

Assimilation Algorithms

Lecture 2: 3D-Var

Sébastien Massart

ECMWF

17 March 2025

Outline

- 1 From Optimal Interpolation to 3D-Var
- 2 The Maximum Likelihood Approach
- 3 Minimisation
- 4 Summary

Outline

- 1 From Optimal Interpolation to 3D-Var
- 2 The Maximum Likelihood Approach
- 3 Minimisation
- 4 Summary

From Optimal Interpolation to 3D-Var

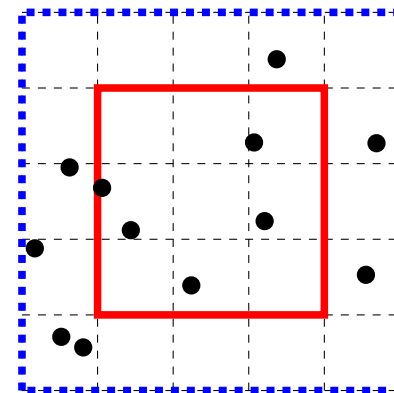
- ✘ Previously in “Assimilation Algorithms”: **linear analysis equation**

$$\mathbf{x}_a = \mathbf{x}_b + \mathbf{K}[\mathbf{y} - \mathcal{H}(\mathbf{x}_b)]$$

where

$$\mathbf{K} = \mathbf{P}^b \mathbf{H}^T [\mathbf{H} \mathbf{P}^b \mathbf{H}^T + \mathbf{R}]^{-1} \equiv [\mathbf{P}^{b-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H}]^{-1} \mathbf{H}^T \mathbf{R}^{-1}$$

- ✘ Optimal Interpolation (OI) applies **direct solution methods** to invert the matrix $[\mathbf{H} \mathbf{P}^b \mathbf{H}^T + \mathbf{R}]$.
- ✘ Data selection is applied to reduce the dimension of the matrix.
- ✘ Direct methods require access to the matrix elements. In particular, $\mathbf{H} \mathbf{P}^b \mathbf{H}^T$ must be available in matrix form.
- ✘ This limits us to very simple observation operators.



Analysis box
Used observations
Selection area

From Optimal Interpolation to 3D-Var

✘ Linear analysis equation: $\mathbf{x}_a = \mathbf{x}_b + \mathbf{K} [\mathbf{y} - \mathcal{H}(\mathbf{x}_b)]$

✘ For $\mathbf{K} = \mathbf{P}^b \mathbf{H}^T [\mathbf{H} \mathbf{P}^b \mathbf{H}^T + \mathbf{R}]^{-1}$

we have $\mathbf{x}_a = \mathbf{x}_b + \mathbf{P}^b \mathbf{H}^T [\mathbf{H} \mathbf{P}^b \mathbf{H}^T + \mathbf{R}]^{-1} [\mathbf{y} - \mathcal{H}(\mathbf{x}_b)]$

if $\mathbf{z} = [\mathbf{H} \mathbf{P}^b \mathbf{H}^T + \mathbf{R}]^{-1} [\mathbf{y} - \mathcal{H}(\mathbf{x}_b)]$

we have to solve $[\mathbf{H} \mathbf{P}^b \mathbf{H}^T + \mathbf{R}] \mathbf{z} = \mathbf{y} - \mathcal{H}(\mathbf{x}_b)$

and then $\mathbf{x}_a = \mathbf{x}_b + \mathbf{P}^b \mathbf{H}^T \mathbf{z}$

From Optimal Interpolation to 3D-Var

✘ Linear analysis equation: $\mathbf{x}_a = \mathbf{x}_b + \mathbf{K}[\mathbf{y} - \mathcal{H}(\mathbf{x}_b)]$

✘ For $\mathbf{K} = \left[\mathbf{P}^{b-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} \right]^{-1} \mathbf{H}^T \mathbf{R}^{-1}$

we have $\mathbf{x}_a = \mathbf{x}_b + \left[\mathbf{P}^{b-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} \right]^{-1} \mathbf{H}^T \mathbf{R}^{-1} [\mathbf{y} - \mathcal{H}(\mathbf{x}_b)]$

if $\delta \mathbf{x} = \left[\mathbf{P}^{b-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} \right]^{-1} \mathbf{H}^T \mathbf{R}^{-1} [\mathbf{y} - \mathcal{H}(\mathbf{x}_b)]$

we have to solve $\left[\mathbf{P}^{b-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} \right] \delta \mathbf{x} = \mathbf{H}^T \mathbf{R}^{-1} [\mathbf{y} - \mathcal{H}(\mathbf{x}_b)]$

and then $\mathbf{x}_a = \mathbf{x}_b + \delta \mathbf{x}$

From Optimal Interpolation to 3D-Var

- ✘ There are two forms to solve the linear analysis equation, depending which expression we adopt for \mathbf{K} :
- ✘ For $\mathbf{K} = \mathbf{P}^b \mathbf{H}^T [\mathbf{H} \mathbf{P}^b \mathbf{H}^T + \mathbf{R}]^{-1}$ we have $\mathbf{x}_a = \mathbf{x}_b + \mathbf{P}^b \mathbf{H}^T \mathbf{z}$ and:

$$[\mathbf{H} \mathbf{P}^b \mathbf{H}^T + \mathbf{R}] \mathbf{z} = \mathbf{y} - \mathcal{H}(\mathbf{x}_b)$$

- ✘ For $\mathbf{K} = [\mathbf{P}^{b^{-1}} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H}]^{-1} \mathbf{H}^T \mathbf{R}^{-1}$, we have $\mathbf{x}_a = \mathbf{x}_b + \delta \mathbf{x}$ and:

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

- ✘ The linear analysis equation could be solved as an equation of the form:

$$\mathbf{A} \mathbf{x} = \mathbf{b} .$$

- ✘ The first of these alternatives is called **PSAS** (Physical-space Statistical Analysis System)
- ✘ The second (although it may not look like it yet) is **3D-Var**

From Optimal Interpolation to 3D-Var

Problem

- ✘ Find the solution \mathbf{x}_a of the linear system:

$$\mathbf{Ax} = \mathbf{b}.$$

Direct methods

- ✘ Direct methods attempt to solve the problem by a finite sequence of operations.
- ✘ In the absence of rounding errors, direct methods would deliver an exact solution \mathbf{x}_a of the linear system.

Iterative methods

- ✘ Beginning with an approximation to the solution \mathbf{x}_0 , an iterative method is a mathematical procedure that generates a sequence of improving approximate solutions $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$.
- ✘ The n-th approximation is derived from the previous ones.
- ✘ The sequence of solutions converges to the exact solution.

