Variational data assimilation I

Background and methods

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The data assimilation problem

- To combine imperfect data from models, from observations distributed in time and space, exploiting any relevant physical constraints, to produce a more accurate and comprehensive picture of the system as it evolves in time.
- Traditionally we are interested in a state of the system.
- This is just a first moment of the posterior PDF.
- "All models are wrong ..." (George Box)
- "All models are wrong and all observations are inaccurate."

Bayes' Theorem

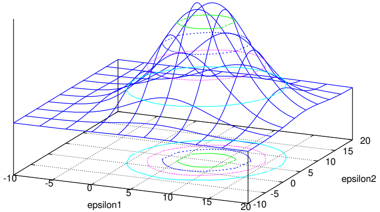
$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{x}) \times p(\mathbf{y}|\mathbf{x})}{p(\mathbf{y})}$$

$$\text{posterior distribution} = \frac{\text{prior distribution} \times \text{likelihood}}{\text{normalizing constant}}$$

- Prior distribution: PDF of the state before observations are considered (e.g. PDF of model forecast).
- Likelihood: PDF of observations given that the state is $\mathbf{x}$.
- Posterior: PDF of the state after the obs. have been considered.

The Gaussian assumption

- PDFs are often described by Gaussians (normal distributions).
- Gaussian PDFs are described by a mean and covariance only.



$\varepsilon = \mathbf{x} - \langle \mathbf{x} \rangle$

For 1 variable (1D): $x \sim N(\langle x \rangle, \sigma^2)$

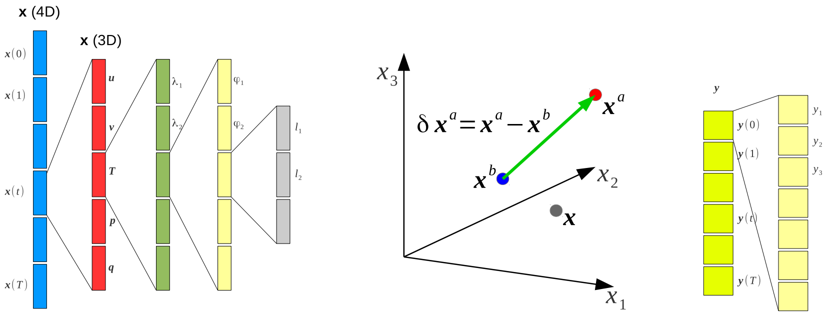
$$P(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp - \frac{(x - \langle x \rangle)^2}{2\sigma^2}$$

For n variables (nD): $\mathbf{x} \sim N(\langle \mathbf{x} \rangle, \mathbf{C})$

$$P(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^n \det(\mathbf{C})}} \times$$

$$\exp - \frac{1}{2} (\mathbf{x} - \langle \mathbf{x} \rangle)^{\mathrm{T}} \mathbf{C}^{-1} (\mathbf{x} - \langle \mathbf{x} \rangle)$$

Meaning of x and y



- $\mathbf{x}^{\mathrm{a}}$ analysis; $\mathbf{x}^{\mathrm{b}}$ background state; $\delta\mathbf{x}$ increment (perturbation).
- $\mathbf{y}$ observations; $\mathbf{y}^{\mathrm{m}} = \mathscr{H}(\mathbf{x})$ model observations.
- $\mathscr{H}(\mathbf{x})$ is the observation operator / forward model.
- Sometimes $\mathbf{x}$ and $\mathbf{y}$ are for only one time (3DVar).
- $\mathbf{x}$-vectors have n elements; $\mathbf{y}$-vectors have p elements.

