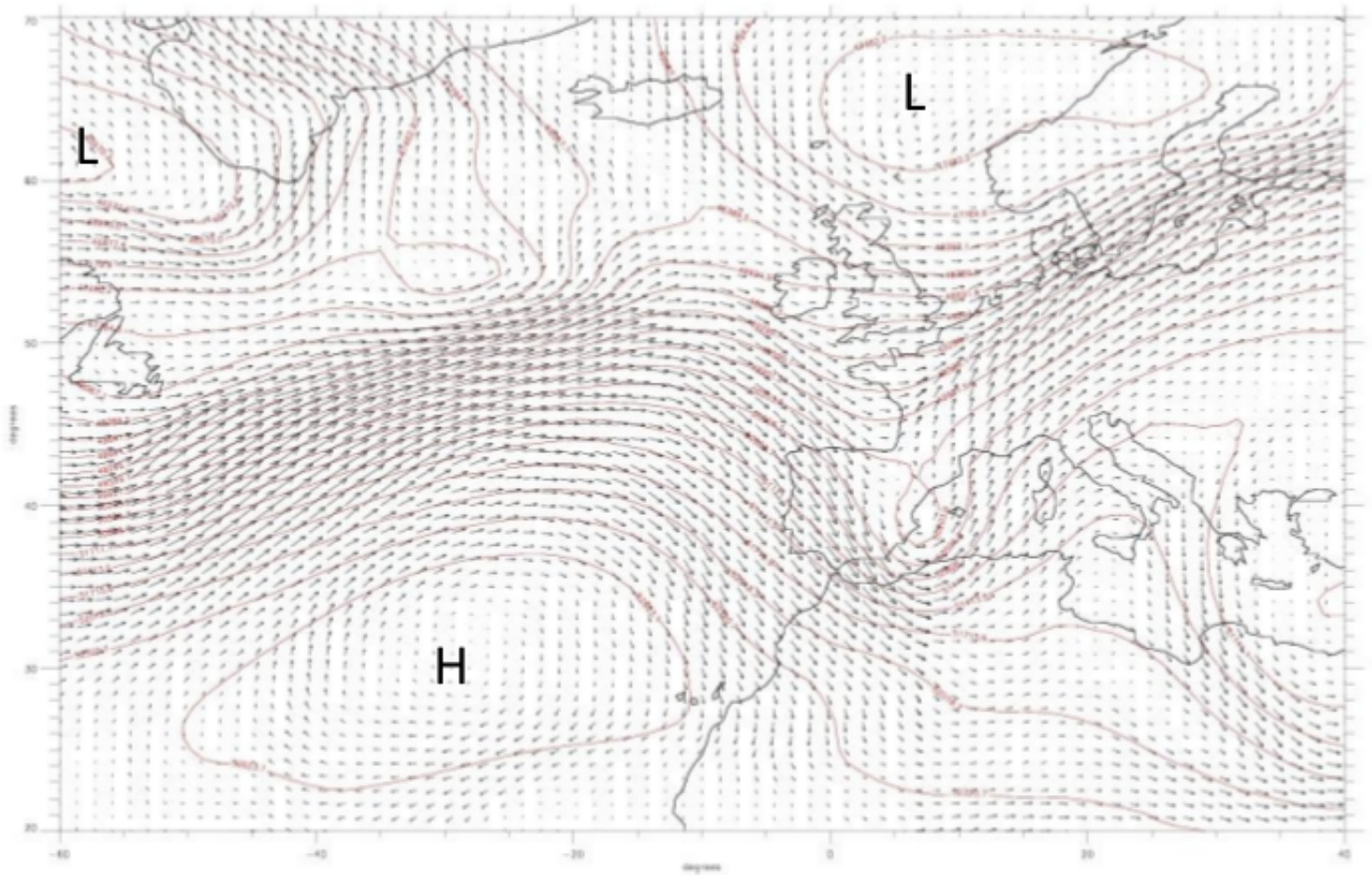
$$\frac{\partial u}{\partial t} + \mathbf{u} \cdot \nabla u = fv - \frac{1}{\rho}\frac{\partial p}{\partial x}, \quad \frac{\partial v}{\partial t} + \mathbf{u} \cdot \nabla v = -fu - \frac{1}{\rho}\frac{\partial p}{\partial y}, \quad \mathbf{u} = \begin{pmatrix} u \\ v \end{pmatrix}.$$

Example with perfect geostrophic balance

For flows with small Rossby number, $\mathrm{Ro} = U/fL \ll 1$, the momentum equations approximate to the following diagnostic equations:

$$v = \frac{1}{f\rho}\frac{\partial p}{\partial x}, \quad u = -\frac{1}{f\rho}\frac{\partial p}{\partial y},$$

(this is geostrophic balance).



Assume:

- Geostrophic balance (in incremental form):

$$\delta v = \frac{1}{f\rho}\frac{\partial \delta p}{\partial x} = \mathbf{G}_v \delta p, \qquad \delta u = -\frac{1}{f\rho}\frac{\partial \delta p}{\partial y} = \mathbf{G}_u \delta p.$$

- Pressure-pressure correlations are homogeneous, isotropic and have correlation length-scale $\sqrt{2}L$. The pressure-pressure correlations between positions i (x_i, y_i) and j (x_j, y_j) are:

$$\mu_{ij} = \exp -\frac{r_{ij}^2}{2L^2}, \qquad r_{ij}^2 = (x_i - x_j)^2 + (y_i - y_j)^2.$$

- Standard deviation of pressure errors: σ_p (constant).
- Constant density, ρ.

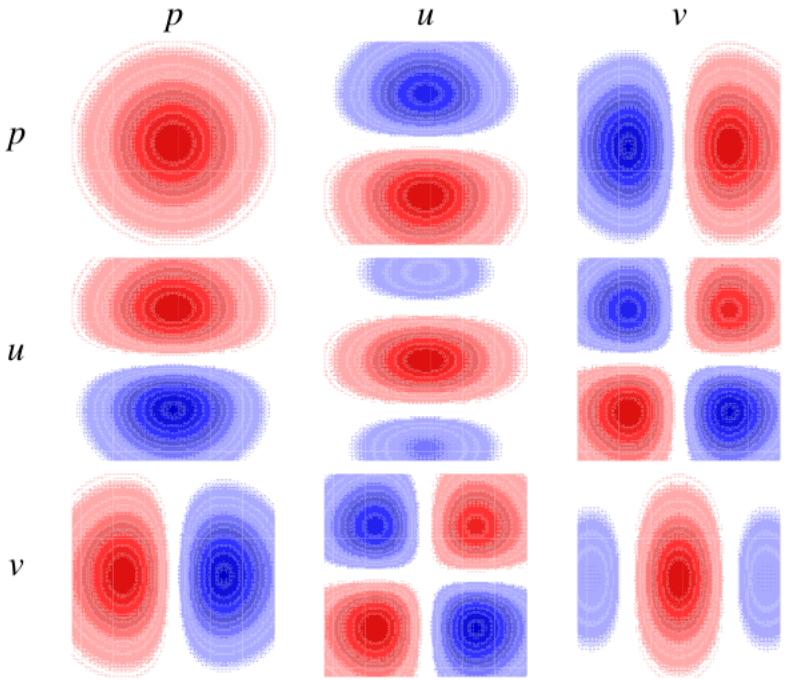
Now derive the multivariate error covariances between positions i and j:

$$
\begin{aligned}
p-p \text{ covs: } \langle \delta p_i \delta p_j \rangle &= \sigma_p^2 \mu_{ij} \text{ (by definition)}, \\
p-u \text{ covs: } \langle \delta p_i \delta u_j \rangle &= -\frac{1}{f\rho} \left\langle \delta p_i \frac{\partial \delta p_j}{\partial y_j} \right\rangle = -\frac{1}{f\rho} \frac{\partial}{\partial y_j} \langle \delta p_i \delta p_j \rangle = -\frac{\sigma_p^2}{f\rho} \frac{\partial \mu_{ij}}{\partial y_j}, \\
p-v \text{ covs: } \langle \delta p_i \delta v_j \rangle &= \frac{1}{f\rho} \left\langle \delta p_i \frac{\partial \delta p_j}{\partial x_j} \right\rangle = \frac{1}{f\rho} \frac{\partial}{\partial x_j} \langle \delta p_i \delta p_j \rangle = \frac{\sigma_p^2}{f\rho} \frac{\partial \mu_{ij}}{\partial x_j}, \\
u-p \text{ covs: } \langle \delta u_i \delta p_j \rangle &= -\frac{1}{f\rho} \left\langle \frac{\partial \delta p_i}{\partial y_i} \delta p_j \right\rangle = -\frac{1}{f\rho} \frac{\partial}{\partial y_i} \langle \delta p_i \delta p_j \rangle = -\frac{\sigma_p^2}{f\rho} \frac{\partial \mu_{ij}}{\partial y_i}, \\
u-u \text{ covs: } \langle \delta u_i \delta u_j \rangle &= \frac{1}{f^2\rho^2} \left\langle \frac{\partial \delta p_i}{\partial y_i} \frac{\partial \delta p_j}{\partial y_j} \right\rangle = \frac{1}{f^2\rho^2} \frac{\partial^2}{\partial y_i \partial y_j} \langle \delta p_i \delta p_j \rangle = \frac{\sigma_p^2}{f^2\rho^2} \frac{\partial^2 \mu_{ij}}{\partial y_i \partial y_j}, \\
u-v \text{ covs: } \langle \delta u_i \delta v_j \rangle &= -\frac{1}{f^2\rho^2} \left\langle \frac{\partial \delta p_i}{\partial y_i} \frac{\partial \delta p_j}{\partial x_j} \right\rangle = -\frac{1}{f^2\rho^2} \frac{\partial^2}{\partial y_i \partial x_j} \langle \delta p_i \delta p_j \rangle = -\frac{\sigma_p^2}{f^2\rho^2} \frac{\partial^2 \mu_{ij}}{\partial y_i \partial x_j}, \\
v-p \text{ covs: } \langle \delta v_i \delta p_j \rangle &= \frac{1}{f\rho} \left\langle \frac{\partial \delta p_i}{\partial x_i} \delta p_j \right\rangle = \frac{1}{f\rho} \frac{\partial}{\partial x_i} \langle \delta p_i \delta p_j \rangle = \frac{\sigma_p^2}{f\rho} \frac{\partial \mu_{ij}}{\partial x_i}, \\
v-u \text{ covs: } \langle \delta v_i \delta u_j \rangle &= -\frac{1}{f^2\rho^2} \left\langle \frac{\partial \delta p_i}{\partial x_i} \frac{\partial \delta p_j}{\partial y_j} \right\rangle = -\frac{1}{f^2\rho^2} \frac{\partial^2}{\partial x_i \partial y_j} \langle \delta p_i \delta p_j \rangle = -\frac{\sigma_p^2}{f^2\rho^2} \frac{\partial^2 \mu_{ij}}{\partial x_i \partial y_j}, \\
v-v \text{ covs: } \langle \delta v_i \delta v_j \rangle &= \frac{1}{f^2\rho^2} \left\langle \frac{\partial \delta p_i}{\partial x_i} \frac{\partial \delta p_j}{\partial x_j} \right\rangle = \frac{1}{f^2\rho^2} \frac{\partial^2}{\partial x_i \partial x_j} \langle \delta p_i \delta p_j \rangle = \frac{\sigma_p^2}{f^2\rho^2} \frac{\partial^2 \mu_{ij}}{\partial x_i \partial x_j}.
\end{aligned}
$$

Note the following first and second derivatives of μ:

$$\begin{aligned}
\frac{\partial \mu_{ij}}{\partial x_i} &= -\mu_{ij}\frac{(x_i - x_j)}{L^2} \\
\frac{\partial \mu_{ij}}{\partial x_j} &= \mu_{ij}\frac{(x_i - x_j)}{L^2}, \\
\frac{\partial \mu_{ij}}{\partial y_i} &= -\mu_{ij}\frac{(y_i - y_j)}{L^2}, \\
\frac{\partial \mu_{ij}}{\partial y_j} &= \mu_{ij}\frac{(y_i - y_j)}{L^2}, \\
\frac{\partial^2 \mu_{ij}}{\partial x_i \partial x_j} &= \frac{\mu_{ij}}{L^2}\left(1 - \frac{(x_i - x_j)^2}{L^2}\right), \\
\frac{\partial^2 \mu_{ij}}{\partial y_i \partial y_j} &= \frac{\mu_{ij}}{L^2}\left(1 - \frac{(y_i - y_j)^2}{L^2}\right), \\
\frac{\partial^2 \mu_{ij}}{\partial y_i \partial x_j} &= -\mu_{ij}\frac{(x_i - x_j)(y_i - y_j)}{L^4}, \\
\frac{\partial^2 \mu_{ij}}{\partial x_i \partial y_j} &= -\mu_{ij}\frac{(x_i - x_j)(y_i - y_j)}{L^4}.
\end{aligned}$$

Example structure functions giving the output field (p, u or v down the side) associated with a point in the centre of the domain (either of p, u or v along the top). Red is positive, blue is negative.



Summary: If we are willing make some assumptions (e.g. that the flow is geostrophic) then we can use various methods to simulate the effect of the background error covariance matrix without the need to store an explicit matrix. There are other methods in addition to those mentioned, e.g. recursive filters.

3(e) Control variable transforms and the implied B-matrix

The method of *control variable transforms* (CVTs) is a general and powerful means of modelling the background error covariance matrix.