From Optimal Interpolation to 3D-Var

Iterative methods have significant advantages over the direct methods used in Optimal Interpolation (OI):

- ✘ They can be applied to much larger problems than direct techniques, so we can avoid data selection.
- ✘ They do not require access to the matrix elements.
- ✘ Typically, to solve $\mathbf{Ax} = \mathbf{b}$, requires only the ability to calculate matrix-vector products: \mathbf{Ax} .
- ✘ This allows us to use operators defined by pieces of code rather than explicitly as matrices.
- ✘ Examples of such operators include radiative-transfer codes, numerical models, Fourier transforms, etc.

Example: Conjugate Gradients

To solve $\mathbf{Ax} = \mathbf{b}$, where \mathbf{A} is real, symmetric and positive-definite:

$$\mathbf{r}_0 := \mathbf{b} - \mathbf{Ax}_0 \quad \mathbf{p}_0 := \mathbf{r}_0 \quad k := 0 ;$$

while \mathbf{r}_{k+1} *is too large* **do**

```
/* Step in the direction of  $\mathbf{p}_k$  */
```

$$\alpha_k := \frac{\mathbf{r}_k^T \mathbf{r}_k}{\mathbf{p}_k^T \mathbf{A} \mathbf{p}_k} ;$$

```
/* New state */
```

$$\mathbf{x}_{k+1} := \mathbf{x}_k + \alpha_k \mathbf{p}_k ;$$

```
/* New residual */
```

$$\mathbf{r}_{k+1} := \mathbf{r}_k - \alpha_k \mathbf{A} \mathbf{p}_k ;$$

```
/* New direction of descent */
```

$$\beta_k := \frac{\mathbf{r}_{k+1}^T \mathbf{r}_{k+1}}{\mathbf{r}_k^T \mathbf{r}_k} ;$$

$$\mathbf{p}_{k+1} := \mathbf{r}_{k+1} + \beta_k \mathbf{p}_k ;$$

```
/* Next iteration */
```

$$k := k + 1 ;$$

end

The result is \mathbf{x}_{k+1}

Outline

- 1 From Optimal Interpolation to 3D-Var
- 2 The Maximum Likelihood Approach**
- 3 Minimisation
- 4 Summary

3D-Var

- ✘ As we have seen, (linear) 3D-Var analysis can be seen as an application of iterative solution methods to the linear analysis equation.
- ✘ Historically, 3D-Var was not developed this way.
- ✘ We will now consider this alternative derivation.
- ✘ We will need to apply **Bayes' theorem**:

$$p(A|B) = \frac{p(B|A)p(A)}{p(B)}$$

where $p(A|B)$ is the probability of A given B , etc.

Maximum Likelihood

- ✘ We developed the linear analysis equation by searching for a linear combination of observation and background that minimised the variance of the error.
- ✘ An alternative approach is to look for the most probable solution \mathbf{x}_a , given the observations \mathbf{Y} and having a prior knowledge \mathbf{x}_b on the solution:

$$\mathbf{x}_a = \arg \max_{\mathbf{x}} [p(\mathbf{x}|\mathbf{y})]$$

- ✘ It will be convenient to define a **cost function**

$$J(\mathbf{x}) = -\log [p(\mathbf{x}|\mathbf{y})] + \text{const.}$$

- ✘ Then, since log is a monotonic function:

$$\mathbf{x}_a = \arg \min_{\mathbf{x}} [J(\mathbf{x})]$$

Maximum Likelihood

- ✘ Applying Bayes' theorem gives:

$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{x})p(\mathbf{x})}{p(\mathbf{y})} \propto p(\mathbf{y}|\mathbf{x})p(\mathbf{x})$$

- ✘ The maximum likelihood approach is applicable to any probability density functions $p(\mathbf{y}|\mathbf{x})$ and $p(\mathbf{x})$.
- ✘ However, let us consider the special case of Gaussian p.d.f's:

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{N/2} |\mathbf{P}|^{1/2}} \exp \left\{ -\frac{1}{2} (\mathbf{x} - \mathbf{x}_b)^T \mathbf{P}^{-1} (\mathbf{x} - \mathbf{x}_b) \right\}$$
$$p(\mathbf{y}|\mathbf{x}) = \frac{1}{(2\pi)^{M/2} |\mathbf{R}|^{1/2}} \exp \left\{ -\frac{1}{2} [\mathbf{y} - \mathcal{H}(\mathbf{x})]^T \mathbf{R}^{-1} [\mathbf{y} - \mathcal{H}(\mathbf{x})] \right\}$$

Maximum Likelihood

✘ Gaussian p.d.f's:

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{N/2} |\mathbf{P}^b|^{1/2}} \exp \left\{ -\frac{1}{2} (\mathbf{x} - \mathbf{x}_b)^T \mathbf{P}^{b-1} (\mathbf{x} - \mathbf{x}_b) \right\}$$
$$p(\mathbf{y}|\mathbf{x}) = \frac{1}{(2\pi)^{M/2} |\mathbf{R}|^{1/2}} \exp \left\{ -\frac{1}{2} [\mathbf{y} - \mathcal{H}(\mathbf{x})]^T \mathbf{R}^{-1} [\mathbf{y} - \mathcal{H}(\mathbf{x})] \right\}$$

✘ Now,

$$\begin{aligned} J(\mathbf{x}) &= -\log [p(\mathbf{x}|\mathbf{y})] + \text{const.} \\ &= -\log [p(\mathbf{y}|\mathbf{x})] - \log [p(\mathbf{x})] + \text{const} \end{aligned}$$

✘ Hence, with an appropriate choice of the constant *const.*:

$$J(\mathbf{x}) = \frac{1}{2} (\mathbf{x} - \mathbf{x}_b)^T \mathbf{P}^{b-1} (\mathbf{x} - \mathbf{x}_b) + \frac{1}{2} [\mathbf{y} - \mathcal{H}(\mathbf{x})]^T \mathbf{R}^{-1} [\mathbf{y} - \mathcal{H}(\mathbf{x})]$$

✘ This is the **3D-Var cost function**

Maximum Likelihood

- ✘ Let us introduce the dot product:

$$\langle \mathbf{x}_1, \mathbf{x}_2 \rangle = \sum_{i=1}^n x_1(i) x_2(i) = \mathbf{x}_1^T \mathbf{x}_2$$

- ✘ The dot product is symmetric:

$$\langle \mathbf{x}_1, \mathbf{x}_2 \rangle = \langle \mathbf{x}_2, \mathbf{x}_1 \rangle$$

- ✘ Let us introduce the matrix \mathbf{A}

$$\begin{aligned} \langle \mathbf{x}_1, \mathbf{A}\mathbf{x}_2 \rangle &= \mathbf{x}_1^T \mathbf{A} \mathbf{x}_2 \\ &= (\mathbf{A}^T \mathbf{x}_1)^T \mathbf{x}_2 \\ &= \langle \mathbf{A}^T \mathbf{x}_1, \mathbf{x}_2 \rangle \end{aligned}$$

