Variational data assimilation

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A brief recap

Assume that we have

- a prior estimate of the state $\mathbf{x}^b$ with error covariance matrix $\mathbf{B}$
- observations $\mathbf{y}$ with error covariance matrix $\mathbf{R}$

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Gaussian assumption

If we assume that the errors are Gaussian then the pdf is defined solely by the mean and covariance.

Prior

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{n/2}|\mathbf{B}|^{1/2}} \exp\{-\frac{1}{2}(\mathbf{x}-\mathbf{x}^b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}^b)\}$$

Likelihood

$$p(\mathbf{y}|\mathbf{x}) = \frac{1}{(2\pi)^{p/2}|\mathbf{R}|^{1/2}} \exp\{-\frac{1}{2}(H(\mathbf{x})-\boldsymbol{y})^T\mathbf{R}^{-1}(H(\mathbf{x})-\boldsymbol{y})\}$$

Posterior

$$p(\mathbf{x}|\mathbf{y}) \propto \exp\{-\frac{1}{2}\{(\mathbf{x}-\mathbf{x}^b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}^b) + (H(\mathbf{x})-\boldsymbol{y})^T\mathbf{R}^{-1}(H(\mathbf{x})-\boldsymbol{y})\}\}$$

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Variational data assimilation – the idea

In variational data assimilation we seek the solution that maximises the *a posterior* probability $p(\mathbf{x}|\mathbf{y})$.

Since

$$p(\mathbf{x}|\mathbf{y}) \propto \exp\{ -\frac{1}{2}\{(\mathbf{x}-\mathbf{x}^b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}^b) + (H(\mathbf{x})-\mathbf{y})^T\mathbf{R}^{-1}(H(\mathbf{x})-\mathbf{y})\} \}$$

we will have the maximum probability when **x** minimises

$$J(\mathbf{x}) = \frac{1}{2}(\mathbf{x}-\mathbf{x}^b)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}^b) + \frac{1}{2}(H(\mathbf{x})-\mathbf{y})^T\mathbf{R}^{-1}(H(\mathbf{x})-\mathbf{y})$$

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We consider two main algorithms

- Three-dimensional variational assimilation (3D-Var)
  - Where we consider 3 space dimensions.
- Four-dimensional variational assimilation (4D-Var)
  - Where we consider 3 space dimensions plus time as the 4^{th} dimension.
  - In this case we can consider the observation operator to include the dynamical model.

We will present 4D-Var first and 3D-Var as a variant of this.

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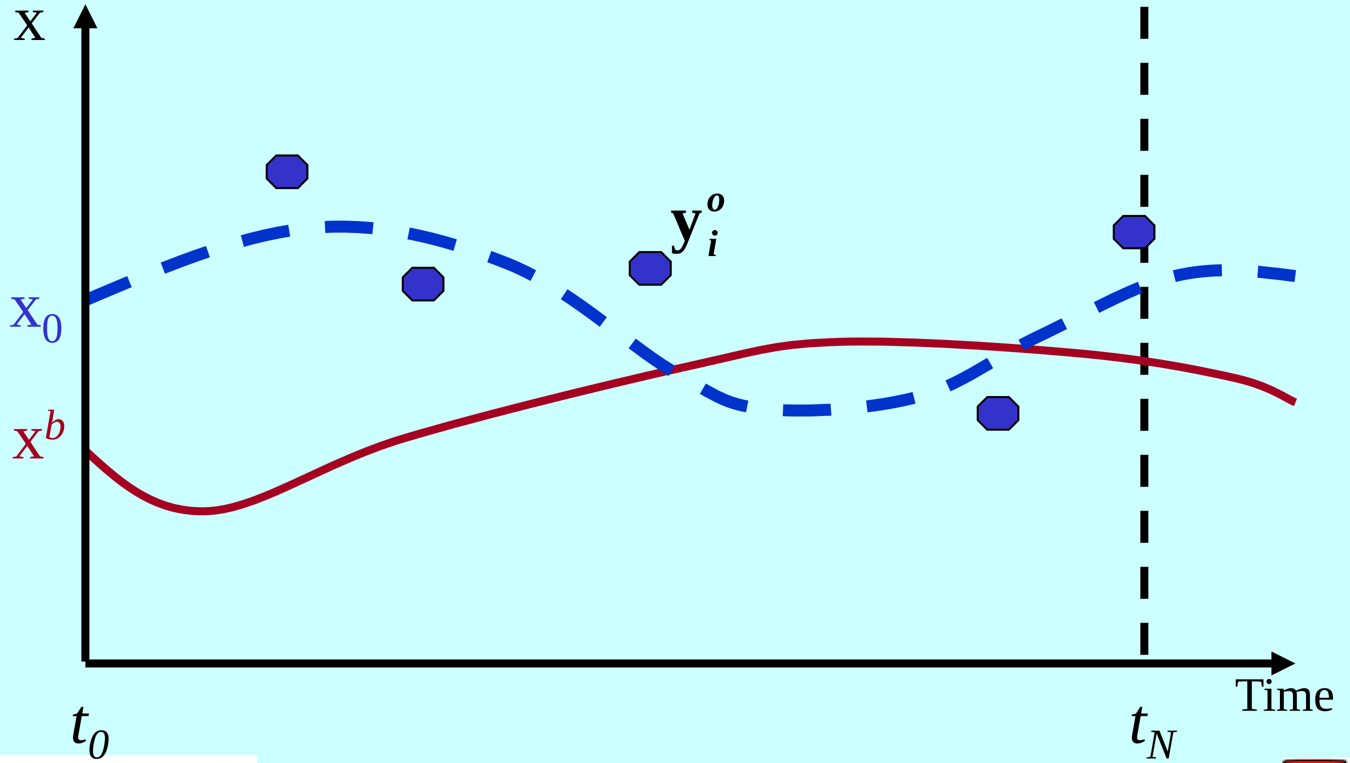
Four-dimensional variational assimilation (4D-Var)