The strong constraint 4D-VAR incremental cost function with the background as the reference state:

$$
\begin{aligned}
J[\delta\mathbf{x}] &= \frac{1}{2}\delta\mathbf{x}^{\mathrm{T}}\mathbf{B}^{-1}\delta\mathbf{x} + \\
&\frac{1}{2}\sum_{t=0}^{T}\left[\delta\mathbf{y}(t) - \mathbf{H}_t\mathbf{M}_{t\leftarrow 0}\delta\mathbf{x}\right]^{\mathrm{T}}\mathbf{R}_t^{-1}\left[\delta\mathbf{y}(t) - \mathbf{H}_t\mathbf{M}_{t\leftarrow 0}\delta\mathbf{x}\right].
\end{aligned}
$$

In this form all variables will inevitably have correlated background errors (the $\mathbf{B}$-matrix is non-diagonal). If we try to minimize this cost function variationally with respect to $\delta\mathbf{x}$, then we have to deal with a prohibitively large $\mathbf{B}$-matrix. Consider the following change of variables:

$$
\begin{aligned}
\delta\mathbf{x} &= \mathbf{U}\delta\boldsymbol{\chi}, \\
\delta\boldsymbol{\chi} &= \mathbf{U}^{-1}\delta\mathbf{x},
\end{aligned}
$$

where $\mathbf{U}$ is the CVT and $\delta\boldsymbol{\chi}$ is new control variable (just a different representation of the increment). The cost function is, in terms of $\delta\boldsymbol{\chi}$:

$$
\begin{aligned}
J[\delta\boldsymbol{\chi}] &= \frac{1}{2}\delta\boldsymbol{\chi}^{\mathrm{T}}\mathbf{U}^{\mathrm{T}}\mathbf{B}^{-1}\mathbf{U}\delta\boldsymbol{\chi} + \\
&\frac{1}{2}\sum_{t=0}^{T}\left[\delta\mathbf{y}(t) - \mathbf{H}_t\mathbf{M}_{t\leftarrow 0}\mathbf{U}\delta\boldsymbol{\chi}\right]^{\mathrm{T}}\mathbf{R}_t^{-1}\left[\delta\mathbf{y}(t) - \mathbf{H}_t\mathbf{M}_{t\leftarrow 0}\mathbf{U}\delta\boldsymbol{\chi}\right].
\end{aligned}
$$

The point of making this transform is to simplify the representation of the background error covariance matrix. Choose $\mathbf{U}$ such that:

$$
\mathbf{U}^{\mathrm{T}}\mathbf{B}^{-1}\mathbf{U} = \mathbf{I}.
$$

What does this mean?

$$
\begin{aligned}
&\text{In model space background error cov matrix is} && \left\langle \delta\boldsymbol{\eta}_{\mathrm{B}}^{\mathbf{x}}\delta\boldsymbol{\eta}_{\mathrm{B}}^{\mathbf{x}^{\mathrm{T}}}\right\rangle = \mathbf{B}, \\
&\text{In control space background error cov matrix is} && \left\langle \delta\boldsymbol{\eta}_{\mathrm{B}}^{\boldsymbol{\chi}}\delta\boldsymbol{\eta}_{\mathrm{B}}^{\boldsymbol{\chi}^{\mathrm{T}}}\right\rangle = \mathbf{I}.
\end{aligned}
$$

These forms imply that $\mathbf{B} = \mathbf{U}\mathbf{U}^{\mathrm{T}}$ ($\mathbf{U}$ is like a 'square-root' of $\mathbf{B}$) (SEE PROBLEM 13 TO SHOW THIS).

Solving a variational problem using CVTs involves the following steps:

- Assume that we know the CVT, $\mathbf{U}$, and its adjoint and that they are practical to apply.
- Minimize $J[\delta\boldsymbol{\chi}]$ with respect to varying $\delta\boldsymbol{\chi}$. The cost function is:

$$J[\delta\boldsymbol{\chi}] = \frac{1}{2}\delta\boldsymbol{\chi}^{\mathrm{T}}\delta\boldsymbol{\chi} + \frac{1}{2}\sum_{t=0}^{T}\left[\delta\mathbf{y}(t) - \mathbf{H}_t\mathbf{M}_{t\leftarrow 0}\mathbf{U}\delta\boldsymbol{\chi}\right]^{\mathrm{T}}\mathbf{R}_t^{-1}\left[\delta\mathbf{y}(t) - \mathbf{H}_t\mathbf{M}_{t\leftarrow 0}\mathbf{U}\delta\boldsymbol{\chi}\right].$$

- The analysis increment in control variable space that minimizes the above is $\delta\boldsymbol{\chi}_{\mathrm{A}}$.
- The analysis in model space is $\mathbf{x}_{\mathrm{A}} = \mathbf{x}_{\mathrm{B}} + \mathbf{U}\delta\boldsymbol{\chi}_{\mathrm{A}}$.
- This is equivalent to minimizing the original cost function $J[\delta\mathbf{x}]$ with the implied background error covariance matrix $\mathbf{B}_{\mathrm{imp}} = \mathbf{U}\mathbf{U}^{\mathrm{T}}$.

A possible form of the CVT is:

$$\mathbf{U} = \mathbf{V}\boldsymbol{\Lambda}^{1/2},$$

where $\mathbf{V}$ is the matrix of eigenvectors (columns of $\mathbf{V}$) of $\mathbf{B}$, and $\boldsymbol{\Lambda}$ is the (diagonal) matrix of eigenvalues, i.e. that $\mathbf{B} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^{\mathrm{T}}$. Check:

$$\mathbf{B}_{\mathrm{imp}} = \mathbf{U}\mathbf{U}^{\mathrm{T}} = \mathbf{V}\boldsymbol{\Lambda}^{1/2}\boldsymbol{\Lambda}^{\mathrm{T}/2}\mathbf{V}^{\mathrm{T}} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^{\mathrm{T}} = \mathbf{B}.$$

Example of the CVT method to model horizontal background error covariances (e.g. for pressure, p)

- Assume that the eigenfunctions are Fourier modes $\sim \exp ikx$ (columns of $\mathbf{V}$). This means that $\mathbf{V}^{\mathrm{T}}$ (actually $\mathbf{V}^{\dagger} \equiv \mathbf{V}^{\mathrm{T}*}$) is the matrix version of the Fourier transform and $\mathbf{V}$ is the matrix version of the inverse Fourier transform ($\mathbf{V}$ is an orthogonal matrix).
- Assume that the eigenvalues are a prescribed function of wavenumber (diagonal elements of $\boldsymbol{\Lambda}_p$).

$$
\begin{aligned}
\text{Matrix form} \quad & \mathbf{U}_p = \mathbf{V}\boldsymbol{\Lambda}_p^{1/2}, \\
\text{Integral form} \quad & \delta\mathbf{x}(\mathbf{r}) = \mathbf{U}_p\delta\boldsymbol{\chi}(\mathbf{k}) = \frac{1}{2\pi}\int\int d\mathbf{k}\exp(i\mathbf{k}\cdot\mathbf{r})\lambda_p^{1/2}(\mathbf{k})\delta\boldsymbol{\chi}(\mathbf{k}), \\
& \mathbf{k} = \text{2D wavenumber} \begin{pmatrix} k_x \\ k_y \end{pmatrix}, \ \mathbf{r} = \text{2D position} \begin{pmatrix} x \\ y \end{pmatrix}, \\
\text{Matrix form (adjoint)} \quad & \mathbf{U}_p^\dagger = \boldsymbol{\Lambda}_p^{1/2}\mathbf{V}^\dagger, \\
\text{Integral form (adjoint)} \quad & \delta\hat{\boldsymbol{\chi}}(\mathbf{k}) = \mathbf{U}_p^\dagger\delta\hat{\mathbf{x}}(\mathbf{r}) = \lambda_p^{1/2}(\mathbf{k})\frac{1}{2\pi}\int\int d\mathbf{r}\exp(-i\mathbf{k}\cdot\mathbf{r})\delta\hat{\mathbf{x}}(\mathbf{r}).
\end{aligned}
$$

(THE INTEGRAL FORM IS USEFUL BECAUSE IT ALLOWS US TO USE FOURIER TRANSFORM FORMULAE.) What is the B-matrix that is implied by this transform?

$$\mathbf{B}_{\text{imp}} = \mathbf{U}_p\mathbf{U}_p^\dagger.$$

$$
\begin{aligned}
\text{Let } \delta\mathbf{x}_2(\mathbf{r}_2) &= \mathbf{B}_{\text{imp}}\delta\mathbf{x}_1(\mathbf{r}_1), \\
&= \mathbf{U}_p\mathbf{U}_p^\dagger\delta\mathbf{x}_1(\mathbf{r}_1), \\
&= \frac{1}{2\pi}\int\int d\mathbf{k}\exp(i\mathbf{k}\cdot\mathbf{r}_2)\lambda_p^{1/2}(\mathbf{k})\ \lambda_p^{1/2}(\mathbf{k})\frac{1}{2\pi}\int\int d\mathbf{r}_1\exp(-i\mathbf{k}\cdot\mathbf{r}_1)\delta\mathbf{x}_1(\mathbf{r}_1), \\
&= \int\int d\mathbf{r}_1\frac{1}{4\pi^2}\int\int d\mathbf{k}\exp(i\mathbf{k}\cdot[\mathbf{r}_2-\mathbf{r}_1])\lambda_p(\mathbf{k})\delta\mathbf{x}_1(\mathbf{r}_1), \\
&= \int\int d\mathbf{r}_1\left(\frac{1}{4\pi^2}\int\int d\mathbf{k}\exp(i\mathbf{k}\cdot[\mathbf{r}_2-\mathbf{r}_1])\lambda_p(\mathbf{k})\right)\delta\mathbf{x}_1(\mathbf{r}_1), \\
&= \int\int d\mathbf{r}_1\mathbf{B}_{\text{imp}}(\mathbf{r}_2,\mathbf{r}_1)\delta\mathbf{x}_1(\mathbf{r}_1),
\end{aligned}
$$

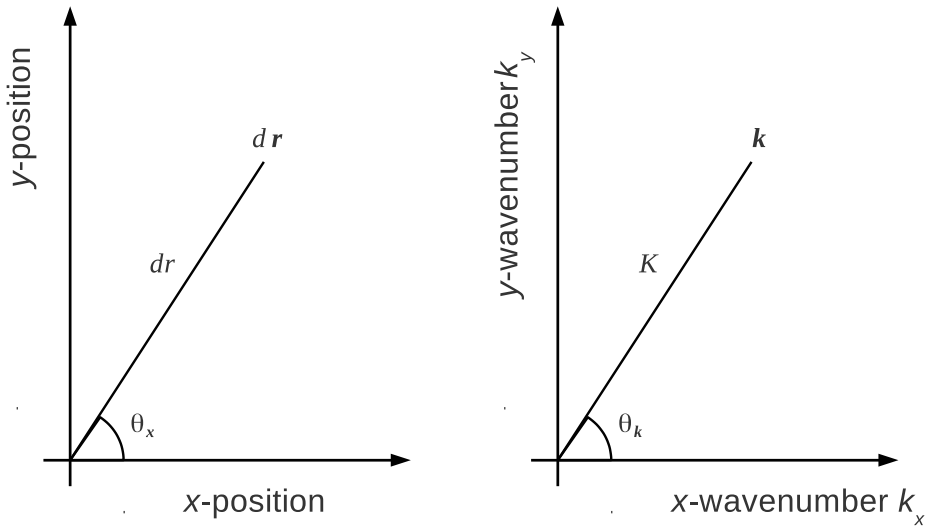
$$\mathbf{B}_{\text{imp}}(\mathbf{r}_2,\mathbf{r}_1) = \text{StrucFunc}(\mathbf{r}_2-\mathbf{r}_1) = \frac{1}{4\pi^2}\int\int d\mathbf{k}\exp(i\mathbf{k}\cdot[\mathbf{r}_2-\mathbf{r}_1])\lambda_p(\mathbf{k}),$$

$$\text{StrucFunc}(\Delta\mathbf{r}) = \frac{1}{4\pi^2}\int\int d\mathbf{k}\exp(i\mathbf{k}\cdot\Delta\mathbf{r})\lambda_p(\mathbf{k}).$$

The structure functions implied by this CVT are homogeneous. They are found to be proportional to the Fourier transform of the function $\lambda_p(\mathbf{k})$ (called the variance spectrum, and which is often prescribed).

- Now assume that $\lambda(\mathbf{k})$ is a function only of the total wavenumber, K: $K^2 = k_x^2 + k_y^2 = \mathbf{k} \cdot \mathbf{k}$.

See Fig. for definitions of angles and lengths in real and Fourier spaces. Note the following:



$$
\begin{aligned}
\Delta\mathbf{r} &= \begin{pmatrix} \Delta x \\ \Delta y \end{pmatrix} = \Delta r \begin{pmatrix} \cos\theta_x \\ \sin\theta_x \end{pmatrix}, \\
\mathbf{k} &= \begin{pmatrix} k_x \\ k_y \end{pmatrix} = K \begin{pmatrix} \cos\theta_k \\ \sin\theta_k \end{pmatrix}, \\
d\mathbf{k} &= K dK d\theta_k.
\end{aligned}
$$

The structure functions in this case become:

$$
\begin{aligned}
\mathrm{StrucFunc}(\Delta r, \theta_x) &= \frac{1}{4\pi^2} \int\int d\mathbf{k} \exp(i\mathbf{k}\cdot\Delta\mathbf{r}) \lambda_p(\mathbf{k}), \\
&= \frac{1}{4\pi^2} \int K dK \lambda_p(K) \int_{\theta_k=0}^{2\pi} d\theta_k \exp iK\Delta r(\cos\theta_x \cos\theta_k + \sin\theta_x \sin\theta_k), \\
&= \frac{1}{4\pi^2} \int K dK \lambda_p(K) \int_{\theta_k=0}^{2\pi} d\theta_k \exp iK\Delta r(\cos[\theta_k - \theta_x]).
\end{aligned}
$$

Since the integral over θ_k is over a full period of the cosine function, it is independent of θ_x. The structure functions implied by this CVT are not just homogeneous but also isotropic. (THIS METHOD IS DEMONSTRATED IN THE COMPUTER PRACTICAL FOR PART I.)

Example of the CVT method to model multivariate (balanced) error covariances

- Assume that the eigenfunctions of the $p-p$ error covariance matrix are Fourier modes, and the eigenvalues are a prescribed function of wavenumber (diagonal elements of $\mathbf{\Lambda}_p$). This is the model of spatial covariances described above, $\mathbf{U}_p$.
- Assume that the pressure and wind increments are in geostrophic balance, $\delta v = \mathbf{G}_v \delta p, \qquad \delta u = \mathbf{G}_u \delta p.$

- Let the model space be $(\delta\mathbf{p}, \delta\mathbf{u}, \delta\mathbf{v})^{\mathrm{T}}$ and the the control variable be just one field, $\delta\boldsymbol{\chi}$ (corresponding to pressure).

This means that $\delta\mathbf{p} = \mathbf{U}_p\delta\boldsymbol{\chi}$. Now, constructing the multivariate CVT and the implied background error covariance matrix:

$$
\begin{aligned}
\delta\mathbf{x} &= \mathbf{U}\delta\boldsymbol{\chi}, \\
\begin{pmatrix} \delta\mathbf{p} \\ \delta\mathbf{u} \\ \delta\mathbf{v} \end{pmatrix} &= \begin{pmatrix} \mathbf{I} \\ \mathbf{G}_u \\ \mathbf{G}_v \end{pmatrix} \mathbf{U}_p\delta\boldsymbol{\chi} \quad , \\
\mathbf{B}_{\mathrm{imp}} &= \mathbf{U}\mathbf{U}^{\mathrm{T}}, \\
&= \begin{pmatrix} \mathbf{I} \\ \mathbf{G}_u \\ \mathbf{G}_v \end{pmatrix} \mathbf{U}_p\mathbf{U}_p^{\mathrm{T}} \begin{pmatrix} \mathbf{I} & \mathbf{G}_u^{\mathrm{T}} & \mathbf{G}_v^{\mathrm{T}} \end{pmatrix} \quad , \\
&= \begin{pmatrix} \mathbf{U}_p\mathbf{U}_p^{\mathrm{T}} & \mathbf{U}_p\mathbf{U}_p^{\mathrm{T}}\mathbf{G}_u^{\mathrm{T}} & \mathbf{U}_p\mathbf{U}_p^{\mathrm{T}}\mathbf{G}_v^{\mathrm{T}} \\ \mathbf{G}_u\mathbf{U}_p\mathbf{U}_p^{\mathrm{T}} & \mathbf{G}_u\mathbf{U}_p\mathbf{U}_p^{\mathrm{T}}\mathbf{G}_u^{\mathrm{T}} & \mathbf{G}_u\mathbf{U}_p\mathbf{U}_p^{\mathrm{T}}\mathbf{G}_v^{\mathrm{T}} \\ \mathbf{G}_v\mathbf{U}_p\mathbf{U}_p^{\mathrm{T}} & \mathbf{G}_v\mathbf{U}_p\mathbf{U}_p^{\mathrm{T}}\mathbf{G}_u^{\mathrm{T}} & \mathbf{G}_v\mathbf{U}_p\mathbf{U}_p^{\mathrm{T}}\mathbf{G}_v^{\mathrm{T}} \end{pmatrix}.
\end{aligned}
$$

$\mathbf{G}_u$, $\mathbf{G}_v$, $\mathbf{G}_u^{\mathrm{T}}$ and $\mathbf{G}_v^{\mathrm{T}}$can each be coded as an algorithm in a subroutine (each has an input field and an output field), avoiding the need to store as explicit matrices.