- ✘ \mathbf{A}^T is the **adjoint** of \mathbf{A} :

$$\langle \mathbf{x}_1, \mathbf{A}\mathbf{x}_2 \rangle = \langle \mathbf{A}^T \mathbf{x}_1, \mathbf{x}_2 \rangle$$

- ✘ If \mathbf{A} is symmetric ($\mathbf{A}^T = \mathbf{A}$):

$$\langle \mathbf{x}_1, \mathbf{A}\mathbf{x}_2 \rangle = \langle \mathbf{A}\mathbf{x}_1, \mathbf{x}_2 \rangle = \langle \mathbf{x}_1, \mathbf{x}_2 \rangle_{\mathbf{A}}$$

Maximum Likelihood

- ✘ The maximum likelihood analysis corresponds to the global minimum of the cost function (using the previously defined dot product):

$$J(\mathbf{x}) = \frac{1}{2} \left\langle \mathbf{x} - \mathbf{x}_b, \mathbf{x} - \mathbf{x}_b \right\rangle_{\mathbf{P}^{b-1}} + \frac{1}{2} \left\langle \mathbf{y} - \mathcal{H}(\mathbf{x}), \mathbf{y} - \mathcal{H}(\mathbf{x}) \right\rangle_{\mathbf{R}^{-1}}$$

- ✘ At the minimum \mathbf{x}_a , the gradient of the cost function is zero:

$$\nabla J(\mathbf{x}) = 0$$

- ✘ The Taylor series of the cost function is (at the first order)

$$J(\mathbf{x} + \delta\mathbf{x}) = J(\mathbf{x}) + \left\langle \delta\mathbf{x}, \nabla J(\mathbf{x}) \right\rangle$$

- ✘ Let introduce a perturbation $\delta\mathbf{x}$ of \mathbf{x} .
- ✘ If \mathcal{H} is linear (or if we neglect second-order terms) then

$$\mathcal{H}(\mathbf{x} + \delta\mathbf{x}) = \mathcal{H}(\mathbf{x}) + \mathbf{H}\delta\mathbf{x}.$$

Maximum Likelihood

✘ The cost function evaluated at $\mathbf{x} + \delta\mathbf{x}$ is

$$J(\mathbf{x} + \delta\mathbf{x}) = \frac{1}{2} \left\langle (\mathbf{x} - \mathbf{x}_b) + \delta\mathbf{x}, (\mathbf{x} - \mathbf{x}_b) + \delta\mathbf{x} \right\rangle_{\mathbf{P}^{b-1}} \\ + \frac{1}{2} \left\langle (\mathbf{y} - \mathcal{H}(\mathbf{x})) - \mathbf{H}\delta\mathbf{x}, (\mathbf{y} - \mathcal{H}(\mathbf{x})) - \mathbf{H}\delta\mathbf{x} \right\rangle_{\mathbf{R}^{-1}}$$

where we will neglect the second order terms $\langle \dots \delta\mathbf{x}, \dots \delta\mathbf{x} \rangle$

Maximum Likelihood

✘ The cost function evaluated at $\mathbf{x} + \delta\mathbf{x}$ is

$$\begin{aligned} J(\mathbf{x} + \delta\mathbf{x}) &\approx \frac{1}{2} \left\langle \mathbf{x} - \mathbf{x}_b, \mathbf{x} - \mathbf{x}_b \right\rangle_{\mathbf{P}^{b-1}} \\ &+ \frac{1}{2} \left\langle \mathbf{x} - \mathbf{x}_b, \delta\mathbf{x} \right\rangle_{\mathbf{P}^{b-1}} + \frac{1}{2} \left\langle \delta\mathbf{x}, \mathbf{x} - \mathbf{x}_b \right\rangle_{\mathbf{P}^{b-1}} \\ &+ \frac{1}{2} \left\langle \mathbf{y} - \mathcal{H}(\mathbf{x}), \mathbf{y} - \mathcal{H}(\mathbf{x}) \right\rangle_{\mathbf{R}^{-1}} \\ &- \frac{1}{2} \left\langle \mathbf{y} - \mathcal{H}(\mathbf{x}), \mathbf{H}\delta\mathbf{x} \right\rangle_{\mathbf{R}^{-1}} - \frac{1}{2} \left\langle \mathbf{H}\delta\mathbf{x}, \mathbf{y} - \mathcal{H}(\mathbf{x}) \right\rangle_{\mathbf{R}^{-1}} \end{aligned}$$

Maximum Likelihood

✘ The cost function evaluated at $\mathbf{x} + \delta\mathbf{x}$ is

$$\begin{aligned} J(\mathbf{x} + \delta\mathbf{x}) &\approx \frac{1}{2} \left\langle \mathbf{x} - \mathbf{x}_b, \mathbf{x} - \mathbf{x}_b \right\rangle_{\mathbf{P}^{b-1}} \\ &+ \frac{1}{2} \left\langle \mathbf{x} - \mathbf{x}_b, \delta\mathbf{x} \right\rangle_{\mathbf{P}^{b-1}} + \frac{1}{2} \left\langle \delta\mathbf{x}, \mathbf{x} - \mathbf{x}_b \right\rangle_{\mathbf{P}^{b-1}} \\ &+ \frac{1}{2} \left\langle \mathbf{y} - \mathcal{H}(\mathbf{x}), \mathbf{y} - \mathcal{H}(\mathbf{x}) \right\rangle_{\mathbf{R}^{-1}} \\ &- \frac{1}{2} \left\langle \mathbf{y} - \mathcal{H}(\mathbf{x}), \mathbf{H}\delta\mathbf{x} \right\rangle_{\mathbf{R}^{-1}} - \frac{1}{2} \left\langle \mathbf{H}\delta\mathbf{x}, \mathbf{y} - \mathcal{H}(\mathbf{x}) \right\rangle_{\mathbf{R}^{-1}} \end{aligned}$$

Maximum Likelihood

✘ The cost function evaluated at $\mathbf{x} + \delta\mathbf{x}$ is

$$\begin{aligned} J(\mathbf{x} + \delta\mathbf{x}) &\approx \frac{1}{2} \left\langle \mathbf{x} - \mathbf{x}_b, \mathbf{x} - \mathbf{x}_b \right\rangle_{\mathbf{P}^{b-1}} \\ &+ \frac{1}{2} \left\langle \mathbf{x} - \mathbf{x}_b, \delta\mathbf{x} \right\rangle_{\mathbf{P}^{b-1}} + \frac{1}{2} \left\langle \delta\mathbf{x}, \mathbf{x} - \mathbf{x}_b \right\rangle_{\mathbf{P}^{b-1}} \\ &+ \frac{1}{2} \left\langle \mathbf{y} - \mathcal{H}(\mathbf{x}), \mathbf{y} - \mathcal{H}(\mathbf{x}) \right\rangle_{\mathbf{R}^{-1}} \\ &- \frac{1}{2} \left\langle \mathbf{y} - \mathcal{H}(\mathbf{x}), \mathbf{H}\delta\mathbf{x} \right\rangle_{\mathbf{R}^{-1}} - \frac{1}{2} \left\langle \mathbf{H}\delta\mathbf{x}, \mathbf{y} - \mathcal{H}(\mathbf{x}) \right\rangle_{\mathbf{R}^{-1}} \end{aligned}$$