Aim: Find the best estimate of the true state of the system (*analysis*), consistent with both observations distributed in time and the system dynamics.



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4D-Var cost function

Minimize

$$\mathcal{J}(\mathbf{x}_0) = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}^b)^{\mathrm{T}}\mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}^b) + \frac{1}{2}\sum_{i=0}^{N}(\mathcal{H}_i(\mathbf{x}_i) - \mathbf{y}_i)^{\mathrm{T}}\mathbf{R}_i^{-1}(\mathcal{H}_i(\mathbf{x}_i) - \mathbf{y}_i)$$

with respect to x_0, subject to

$$\mathbf{x}_{i+1} = \mathcal{M}_i(\mathbf{x}_i),$$

x^b - *a priori* (background) state – Size of order 10^8 - 10^9

y_i - Observations – Size of order 10^6 - 10^7

H_i - Observation operator

B - Background error covariance matrix

R_i - Observation error covariance matrix

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For N=0 we have 3D-Var

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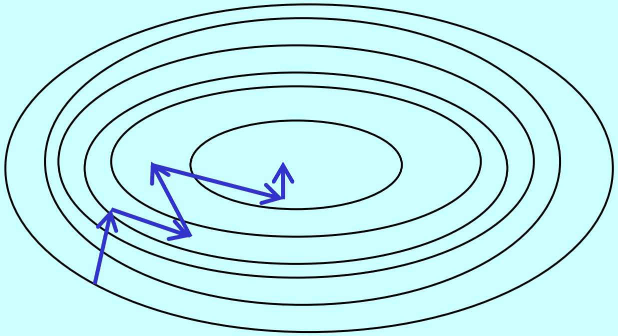
Numerical minimization - Gradient descent methods

Iterative methods, where each successive iteration is based on the value of the function and its gradient at the current iteration.



$$\mathbf{x}_0^{(k+1)} = \mathbf{x}_0^{(k)} - \alpha\, \varphi(\mathbf{x}_0^{(k)})$$

where α is a step length and φ is a direction that depends on $J(\mathbf{x}_0^{(k)})$ and its gradient.

Problem: How do we calculate the gradient of $J(\mathbf{x}_0^{(k)})$ with respect to $\mathbf{x}_0^{(k)}$?