What is the saving of this CVT method of modelling B compared to an explicit matrix method?

- No. of grid points: $n_x \times n_y$.
- No. of pieces of information in $\delta\mathbf{x}$: $3 \times n_x \times n_y$.
- No. of pieces of information in $\delta\boldsymbol{\chi}$: $n_x \times n_y$.
- No. of independent elements in explicit $\mathbf{B}$: $\sim \frac{1}{2}\left(3 \times n_x \times n_y\right)^2 \sim \frac{9}{2}n_x^4$ (assuming $n_x \sim n_y$).
- No. of pieces of information needed for CVT: $\sim$ No. of total wavenumbers needed to know $\lambda_p(K)$ $\sim \sqrt{2}n_x$.

If $n_x = 1000$, then

- No. of independent elements in explicit $\mathbf{B}$: $\sim 5 \times 10^{12}$.
- No. of pieces of information needed for CVT: ~ 1500.

Operational CVTs

- The Met Office use a similar approach in its operational 4D-VAR and 3DFGAT systems. Geostrophic balance (imposed weakly) and hydrostatic balance are used. The spatial component includes a similar approach as shown above (spectral space) for the horizontal structure of background error covariances, and vertical modes (empirical orthogonal functions) for the vertical structure. *Lorenc A.C., Ballard S.P., Bell R.S., Ingleby N.B., Andrews P.L.F., Barker D.M., Bray J.R., Clayton A.M., Dalby T., Li D., Payne T.J., Saunders F.W., The Met Office global 3-dimensional variational data assimilation scheme, Q.J.R.Meteor.Soc. 126 pp.2991-3012 (2000).*

- The ECMWF use similar balance relationships, but use a spatial component that makes use of wavelets. *Fisher M., Andersson E., Developments in 4d-Var and Kalman filtering, ECMWF Research Report No. 347 pp.36 (2001).*

- The diffusion operator approach is used in ocean data assimilation systems. *Weaver A.T., Deltel C., Machu E., Ricci S., Daget N., A multivariate balance operator for variational ocean data assimilation, Q.J.R.Meteor.Soc. 131 pp.3605-3626 (2005).*

3(f) Conditioning of the variational problem

The rate of convergence of the variational problem is affected strongly by the *conditioning* of the variational problem. Consider the case when $\delta\mathbf{x}$ is the control variable. A Taylor expansion of $J(\mathbf{x})$ with respect to perturbations $\delta\mathbf{x}$ about $\mathbf{x}$ is:

$$\begin{array}{ccccccc} J(\mathbf{x}+\delta\mathbf{x}) & = & J(\mathbf{x}) & + & \left.\dfrac{\partial J}{\partial \delta\mathbf{x}}\right|_{\mathbf{x}} \delta\mathbf{x} & + & \dfrac{1}{2}\delta\mathbf{x}^{\mathrm{T}} \left.\dfrac{\partial^2 J}{\partial \delta\mathbf{x}^2}\right|_{\mathbf{x}} \delta\mathbf{x}. \\ & & & & \text{gradient} & & \text{Hessian} \\ & & & & \text{vector} & & \text{matrix} \\ & & (1\times 1) & & (1\times n)(n\times 1) & & (1\times n)(n\times n)(n\times 1) \end{array}$$

The Hessian matrix is an $n \times n$ matrix that describes all possible second derivatives of J with respect to the control variable elements:

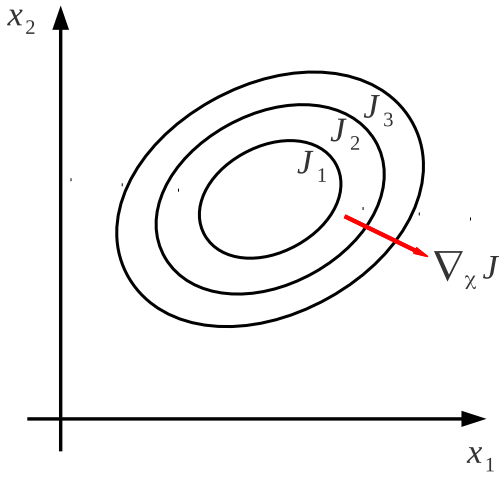
$$\frac{\partial^2 J}{\partial \delta\mathbf{x}^2} = \begin{pmatrix} \frac{\partial^2 J}{\partial x_1^2} & \frac{\partial^2 J}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 J}{\partial x_1 \partial x_n} \\ \frac{\partial^2 J}{\partial x_2 \partial x_1} & \frac{\partial^2 J}{\partial x_2^2} & \cdots & \frac{\partial^2 J}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 J}{\partial x_n \partial x_1} & \frac{\partial^2 J}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 J}{\partial x_n^2} \end{pmatrix},$$

and describes the eccentricity and orientation of the ellipsoids that describe surfaces of constant J in phase space. In particular, the condition number is important:

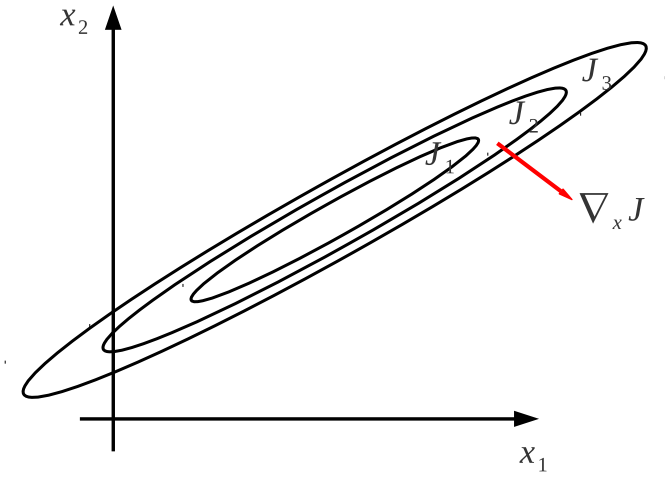
$$\kappa = \text{condition number} = \frac{\text{maximum eigenvalue of the Hessian}}{\text{minimum eigenvalue of the Hessian}}.$$

- If $\kappa \approx 1$, then the variational problem is well conditioned and it will be possible for the solution to be found to a high accuracy.
- If $\kappa \gg 1$, then the variational problem will converge slowly and it is hard for the solution to be found to a high accuracy.

Low condition number



High condition number

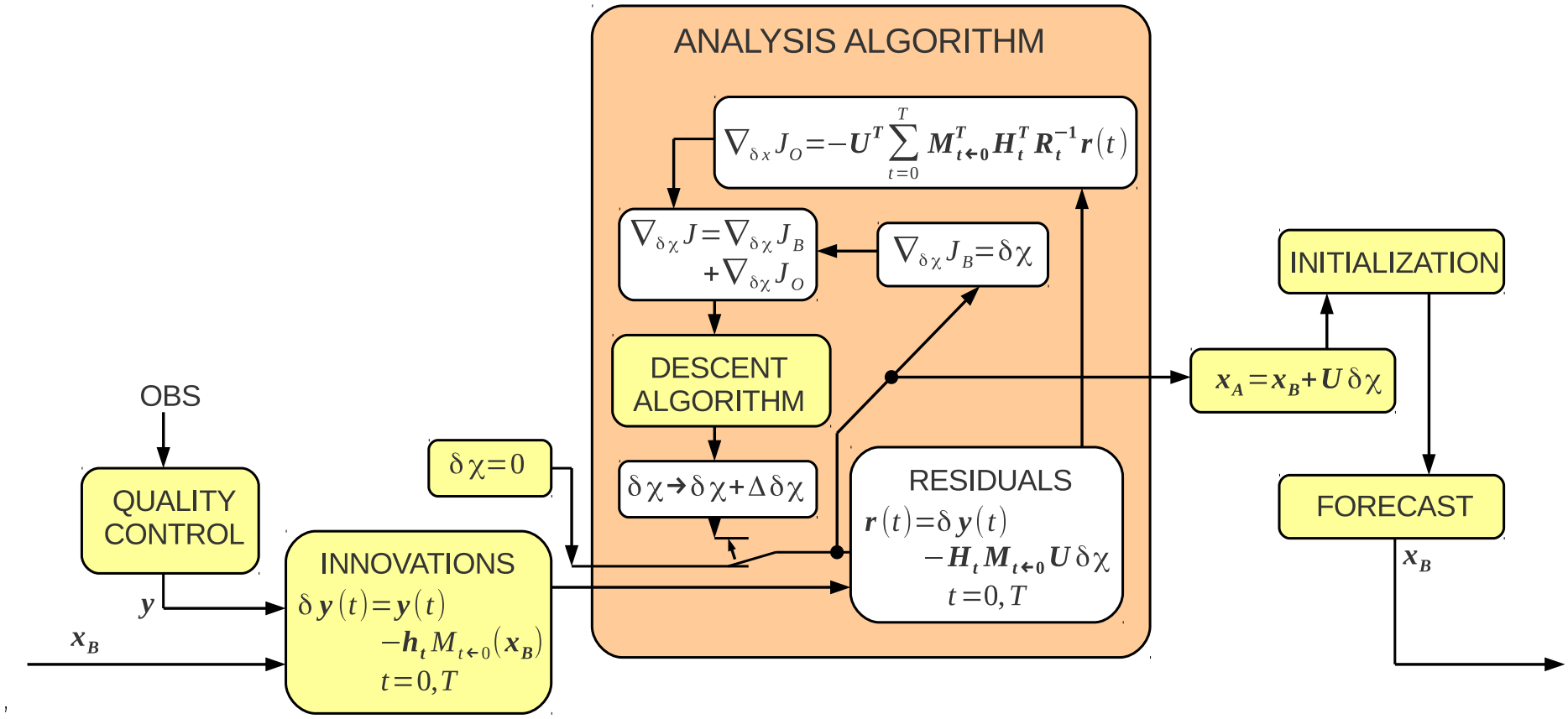


The gradient vectors are the direction in phase space (either $\delta\boldsymbol{\chi}$ or $\delta\mathbf{x}$) that points in the direction of steepest ascent at the particular position. It is thought that κ is extremely large for operational problems posed in the $\delta\mathbf{x}$ formulation. If the problem is posed in the $\delta\boldsymbol{\chi}$ formulation then the principle is the same (but replace $\delta\mathbf{x} \rightarrow \delta\boldsymbol{\chi}$ in the above formulae). The following table compares weak constraint 4D-VAR with $\delta\boldsymbol{\chi}$ and $\delta\mathbf{x}$ as the control variable.

	$\delta\boldsymbol{\chi}$	$\delta\mathbf{x}$
Hessian	$\mathbf{I} + \sum_{t=0}^{T} \mathbf{U}^{\mathrm{T}}\mathbf{M}_{t\leftarrow 0}^{\mathrm{T}}\mathbf{H}_t^{\mathrm{T}}\mathbf{R}_t^{-\mathrm{T}}\mathbf{H}_t\mathbf{M}_{t\leftarrow 0}\mathbf{U}$	$\mathbf{B}^{-1} + \sum_{t=0}^{T} \mathbf{M}_{t\leftarrow 0}^{\mathrm{T}}\mathbf{H}_t^{\mathrm{T}}\mathbf{R}_t^{-\mathrm{T}}\mathbf{H}_t\mathbf{M}_{t\leftarrow 0}$
min eigenvalue	$\lambda_{\min}^{\boldsymbol{\chi}} \gtrsim 1$	$\lambda_{\min}^{\mathbf{x}} \geq 0$
max eigenvalue	$\lambda_{\max}^{\boldsymbol{\chi}}$	$\lambda_{\max}^{\mathbf{x}} \gg 1$ in practice
condition No.	$\lambda_{\max}^{\boldsymbol{\chi}}/1 \sim \lambda_{\max}^{\boldsymbol{\chi}}$	$\lambda_{\max}^{\mathbf{x}}/0^{+} \rightarrow \infty$

4. Operational algorithms

We now have enough information to understand the standard operational algorithm using a CVT, given in the Fig. for incremental strong constraint 4D-VAR. The descent algorithm is a method to use the gradient vector to adjust $\delta\chi$ to reduce the value of J. Examples of descent algorithms are: method of steepest descent (very inefficient), conjugate gradient method (quite efficient).



(STEP 4 BELOW IS DONE IN PROBLEM 14. A VERSION OF THE GRADIENT FORMULA THAT IS EXTREMELY EFFICIENT TO COMPUTE IS DEVELOPED IN PROBLEM 15.)

1. Run $\mathbf{x}_{\mathrm{B}}$ forward in time $0 \rightarrow T$. Calculate the model observations, $\mathbf{y}^{\mathrm{mo}}(t) = \mathbf{h}_t(\boldsymbol{\mathcal{M}}_{t\leftarrow 0}(\mathbf{x}_{\mathrm{B}}))$, and the innovations, $\delta\mathbf{y}(t) = \mathbf{y}(t) - \mathbf{y}^{\mathrm{mo}}(t)$.

2. Set the initial value of $\delta\boldsymbol{\chi} = 0$, and the loop counter $l = 0$.

3. Calculate the residual vector at time t and for loop l in the time window, $\mathbf{r}(t) = \delta\mathbf{y}(t) - \mathbf{H}_t\mathbf{M}_{t\leftarrow 0}\mathbf{U}\delta\boldsymbol{\chi}$.
4. Calculate the gradient of J_O for loop l.
5. Calculate the gradient of J for loop l.
6. Use a descent algorithm to calculate a change to the control variable increment, $\Delta\delta\boldsymbol{\chi}$, such that $\delta\boldsymbol{\chi} + \Delta\delta\boldsymbol{\chi}$ reduces the value of the cost function.
7. Update $\delta\boldsymbol{\chi} \rightarrow \delta\boldsymbol{\chi} + \Delta\delta\boldsymbol{\chi}$ and increment l: $l \rightarrow l + 1$.
8. If we decide that we have 'converged', go to step 9, otherwise go to step 3.
9. Obtain the analysis, $\mathbf{x}_\mathrm{A} = \mathbf{x}_\mathrm{B} + \mathbf{U}\delta\boldsymbol{\chi}$.
10. Make a weather forecast for x days ahead and store the forecast after time T (e.g. 1, 3, 6, 12 hours) as the background state for the next cycle.