Maximum Likelihood

✘ The cost function evaluated at $\mathbf{x} + \delta\mathbf{x}$ is

$$\begin{aligned} J(\mathbf{x} + \delta\mathbf{x}) &\approx \frac{1}{2} \left\langle \mathbf{x} - \mathbf{x}_b, \mathbf{x} - \mathbf{x}_b \right\rangle_{\mathbf{P}^{b-1}} \\ &+ \frac{1}{2} \left\langle \mathbf{x} - \mathbf{x}_b, \delta\mathbf{x} \right\rangle_{\mathbf{P}^{b-1}} + \frac{1}{2} \left\langle \delta\mathbf{x}, \mathbf{x} - \mathbf{x}_b \right\rangle_{\mathbf{P}^{b-1}} \\ &+ \frac{1}{2} \left\langle \mathbf{y} - \mathcal{H}(\mathbf{x}), \mathbf{y} - \mathcal{H}(\mathbf{x}) \right\rangle_{\mathbf{R}^{-1}} \\ &- \frac{1}{2} \left\langle \mathbf{y} - \mathcal{H}(\mathbf{x}), \mathbf{H}\delta\mathbf{x} \right\rangle_{\mathbf{R}^{-1}} - \frac{1}{2} \left\langle \mathbf{H}\delta\mathbf{x}, \mathbf{y} - \mathcal{H}(\mathbf{x}) \right\rangle_{\mathbf{R}^{-1}} \end{aligned}$$

Maximum Likelihood

✘ The cost function evaluated at $\mathbf{x} + \delta\mathbf{x}$ is

$$\begin{aligned} J(\mathbf{x} + \delta\mathbf{x}) &\approx \frac{1}{2} \left\langle \mathbf{x} - \mathbf{x}_b, \mathbf{x} - \mathbf{x}_b \right\rangle_{\mathbf{P}^{b-1}} \\ &+ \frac{1}{2} \left\langle \mathbf{x} - \mathbf{x}_b, \delta\mathbf{x} \right\rangle_{\mathbf{P}^{b-1}} + \frac{1}{2} \left\langle \delta\mathbf{x}, \mathbf{x} - \mathbf{x}_b \right\rangle_{\mathbf{P}^{b-1}} \\ &+ \frac{1}{2} \left\langle \mathbf{y} - \mathcal{H}(\mathbf{x}), \mathbf{y} - \mathcal{H}(\mathbf{x}) \right\rangle_{\mathbf{R}^{-1}} \\ &- \frac{1}{2} \left\langle \mathbf{y} - \mathcal{H}(\mathbf{x}), \mathbf{H}\delta\mathbf{x} \right\rangle_{\mathbf{R}^{-1}} - \frac{1}{2} \left\langle \mathbf{H}\delta\mathbf{x}, \mathbf{y} - \mathcal{H}(\mathbf{x}) \right\rangle_{\mathbf{R}^{-1}} \end{aligned}$$

$$\begin{aligned} J(\mathbf{x} + \delta\mathbf{x}) &\approx J(\mathbf{x}) \\ &+ \left\langle \delta\mathbf{x}, \mathbf{x} - \mathbf{x}_b \right\rangle_{\mathbf{P}^{b-1}} \\ &- \left\langle \delta\mathbf{x}, \mathbf{H}^T [\mathbf{y} - \mathcal{H}(\mathbf{x})] \right\rangle_{\mathbf{R}^{-1}} \end{aligned}$$

Maximum Likelihood

✘ The cost function evaluated at $\mathbf{x} + \delta\mathbf{x}$ is

$$\begin{aligned} J(\mathbf{x} + \delta\mathbf{x}) &\approx \frac{1}{2} \left\langle \mathbf{x} - \mathbf{x}_b, \mathbf{x} - \mathbf{x}_b \right\rangle_{\mathbf{P}^{b-1}} \\ &+ \frac{1}{2} \left\langle \mathbf{x} - \mathbf{x}_b, \delta\mathbf{x} \right\rangle_{\mathbf{P}^{b-1}} + \frac{1}{2} \left\langle \delta\mathbf{x}, \mathbf{x} - \mathbf{x}_b \right\rangle_{\mathbf{P}^{b-1}} \\ &+ \frac{1}{2} \left\langle \mathbf{y} - \mathcal{H}(\mathbf{x}), \mathbf{y} - \mathcal{H}(\mathbf{x}) \right\rangle_{\mathbf{R}^{-1}} \\ &- \frac{1}{2} \left\langle \mathbf{y} - \mathcal{H}(\mathbf{x}), \mathbf{H}\delta\mathbf{x} \right\rangle_{\mathbf{R}^{-1}} - \frac{1}{2} \left\langle \mathbf{H}\delta\mathbf{x}, \mathbf{y} - \mathcal{H}(\mathbf{x}) \right\rangle_{\mathbf{R}^{-1}} \end{aligned}$$

$$\begin{aligned} J(\mathbf{x} + \delta\mathbf{x}) &\approx J(\mathbf{x}) \\ &+ \left\langle \delta\mathbf{x}, \mathbf{x} - \mathbf{x}_b \right\rangle_{\mathbf{P}^{b-1}} \\ &- \left\langle \delta\mathbf{x}, \mathbf{H}^T [\mathbf{y} - \mathcal{H}(\mathbf{x})] \right\rangle_{\mathbf{R}^{-1}} \end{aligned}$$

$$\begin{aligned} J(\mathbf{x} + \delta\mathbf{x}) &\approx J(\mathbf{x}) \\ &+ \left\langle \delta\mathbf{x}, \mathbf{P}^{b-1} [\mathbf{x} - \mathbf{x}_b] - \mathbf{R}^{-1} \mathbf{H}^T [\mathbf{y} - \mathcal{H}(\mathbf{x})] \right\rangle \end{aligned}$$

Maximum Likelihood

- ✘ The maximum likelihood analysis corresponds to the global minimum of the cost function (using the previously defined dot product):

$$J(\mathbf{x}) = \frac{1}{2} \left\langle \mathbf{x} - \mathbf{x}_b, \mathbf{x} - \mathbf{x}_b \right\rangle_{\mathbf{P}^{b-1}} + \frac{1}{2} \left\langle \mathbf{y} - \mathcal{H}(\mathbf{x}), \mathbf{y} - \mathcal{H}(\mathbf{x}) \right\rangle_{\mathbf{R}^{-1}}$$