Back to the Gaussian assumption

Prior: mean $\mathbf{x}^{\mathrm{b}}$, covariance $\mathbf{B}$

$$P(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^n \det(\mathbf{B})}} \exp -\frac{1}{2}\left(\mathbf{x}-\mathbf{x}^{\mathrm{b}}\right)^{\mathrm{T}} \mathbf{B}^{-1}\left(\mathbf{x}-\mathbf{x}^{\mathrm{b}}\right)$$

Likelihood: mean $\mathscr{H}(\mathbf{x})$, covariance $\mathbf{R}$

$$P(\mathbf{y}|\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^p \det(\mathbf{R})}} \exp -\frac{1}{2}\left(\mathbf{y}-\mathscr{H}(\mathbf{x})\right)^{\mathrm{T}} \mathbf{R}^{-1}\left(\mathbf{y}-\mathscr{H}(\mathbf{x})\right)$$

Posterior

$$\begin{aligned} p(\mathbf{x}|\mathbf{y}) \quad = \quad \frac{p(\mathbf{x}) \times p(\mathbf{y}|\mathbf{x})}{p(\mathbf{y})} &\propto \exp -\frac{1}{2}\left[\left(\mathbf{x}-\mathbf{x}^{\mathrm{b}}\right)^{\mathrm{T}} \mathbf{B}^{-1}\left(\mathbf{x}-\mathbf{x}^{\mathrm{b}}\right)\right. \\ &\left. + \left(\mathbf{y}-\mathscr{H}(\mathbf{x})\right)^{\mathrm{T}} \mathbf{R}^{-1}\left(\mathbf{y}-\mathscr{H}(\mathbf{x})\right)\right] \end{aligned}$$

Variational DA – the idea

- In Var., we seek a solution that maximizes the posterior probability $p(\mathbf{x}|\mathbf{y})$ (maximum-a-posteriori).
  - This is the most likely state given the observations (and the background), called the analysis, $\mathbf{x}^{\mathrm{a}}$.
  - Maximizing $p(\mathbf{x}|\mathbf{y})$ is equivalent to minimizing $-\ln p(\mathbf{x}|\mathbf{y}) \equiv J(\mathbf{x})$ (a least-squares problem).

$$
\begin{aligned}
p(\mathbf{x}|\mathbf{y}) &= C \exp -\frac{1}{2}\Big[\left(\mathbf{x}-\mathbf{x}^{\mathrm{b}}\right)^{\mathrm{T}} \mathbf{B}^{-1}\left(\mathbf{x}-\mathbf{x}^{\mathrm{b}}\right) \\
&\qquad + (\mathbf{y}-\mathscr{H}(\mathbf{x}))^{\mathrm{T}} \mathbf{R}^{-1} (\mathbf{y}-\mathscr{H}(\mathbf{x}))\Big] \\
J(\mathbf{x}) &= -\ln C + \frac{1}{2}\left(\mathbf{x}-\mathbf{x}^{\mathrm{b}}\right)^{\mathrm{T}} \mathbf{B}^{-1}\left(\mathbf{x}-\mathbf{x}^{\mathrm{b}}\right) \\
&\qquad + \frac{1}{2}(\mathbf{y}-\mathscr{H}(\mathbf{x}))^{\mathrm{T}} \mathbf{R}^{-1} (\mathbf{y}-\mathscr{H}(\mathbf{x})) \\
&= \text{constant (ignored)} + J^{\mathrm{b}}(\mathbf{x}) + J^{\mathrm{o}}(\mathbf{x})
\end{aligned}
$$

Exercises – practise the 'short hand' algebra

- $\mathbf{u}^{\mathrm{T}}\mathbf{v}$ (product of $1 \times n$ and $n \times 1$ vectors [an inner product], result is 1×1 [a scalar])

$$\begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix} = \begin{pmatrix} u_1 & \cdots & u_n \end{pmatrix} \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix} = u_1 v_1 + \cdots + u_n v_n$$