(THE ITERATIVE NATURE IS THE VARIATIONAL ASPECT OF THE METHOD.)

5. Measuring the B-matrix

- We now have techniques to compress the $n \times n$ $\mathbf{B}$ or $\mathbf{P}^\mathrm{f}$ matrix, as long as we are willing to make assumptions about its properties (e.g. homogeneous, isotropic, balanced). These are called error covariance models.
- We still have the problem of determining the parameters in a covariance model (e.g. the $\lambda(K)$)?
- Need a population of sample forecast error states. Ideally we have N samples of forecast error, $\boldsymbol{\eta}_\mathrm{B}^{(i)} = \mathbf{x}_\mathrm{B}^{(i)} - \mathbf{x}^\mathrm{t}$, $1 \leq i \leq N$. Focus now not on determining $\lambda(K)$, but instead on how we can estimate $\mathbf{B}$ explicitly from data. There are two problems:
  - Have background states available, but don't know the truth. This is a fundamental problem. Instead propose members that are *proxies* for forecast error.

– Need sufficient members of the sample to determine $\mathbf{B}$ well enough ($N \gtrsim n$). This is a practical problem. Practically, we will never have enough members, so there will be consequences (e.g. see Sec. 3b). (If we are determining $\lambda(K)$ from the data then fewer members are needed.)

Recall:

$$\mathbf{P}^{\mathrm{f}} = \left\langle \boldsymbol{\eta}_{\mathrm{B}} \boldsymbol{\eta}_{\mathrm{B}}^{\mathrm{T}} \right\rangle \approx \mathbf{P}^{\mathrm{f}}_{(N)} = \frac{1}{N-1} \sum_{i=1}^{N} \boldsymbol{\eta}_{\mathrm{B}}^{(i)} \boldsymbol{\eta}_{\mathrm{B}}^{(i)\mathrm{T}}.$$

We will here focus on methods of generating proxies of forecast error. Here background states (and hence background error states) are valid at $t = 0$. For the purposes of this section, we will assume linear (and perfect) observation operators.

5(a) Analysis of innovations

$$\left.\begin{array}{c} \text{Innovation "O-B"} = \delta\mathbf{y} = \mathbf{y} - \mathbf{H}\mathbf{x}_{\mathrm{B}}, \\ \mathbf{y} = \mathbf{H}\mathbf{x}^{\mathrm{t}} + \boldsymbol{\epsilon}, \\ \mathbf{x}_{\mathrm{B}} = \mathbf{x}^{\mathrm{t}} + \boldsymbol{\eta}_{\mathrm{B}}, \end{array}\right\} \begin{array}{c} \mathbf{y} - \mathbf{H}\mathbf{x}_{\mathrm{B}} = \mathbf{H}\mathbf{x}^{\mathrm{t}} + \boldsymbol{\epsilon} - \mathbf{H}\left(\mathbf{x}^{\mathrm{t}} + \boldsymbol{\eta}_{\mathrm{B}}\right), \\ \mathbf{y} - \mathbf{H}\mathbf{x}_{\mathrm{B}} = \boldsymbol{\epsilon} - \mathbf{H}\boldsymbol{\eta}_{\mathrm{B}}. \\ \text{measureable} \qquad \text{unmeasureable} \end{array}$$

Then:

$$\begin{aligned} \left\langle \left(\mathbf{y} - \mathbf{H}\mathbf{x}_{\mathrm{B}}\right)\left(\mathbf{y} - \mathbf{H}\mathbf{x}_{\mathrm{B}}\right)^{\mathrm{T}} \right\rangle &= \left\langle \left(\boldsymbol{\epsilon} - \mathbf{H}\boldsymbol{\eta}_{\mathrm{B}}\right)\left(\boldsymbol{\epsilon} - \mathbf{H}\boldsymbol{\eta}_{\mathrm{B}}\right)^{\mathrm{T}} \right\rangle, \\ &= \mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}, \end{aligned}$$

(assuming that observation and background errors are uncorrelated). In order to see this more clearly, let us move away from the vector/matrix notation and assume that when $\mathbf{H} = \mathbf{H}_i$, the observation operator represents a direct measurement of a model variable (v_i at position $\mathbf{r}_i$), i.e. $\mathbf{H}_i\mathbf{x}_{\mathrm{B}} = v_i(\mathbf{r}_i)$. Now consider two measurements as follows.

	model variable	position	observation	innovation
measurement 1	v_1	$\mathbf{r}$	y_1	$y_1 - v_1(\mathbf{r}) = \epsilon_1 - \eta^{v_1}(\mathbf{r})$
measurement 2	v_2	$\mathbf{r} + \Delta\mathbf{r}$	y_2	$y_2 - v_2(\mathbf{r} + \Delta\mathbf{r}) = \epsilon_2 - \eta^{v_2}(\mathbf{r} + \Delta\mathbf{r})$

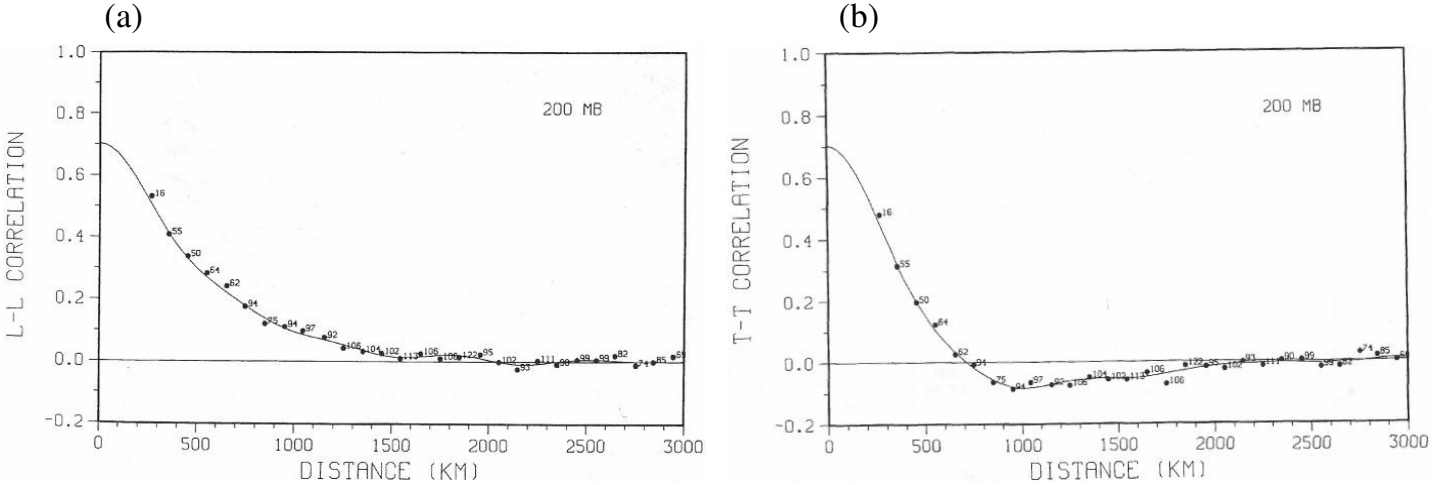
If we make repeat measurements and repeat draws from an equivalent background state then the expectation of the product of these innovations is

$$\left\langle \left(y_1 - v_1(\mathbf{r})\right)\left(y_2 - v_2(\mathbf{r} + \Delta\mathbf{r})\right) \right\rangle = \left\langle \left(\epsilon_1 - \eta^{v_1}(\mathbf{r})\right)\left(\epsilon_2 - \eta^{v_2}(\mathbf{r} + \Delta\mathbf{r})\right) \right\rangle.$$

Then for $\Delta\mathbf{r} \neq 0$ or $v_1 \neq v_2$, assuming that observation and background errors are uncorrelated, and assuming that observation errors at different positions are uncorrelated leads to:

$$\langle (y_1 - v_1(\mathbf{r}))\,(y_2 - v_2(\mathbf{r}+\Delta\mathbf{r}))\rangle = \langle \eta^{v_1}(\mathbf{r})\eta^{v_2}(\mathbf{r}+\Delta\mathbf{r})\rangle\,,$$

(background errors at different positions are fundamentally correlated). This method of estimating the structure of background error covariances is called the *analysis of innovation method* or the *Hollingsworth and Lonnberg method*.



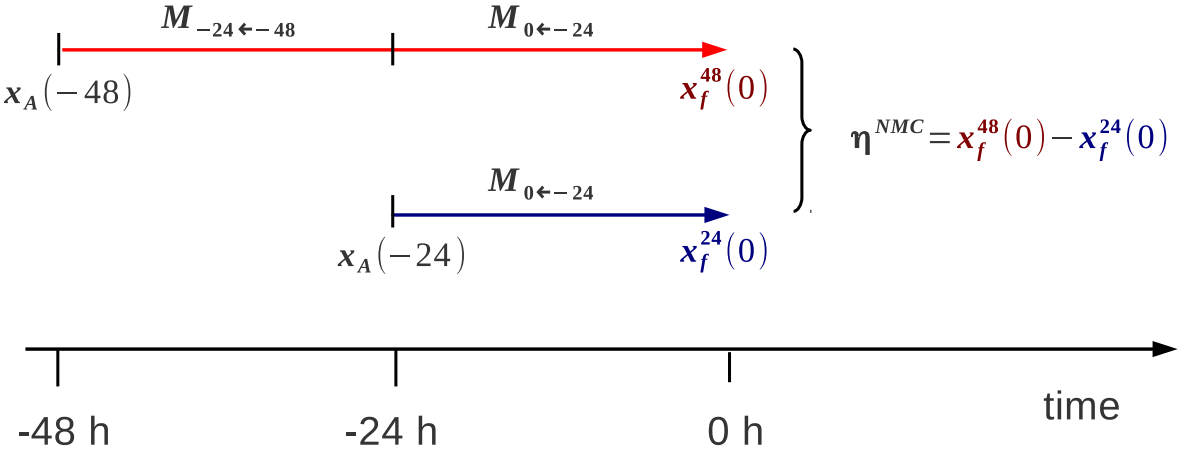
- The H+L method was popular in the 1980s and 1990s.
- It replies on a huge number of direct (in-situ) observations.
- Not useful in practice to probe flow dependence of $\mathbf{B}$, or $\mathbf{B}$ in unobserved regions.
- *Hollingsworth A., Lonnberg P., The statistical structure of short-range forecast errors as determined from radiosonde data. Part I: The wind field, Tellus 38A pp.111-136 (1986). Lonnberg P., Hollingsworth A., The statistical structure of short-range forecast errors as determined from radiosonde data. Part II: The covariance of height and wind errors, Tellus 38A pp.137-161 (1986).*

5(b) The NMC method

THIS IS NAMED AFTER THE NATIONAL METEOROLOGICAL CENTRE IN THE USA (NOW CALLED NCEP - THE NATIONAL CENTER FOR ENVIRONMENTAL PREDICTION).

Propose a proxy for forecast error:

$$\boldsymbol{\eta}^{\mathrm{NMC}} \approx \mathbf{x}_{\mathrm{f}}^{48}(0) - \mathbf{x}_{\mathrm{f}}^{24}(0).$$



The difference between two forecasts, starting from analyses at different times, but valid at the same time. Use a population of such forecast differences over a time period to estimate forecast errors:

$$\mathbf{B} \approx \frac{1}{2} \left\langle \left(\mathbf{x}_{\mathrm{f}}^{48}(0) - \mathbf{x}_{\mathrm{f}}^{24}(0)\right) \left(\mathbf{x}_{\mathrm{f}}^{48}(0) - \mathbf{x}_{\mathrm{f}}^{24}(0)\right)^{\mathrm{T}} \right\rangle .$$

This assumes ergodicity (that taking forecast errors over time is equivalent to sampling from the PDF at one time). SEE PROBLEM 16 TO SEE HOW THE FACTOR OF 1/2 APPEARS. Notes:

- The averaging over time means that only a climatological estimate of forecast errors is possible with the NMC method.
- The usual forecast length of a background state is 6 or 12 hours (or shorter for some applications). The NMC usually uses 12 and 24-hour forecasts. We might therefore expect the forecast difference to overestimate forecast error variances and overestimate correlation length-scales.
- In poorly observed regions however, the NMC method is likely to underestimate forecast error variances for the following reason:

$$\begin{aligned}
\mathbf{x}_{\mathrm{f}}^{24}(0) &= \boldsymbol{\mathcal{M}}_{0\leftarrow-24}\left(\mathbf{x}_{\mathrm{A}}(-24)\right), \\
\mathbf{x}_{\mathrm{f}}^{48}(0) &= \boldsymbol{\mathcal{M}}_{0\leftarrow-24}\left(\boldsymbol{\mathcal{M}}_{-24\leftarrow-48}\left(\mathbf{x}_{\mathrm{A}}(-48)\right)\right), \\
\text{but } \mathbf{x}_{\mathrm{A}}(-24) &= \boldsymbol{\mathcal{K}}_{-24}\left(\boldsymbol{\mathcal{M}}_{-24\leftarrow-48}\left(\mathbf{x}_{\mathrm{A}}(-48)\right)\right), \\
\text{where } \boldsymbol{\mathcal{K}}_{-24}(\mathbf{x}_{\mathrm{B}}) & \quad \text{represents the result of doing DA at } t = -24 \text{ with background } \mathbf{x}_{\mathrm{B}}.
\end{aligned}$$

Note the expected properties of $\boldsymbol{\mathcal{K}}_{-24}$:

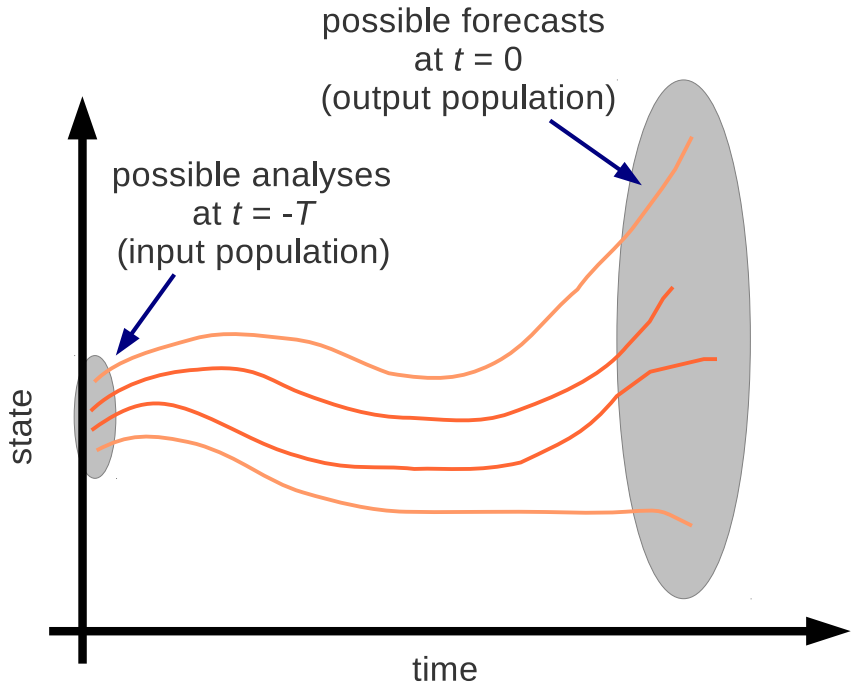
$$\boldsymbol{\mathcal{K}}_{-24}(\mathbf{x}_{\mathrm{B}}) = \begin{cases} \approx \mathbf{x}_{\mathrm{B}} & \Delta r \gg L \\ \text{background state modified by observations} & \text{elsewhere} \end{cases}$$

where $\Delta r \gg L$ means regions that are a distance from the nearest observations much greater than the background error correlation length-scale. These regions are largely unaffected by the data assimilation. Focusing on these regions only:

$$\begin{aligned} \mathbf{x}_{\mathrm{A}}(-24) &\approx \boldsymbol{\mathcal{M}}_{-24\leftarrow-48}\left(\mathbf{x}_{\mathrm{A}}(-48)\right), \\ \therefore \mathbf{x}_{\mathrm{f}}^{24}(0) &\approx \boldsymbol{\mathcal{M}}_{0\leftarrow-24}\left(\boldsymbol{\mathcal{M}}_{-24\leftarrow-48}\left(\mathbf{x}_{\mathrm{A}}(-48)\right)\right) = \mathbf{x}_{\mathrm{f}}^{48}(0), \\ \therefore \boldsymbol{\eta}^{\mathrm{NMC}} &\approx 0. \end{aligned}$$

5(c) Monte-Carlo (ensemble) method

Generate an ensemble that ideally simulates all known sources of forecast error.