- ✘ The cost function evaluated at $\mathbf{x} + \delta\mathbf{x}$ is (at the first order)

$$J(\mathbf{x} + \delta\mathbf{x}) = J(\mathbf{x}) + \left\langle \delta\mathbf{x}, \mathbf{P}^{b-1} [\mathbf{x} - \mathbf{x}_b] - \mathbf{R}^{-1} \mathbf{H}^T [\mathbf{y} - \mathcal{H}(\mathbf{x})] \right\rangle.$$

- ✘ The Taylor series of the cost function is (at the first order)

$$J(\mathbf{x} + \delta\mathbf{x}) = J(\mathbf{x}) + \left\langle \delta\mathbf{x}, \nabla J(\mathbf{x}) \right\rangle$$

- ✘ We deduce the **gradient** of the cost function

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

Maximum Likelihood

- ✘ At the minimum \mathbf{x}_a , the gradient of the cost function ($\nabla J(\mathbf{x})$) is zero:

$$\nabla J(\mathbf{x}_a) = \mathbf{P}^{b-1} [\mathbf{x}_a - \mathbf{x}_b] + \mathbf{H}^T \mathbf{R}^{-1} [\mathcal{H}(\mathbf{x}_a) - \mathbf{y}] = \mathbf{0}$$

- ✘ Now, if \mathcal{H} is linear (or if we neglect second-order terms) then

$$\mathcal{H}(\mathbf{x}_a) = \mathcal{H}(\mathbf{x}_b) + \mathbf{H} \delta \mathbf{x}_a \quad \text{where} \quad \delta \mathbf{x}_a = \mathbf{x}_a - \mathbf{x}_b$$

- ✘ Hence:

$$\mathbf{P}^{b-1} \delta \mathbf{x}_a + \mathbf{H}^T \mathbf{R}^{-1} [\mathcal{H}(\mathbf{x}_b) - \mathbf{y}] + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} \delta \mathbf{x}_a = \mathbf{0}$$

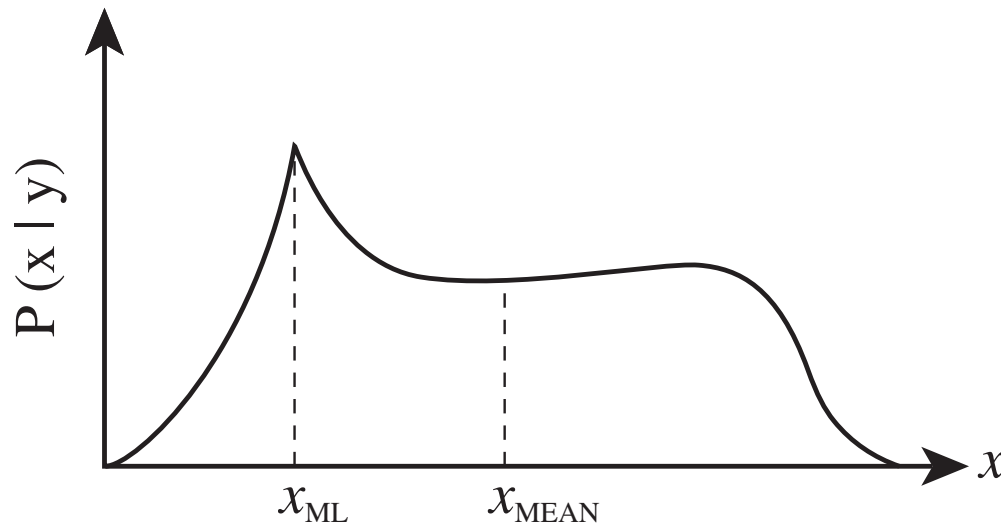
- ✘ Rearranging a little gives:

$$\left[\mathbf{P}^{b-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} \right] \delta \mathbf{x}_a = \mathbf{H}^T \mathbf{R}^{-1} [\mathbf{y} - \mathcal{H}(\mathbf{x}_b)]$$

- ✘ This is exactly the equation for the minimum-variance analysis we derived at the start of the lecture!

Maximum Likelihood

- ✘ We have shown that the **maximum likelihood** approach is naturally expressed in terms of a **cost function** representing minus the log of the probability of the analysis state.
- ✘ The minimum of the cost function corresponds to the maximum likelihood (probability) solution.
- ✘ For Gaussian errors and linear observation operators, the maximum likelihood analysis coincides with the minimum variance solution.
- ✘ This is not the case in general:



Maximum Likelihood

- ✘ In the nonlinear case, the minimum variance approach is difficult to apply.
- ✘ The maximum-likelihood approach is much more generally applicable
- ✘ As long as we know the p.d.f.'s, we can define the cost function
 - ⇒ However, finding the global minimum may not be easy for highly non-Gaussian p.d.f.'s.
- ✘ In practice, background errors are usually assumed to be Gaussian (or a nonlinear transformation is applied to *make* them Gaussian).
 - ⇒ This makes the background-error term of the cost function quadratic.
- ✘ However, non-Gaussian observation errors are taken into account. For example:
 - ⇒ Directionally-ambiguous wind observations from scatterometers
 - ⇒ Observations contaminated by occasional gross errors, which make outliers much more likely than implied by a Gaussian model.

Outline

- 1 From Optimal Interpolation to 3D-Var
- 2 The Maximum Likelihood Approach
- 3 Minimisation**
- 4 Summary

Minimisation

- ✘ In 3D-Var, the analysis is found by minimising the cost function:

$$J(\mathbf{x}) = \frac{1}{2} (\mathbf{x} - \mathbf{x}_b)^T \mathbf{P}^{b-1} (\mathbf{x} - \mathbf{x}_b) + \frac{1}{2} [\mathbf{y} - \mathcal{H}(\mathbf{x})]^T \mathbf{R}^{-1} [\mathbf{y} - \mathcal{H}(\mathbf{x})]$$

- ✘ This is a very large-scale ($\dim(\mathbf{x}) \approx 10^8$) minimisation problem.
- ✘ The size of the problem restricts on the algorithms we can use.
- ✘ Derivative-free algorithms (which require only the ability to calculate $J(\mathbf{x})$ for arbitrary \mathbf{x}) are too slow.
- ✘ This is because each function evaluation gives very limited information about the shape of the cost function.
 - ⇒ E.g. a finite difference, $J(\mathbf{x} + \delta\mathbf{v}) - J(\mathbf{x}) \approx \delta\mathbf{v}^T \nabla J(\mathbf{x})$, gives a single component of the gradient.
 - ⇒ We need $O(10^8)$ components to work out which direction is “downhill”.