Method of Lagrange multipliers

We introduce Lagrange multipliers $\boldsymbol{\lambda}_i$ at time t_i and define the Lagrangian

$$\mathcal{L}(\mathbf{x}_i, \boldsymbol{\lambda}_i) = \mathcal{J}(\mathbf{x}_0) + \sum_{i=0}^{N-1} \boldsymbol{\lambda}_{i+1}^{\mathrm{T}} (\mathbf{x}_{i+1} - \mathcal{M}_i(\mathbf{x}_i))$$

Then necessary conditions for a minimum of the cost function subject to the constraint are found by taking variations with respect to $\boldsymbol{\lambda}_i$ and $\mathbf{x}_i$.

Variations with respect to $\boldsymbol{\lambda}_i$ simply give the original constraint.

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$$\mathcal{L}(\mathbf{x}_i, \boldsymbol{\lambda}_i) = \mathcal{J}(\mathbf{x}_0) + \sum_{i=0}^{N-1} \boldsymbol{\lambda}_{i+1}^{\mathrm{T}}(\mathbf{x}_{i+1} - \mathcal{M}_i(\mathbf{x}_i))$$

Variations with respect to $\mathbf{x}_i$ give the *adjoint* equations

$$\boldsymbol{\lambda}_i = \mathbf{M}_i^T \boldsymbol{\lambda}_{i+1} - \mathbf{H}_i^T \mathbf{R}_i^{-1}(\mathcal{H}_i(\mathbf{x}_i) - \mathbf{y}_i)$$

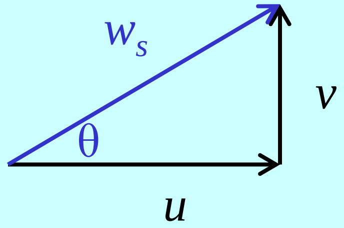
with boundary condition $\boldsymbol{\lambda}_{N+1} = 0$.

Then at initial time we have

$$\nabla \mathcal{J}(\mathbf{x}_0) = -\boldsymbol{\lambda}_0 + \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}^b).$$

An aside – What are the linear operators **H** & **M**?

Suppose we observe the wind speed w_s.



Then we have $\mathbf{x} = \begin{pmatrix} u \\ v \end{pmatrix}$, $\mathbf{y} = w_s$ and $\mathbf{y} = H(\mathbf{x})$

with

$$H(\mathbf{x}) = \sqrt{u^2 + v^2}$$

Then

$$\mathbf{H} = \begin{pmatrix} \frac{\partial H}{\partial u} & \frac{\partial H}{\partial v} \end{pmatrix} = \begin{pmatrix} \frac{u}{\sqrt{u^2+v^2}} & \frac{v}{\sqrt{u^2+v^2}} \end{pmatrix}$$

So where have we got to?

We wish to minimize

$$\mathcal{J}(\mathbf{x}_0) = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}^b)^{\mathrm{T}}\mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}^b) + \frac{1}{2}\sum_{i=0}^{N}(\mathcal{H}_i(\mathbf{x}_i) - \mathbf{y}_i)^{\mathrm{T}}\mathbf{R}_i^{-1}(\mathcal{H}_i(\mathbf{x}_i) - \mathbf{y}_i)$$

with respect to x_0, subject to

$$\mathbf{x}_{i+1} = \mathcal{M}_i(\mathbf{x}_i),$$

On each iteration we have to calculate *J* and its gradient

- To calculate *J* we need to run the nonlinear model
- To calculate the gradient of *J* we need one run of the adjoint model (backward in time)