For the ith ensemble member ($1 \leq i \leq N$):

$$\mathbf{x}^{(i)}(t+\delta t) = \boldsymbol{\mathcal{M}}_{t+\delta t \leftarrow t}\left(\mathbf{x}^{(i)}(t)\right) + \mathbf{e}^{(i)}(t),$$

integrated from $t = -T$ to $t = 0$. The following sources of error are considered:

- Initial condition error, $\delta\mathbf{x}_{\mathrm{A}}^{(i)}(-T)$, e.g.:

  $$\mathbf{x}^{(i)}(-T) = \mathbf{x}_{\mathrm{A}}(-T) + \delta\mathbf{x}_{\mathrm{A}}^{(i)}(-T),$$

  where

  $$\frac{1}{N-1}\sum_{i=1}^{N} \delta\mathbf{x}_{\mathrm{A}}^{(i)}(-T)\delta\mathbf{x}_{\mathrm{A}}^{(i)\mathrm{T}}(-T) \approx \mathbf{P}_{\mathrm{A}}(-T).$$

  All errors inherited from previous DA cycles are represented as initial condition errors.

- Model error, the integrated effect of $\mathbf{e}^{(i)}(t)$. The model error is unknown, but can be included stochastically during the integration of the model. Practical methods of implicitly approximating model error include:
  - Multi-model/multi-physics methods (these use different models, different parameterizations or different parameter values of the parameterizations for each ensemble methods to approximate the effect of $\mathbf{e}^{(i)}(t)$).
  - Stochastic kinetic energy backscatter (SKEB) methods (forecast models do not represent the energy well at scales close to the grid-scale - leading to significant model errors; SKEB injects kinetic energy into the model to try to make up for this).
  - Stochastically perturbed tendencies (SPT) (tendencies from the - imperfect - parametrization schemes are scaled and added as possible model errors).
- Other errors (e.g. boundary condition perturbations for limited area models, perturbations to the unknown forcings of the model).

This is called the system simulation method, which attempts to represent the unknowns as an ensemble of possibilities. This

has parallels to ensemble Kalman filter methods, but here we are generating possible forecasts to help estimate $\mathbf{P}_{\rm f}$ or $\mathbf{B}$:

$$\begin{aligned}
\mathbf{P}^{\rm f}_{(N)}(0) &= \frac{1}{N-1}\sum_{i=1}^{N}\boldsymbol{\eta}^{(i)}(0)\boldsymbol{\eta}^{(i)\rm T}(0) \qquad \text{(flow dependent)},\\
\text{where, e.g. } \boldsymbol{\eta}^{(i)}(0) &= \mathbf{x}^{(i)}(t) - \frac{1}{N}\sum_{i=1}^{N}\mathbf{x}^{(i)}(t) \text{ is the } i\text{th forecast error},\\
\text{or } \mathbf{B} &\approx \frac{1}{NC-1}\sum_{i=1}^{N}\sum_{c=1}^{C}\boldsymbol{\eta}^{(i,c)}(0)\boldsymbol{\eta}^{(i,c)\rm T}(0) \qquad \text{(flow independent)},\\
\text{where, e.g. } \boldsymbol{\eta}^{(i,c)} &= \mathbf{x}^{(i,c)}(t) - \frac{1}{N}\sum_{i=1}^{N}\mathbf{x}^{(i,c)}(t) \text{ is the } i\text{th forecast error of the } c\text{th cycle}.
\end{aligned}$$

This is a very expensive method and relies on being able to simulate well the possible errors.

6. Hybrid (var/ensemble) formations

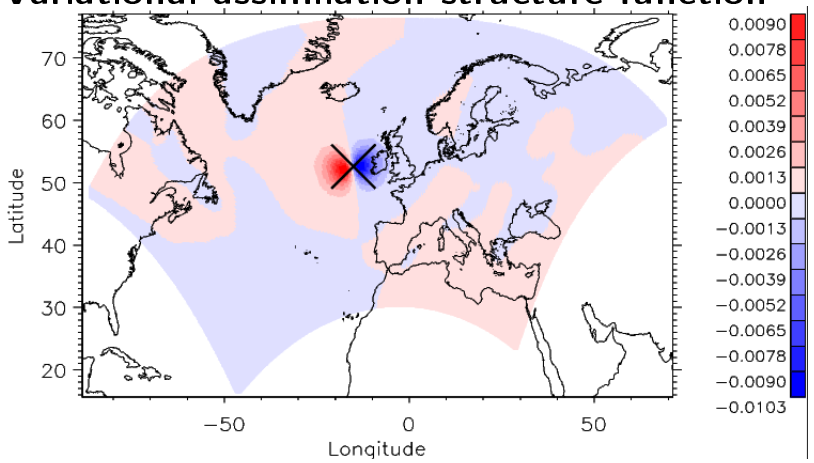
6(a) Basic ideas

Let us consider the pros and cons of variational data assimilation and ensemble data assimilation (such as the ensemble Kalman filter discussed in part II of this course).

	VARIATIONAL DATA ASSIMILATION	ENSEMBLE KALMAN FILTER	
1. Efficiency	Good	Good	
2. Data voids	Reverts to the background state, $\mathbf{x}_{\mathrm{B}}$	Reverts to the background state, $\mathbf{x}_{\mathrm{B}}$	
3. Processing	Continuous (within assimilation window)	Intermittent	
4. Scaling for parallel computing	Limits to scaling	No limits to scaling	
5. Errors in inputs	Allows for errors in $\mathbf{x}_{\mathrm{B}}$ and $\mathbf{y}$	Allows for errors in $\mathbf{x}_{\mathrm{B}}$ and $\mathbf{y}$	
6. Errors in model	Accounted for in WC 4D-VAR	Accounted for	
7. Indirect observations	Yes	Yes	
8. Balance and smoothness of analysis	Yes	No, unless N is sufficiently large	*
9. Flow dependent background error covariance matrix	No, $\mathbf{P}^{\mathrm{f}}$ is approximated by $\mathbf{B}$	Yes, $\mathbf{P}^{\mathrm{f}}$ is approximated by $\mathbf{P}^{\mathrm{f}}_{(N)}$	*
10. Rank of background error covariance matrix	Full rank	$\mathrm{rank} \leq N$	*

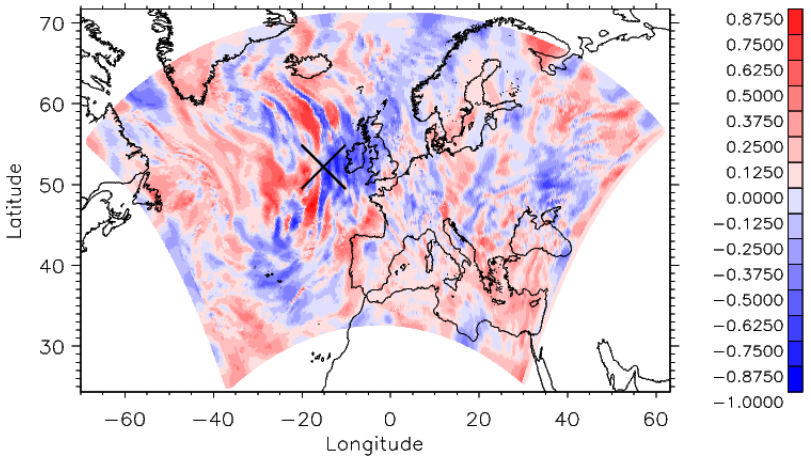
* These issues are related. The aim of hybrid data assimilation is to combine VAR with an ensemble to get the best bits of each approach.

Variational assimilation structure function

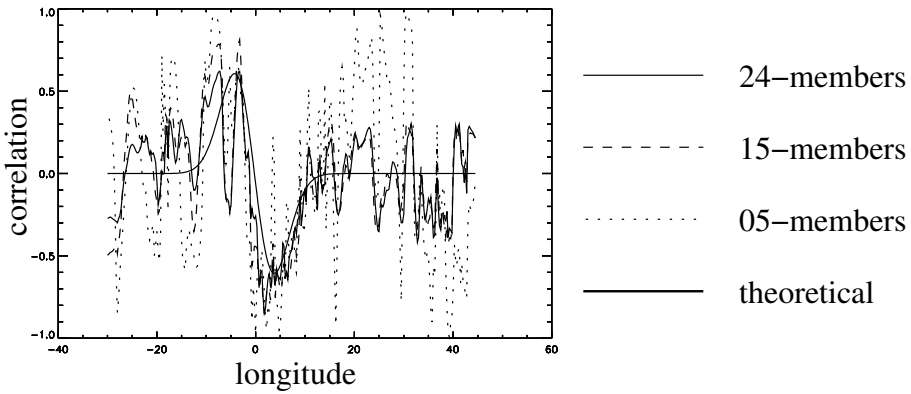


- Full rank, but not flow dependent.

Ensemble-derived structure function ($N = 24$)



(c) v–p correlation (NAE)



- Flow dependent, but rank deficient.

In the hybrid solution, we solve a VAR-like problem but $\mathbf{B} \rightarrow \mathbf{P}^{\mathrm{H}}$:

$$\mathbf{P}^{\mathrm{H}} = \alpha\mathbf{B} + (1-\alpha)\mathbf{P}^{\mathrm{f}}_{(N)}, \text{ where } 0 \leq \alpha \leq 1.$$

6(b) Incorporating a simple hybrid scheme in VAR

In order to use $\mathbf{P}^{\mathrm{H}} = \alpha\mathbf{B} + (1-\alpha)\mathbf{P}^{\mathrm{f}}_{(N)}$ in variational assimilation, $\mathbf{P}^{\mathrm{H}}$ needs to be made compatible with the control variable transform (CVT).

Recall from 3(e), $\mathbf{B}$ is modelled by minimizing the cost function with respect to a control variable $\delta\boldsymbol{\chi}$:

$$\begin{aligned} J[\delta\boldsymbol{\chi}] &= \frac{1}{2}\delta\boldsymbol{\chi}^{\mathrm{T}}\delta\boldsymbol{\chi} + \\ &\quad \frac{1}{2}\sum_{t=0}^{T}\left[\delta\mathbf{y}(t) - \mathbf{H}_t\mathbf{M}_{t\leftarrow 0}\mathbf{U}\delta\boldsymbol{\chi}\right]^{\mathrm{T}}\mathbf{R}_t^{-1}\times \\ &\quad\quad \left[\delta\mathbf{y}(t) - \mathbf{H}_t\mathbf{M}_{t\leftarrow 0}\mathbf{U}\delta\boldsymbol{\chi}\right], \\ \text{where } \delta\mathbf{x} &= \mathbf{U}\delta\boldsymbol{\chi}, \\ \text{and } \left\langle\delta\boldsymbol{\chi}\delta\boldsymbol{\chi}^{\mathrm{T}}\right\rangle &= \mathbf{I}, \end{aligned}$$

and the implied background error covariance matrix is:

$$\mathbf{B}_{\mathrm{imp}} = \mathbf{U}\mathbf{U}^{\mathrm{T}}.$$

Now consider the following cost function and modification to the control variable and its CVT:

$$\begin{aligned} J^{\mathrm{H}}[\delta\boldsymbol{\chi}^{\mathrm{H}}] &= \frac{1}{2}\delta\boldsymbol{\chi}_{\mathrm{var}}^{\mathrm{T}}\delta\boldsymbol{\chi}_{\mathrm{var}} + \frac{1}{2}\delta\boldsymbol{\chi}_{\mathrm{ens}}^{\mathrm{T}}\delta\boldsymbol{\chi}_{\mathrm{ens}} + \\ &\quad \frac{1}{2}\sum_{t=0}^{T}\left[\delta\mathbf{y}(t) - \mathbf{H}_t\mathbf{M}_{t\leftarrow 0}\mathbf{U}^{\mathrm{H}}\delta\boldsymbol{\chi}^{\mathrm{H}}\right]^{\mathrm{T}}\mathbf{R}_t^{-1}\times \\ &\quad\quad \left[\delta\mathbf{y}(t) - \mathbf{H}_t\mathbf{M}_{t\leftarrow 0}\mathbf{U}^{\mathrm{H}}\delta\boldsymbol{\chi}^{\mathrm{H}}\right], \\ \text{where } \delta\mathbf{x} &= \mathbf{U}^{\mathrm{H}}\delta\boldsymbol{\chi}^{\mathrm{H}}, \\ \text{and } \left\langle\delta\boldsymbol{\chi}^{\mathrm{H}}\delta\boldsymbol{\chi}^{\mathrm{HT}}\right\rangle &= \mathbf{I}, \\ \text{but now } \delta\boldsymbol{\chi}^{\mathrm{H}} &= \begin{pmatrix}\delta\boldsymbol{\chi}_{\mathrm{var}} \\ \delta\boldsymbol{\chi}_{\mathrm{ens}}\end{pmatrix}, \qquad \delta\boldsymbol{\chi}_{\mathrm{var}}\in\mathbb{R}^n,\ \delta\boldsymbol{\chi}_{\mathrm{ens}}\in\mathbb{R}^N, \\ \text{and } \mathbf{U}^{\mathrm{H}} &= \begin{pmatrix}\sqrt{\alpha}\mathbf{U} & \sqrt{\frac{1-\alpha}{N-1}}\mathbf{X}\end{pmatrix}. \end{aligned}$$

What is the implied background error covariance matrix of this scheme?

$$\begin{aligned} \mathbf{B}^{\mathrm{H}}_{\mathrm{imp}} &= \left\langle\delta\mathbf{x}\delta\mathbf{x}^{\mathrm{T}}\right\rangle = \mathbf{U}^{\mathrm{H}}\left\langle\delta\boldsymbol{\chi}^{\mathrm{H}}\delta\boldsymbol{\chi}^{\mathrm{HT}}\right\rangle\mathbf{U}^{\mathrm{HT}} = \mathbf{U}^{\mathrm{H}}\mathbf{U}^{\mathrm{HT}}, \\ &= \begin{pmatrix}\sqrt{\alpha}\mathbf{U} & \sqrt{\frac{1-\alpha}{N-1}}\mathbf{X}\end{pmatrix}\begin{pmatrix}\sqrt{\alpha}\mathbf{U}^{\mathrm{T}} \\ \sqrt{\frac{1-\alpha}{N-1}}\mathbf{X}^{\mathrm{T}}\end{pmatrix} = \alpha\mathbf{U}\mathbf{U}^{\mathrm{T}} + \frac{1-\alpha}{N-1}\mathbf{X}\mathbf{X}^{\mathrm{T}}, \\ &= \alpha\mathbf{B} + (1-\alpha)\mathbf{P}^{\mathrm{f}}_{(N)}. \end{aligned}$$

The first term contains $\mathbf{U}\mathbf{U}^{\mathrm{T}}$, which is the implied background error covariance matrix from the pure variational scheme, and the second term contains $\mathbf{X}\mathbf{X}^{\mathrm{T}}/(N-1)$, which is the ensemble-derived background error covariance matrix (we used this notation in section 3(b), and in problem 12).