Minimisation

- ✘ Practical algorithms for minimising the 3D-Var cost function require us to calculate its gradient:

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

- ✘ The simplest gradient-based minimisation algorithm is called **steepest descent**:

Let \mathbf{x}_0 be an initial guess of the analysis;

while *gradient is not sufficiently small* **do**

```
/* Define a descent direction */
```

```
 $\mathbf{d}_k = -\nabla J(\mathbf{x}_k);$ 
```

```
/* Find a step  $\alpha_k$ , e.g. by line minimisation of the  
function  $J(\mathbf{x}_k + \alpha \mathbf{d}_k)$ , for which  $J(\mathbf{x}_k + \alpha \mathbf{d}_k) < J(\mathbf{x}_k)$  */
```

```
 $\alpha_k = \dots;$ 
```

```
/* Compute the new estimate */
```

```
 $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha \mathbf{d}_k;$ 
```

```
/* Next step */
```

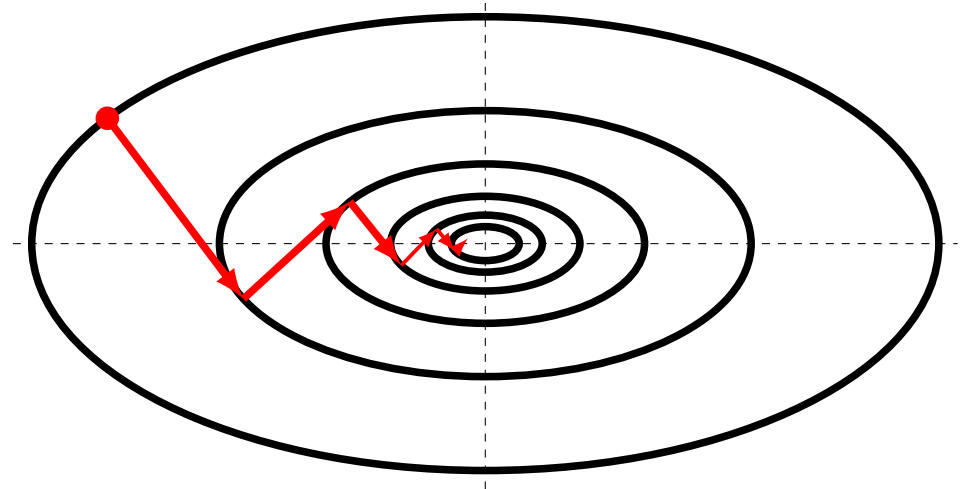
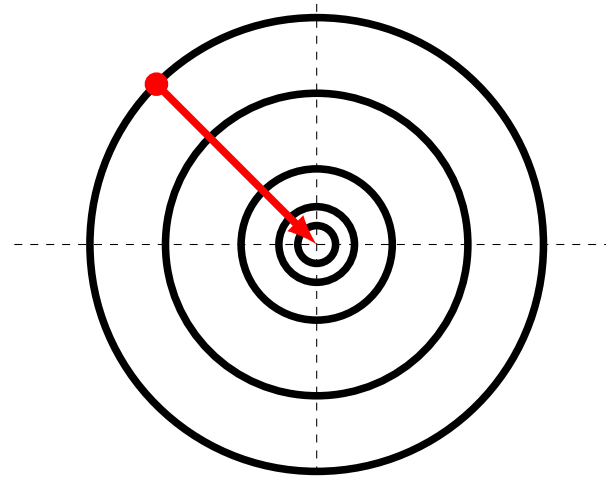
```
 $k = k + 1$ 
```

end

Minimisation

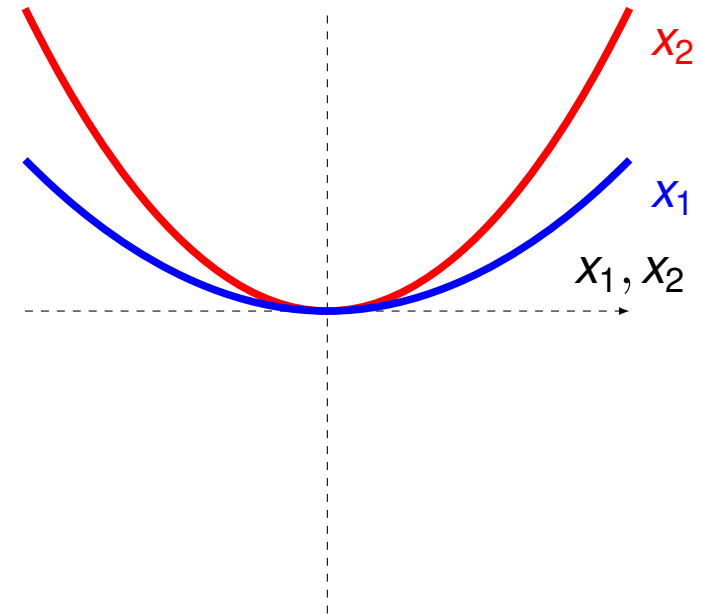
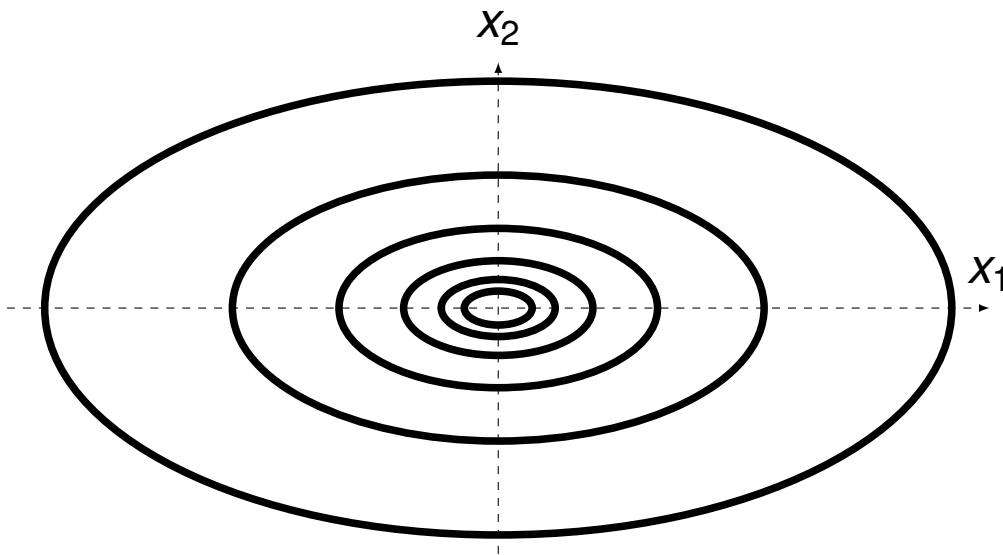
- ✘ Steepest descent can work well on problems in which the iso-surfaces of the cost function are nearly spherical.
 - ⇒ In this case, the steepest descent direction points towards the minimum.
 - ⇒ They are very well conditioned problems.

- ✘ For problems with ellipsoidal iso-surfaces, steepest descent is not efficient.
 - ⇒ They are poorly conditioned problems.



