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

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From Optimal Interpolation to 3D-Var

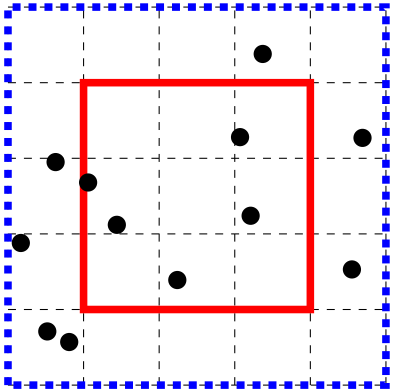
- ✘ Previously in “Assimilation Algorithms”: linear analysis equation

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

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

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

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

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

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

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

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 $\mathbf{K} = \mathbf{P}^b\mathbf{H}^{\mathrm{T}}\left[\mathbf{H}\mathbf{P}^b\mathbf{H}^{\mathrm{T}} + \mathbf{R}\right]^{-1}$ 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
- ✘ 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 $\mathbf{x}_1, \mathbf{x}_2, \cdots \mathbf{x}_n$.
- ✗ 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 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:

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

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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:

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

- ✗ It will be convenient to define a cost function

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

- ✗ Then, since log is a monotonic function:

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

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:

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

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

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

- ✘ 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 ($\mathbf{A}^{\mathrm{T}} = \mathbf{A}$):

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

Maximum Likelihood

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

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

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

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

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

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

- 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:

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

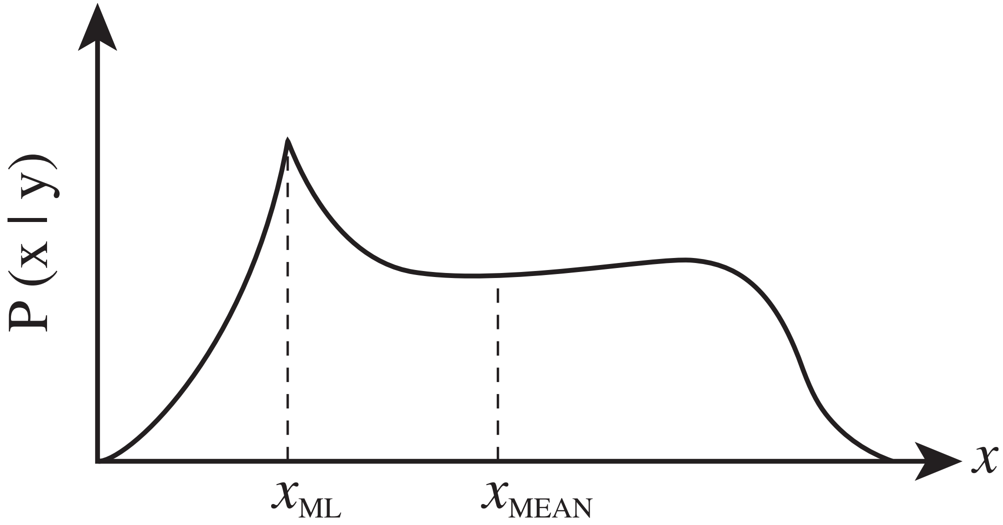
- Rearranging a little gives:

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

- 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.

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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:

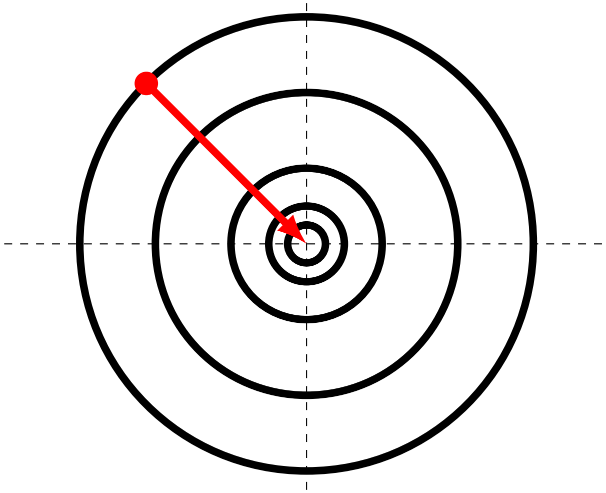
$$\nabla J(\mathbf{x}) = \mathbf{P}^{b^{-1}}(\mathbf{x}-\mathbf{x}_b) + \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\left[\mathcal{H}(\mathbf{x}) - \mathbf{y}\right]$$