6(c) Incorporating a localized hybrid scheme in VAR

The ensemble contribution to the hybrid covariance is noisy when N is small. How can we mitigate this noise?

- A statistical result tells us that the error in the sample correlation between two variables x and y has expectation $(1 - \mathrm{cor}^2(x, y))/\sqrt{N-1}$.
- For a given N, sampling errors are expected to be largest when the correlations are close to zero.
- Correlations are expected to be smaller at larger separations.
- 'Localization' artificially reduces covariances between variables separated by large distances.

Let $x = \boldsymbol{\eta}_{\mathrm{B}}(\mathbf{r}_1)$ and $y = \boldsymbol{\eta}_{\mathrm{B}}(\mathbf{r}_2)$. The raw covariance between x and y is:

$$\mathbf{P}^{\mathrm{f}}_{(N)}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{N-1} \sum_{i=1}^{N} \boldsymbol{\eta}^{(i)}_{\mathrm{B}}(\mathbf{r}_1) \boldsymbol{\eta}^{(i)}_{\mathrm{B}}(\mathbf{r}_2).$$

For the covariance actually used in the hybrid scheme, we wish to multiply this by a moderation function that decreases with separation between $\mathbf{r}_1$ and $\mathbf{r}_2$: $\boldsymbol{\Omega}(\mathbf{r}_1, \mathbf{r}_2)$ = prescribed function of $|\mathbf{r}_1 - \mathbf{r}_2|$, $0 \leq \boldsymbol{\Omega}(\mathbf{r}_1, \mathbf{r}_2) \leq 1$. The covariance used is then:

$$\mathbf{P}^{\mathrm{f,l}}_{(N)}(\mathbf{r}_1, \mathbf{r}_2) = \mathbf{P}^{\mathrm{f}}_{(N)}(\mathbf{r}_1, \mathbf{r}_2) \boldsymbol{\Omega}(\mathbf{r}_1, \mathbf{r}_2).$$

This is for a particular matrix element. For the whole covariance matrix, introduce the Schur product of matrices:

$$\mathbf{P}^{\mathrm{f,l}}_{(N)} = \mathbf{P}^{\mathrm{f}}_{(N)} \circ \boldsymbol{\Omega}, \qquad \boldsymbol{\Omega} \in \mathbb{R}^{n \times n}.$$

How do we incorporate this into the CVT?

This section is provided for information only. In outline:

- We know that $\mathbf{P}^{\mathrm{f}}_{(N)} = \frac{1}{N-1} \mathbf{X}\mathbf{X}^{\mathrm{T}}$, $\mathbf{P}^{\mathrm{f}}_{(N)} \in \mathbb{R}^{n \times n}$, $\mathbf{X} \in \mathbb{R}^{n \times N}$.
- Now suppose that we can decompose $\boldsymbol{\Omega}$ in terms of M members in $\mathbf{Y}$: $\boldsymbol{\Omega} = \frac{1}{M-1} \mathbf{Y}\mathbf{Y}^{\mathrm{T}}$, $\boldsymbol{\Omega} \in \mathbb{R}^{n \times n}$, $\mathbf{Y} \in \mathbb{R}^{n \times M}$.

- Then the localized background error covariance matrix is:

$$\begin{aligned}\mathbf{P}^{\mathrm{f,l}}_{(N)} &= \mathbf{P}^{\mathrm{f}}_{(N)} \circ \mathbf{\Omega}, \\ &= \left(\frac{1}{N-1}\mathbf{X}\mathbf{X}^{\mathrm{T}}\right) \circ \left(\frac{1}{M-1}\mathbf{Y}\mathbf{Y}^{\mathrm{T}}\right), \\ &= \frac{1}{(M-1)(N-1)}\left(\mathbf{X}\mathbf{X}^{\mathrm{T}}\right) \circ \left(\mathbf{Y}\mathbf{Y}^{\mathrm{T}}\right).\end{aligned}$$

- It is possible to construct a new matrix $\mathbf{X}_\Omega$ such that $\mathbf{P}^{\mathrm{f,l}}_{(N)} = \frac{1}{(N-1)(M-1)}\mathbf{X}_\Omega\mathbf{X}_\Omega^{\mathrm{T}}$, $\mathbf{X}_\Omega \in \mathbb{R}^{n\times NM}$.

- This new matrix has the form:

$$\mathbf{X}_\Omega = \left(\begin{array}{cccccccccc} \uparrow & \uparrow & & \uparrow & \uparrow & & \uparrow & & & \uparrow \\ \boldsymbol{\eta}_{\mathrm{B}}^{(1)} \circ \mathbf{y}^{(1)} & \boldsymbol{\eta}_{\mathrm{B}}^{(1)} \circ \mathbf{y}^{(2)} & \cdots & \boldsymbol{\eta}_{\mathrm{B}}^{(1)} \circ \mathbf{y}^{(M)} & \boldsymbol{\eta}_{\mathrm{B}}^{(2)} \circ \mathbf{y}^{(1)} & \cdots & \boldsymbol{\eta}_{\mathrm{B}}^{(2)} \circ \mathbf{y}^{(M)} & \cdots & \cdots & \boldsymbol{\eta}_{\mathrm{B}}^{(N)} \circ \mathbf{y}^{(M)} \\ \downarrow & \downarrow & & \downarrow & \downarrow & & \downarrow & & & \downarrow \end{array} \right),$$

  where $\boldsymbol{\eta}_{\mathrm{B}}^{(i)}$ is the ith column of $\mathbf{X}$ and $\mathbf{y}^{(j)}$ is the jth column of $\mathbf{X}_\Omega$. There are other compact ways to write this matrix: Buehner M., Ensemble derived stationary and flow dependent background error covariances: Evaluation in a quasi-operational NWP setting, Q.J.R.Meteor.Soc. 131 pp.1013-1043 (2005).

- The localized hybrid scheme is then the same as the unlocalized one, but with
  - the N-element part of the control vector $\delta\boldsymbol{\chi}^{\mathrm{H}}$ relaced with an NM-element control vector, and
  - $\sqrt{\frac{1-\alpha}{N-1}}\mathbf{X}$ in the CVT replaced with $\sqrt{\frac{1-\alpha}{(N-1)(M-1)}}\mathbf{X}_\Omega$.

N.B. There are other ways of representing a hyrid system in terms of control variables: Lorenc A.C., The potential of the ensemble Kalman filter for NWP - a comparison with 4d-Var, Q.J.R.Meteor.Soc. 129 pp.3183-3203 (2003).

7. Data assimilation diagnostics

- What can go wrong with a data assimilation scheme? For a strong constraint 4D-VAR, e.g.:

  - Incorrect error covariance matrices.
  - Non-Gaussian or biased errors in the background or the observations.
  - Errors in $\boldsymbol{\mathcal{M}}$, $\mathbf{h}$, $\mathbf{M}$ or $\mathbf{H}$.
  - Strong non-linearities in $\boldsymbol{\mathcal{M}}$ or $\mathbf{h}$.
  - Variational procedure not converged to the minimum.
  - Background and observation errors are correlated.

- How can we assess if a given data assimilation scheme is sub-optimal? E.g. for variational data assimilation:

  - Bennett-Talagrand diagnostic.
  - Desrozier's diagnostics.

7(a) The Bennett-Talagrand theorem[1]

Twice the cost function value at the minimum (i.e. at the analysis) for an optimal assimilation system is a random variable that obeys χ^2 statistics and therefore has a particular expectation value[2]. Statistics tells us that the expectation value of a χ^2 distribution that results from a fit of ν degrees of freedom to q pieces of data is $\mathcal{E}(2J_{\min}) = q - \nu$. The data assimilation problem tries to fit $\nu = n$ pieces of information to $q = n + p$ pieces of information (the background state and the observations). Then, $\mathcal{E}(2J_{\min}) = n + p - n = p$. Therefore the expected value of $J_{\min}$ is

$$\mathcal{E}(J_{\min}) = \frac{p}{2}.$$

If a given assimilation run does not give a value of $J_{\min}$ close to this value then it is an indication that something is wrong with the data assimilation. This can also be proved directly for the data assimilation problem (the Bennet-Talagrand theorem).

[1] Based on notes by T. Payne, Met Office

[2] For any one assimilation, there will be one value of the cost function at the minimum, so what do we mean by the "expected value of the cost function at the minimum"? Imagine doing a very large number of assimilations of the same situation, but each with slightly different backgrounds and observations (where perturbations are consistent with the background and observations error covariance matrices). This is like doing different data assimilation runs in parallel universes. The expected value of the cost function at the minimum is the average of these experiments.

This section is provided for information only. Assume a data assimilation system that is optimal (e.g. all error covariance matrices are correctly specified). Then

$$\mathbf{x}_\mathrm{a} - \mathbf{x}_\mathrm{b} = \mathbf{K}(\mathbf{y} - \mathbf{H}\mathbf{x}_\mathrm{b}) \text{ where } \mathbf{K} = \mathbf{B}\mathbf{H}^\mathrm{T}\left(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^\mathrm{T}\right). \tag{27}$$

We wish to evaluate the expected value of the cost function at its minimum, $\mathbf{x} = \mathbf{x}_\mathrm{a}$. This expected value is written $\mathcal{E}[J(\mathbf{x}_\mathrm{a})]$ and the cost function at the analysis is (given a specific background state and set of observations)

$$\begin{aligned} J(\mathbf{x}_\mathrm{a}) &= J_\mathrm{b}(\mathbf{x}_\mathrm{a}) + J_\mathrm{o}(\mathbf{x}_\mathrm{a}), & (28)\\ \text{where } J_\mathrm{b}(\mathbf{x}_\mathrm{a}) &= \frac{1}{2}\left(\mathbf{x}_\mathrm{a} - \mathbf{x}_\mathrm{b}\right)^\mathrm{T}\mathbf{B}^{-1}\left(\mathbf{x}_\mathrm{a} - \mathbf{x}_\mathrm{b}\right), & (29)\\ \text{and } J_\mathrm{o}(\mathbf{x}_\mathrm{a}) &= \frac{1}{2}\left(\mathbf{y} - \mathbf{H}\mathbf{x}_\mathrm{a}\right)^\mathrm{T}\mathbf{R}^{-1}\left(\mathbf{y} - \mathbf{H}\mathbf{x}_\mathrm{a}\right). & (30) \end{aligned}$$

The analysis, background and observation errors are (again given a specific background state and set of observations)

$$\varepsilon_\mathrm{a} = \mathbf{x}_\mathrm{a} - \mathbf{x}_\mathrm{t}, \quad \varepsilon_\mathrm{b} = \mathbf{x}_\mathrm{b} - \mathbf{x}_\mathrm{t}, \quad \varepsilon_\mathrm{o} = \mathbf{y} - \mathbf{H}\mathbf{x}_\mathrm{t}. \tag{31}$$

The analysis error can be developed as follows using (27) and (31):

$$\begin{aligned} \varepsilon_\mathrm{a} &= \mathbf{x}_\mathrm{a} - \mathbf{x}_\mathrm{b} + \varepsilon_\mathrm{b} = \mathbf{K}\left(\mathbf{y} - \mathbf{H}\mathbf{x}_\mathrm{b}\right) + \varepsilon_\mathrm{b},\\ &= \mathbf{K}\left(\mathbf{y} - \mathbf{H}(\mathbf{x}_\mathrm{b} - \mathbf{x}_\mathrm{t}) - \mathbf{H}\mathbf{x}_\mathrm{t}\right) + \varepsilon_\mathrm{b},\\ &= \mathbf{K}\left(\varepsilon_\mathrm{o} - \mathbf{H}\varepsilon_\mathrm{b}\right) + \varepsilon_\mathrm{b} = \left(\mathbf{I} - \mathbf{K}\mathbf{H}\right)\varepsilon_\mathrm{b} + \mathbf{K}\varepsilon_\mathrm{o}. \end{aligned} \tag{32}$$

Equations (29) and (30) are inner products. To evaluate them, the following identity is useful

$$\mathbf{u}^\mathrm{T}\mathbf{C}\mathbf{v} = \sum_{i,j} u_i C_{ij} v_j = \mathrm{tr}\left(\mathbf{C}\mathbf{v}\mathbf{u}^\mathrm{T}\right). \tag{33}$$