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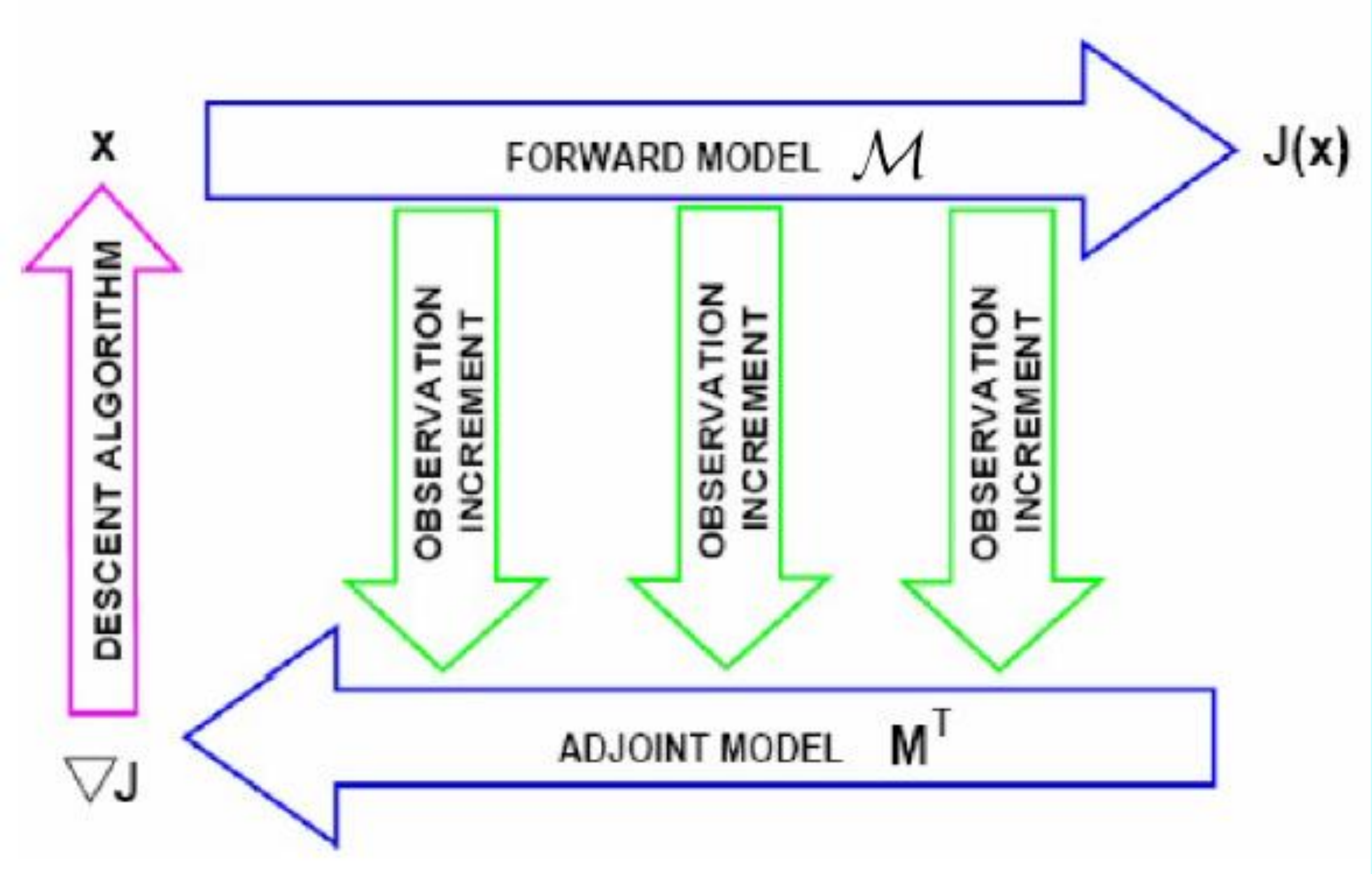

BUT this can be computationally expensive!