- $\mathbf{u}^{\mathrm{T}}\mathbf{A}\mathbf{v}$ (product of a $1 \times n$, an $n \times n$ matrix, and a $n \times 1$ vector [an inner product in a particular norm], result is 1×1 [a scalar])

$$\begin{pmatrix} u_1 & \cdots & u_n \end{pmatrix} \begin{pmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \cdots & A_{nn} \end{pmatrix} \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix} = \begin{pmatrix} u_1 & \cdots & u_n \end{pmatrix} \begin{pmatrix} A_{11} v_1 + \cdots + A_{1n} v_n \\ \vdots \\ A_{n1} v_1 + \cdots + A_{nn} v_n \end{pmatrix}$$

$$u_1 \left[A_{11} v_1 + \cdots + A_{1n} v_n \right] + \ldots + u_n \left[A_{n1} v_1 + \cdots + A_{nn} v_n \right]$$

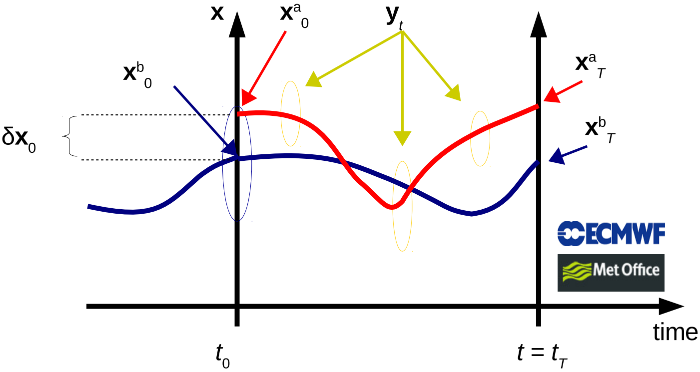
- $\mathbf{u}\mathbf{v}^{\mathrm{T}}$ (product of $n \times 1$ and $1 \times m$ vectors [an outer product], result is $n \times m$ matrix)

$$\begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix} \begin{pmatrix} v_1 & \cdots & v_m \end{pmatrix} = \begin{pmatrix} u_1 v_1 & \cdots & u_1 v_m \\ \vdots & \ddots & \vdots \\ u_n v_1 & & u_n v_m \end{pmatrix}$$

Four-dimensional Var (4DVar)

Aim

To find the 'best' estimate of the true state of the system (analysis), consistent with the observations, the background, and the system dynamics.



Towards a 4DVar cost function

Consider the observation operator in this case:

$$\mathscr{H}(\mathbf{x}) = \mathscr{H}\begin{pmatrix} \mathbf{x}_0 \\ \vdots \\ \mathbf{x}_T \end{pmatrix} = \begin{pmatrix} \mathscr{H}_0(\mathbf{x}_0) \\ \vdots \\ \mathscr{H}_T(\mathbf{x}_T) \end{pmatrix}$$

So the J^{o} is (assume that $\mathbf{R}$ is block diagonal):

$$J^{\mathrm{o}} = \frac{1}{2}(\mathbf{y} - \mathscr{H}(\mathbf{x}))^{\mathrm{T}}\mathbf{R}^{-1}(\mathbf{y} - \mathscr{H}(\mathbf{x})) =$$

$$\frac{1}{2}\begin{pmatrix} \mathbf{y}_0 - \mathscr{H}_0(\mathbf{x}_0) \\ \vdots \\ \mathbf{y}_T - \mathscr{H}_T(\mathbf{x}_T) \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} \mathbf{R}_0 & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \ddots & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{R}_T \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{y}_0 - \mathscr{H}_0(\mathbf{x}_0) \\ \vdots \\ \mathbf{y}_T - \mathscr{H}_T(\mathbf{x}_T) \end{pmatrix}$$

$$= \frac{1}{2}\sum_{i=0}^{T}(\mathbf{y}_i - \mathscr{H}_i(\mathbf{x}_i))^{\mathrm{T}}\mathbf{R}_i^{-1}(\mathbf{y}_i - \mathscr{H}_i(\mathbf{x}_i))$$

subject to the constraint $\mathbf{x}_{i+1} = \mathscr{M}_i(\mathbf{x}_i)$

The 4DVar cost function ('full 4DVar')