The background term

The expectation of the background term (29) is, using (33):

$$\begin{aligned} \mathcal{E}[J_\mathrm{b}(\mathbf{x}_\mathrm{a})] &= \frac{1}{2}\mathcal{E}\left[\mathrm{tr}\left(\mathbf{B}^{-1}(\mathbf{x}_\mathrm{a} - \mathbf{x}_\mathrm{b})(\mathbf{x}_\mathrm{a} - \mathbf{x}_\mathrm{b})^\mathrm{T}\right)\right] = \frac{1}{2}\mathrm{tr}\left(\mathbf{B}^{-1}\mathcal{E}\left[(\mathbf{x}_\mathrm{a} - \mathbf{x}_\mathrm{b})(\mathbf{x}_\mathrm{a} - \mathbf{x}_\mathrm{b})^\mathrm{T}\right]\right),\\ &= \frac{1}{2}\mathrm{tr}\left(\mathbf{B}^{-1}\mathcal{E}\left[(\varepsilon_\mathrm{a} - \varepsilon_\mathrm{b})(\varepsilon_\mathrm{a} - \varepsilon_\mathrm{b})^\mathrm{T}\right]\right), \end{aligned} \tag{34}$$

where (31) have been used for the last line. Part of the last line is the expression $\mathcal{E}[(\varepsilon_\mathrm{a}-\varepsilon_\mathrm{b})(\varepsilon_\mathrm{a}-\varepsilon_\mathrm{b})^\mathrm{T}]$ which may be developed using (32)

$$\begin{aligned}
\mathcal{E}\left[(\varepsilon_\mathrm{a}-\varepsilon_\mathrm{b})(\varepsilon_\mathrm{a}-\varepsilon_\mathrm{b})^\mathrm{T}\right] &= \mathcal{E}\left[\varepsilon_\mathrm{a}\varepsilon_\mathrm{a}^\mathrm{T}+\varepsilon_\mathrm{b}\varepsilon_\mathrm{b}^\mathrm{T}-\varepsilon_\mathrm{a}\varepsilon_\mathrm{b}^\mathrm{T}-\varepsilon_\mathrm{b}\varepsilon_\mathrm{a}^\mathrm{T}\right], \\
&= (\mathbf{I}-\mathbf{KH})\mathcal{E}\left[\varepsilon_\mathrm{b}\varepsilon_\mathrm{b}^\mathrm{T}\right](\mathbf{I}-\mathbf{KH})^\mathrm{T}+\mathbf{K}\mathcal{E}\left[\varepsilon_\mathrm{o}\varepsilon_\mathrm{o}^\mathrm{T}\right]\mathbf{K}^\mathrm{T}+\mathcal{E}\left[\varepsilon_\mathrm{b}\varepsilon_\mathrm{b}^\mathrm{T}\right] \\
&\quad -(\mathbf{I}-\mathbf{KH})\mathcal{E}\left[\varepsilon_\mathrm{b}\varepsilon_\mathrm{b}^\mathrm{T}\right]-\mathcal{E}\left[\varepsilon_\mathrm{b}\varepsilon_\mathrm{b}^\mathrm{T}\right](\mathbf{I}-\mathbf{KH})^\mathrm{T}, \\
&= (\mathbf{I}-\mathbf{KH})\mathbf{B}(\mathbf{I}-\mathbf{KH})^\mathrm{T}+\mathbf{KRK}^\mathrm{T}+\mathbf{B}-(\mathbf{I}-\mathbf{KH})\mathbf{B}-\mathbf{B}(\mathbf{I}-\mathbf{KH})^\mathrm{T}, \\
&= \mathbf{B}+\mathbf{KHB}(\mathbf{KH})^\mathrm{T}-\mathbf{B}(\mathbf{KH})^\mathrm{T}-\mathbf{KHB}+\mathbf{KRK}^\mathrm{T}+\mathbf{B}-\mathbf{B} \\
&\quad +\mathbf{KHB}-\mathbf{B}+\mathbf{B}(\mathbf{KH})^\mathrm{T}, \\
&= \mathbf{KHB}(\mathbf{KH})^\mathrm{T}+\mathbf{KRK}^\mathrm{T}.
\end{aligned}$$

These steps assume that background and observation errors are mutually uncorrelated. Using the definition of $\mathbf{K}$ (27) turns the above into:

$$\begin{aligned}
\mathcal{E}\left[(\varepsilon_\mathrm{a}-\varepsilon_\mathrm{b})(\varepsilon_\mathrm{a}-\varepsilon_\mathrm{b})^\mathrm{T}\right] &= \mathbf{BH}^\mathrm{T}(\mathbf{HBH}^\mathrm{T}+\mathbf{R})^{-1}\mathbf{HB}(\mathbf{BH}^\mathrm{T}(\mathbf{HBH}^\mathrm{T}+\mathbf{R})^{-1}\mathbf{H})^\mathrm{T} \\
&\quad +\mathbf{BH}^\mathrm{T}(\mathbf{HBH}^\mathrm{T}+\mathbf{R})^{-1}\mathbf{R}(\mathbf{BH}^\mathrm{T}(\mathbf{HBH}^\mathrm{T}+\mathbf{R})^{-1})^\mathrm{T}, \\
&= \mathbf{BH}^\mathrm{T}(\mathbf{HBH}^\mathrm{T}+\mathbf{R})^{-1}\mathbf{HBH}^\mathrm{T}(\mathbf{HBH}^\mathrm{T}+\mathbf{R})^{-1}\mathbf{HB} \\
&\quad +\mathbf{BH}^\mathrm{T}(\mathbf{HBH}^\mathrm{T}+\mathbf{R})^{-1}\mathbf{R}(\mathbf{HBH}^\mathrm{T}+\mathbf{R})^{-1}\mathbf{HB}, \\
&= \mathbf{BH}^\mathrm{T}(\mathbf{HBH}^\mathrm{T}+\mathbf{R})^{-1}\mathbf{HB}=\mathbf{KHB}.
\end{aligned}$$

Inserting this into (34) gives

$$\mathcal{E}[J_\mathrm{b}(\mathbf{x}_\mathrm{a})] = \frac{1}{2}\mathrm{tr}(\mathbf{B}^{-1}\mathbf{KHB}). \tag{35}$$

Note the following identity, which holds for matrices $\mathbf{E}$ and $\mathbf{F}$, where $\mathbf{E}$ is $r\times s$ and $\mathbf{F}$ is $s\times r$

$$\mathrm{tr}(\mathbf{EF})=\sum_{j=1}^{r}\sum_{i=1}^{s}E_{ji}F_{ij}=\sum_{i=1}^{s}\sum_{j=1}^{r}F_{ij}E_{ji}=\mathrm{tr}(\mathbf{FE}), \tag{36}$$

i.e., the order of the operators inside the trace can be reversed. Applying this to (35) gives

$$E[J_\mathrm{b}(\mathbf{x}_\mathrm{a})]=\frac{1}{2}\mathrm{tr}(\mathbf{KH}). \tag{37}$$

The observation term

The expectation of the observation term (30) is, using (33):

$$\begin{aligned}
\mathcal{E}[J_{\rm o}(\mathbf{x}_{\rm a})] &= \frac{1}{2}\mathcal{E}\left[\mathrm{tr}\left(\mathbf{R}^{-1}(\mathbf{y}-\mathbf{H}\mathbf{x}_{\rm a})(\mathbf{y}-\mathbf{H}\mathbf{x}_{\rm a})^{\rm T}\right)\right], \\
&= \frac{1}{2}\mathrm{tr}\left(\mathbf{R}^{-1}\mathcal{E}\left[(\mathbf{y}-\mathbf{H}\mathbf{x}_{\rm a})(\mathbf{y}-\mathbf{H}\mathbf{x}_{\rm a})^{\rm T}\right]\right), \\
&= \frac{1}{2}\mathrm{tr}\left(\mathbf{R}^{-1}\mathcal{E}\left[(\varepsilon_{\rm o}-\mathbf{H}\varepsilon_{\rm a})(\varepsilon_{\rm o}-\mathbf{H}\varepsilon_{\rm a})^{\rm T}\right]\right). \qquad (38)
\end{aligned}$$

where (31) have been used for the last line. Part of the last line is the expression $\mathcal{E}[(\varepsilon_{\rm o}-\mathbf{H}\varepsilon_{\rm a})(\varepsilon_{\rm o}-\mathbf{H}\varepsilon_{\rm a})^{\rm T}]$ which may be developed using (32):

$$\begin{aligned}
\mathcal{E}[(\varepsilon_{\rm o}-\mathbf{H}\varepsilon_{\rm a})(\varepsilon_{\rm o}-\mathbf{H}\varepsilon_{\rm a})^{\rm T}] &= \mathbf{H}\mathcal{E}[\varepsilon_{\rm a}\varepsilon_{\rm a}^{\rm T}]\mathbf{H}^{\rm T}+\mathcal{E}[\varepsilon_{\rm o}\varepsilon_{\rm o}^{\rm T}]-\mathbf{H}\mathcal{E}[\varepsilon_{\rm a}\varepsilon_{\rm o}^{\rm T}]-\mathcal{E}[\varepsilon_{\rm o}\varepsilon_{\rm a}^{\rm T}]\mathbf{H}^{\rm T}, \\
&= \mathbf{H}\{(\mathbf{I}-\mathbf{K}\mathbf{H})\mathcal{E}[\varepsilon_{\rm b}\varepsilon_{\rm b}^{\rm T}](\mathbf{I}-\mathbf{K}\mathbf{H})^{\rm T}+\mathbf{K}\mathcal{E}[\varepsilon_{\rm o}\varepsilon_{\rm o}^{\rm T}]\mathbf{K}^{\rm T}\}\mathbf{H}^{\rm T} \\
&\quad +\mathcal{E}[\varepsilon_{\rm o}\varepsilon_{\rm o}^{\rm T}]-\mathbf{H}\mathbf{K}\mathcal{E}[\varepsilon_{\rm o}\varepsilon_{\rm o}^{\rm T}]-\mathcal{E}[\varepsilon_{\rm o}\varepsilon_{\rm o}^{\rm T}]\mathbf{K}^{\rm T}\mathbf{H}^{\rm T}, \\
&= \mathbf{H}\{(\mathbf{I}-\mathbf{K}\mathbf{H})\mathbf{B}(\mathbf{I}-\mathbf{K}\mathbf{H})^{\rm T}+\mathbf{K}\mathbf{R}\mathbf{K}^{\rm T}\}\mathbf{H}^{\rm T}+\mathbf{R}-\mathbf{H}\mathbf{K}\mathbf{R}-\mathbf{R}\mathbf{K}^{\rm T}\mathbf{H}^{\rm T}, \\
&= \mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}+\mathbf{H}\mathbf{K}\mathbf{H}\mathbf{B}(\mathbf{K}\mathbf{H})^{\rm T}\mathbf{H}^{\rm T}-\mathbf{H}\mathbf{B}(\mathbf{K}\mathbf{H})^{\rm T}\mathbf{H}^{\rm T}-\mathbf{H}\mathbf{K}\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T} \\
&\quad +\mathbf{H}\mathbf{K}\mathbf{R}\mathbf{K}^{\rm T}\mathbf{H}^{\rm T}+\mathbf{R}-\mathbf{H}\mathbf{K}\mathbf{R}-\mathbf{R}\mathbf{K}^{\rm T}\mathbf{H}^{\rm T}.
\end{aligned}$$

These steps assume that background and observation errors are mutually uncorrelated. Using the definition of $\mathbf{K}$ (27):

$$\begin{aligned}
\mathcal{E}[(\varepsilon_{\rm o}-\mathbf{H}\varepsilon_{\rm a})(\varepsilon_{\rm o}-\mathbf{H}\varepsilon_{\rm a})^{\rm T}] &= \mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}+\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}(\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}+\mathbf{R})^{-1}\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}(\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}+\mathbf{R})^{-1}\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T} \\
&\quad -\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}(\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}+\mathbf{R})^{-1}\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}-\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}(\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}+\mathbf{R})^{-1}\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T} \\
&\quad +\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}(\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}+\mathbf{R})^{-1}\mathbf{R}(\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}+\mathbf{R})^{-1}\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}+\mathbf{R} \\
&\quad -\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}(\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}+\mathbf{R})^{-1}\mathbf{R}-\mathbf{R}(\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}+\mathbf{R})^{-1}\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}.
\end{aligned}$$

Merging the 2nd and 5th terms leads to

$$\begin{aligned}
\mathcal{E}[(\varepsilon_{\rm o}-\mathbf{H}\varepsilon_{\rm a})(\varepsilon_{\rm o}-\mathbf{H}\varepsilon_{\rm a})^{\rm T}] &= \mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}+\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}(\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}+\mathbf{R})^{-1}\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T} \\
&\quad -\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}(\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}+\mathbf{R})^{-1}\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}-\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}(\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}+\mathbf{R})^{-1}\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T} \\
&\quad +\mathbf{R}-\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}(\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}+\mathbf{R})^{-1}\mathbf{R}-\mathbf{R}(\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}+\mathbf{R})^{-1}\mathbf{H}\mathbf{B}\mathbf{H}^{\rm T}.
\end{aligned}$$

Further simplifications can be made by merging the 3rd and 6th terms and the 4th and 7th terms

$$\begin{aligned}\mathcal{E}[(\varepsilon_{\rm o}-\mathbf{H}\varepsilon_{\rm a})(\varepsilon_{\rm o}-\mathbf{H}\varepsilon_{\rm a})^{\rm T}] &= \mathbf{HBH}^{\rm T}+\mathbf{HBH}^{\rm T}(\mathbf{HBH}^{\rm T}+\mathbf{R})^{-1}\mathbf{HBH}^{\rm T}-\mathbf{HBH}^{\rm T}-\mathbf{HBH}^{\rm T}+\mathbf{R},\\ &= \mathbf{HBH}^{\rm T}\left\{(\mathbf{HBH}^{\rm T}+\mathbf{R})^{-1}\mathbf{HBH}^{\rm T}-\mathbf{I}\right\}+\mathbf{R}. \end{aligned} \tag{39}$$

Consider the term inside the curly brackets in the above:

$$\begin{aligned}(\mathbf{HBH}^{\rm T}+\mathbf{R})^{-1}\mathbf{HBH}^{\rm T}-\mathbf{I} &= (\mathbf{HBH}^{\rm T}+\mathbf{R})^{-1}\mathbf{HBH}^{\rm T}-(\mathbf{HBH}^{\rm T}+\mathbf{R})^{-1}(\mathbf{HBH}^{\rm T}+\mathbf{R}),\\ &= (\mathbf{HBH}^{\rm T}+\mathbf{R})^{-1}[\mathbf{HBH}^{\rm T}-\mathbf{HBH}^{\rm T}-\mathbf{R}],\\ &= -(\mathbf{HBH}^{\rm T}+\mathbf{R})^{-1}\mathbf{R}.\end{aligned}$$

Using this to rewrite (39):

$$\mathcal{E}[(\varepsilon_{\rm o}-\mathbf{H}\varepsilon_{\rm a})(\varepsilon_{\rm o}-\mathbf{H}\varepsilon_{\rm a})^{\rm T}] = -\mathbf{HBH}^{\rm T}(\mathbf{HBH}^{\rm T}+\mathbf{R})^{-1}\mathbf{R}+\mathbf{R},$$

and then substituting this into (38) and then using (36) gives

$$\begin{aligned}\mathcal{E}[J_{\rm o}(\mathbf{x}_{\rm a})] &= \frac{1}{2}{\rm tr}\left(\mathbf{R}^{-1}[-\mathbf{HBH}^{\rm T}(\mathbf{HBH}^{\rm T}+\mathbf{R})^{-1}\mathbf{R}+\mathbf{R}]\right),\\ &= \frac{1}{2}{\rm tr}\left(-\mathbf{HBH}^{\rm T}(\mathbf{HBH}^{\rm T}+\mathbf{R})^{-1}+\mathbf{I}\right),\\ &= \frac{1}{2}{\rm tr}\left(-\mathbf{HK}+\mathbf{I}\right)=\frac{1}{2}\left(-{\rm tr}(\mathbf{HK})+p\right)=\frac{1}{2}\left(-{\rm tr}(\mathbf{KH})+p\right),\end{aligned} \tag{40}$$

where p is the number of observations.