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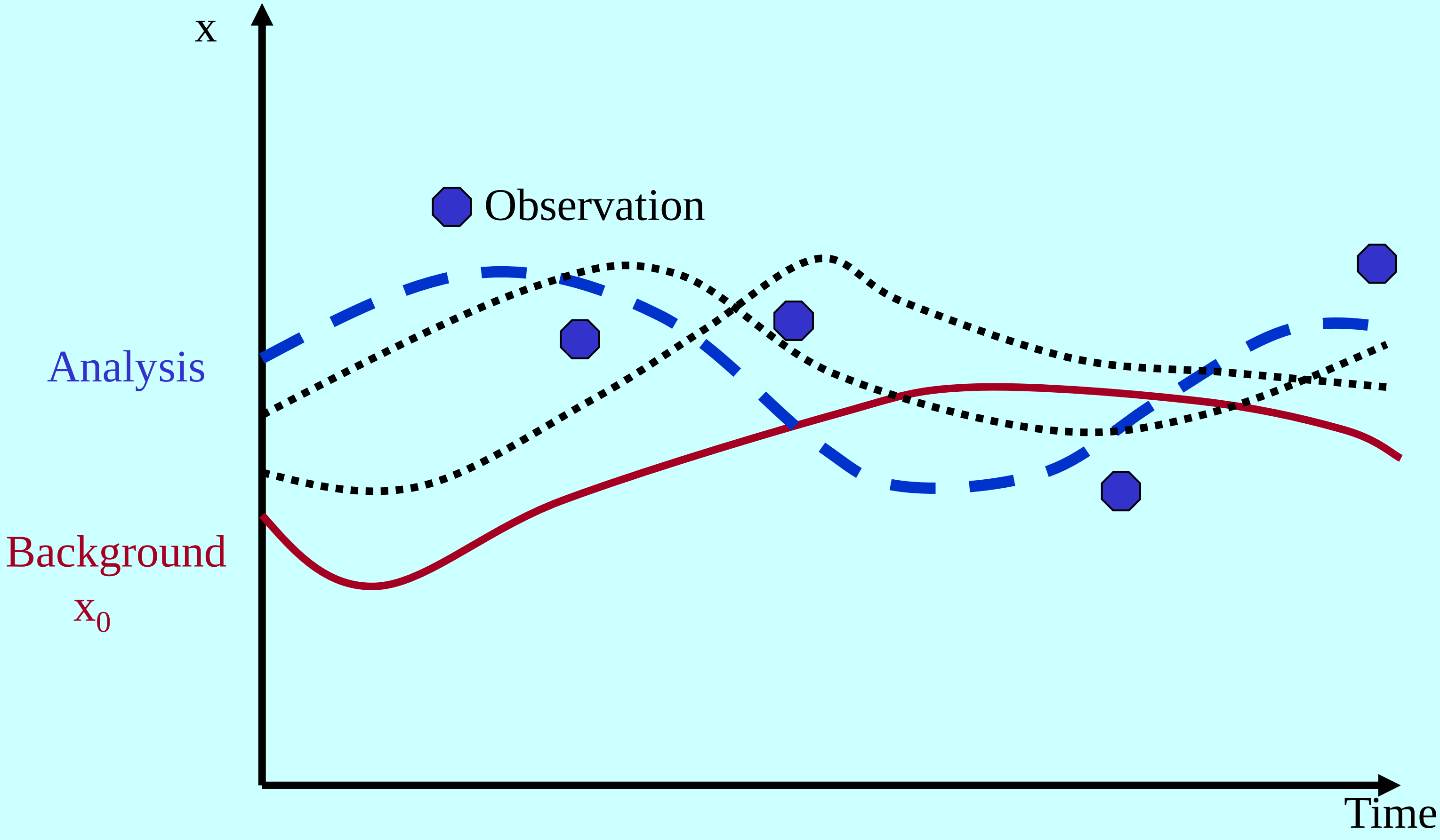
Incremental 4D-Var



Incremental 4D-Var

We solve a series of linearized minimization problems

$$\begin{aligned}\tilde{\mathcal{J}}^{(k)}[\delta\mathbf{x}_0^{(k)}] &= \frac{1}{2}(\delta\mathbf{x}_0^{(k)} - [\mathbf{x}^b - \mathbf{x}_0{}^{(k)}])^{\mathrm{T}}\mathbf{B}^{-1}(\delta\mathbf{x}_0^{(k)} - [\mathbf{x}^b - \mathbf{x}_0{}^{(k)}]) \\ &+ \frac{1}{2}\sum_{i=0}^{N}(\mathbf{H}_i\delta\mathbf{x}_i^{(k)} - \mathbf{d}_i^{(k)})^{\mathrm{T}}\mathbf{R}_i^{-1}(\mathbf{H}_i\delta\mathbf{x}_i^{(k)} - \mathbf{d}_i^{(k)})\end{aligned}$$

with

$$\begin{aligned}\mathbf{d}_i &= \mathbf{y}_i - \mathcal{H}_i[\mathbf{x}_i^{(k)}] \\ \delta\mathbf{x}_{i+1} &= \mathbf{M}_i\delta\mathbf{x}_i\end{aligned}$$

and update using

$$\mathbf{x}_0^{(k+1)} = \mathbf{x}_0^{(k)} + \delta\mathbf{x}_0^{(k)}$$

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Comments on incremental formulation

- Inner loop cost function is linear quadratic, so has a unique minimum.
- Can simplify the linear model (low resolution, simplified physics) in order to save computational time.
- Equivalent to an approximate Gauss-Newton procedure – Convergence results proved by *Lawless, Gratton & Nichols, QJRMS, 2005; Gratton, Lawless & Nichols, SIAM J. on Optimization, 2007.*
- Used in several operational centres, including ECMWF and Met Office.

