Assimilation Algorithms
Lecture 2: 3D-Var

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Outline

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

Outline

From Optimal Interpolation to 3D-Var

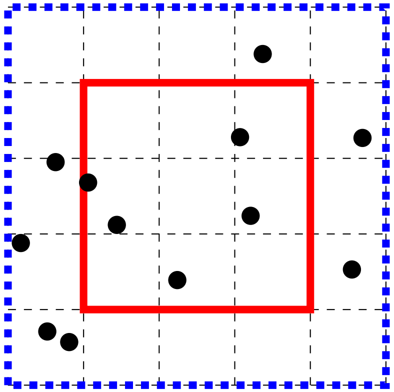
- Previously in "Assimilation Algorithms": linear analysis equation

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

where

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

- Optimal Interpolation (OI) applies direct solution methods to invert the matrix $\left[\mathbf{H}\mathbf{P}^b\mathbf{H}^\mathrm{T} + \mathbf{R}\right]$.
- Data selection is applied to reduce the dimension of the matrix.
- Direct methods require access to the matrix elements. In particular, $\mathbf{H}\mathbf{P}^b\mathbf{H}^\mathrm{T}$ 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: $\mathbf{x}_a = \mathbf{x}_b + \mathbf{K}\left[\mathbf{y} - \mathcal{H}(\mathbf{x}_b)\right]$
- For $\mathbf{K} = \mathbf{P}^b\mathbf{H}^\mathrm{T}\left[\mathbf{H}\mathbf{P}^b\mathbf{H}^\mathrm{T} + \mathbf{R}\right]^{-1}$

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

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

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

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

From Optimal Interpolation to 3D-Var

- Linear analysis equation: $\mathbf{x}_a = \mathbf{x}_b + \mathbf{K}\left[\mathbf{y} - \mathcal{H}(\mathbf{x}_b)\right]$
- For $\mathbf{K} = \left[\mathbf{P}^{b^{-1}} + \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\right]^{-1}\mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}$

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

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

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

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 **K**:
- For $\mathbf{K} = \mathbf{P}^b\mathbf{H}^\mathrm{T}\left[\mathbf{H}\mathbf{P}^b\mathbf{H}^\mathrm{T} + \mathbf{R}\right]^{-1}$ we have $\mathbf{x}_a = \mathbf{x}_b + \mathbf{P}^b\mathbf{H}^\mathrm{T}\mathbf{z}$ and:

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

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

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

- 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:

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

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 $\mathbf{x}_1, \mathbf{x}_2, \cdots \mathbf{x}_n$.
- ✗ 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:

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

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

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

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

`/* New state */`

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

`/* New residual */`

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

`/* New direction of descent */`

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

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

`/* Next iteration */`

$$k := k + 1 ;$$

end

The result is x_{k+1}

Outline

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:

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

- It will be convenient to define a cost function

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

- Then, since log is a monotonic function:

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

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:

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

Maximum Likelihood

- Gaussian p.d.f's:

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{N/2}|\mathbf{P}^b|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\mathbf{x}_b)^{\mathrm{T}} \mathbf{P}^{b^{-1}} (\mathbf{x}-\mathbf{x}_b)\right\}$$

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

- Now,

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

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

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

- This is the 3D-Var cost function

Maximum Likelihood

- Let us introduce the dot product:

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

- 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 **A**

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

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

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

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

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

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

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

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

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

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

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

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)

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

- 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

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

Maximum Likelihood

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

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

- 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:

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

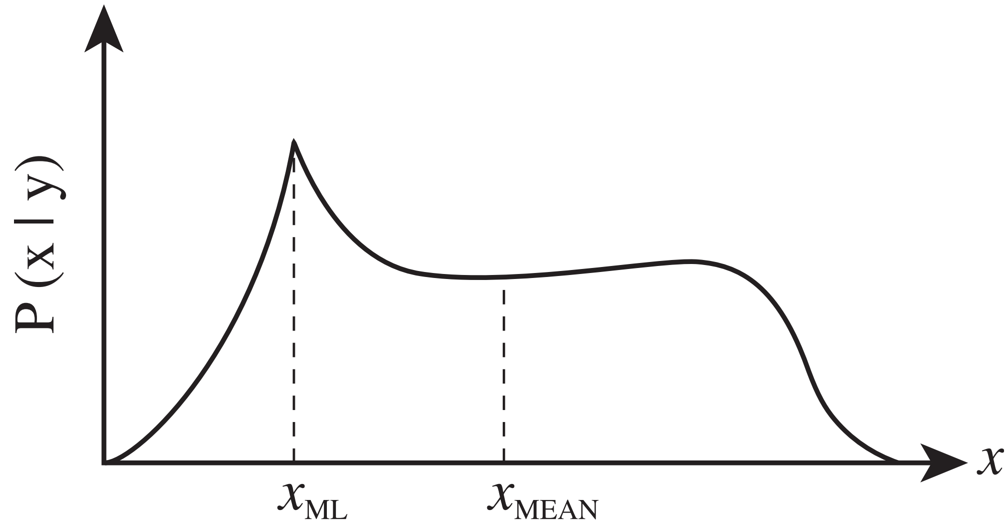
- Rearranging a little gives:

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

- 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

Minimisation

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

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

- 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, $J(\mathbf{x}+\delta\mathbf{v}) - J(\mathbf{x}) \approx \delta\mathbf{v}^{\mathrm{T}}\nabla J(\mathbf{x})$, 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:

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

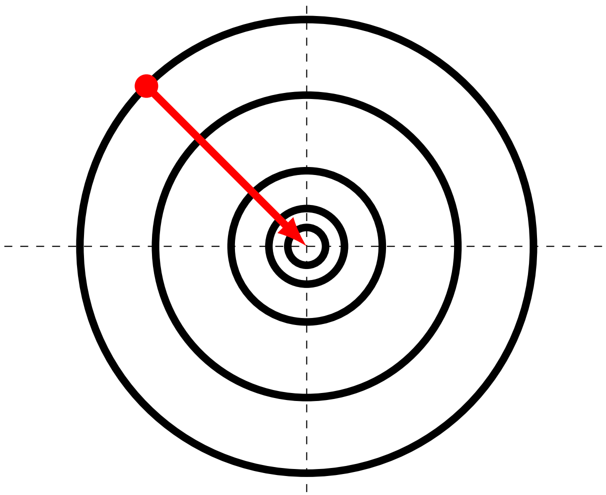
- The simplest gradient-based minimisation algorithm is called steepest descent:

Let $\mathbf{x}_0$ be an initial guess of the analysis;
while *gradient is not sufficiently small* **do**