Curvature

- ✘ The degree of sphericity of the cost function can be measured by the eigenvalues of the Hessian (matrix J'' of second derivatives of J).
- ✘ Each eigenvalue corresponds to the **curvature** in the direction of the corresponding eigenvector.
- ✘ the curvature is defined as the amount by which a line deviates from being straight.



Preconditioning

- ✘ The steepest descent method works best if the iso-surfaces of the cost function are approximately spherical.
- ✘ This is generally true of all minimisation algorithms.
- ✘ In particular, the convergence rate will depend on the **condition number**:

$$\kappa = \frac{\lambda_{\max}}{\lambda_{\min}},$$

where λ_{\max} and λ_{\min} are the maximum and minimum eigenvalues respectively.

- ✘ In general, expressing the cost function directly in terms of \mathbf{x} will not lead to spherical iso-surfaces.

Preconditioning

✘ We can speed up the convergence of the minimisation by a **change of variables** $\boldsymbol{\chi} = \mathbf{L}^{-1}(\mathbf{x} - \mathbf{x}_b)$, where \mathbf{L} is chosen to make the cost function more spherical.

✘ A common choice is $\mathbf{L} = \mathbf{P}^{b^{1/2}}$. The cost function becomes:

$$\begin{aligned} J(\boldsymbol{\chi}) &= \frac{1}{2}\boldsymbol{\chi}^T\boldsymbol{\chi} + \frac{1}{2}[\mathbf{y} - \mathcal{H}(\mathbf{x}_b + \mathbf{L}\boldsymbol{\chi})]^T \mathbf{R}^{-1} [\mathbf{y} - \mathcal{H}(\mathbf{x}_b + \mathbf{L}\boldsymbol{\chi})] \\ &\approx \frac{1}{2}\boldsymbol{\chi}^T\boldsymbol{\chi} + \frac{1}{2}[\mathbf{y} - \mathcal{H}(\mathbf{x}_b) + \mathbf{H}\mathbf{L}\boldsymbol{\chi}]^T \mathbf{R}^{-1} [\mathbf{y} - \mathcal{H}(\mathbf{x}_b) + \mathbf{H}\mathbf{L}\boldsymbol{\chi}] \end{aligned}$$

✘ With this change of variables, the Hessian becomes:

$$J''_{\boldsymbol{\chi}} = \mathbf{I} + \mathbf{L}^T \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} \mathbf{L} \text{ (plus higher order terms)}$$

✘ The presence of the identity matrix in this expression guarantees that the minimum eigenvalue is ≥ 1 .

✘ There are no small eigenvalues to destroy the conditioning of the problem.

Newton's methods

- ✘ Steepest Descent is inefficient because it does not use information about the curvature of the cost function.
- ✘ The simplest algorithms that use curvature are in the family of **Newton's methods**.
- ✘ Newton's methods use a local quadratic approximation:

$$J(\mathbf{x} + \delta\mathbf{x}) \approx J(\mathbf{x}) + \delta\mathbf{x}^T \nabla J(\mathbf{x}) + \frac{1}{2} \delta\mathbf{x}^T J'' \delta\mathbf{x}$$

- ✘ Taking the gradient gives:

$$\nabla J(\mathbf{x} + \delta\mathbf{x}) \approx \nabla J(\mathbf{x}) + J'' \delta\mathbf{x}$$

- ✘ Since the gradient is zero at the minimum, Newton's method chooses the step at each iteration by solving:

$$J'' \delta\mathbf{x} = -\nabla J(\mathbf{x})$$

Newton's methods

✘ Newton's method:

Start with an initial guess, \mathbf{x}_0 ;

while *gradient is not sufficiently small* **do**

```
/* Solve  $J''\delta\mathbf{x}_k = -\nabla J(\mathbf{x}_k)$  */
```

```
*/
```

```
 $\delta\mathbf{x}_k = \dots$ ;
```

```
/* Compute the new estimate */
```

```
*/
```

```
 $\mathbf{x}_{k+1} = \mathbf{x}_k + \delta\mathbf{x}_k$ ;
```

```
/* Next step */
```

```
*/
```

```
 $k = k + 1$ 
```

end

✘ Newton's method works well for cost functions that are well approximated by a quadratic — i.e. for quasi-linear observation operators.

✘ However, it suffers from several problems ...

⇒ There is no control on the step length $\|\delta\mathbf{x}\|$.

⇒ The method can make huge jumps into regions where the local quadratic approximation is poor.

✘ This can be controlled using line searches, or by **trust region** methods that limit the step size to a region where the approximation is valid.

Newton's methods

- ✘ Newton's method requires us to solve $J''\delta\mathbf{x}_k = -\nabla J(\mathbf{x}_k)$ at every iteration.
- ✘ Now, J'' is a $\sim 10^8 \times 10^8$ matrix! Clearly, we cannot explicitly construct the matrix, or use direct methods to invert it.
- ✘ However, if we have a code that calculates Hessian-vector products, then we can use an iterative method (e.g. conjugate gradients) to solve for $\delta\mathbf{x}_k$.
- ✘ Such a code is called a **second order adjoint**. See Wang, Navon, LeDimet, Zou, 1992 Meteor. and Atmos. Phys. 50, pp3-20 for details.
- ✘ Alternatively, we can use a method that constructs an approximation to $(J'')^{-1}$.
- ✘ Methods based on approximations of J'' or $(J'')^{-1}$ are called **quasi-Newton** methods.

Newton's methods

- ✘ By far the most popular quasi-Newton method is the BFGS algorithm, named after its creators Broyden, Fletcher, Goldfarb and Shanno.
- ✘ The BFGS method builds up an approximation to the Hessian:

$$\mathbf{B}_{k+1} = \mathbf{B}_k + \frac{\mathbf{y}_k \mathbf{y}_k^T}{\mathbf{y}_k \mathbf{s}_k^T} - \frac{\mathbf{B}_k \mathbf{s}_k (\mathbf{B}_k \mathbf{s}_k)^T}{\mathbf{s}_k \mathbf{B}_k \mathbf{s}_k^T}$$

where $\mathbf{s}_k = \mathbf{x}_{k+1} - \mathbf{x}_k$ and $\mathbf{y}_k = \nabla J(\mathbf{x}_{k+1}) - \nabla J(\mathbf{x}_k)$.

- ✘ The approximation is symmetric and positive definite, and satisfies

$$\nabla J(\mathbf{x}_{j+1}) - \nabla J(\mathbf{x}_j) = \mathbf{J}''(\mathbf{x}_{j+1} - \mathbf{x}_j) \quad \text{for } j = 0, 1, \dots, k$$

- ✘ There is an explicit expression for the inverse of \mathbf{B}_k , which allows Newton's equation to be solved at the cost of $O(Nk)$ operations.