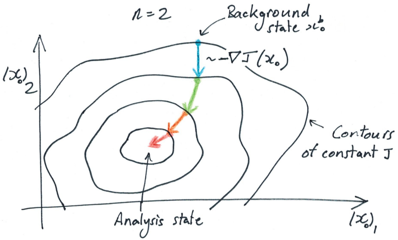
$$\text{Let } (\mathbf{a})^{\mathrm{T}} \mathbf{A}^{-1} (\mathbf{a}) \equiv (\mathbf{a})^{\mathrm{T}} \mathbf{A}^{-1} (\bullet)$$

$$\begin{aligned} J(\mathbf{x}) &= \frac{1}{2}\left(\mathbf{x}_0 - \mathbf{x}_0^{\mathrm{b}}\right)^{\mathrm{T}} \mathbf{B}_0^{-1} (\bullet) + \frac{1}{2}(\mathbf{y} - \mathscr{H}(\mathbf{x}))^{\mathrm{T}} \mathbf{R}^{-1} (\bullet) \\ &= \frac{1}{2}\left(\mathbf{x}_0 - \mathbf{x}_0^{\mathrm{b}}\right)^{\mathrm{T}} \mathbf{B}_0^{-1} (\bullet) + \frac{1}{2}\sum_{i=0}^{T} (\mathbf{y}_i - \mathscr{H}_i(\mathbf{x}_i))^{\mathrm{T}} \mathbf{R}_i^{-1} (\bullet) \end{aligned}$$

$$\text{subject to the constraint } \mathbf{x}_{i+1} = \mathscr{M}_i(\mathbf{x}_i)$$

- $\mathbf{x}_0^{\mathrm{b}}$ a-priori (background) state at t_0.
- $\mathbf{y}_i$ observations at t_i.
- $\mathscr{H}_i(\mathbf{x}_i)$ observation operator at t_i.
- $\mathbf{B}_0$ background error covariance matrix at t_0.
- $\mathbf{R}_i$ observation error covariance matrix at t_i.

Minimize $J(\mathbf{x})$ iteratively



Use the gradient of J at each iteration:

$$\mathbf{x}_0^{k+1} = \mathbf{x}_0^k + \alpha \nabla J(\mathbf{x}_0^k)$$

The gradient of the cost function

$$\nabla J(\mathbf{x}_0) = \begin{pmatrix} \partial J / \partial (\mathbf{x}_0)_1 \\ \vdots \\ \partial J / \partial (\mathbf{x}_0)_n \end{pmatrix}$$

$-\nabla J$ points in the direction of steepest descent.

Methods: steepest descent (inefficient), conjugate gradient (more efficient), . . .

The gradient of the cost function (wrt $\mathbf{x}(t_0)$)

Either:

1. Minimise $J(\mathbf{x}_0)$ w.r.t. $\mathbf{x}_0$ with $\mathbf{x}_i = \mathscr{M}_{i-1}(\mathscr{M}_{i-2}(\cdots \mathscr{M}_0(\mathbf{x}_0)))$.
2. Minimise $J(\mathbf{x}) = J(\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_T)$ w.r.t. $\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_T$ subject to the constraint

$$\mathbf{x}_{i+1} - \mathscr{M}_i(\mathbf{x}_i) = 0$$

$$L(\mathbf{x}, \lambda) = J(\mathbf{x}) + \sum_{i=0}^{T-1} \lambda_{i+1}^{\mathrm{T}} (\mathbf{x}_{i+1} - \mathscr{M}_i(\mathbf{x}_i)).$$

Each approach leads to the **adjoint method**

- An efficient means of computing the gradient.
- Uses the linearised/adjoint of $\mathscr{M}_i$ and $\mathscr{H}_i$: $\mathbf{M}_i^{\mathrm{T}}$ and $\mathbf{H}_i^{\mathrm{T}}$ (see next slides).