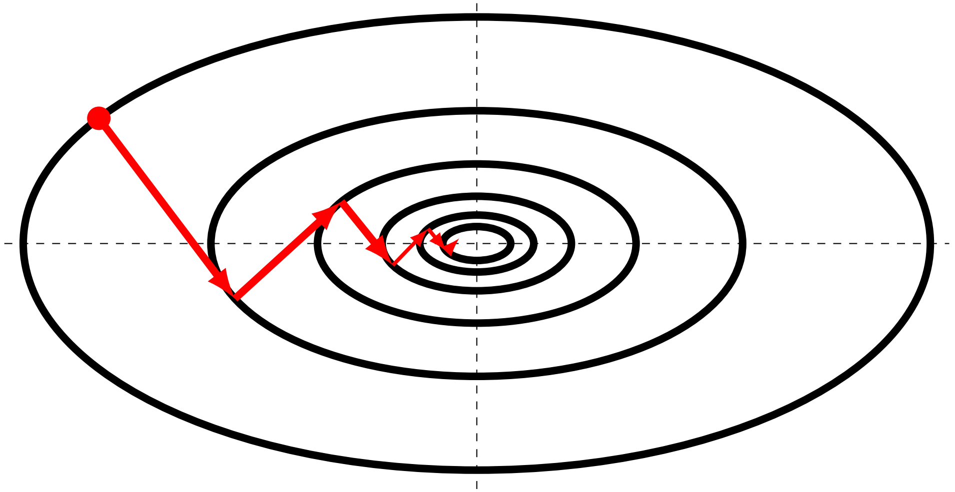
```
    /* Define a descent direction                                        */
    d_k = −∇J(x_k);
    /* Find a step α_k, e.g. by line minimisation of the
       function J(x_k + αd_k), for which J(x_k + αd_k) < J(x_k)          */
    α_k = ··· ;
    /* Compute the new estimate                                          */
    x_{k+1} = x_k + αd_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.

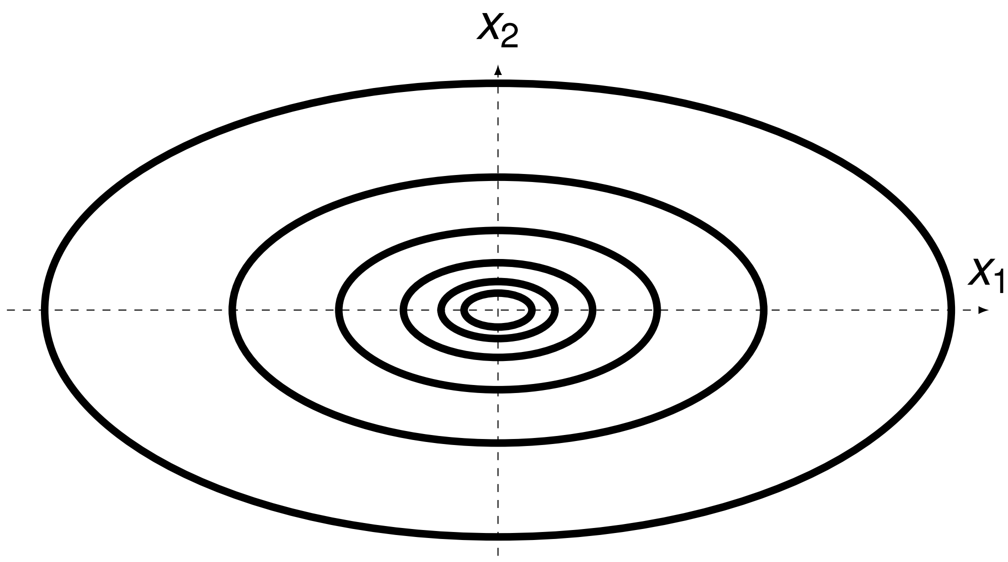


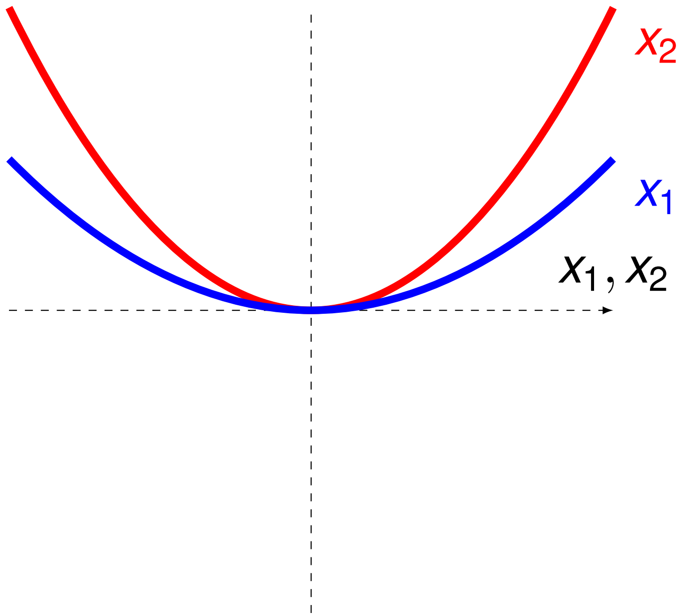
- For problems with ellipsoidal iso-surfaces, steepest descent is not efficient.
  - They are poorly conditioned problems.



Curvature

- We define the curvature as the amount by which a line deviates from being straight.





- 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.

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 $\lambda_{\max}$ and $\lambda_{\min}$ 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 $\chi = \mathbf{L}^{-1}(\mathbf{x} - \mathbf{x}_b)$, 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:

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

- With this change of variables, the Hessian becomes:

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

- 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:

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

- 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''δx_k = −∇J(x_k)                  */
    δx_k = ···;
    /* Compute the new estimate                  */
    x_{k+1} = x_k + δx_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 call 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:

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

  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

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

- 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. */
  >
  > $\delta \mathbf{x}_k = \cdots;$
  >
  > /* Perform a line search to find a step α_k for which for which $J(\mathbf{x}_k + \alpha_k \delta \mathbf{x}_k) < J(\mathbf{x}_k)$ */
  >
  > $\alpha_k = \cdots;$
  >
  > /* Compute the new estimate */
  >
  > $\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \delta \mathbf{x}_k;$
  >
  > /* Generate an updated approximation to the Hessian */
  >
  > $\mathbf{B}_{k+1} = \cdots;$
  >
  > /* 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:

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

- 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 $\left[\mathbf{P}^{b^{-1}} + \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\right]$ 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:

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

- We use the conjugate gardient to solve

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

- 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 congugate gradient and the Lanczos algorithm

- We can use as a new preconditioning

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

Calculating the operators

- We use the conjugate gardient to solve

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

- Typically, **R** is diagonal — observation errors are treated as being mutually uncorrelated.
- However, the matrices $\mathbf{H}^{\mathrm{T}}$, $\mathbf{L}^{\mathrm{T}}$ and **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

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

- 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 $\mathcal{H}$

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

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

Tangent Linear and Adjoints

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

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.