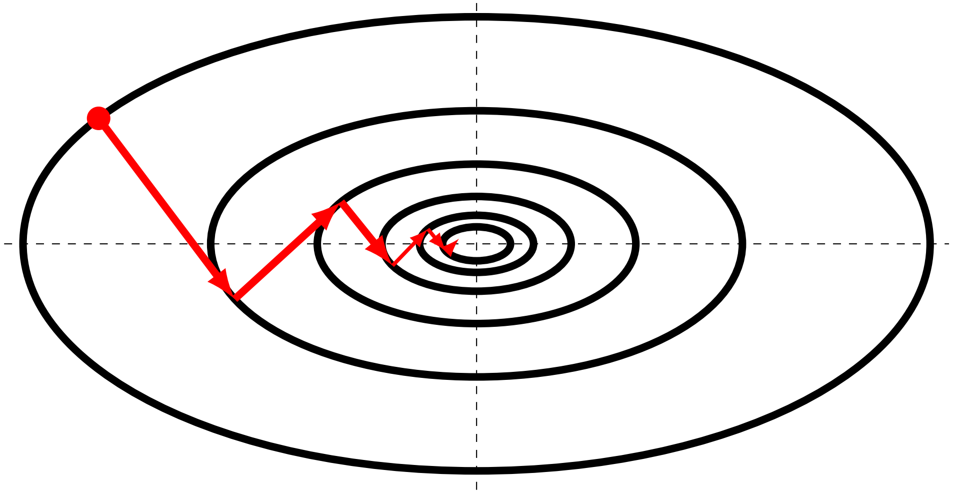
- ✗ The simplest gradient-based minimisation algorithm is called steepest descent:

```
Let $\mathbf{x}_0$ be an initial guess of the analysis;
while gradient is not sufficiently small do
    /* Define a descent direction                                          */
    $\mathbf{d}_k = -\nabla J(\mathbf{x}_k)$;
    /* Find a step $\alpha_k$, e.g. by line minimisation of the
       function $J(\mathbf{x}_k + \alpha\mathbf{d}_k)$, for which $J(\mathbf{x}_k + \alpha\mathbf{d}_k) < J(\mathbf{x}_k)$     */
    $\alpha_k = \cdots$ ;
    /* 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.
- ✗ We define the curvature as the amount by which a line deviates from being straight.





Preconditioning

- ✘ 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 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:

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

- ✘ 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 $J''\delta\mathbf{x}_k = -\nabla J(\mathbf{x}_k)$ */
    $\delta\mathbf{x}_k = \cdots$;
    /* 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 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 $\alpha_k$ 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 if the observation operator $\mathcal{H}$ is linear. In this case, the cost function is strictly quadratic, and the gradient is linear:

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

- ✘ 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 method can be found online: Shewchuk (1994) "An Introduction to the Conjugate Gradient Method Without the Agonizing pain".

Calculating the Gradient

- To minimise the cost function, we must be able to calculate gradients.
- If we precondition using $\mathbf{L} = {\mathbf{P}^b}^{-1}$, the gradient (with respect to χ) is:

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

- 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 Gradient

- 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 $\mathbf{h}_k$. Each of these is extremely simple, and can be represented by a one or two lines of code.
- 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, $\mathbf{H}^{\mathrm{T}}(\mathbf{x}) \equiv \mathbf{h}_1^{\mathrm{T}} \mathbf{h}_2^{\mathrm{T}} \cdots \mathbf{h}_K^{\mathrm{T}} \mathbf{x}$, is called the adjoint of $\mathcal{H}$.
- Again, each $\mathbf{h}_k^{\mathrm{T}}$ 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

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.