Newton's methods

✘ The BFGS quasi-Newton method:

Start with an initial guess, \mathbf{x}_0 ;

Start with an initial approximation of the Hessian (typically, $\mathbf{B}_0 = \mathbf{I}$);

while *gradient is not sufficiently small* **do**

```
/* Solve the approximate Newton's equation,  
    $\mathbf{B}_k \delta \mathbf{x}_k = -\nabla J(\mathbf{x}_k)$ , to determine the search direction.  
*/
```

```
 $\delta \mathbf{x}_k = \dots;$ 
```

```
/* Perform a line search to find a step  $\alpha_k$  for which for  
   which  $J(\mathbf{x}_k + \alpha_k \delta \mathbf{x}_k) < J(\mathbf{x}_k)$  */
```

```
 $\alpha_k = \dots;$ 
```

```
/* Compute the new estimate */
```

```
 $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \delta \mathbf{x}_k;$ 
```

```
/* Generate an updated approximation to the Hessian */
```

```
 $\mathbf{B}_{k+1} = \dots;$ 
```

```
/* Next step */
```

```
 $k = k + 1$ 
```

end

Newton's methods

The BFGS quasi-Newton method

- ✘ As k increases, the cost of storing and applying the approximate Hessian increases linearly.
- ✘ Moreover, the vectors \mathbf{s}_k and \mathbf{y}_k generated many iterations ago no longer provide accurate information about the Hessian.
- ✘ It is usual to construct \mathbf{B}_k from only the $O(10)$ most recent iterations.
- ✘ The algorithm is then called the **limited memory BFGS method**.

Newton's methods

- ✘ The methods presented so far apply to general nonlinear functions.
- ✘ An important special case occurs when the cost function is strictly quadratic, and the gradient is linear:

$$\begin{aligned}\nabla J(\mathbf{x}) &= \mathbf{P}^{b-1} \delta \mathbf{x} + \mathbf{H}^T \mathbf{R}^{-1} [\mathbf{H} \mathbf{x}_b + \mathbf{H} \delta \mathbf{x} - \mathbf{y}] \\ &= \left[\mathbf{P}^{b-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} \right] \delta \mathbf{x} + \mathbf{H}^T \mathbf{R}^{-1} [\mathbf{H} \mathbf{x}_b - \mathbf{y}]\end{aligned}$$

- ✘ We will see tomorrow that ECMWF 4DVAR falls into this situation
- ✘ In this case, it makes sense to determine the analysis by solving the **linear** equation $\nabla J(\mathbf{x}) = \mathbf{0}$.
- ✘ Since the matrix $\left[\mathbf{P}^{b-1} + \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} \right]$ is symmetric and positive definite, the best algorithm to use is **conjugate gradients**. The algorithm was presented earlier in this lecture.
- ✘ A good introduction to the conjugate gradient method can be found online: Shewchuk (1994) "An Introduction to the Conjugate Gradient Method Without the Agonizing pain".

ECMWF Lanczos algorithm

- ✘ We precondition using $\mathbf{L} = \mathbf{P}^{b^{1/2}}$, the gradient (with respect to χ) is:

$$\nabla_{\chi} J(\chi) = \chi + \mathbf{L}^T \mathbf{H}^T \mathbf{R}^{-1} (\mathbf{y} - \mathcal{H}(\mathbf{x}_b) + \mathbf{H}\mathbf{L}\chi)$$

- ✘ We use the conjugate gradient to solve

$$[\mathbf{I} + \mathbf{L}^T \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H}\mathbf{L}] \chi = \mathbf{L}^T \mathbf{H}^T \mathbf{R}^{-1} [\mathbf{y} - \mathcal{H}(\mathbf{x}_b)]$$

- ✘ This allows the hessian matrix to be approximated by

$$J'' = \mathbf{I} + \sum_{i=1}^K (\lambda_i - 1) \mathbf{v}_i \mathbf{v}_i^T$$

where λ_i and \mathbf{v}_i are the eigenvalues and eigenvectors determined by the conjugate gradient and the Lanczos algorithm

- ✘ We can use as a new preconditioning

$$(J'')^{-1/2} = \mathbf{I} + \sum_{i=1}^K (\lambda_i^{-1/2} - 1) \mathbf{v}_i \mathbf{v}_i^T$$

Calculating the operators

- ✘ We use the conjugate gradient to solve

$$[\mathbf{I} + \mathbf{L}^T \mathbf{H}^T \mathbf{R}^{-1} \mathbf{H} \mathbf{L}] \boldsymbol{\chi} = \mathbf{L}^T \mathbf{H}^T \mathbf{R}^{-1} [\mathbf{y} - \mathcal{H}(\mathbf{x}_b)]$$

- ✘ Typically, \mathbf{R} is diagonal — observation errors are treated as being mutually uncorrelated.
- ✘ However, the matrices \mathbf{H}^T , \mathbf{L}^T and \mathbf{L} are not diagonal, and are much too large to be represented explicitly.
- ✘ We must represent these as operators (subroutines) that calculate matrix-vector products.

Calculating the operators

- ✘ Take \mathcal{H} as an example. Each line of the subroutine that applies \mathcal{H} can be considered as a function h_k , so that

$$\mathcal{H}(\mathbf{x}) \equiv h_K(h_{K-1}(\cdots(h_1(\mathbf{x}))))$$

- ✘ Each of the functions h_k can be linearised, to give the corresponding linear function \mathbf{h}_k . The resulting code is called the **tangent linear** of \mathcal{H} .

$$\mathbf{H}\mathbf{x} \equiv \mathbf{h}_K\mathbf{h}_{K-1}\cdots\mathbf{h}_1\mathbf{x}$$

- ✘ The transpose is called the **adjoint** of \mathcal{H}

$$\mathbf{H}^T\mathbf{x} \equiv \mathbf{h}_1^T\mathbf{h}_2^T\cdots\mathbf{h}_K^T\mathbf{x}$$

- ✘ Each \mathbf{h}_k and \mathbf{h}_k^T is extremely simple — just to a few lines of code.

Tangent Linear and Adjoint

There is a whole 1-hour lecture on tangent linear and adjoint operators Tuesday when you will learn to derive tangent linear and adjoint equations for a simple nonlinear equation.

Outline

- 1 From Optimal Interpolation to 3D-Var
- 2 The Maximum Likelihood Approach
- 3 Minimisation
- 4 Summary

Summary

- ✘ We showed that 3D-Var can be considered as an iterative procedure for solving the linear (minimum variance) analysis equation.
- ✘ We also derived 3D-Var from the **maximum likelihood principle**.
- ✘ The Maximum Likelihood approach can be applied to non-Gaussian, nonlinear analysis.
- ✘ We introduced the 3D-Var **cost function**.
- ✘ We considered how to minimise the cost function using algorithms based on knowledge of its gradient.
- ✘ We looked at a simple preconditioning.
- ✘ Finally, we saw how it is possible to write code that computes the gradient.