The sum of the background and observation terms

The sum of the background and observation terms is (using (28), (37) and (40)):

$$\mathcal{E}(J(\mathbf{x}_{\rm a})) = \mathcal{E}(J_{\rm b}(\mathbf{x}_{\rm a}))+\mathcal{E}(J_{\rm o}(\mathbf{x}_{\rm a}))=\frac{1}{2}\left({\rm tr}(\mathbf{KH})-{\rm tr}(\mathbf{KH})+p\right)=\frac{p}{2}.$$

This is a very involved derivation, but leads to the very simple result that the expectation of the minimum of the cost function has value equal to half the number of observations. Some people have called this the Bennett-Talagrand theorem. If the value of the cost function at the minimum does not have this value in practice then this is an indication that the error characteristics of the data assimilation do not match those of the actual data, or other things are wrong with the set-up like the forward operator, $\mathbf{H}$. Note that this result applies to systems that are Gaussian and linear.

Desrozier's Diagnostics[3]

Desrozier diagnostics use the following quantities calculated for a data assimilation run (all in observation space):

- Innovations (observation minus background): $\mathbf{d}_{\mathrm{b}}^{\mathrm{o}} = \mathbf{y} - \mathbf{H}\mathbf{x}_{\mathrm{b}}$.
- Analysis increment (analysis minus background):$\mathbf{d}_{\mathrm{b}}^{\mathrm{a}} = \mathbf{H}\delta\mathbf{x}_{\mathrm{a}}$.
- Residuals (observation minus analysis): $\mathbf{d}_{\mathrm{a}}^{\mathrm{o}} = \mathbf{y} - \mathbf{H}\mathbf{x}_{\mathrm{a}}$.

The covariances of these quantities reveals the consistency (or inconsistency) of the data assimilation. E.g. for 3D-VAR:

Covariance	Actual result (sub-optimal)	Result if optimal
$\mathcal{E}\{\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}\mathrm{T}}\}$	$\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}$	$\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}$
$\mathcal{E}\{\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}\mathrm{T}}\}$	$\mathbf{H}\hat{\mathbf{B}}\mathbf{H}^{\mathrm{T}}(\mathbf{H}\hat{\mathbf{B}}\mathbf{H}^{\mathrm{T}} + \hat{\mathbf{R}})^{-1}(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}})$	$\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}$
$\mathcal{E}\{\mathbf{d}_{\mathrm{a}}^{\mathrm{o}}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}\mathrm{T}}\}$	$(\mathbf{I} - \mathbf{H}\hat{\mathbf{B}}\mathbf{H}^{\mathrm{T}}(\mathbf{H}\hat{\mathbf{B}}\mathbf{H}^{\mathrm{T}} + \hat{\mathbf{R}})^{-1})(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}})$	$\mathbf{R}$
$\mathcal{E}\{\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}\mathbf{d}_{\mathrm{a}}^{\mathrm{o}\mathrm{T}}\}$	$\mathbf{H}\hat{\mathbf{B}}\mathbf{H}^{\mathrm{T}}(\mathbf{H}\hat{\mathbf{B}}\mathbf{H}^{\mathrm{T}} + \hat{\mathbf{R}})^{-1}(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}})(\mathbf{I} - \mathbf{H}\hat{\mathbf{B}}\mathbf{H}^{\mathrm{T}}(\mathbf{H}\hat{\mathbf{B}}\mathbf{H}^{\mathrm{T}} + \hat{\mathbf{R}})^{-1})^{\mathrm{T}}$	$\mathbf{H}\mathbf{A}\mathbf{H}^{\mathrm{T}}$

Here $\mathbf{B}$ and $\mathbf{R}$ are the true background and observation error covariances matrices, and $\hat{\mathbf{B}}$ and $\hat{\mathbf{R}}$ are the ones assumed for the data assimilation. $\mathbf{H}$ is assumed perfect.

This section is provided for information only. Proofs of these results are as follows. Consider a sub-optimal variational data assimilation scheme where the specified statistics (indicated with hats) may have been given incorrectly. Consider the following analysis increment that result:

$$\delta\mathbf{x}_{\mathrm{a}} = \mathbf{x}_{\mathrm{a}} - \mathbf{x}_{\mathrm{b}} = \hat{\mathbf{K}}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}},$$

where the Kalman gain used in the assimilation is

$$\hat{\mathbf{K}} = \hat{\mathbf{B}}\mathbf{H}^{\mathrm{T}}(\mathbf{H}\hat{\mathbf{B}}\mathbf{H}^{\mathrm{T}} + \hat{\mathbf{R}})^{-1}, \tag{41}$$

and $\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}$ is the innovation vector (observation minus background - see below). $\hat{\mathbf{B}}$ and $\hat{\mathbf{R}}$ are the (potentially incorrect) background and observation error covariance matrices that are actually specified in the data assimilation (and $\hat{\mathbf{K}}$ is the Kalman gain that

[3]Desroziers G., Berre L., Chapnik B., Poli P., 2005, Diagnostics of observation, background and analysis-error statistics in observation space. Q.J.R. Meteorol. Soc. 131, 3385-3396.

follows). $\mathbf{B}$ and $\mathbf{R}$ (without the hats) are the correct background and observation error covariance matrices and $\mathbf{K}$ is the correct Kalman gain (27) that follows. We now examine various 'difference statistics' in observation space.

O-B, A-B, O-A expressions

The 'observation minus background' difference in observation space is:

$$\mathbf{d}^{\mathrm{o}}_{\mathrm{b}} = \mathbf{y} - \mathbf{H}\mathbf{x}_{\mathrm{b}} \approx \varepsilon_{\mathrm{o}} - \mathbf{H}\varepsilon_{\mathrm{b}}, \tag{42}$$

where ε_{o} is the observation error, and ε_{b} is the background error as in (31). We now express other important differences in terms of the innovations. The 'analysis minus background' difference in observation space is:

$$\mathbf{d}^{\mathrm{a}}_{\mathrm{b}} = \mathbf{H}\delta\mathbf{x}_{\mathrm{a}} = \mathbf{H}\hat{\mathbf{K}}\mathbf{d}^{\mathrm{o}}_{\mathrm{b}}, \tag{43}$$

and the 'observation minus analysis' difference in observation space is:

$$\begin{aligned} \mathbf{d}^{\mathrm{o}}_{\mathrm{a}} &= \mathbf{y} - \mathbf{H}\mathbf{x}_{\mathrm{a}} = \mathbf{y} - \mathbf{H}(\mathbf{x}_{\mathrm{b}} + \delta\mathbf{x}_{\mathrm{a}}) \\ &= \mathbf{d}^{\mathrm{o}}_{\mathrm{b}} - \mathbf{H}\hat{\mathbf{K}}\mathbf{d}^{\mathrm{o}}_{\mathrm{b}} = (\mathbf{I} - \mathbf{H}\hat{\mathbf{K}})\mathbf{d}^{\mathrm{o}}_{\mathrm{b}}. \end{aligned} \tag{44}$$

The vector $\mathbf{d}^{\mathrm{o}}_{\mathrm{b}}$ is otherwise known as the 'innovation vector' and the vector $\mathbf{d}^{\mathrm{o}}_{\mathrm{a}}$ is otherwise known as the 'residual vector'. The key thing is that these vectors are measurable directly from an existing data assimilation system. We will now use their equivalents in the above to see what we can learn about the system.

Measured statistics

Now we have these expressions, let us look at their covariance statistics.

O-B \ O-B statistics Assuming that background and observation errors are uncorrelated, the covariance matrix between $\mathbf{d}^{\mathrm{o}}_{\mathrm{b}}$ and $\mathbf{d}^{\mathrm{o}}_{\mathrm{b}}$ are[4]:

$$\begin{aligned} \mathcal{E}\{\mathbf{d}^{\mathrm{o}}_{\mathrm{b}}\mathbf{d}^{\mathrm{o}\mathrm{T}}_{\mathrm{b}}\} &= \mathcal{E}\{(\varepsilon_{\mathrm{o}} - \mathbf{H}\varepsilon_{\mathrm{b}})(\varepsilon_{\mathrm{o}} - \mathbf{H}\varepsilon_{\mathrm{b}})^{\mathrm{T}}\}, \\ &= \mathcal{E}\{\varepsilon_{\mathrm{o}}\varepsilon^{\mathrm{T}}_{\mathrm{o}}\} - \mathcal{E}\{\varepsilon_{\mathrm{o}}\varepsilon^{\mathrm{T}}_{\mathrm{b}}\}\mathbf{H}^{\mathrm{T}} - \mathbf{H}\mathcal{E}\{\varepsilon_{\mathrm{b}}\varepsilon^{\mathrm{T}}_{\mathrm{o}}\} + \mathbf{H}\mathcal{E}\{\varepsilon_{\mathrm{b}}\varepsilon^{\mathrm{T}}_{\mathrm{b}}\}\mathbf{H}^{\mathrm{T}}, \\ &= \mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}. \end{aligned} \tag{45}$$

[4]The $\mathcal{E}$ operator performs an average over a population of realizations of the assimilation system (as though we had access to results from parallel universes). In practice though we do not have access to parallel universes so instead the average is taken between pairs of different observations that have (say) similar separations.

A-B \ O-B statistics Using (43), (45) and (41), the covariance matrix between $\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}$ and $\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}$ are:

$$\begin{aligned}\mathcal{E}\{\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}\mathrm{T}}\} &= \mathbf{H}\hat{\mathbf{K}}\mathcal{E}\{\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}\mathrm{T}}\} = \mathbf{H}\hat{\mathbf{K}}(\mathbf{R}+\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}),\\ &= \mathbf{H}\hat{\mathbf{B}}\mathbf{H}^{\mathrm{T}}(\mathbf{H}\hat{\mathbf{B}}\mathbf{H}^{\mathrm{T}}+\hat{\mathbf{R}})^{-1}(\mathbf{R}+\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}).\end{aligned}$$

If $\hat{\mathbf{B}} = \mathbf{B}$ and $\hat{\mathbf{R}} = \mathbf{R}$ then this becomes

$$\mathcal{E}\{\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}\mathrm{T}}\} = \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}(\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}+\mathbf{R})^{-1}(\mathbf{R}+\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}) = \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}. \tag{46}$$

O-A \ O-B statistics Using (44), (45) and (41), the covariance matrix between $\mathbf{d}_{\mathrm{a}}^{\mathrm{o}}$ and $\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}$ are:

$$\begin{aligned}\mathcal{E}\{\mathbf{d}_{\mathrm{a}}^{\mathrm{o}}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}\mathrm{T}}\} &= (\mathbf{I}-\mathbf{H}\hat{\mathbf{K}})\mathcal{E}\{\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}\mathrm{T}}\} = (\mathbf{I}-\mathbf{H}\hat{\mathbf{K}})(\mathbf{R}+\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}),\\ &= (\mathbf{I}-\mathbf{H}\hat{\mathbf{B}}\mathbf{H}^{\mathrm{T}}(\mathbf{H}\hat{\mathbf{B}}\mathbf{H}^{\mathrm{T}}+\hat{\mathbf{R}})^{-1})(\mathbf{R}+\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}).\end{aligned}$$

If $\hat{\mathbf{B}} = \mathbf{B}$ and $\hat{\mathbf{R}} = \mathbf{R}$ then this becomes:

$$\mathcal{E}\{\mathbf{d}_{\mathrm{a}}^{\mathrm{o}}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}\mathrm{T}}\} = (\mathbf{I}-\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}(\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}+\mathbf{R})^{-1})(\mathbf{R}+\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}) = \mathbf{R}. \tag{47}$$

A-B \ O-A statistics Using (43), (44), (45) and (41), the covariance matrix between $\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}$ and $\mathbf{d}_{\mathrm{a}}^{\mathrm{o}}$ are:

$$\begin{aligned}\mathcal{E}\{\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}\mathbf{d}_{\mathrm{a}}^{\mathrm{o}\mathrm{T}}\} &= \mathbf{H}\hat{\mathbf{K}}\mathcal{E}\{\mathbf{d}_{\mathrm{b}}^{\mathrm{o}}\mathbf{d}_{\mathrm{b}}^{\mathrm{o}\mathrm{T}}\}(\mathbf{I}-\mathbf{H}\hat{\mathbf{K}})^{\mathrm{T}} = \mathbf{H}\hat{\mathbf{K}}(\mathbf{R}+\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}})(\mathbf{I}-\mathbf{H}\hat{\mathbf{K}})^{\mathrm{T}},\\ &= \mathbf{H}\hat{\mathbf{B}}\mathbf{H}^{\mathrm{T}}(\mathbf{H}\hat{\mathbf{B}}\mathbf{H}^{\mathrm{T}}+\hat{\mathbf{R}})^{-1}(\mathbf{R}+\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}})(\mathbf{I}-\mathbf{H}\hat{\mathbf{B}}\mathbf{H}^{\mathrm{T}}(\mathbf{H}\hat{\mathbf{B}}\mathbf{H}^{\mathrm{T}}+\hat{\mathbf{R}})^{-1})^{\mathrm{T}}.\end{aligned}$$

If $\hat{\mathbf{B}} = \mathbf{B}$ and $\hat{\mathbf{R}} = \mathbf{R}$ then this becomes:

$$\mathcal{E}\{\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}\mathbf{d}_{\mathrm{a}}^{\mathrm{o}\mathrm{T}}\} = \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}(\mathbf{I}-\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}(\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}+\mathbf{R})^{-1})^{\mathrm{T}}.$$

By writing $\mathbf{I} = (\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}+\mathbf{R})(\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}+\mathbf{R})^{-1}$ then the above becomes:

$$\begin{aligned}\mathcal{E}\{\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}\mathbf{d}_{\mathrm{a}}^{\mathrm{o}\mathrm{T}}\} &= \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}((\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}+\mathbf{R})(\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}+\mathbf{R})^{-1}-\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}(\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}+\mathbf{R})^{-1})^{\mathrm{T}},\\ &= \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}([\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}+\mathbf{R}-\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}](\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}+\mathbf{R})^{-1})^{\mathrm{T}},\\ &= \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}(\mathbf{R}(\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}+\mathbf{R})^{-1})^{\mathrm{T}},\\ &= \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}(\mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}+\mathbf{R})^{-1}\mathbf{R}.\end{aligned}$$

Note that the inverse Hessian has the form $\mathbf{A}^{-1} = \mathbf{B}^{-1} + \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}$ and the Sherman-Morrison-Woodbury formula in terms of $\mathbf{A}^{-1}$ is $\mathbf{A}^{-1}\mathbf{B}\mathbf{H}^{\mathrm{T}} = \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}})$. This makes the above into:

$$\mathcal{E}\{\mathbf{d}_{\mathrm{b}}^{\mathrm{a}}\mathbf{d}_{\mathrm{a}}^{\mathrm{o}\mathrm{T}}\} = \mathbf{H}\mathbf{A}\mathbf{H}^{\mathrm{T}}, \tag{48}$$

which is the analysis error covariance matrix in observation space.

These results are important because they allow the error statistics to be checked. If (46), (47) or (48) are not satisfied then the assumptions that $\hat{\mathbf{B}} = \mathbf{B}$ and $\hat{\mathbf{R}} = \mathbf{R}$ may not be correct. Even in this case, these equations can help us to improve the error statistics in the ways discussed in the Desroziers et al. paper.