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3D-FGAT (First guess at appropriate time)

We solve a series of linearized minimization problems

$$
\begin{aligned}
\tilde{\mathcal{J}}^{(k)}[\delta \mathbf{x}_0^{(k)}] &= \frac{1}{2}(\delta \mathbf{x}_0^{(k)} - [\mathbf{x}^b - \mathbf{x}_0{}^{(k)}])^{\mathrm{T}} \mathbf{B}^{-1} (\delta \mathbf{x}_0^{(k)} - [\mathbf{x}^b - \mathbf{x}_0{}^{(k)}]) \\
&+ \frac{1}{2} \sum_{i=0}^{N} (\mathbf{H}_i \delta \mathbf{x}_i^{(k)} - \mathbf{d}_i^{(k)})^{\mathrm{T}} \mathbf{R}_i^{-1} (\mathbf{H}_i \delta \mathbf{x}_i^{(k)} - \mathbf{d}_i^{(k)})
\end{aligned}
$$

with

$$
\begin{aligned}
\mathbf{d}_i &= \mathbf{y}_i - \mathcal{H}_i[\mathbf{x}_i^{(k)}] \\
\delta \mathbf{x}_{i+1} &= \mathbf{M}_i \delta \mathbf{x}_i
\end{aligned}
$$

Replace this equation with $\delta \mathbf{x}_{i+1} = \delta \mathbf{x}_i$

and update using

$$
\mathbf{x}_0^{(k+1)} = \mathbf{x}_0^{(k)} + \delta \mathbf{x}_0^{(k)}
$$

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Properties of 4D-Var

- Observations are treated at correct time.
- Use of dynamics means that more information can be obtained from observations.
- Covariances are implicitly evolved.
- In practice development of linear and adjoint models may be complex, but can be done at level of code.
- Standard formulation assumes model is perfect. Weak-constraint 4D-Var being developed to relax this assumption.

Weak-constraint 4D-Var

- The difference between the observation and the model trajectory may be due to model error rather than observation error.
- In weak constraint 4D-Var we do not assume that the model is correct, but assume

$$\mathbf{x}_{i+1} = \mathcal{M}_i(\mathbf{x}_i) + \eta_{i+1}, \qquad \eta \sim \mathcal{N}(\mathbf{Q}_i)$$

- Then we can either solve for $\mathbf{x}$ at each time, or for the initial $\mathbf{x}_0$ and all the η_i.

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Error formulation

$$J(\mathbf{x}_0, \eta_1, \ldots, \eta_N) = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}^b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}^b) + \frac{1}{2}\sum_{i=0}^{N}(\mathbf{y}_i - \mathcal{H}_i(\mathbf{x}_i))^T \mathbf{R}_i^{-1}(\mathbf{y}_i - \mathcal{H}_i(\mathbf{x}_i)) + \frac{1}{2}\sum_{i=1}^{N}\eta_i^T \mathbf{Q}_i^{-1}\eta_i.$$

State formulation

$$J(\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_N) = \frac{1}{2}(\mathbf{x}_0 - \mathbf{x}^b)^T \mathbf{B}^{-1}(\mathbf{x}_0 - \mathbf{x}^b) + \frac{1}{2}\sum_{i=0}^{N}(\mathbf{y}_i - \mathcal{H}_i(\mathbf{x}_i))^T \mathbf{R}_i^{-1}(\mathbf{y}_i - \mathcal{H}_i(\mathbf{x}_i)) + \frac{1}{2}\sum_{i=1}^{N}(\mathbf{x}_i - \mathbf{x}_{i-1})^T \mathbf{Q}_i^{-1}(\mathbf{x}_i - \mathbf{x}_{i-1}).$$

Comments on weak-constraint formulation

- No longer assumes that the model is perfect, so in theory is more realistic.
- The problem becomes much bigger and more complicated to solve.
- We don't really know how to specify the model error covariance matrix **Q**.
- Even though the two formulations are equivalent, they have different mathematical properties.

References – Variational methods

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