The adjoint method

Equivalent gradient formula:

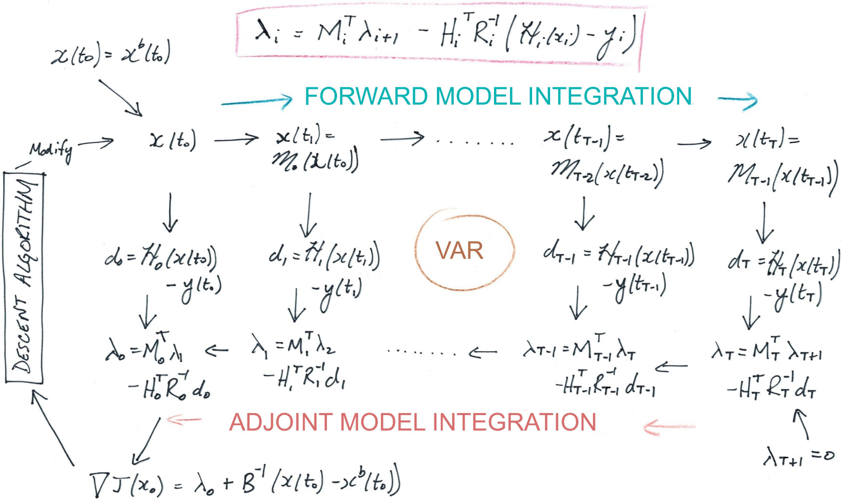
1.

$$\begin{aligned}
\nabla J \equiv \nabla J(\mathbf{x}_0) &= \nabla J_\mathrm{b}(\mathbf{x}_0) + \nabla J_\mathrm{o}(\mathbf{x}_0) \\
&= \mathbf{B}_0^{-1}\left(\mathbf{x}_0 - \mathbf{x}_0^\mathrm{b}\right) \\
&\quad - \sum_{i=0}^{T} \mathbf{M}_0^\mathrm{T} \ldots \mathbf{M}_{i-1}^\mathrm{T} \mathbf{H}_i^\mathrm{T} \mathbf{R}_i^{-1}\left(\mathbf{y}_i - \mathscr{H}_i(\mathbf{x}_i)\right) \\
\text{where } \mathbf{M}_i &= \partial \mathscr{M}_i(\mathbf{x}_i)/\partial \mathbf{x}_i \text{ and } \mathbf{H}_i = \partial \mathscr{H}_i(\mathbf{x}_i)/\partial \mathbf{x}_i
\end{aligned}$$

2.

$$\begin{aligned}
\lambda_{T+1} &= 0 \\
\lambda_i &= \mathbf{H}_i^\mathrm{T} \mathbf{R}_i^{-1}\left(\mathbf{y}_i - \mathscr{H}_i(\mathbf{x}_i)\right) + \mathbf{M}_i^\mathrm{T} \lambda_{i+1} \\
\lambda_0 &= \nabla J_\mathrm{o} \\
\therefore \nabla J &= \nabla J_\mathrm{b} + \nabla J_\mathrm{o} \\
&= \mathbf{B}_0^{-1}\left(\mathbf{x}_0 - \mathbf{x}_0^\mathrm{b}\right) + \lambda_0
\end{aligned}$$

The adjoint method



Simplifications and complications

- The full 4DVar method is expensive and difficult to solve.
- Model $\mathscr{M}_i$ is non-linear.
- Observation operators, $\mathscr{H}_i$ can be non-linear.
- Linear $\mathscr{H} \rightarrow$ quadratic cost function – easy(er) to minimize, $J^{\mathrm{o}} \sim \frac{1}{2}(y - ax)^2/\sigma_{\mathrm{o}}^2$.
- Non-linear $\mathscr{H} \rightarrow$ non-quadratic cost function – hard to minimize, $J^{\mathrm{o}} \sim \frac{1}{2}(y - f(x))^2/\sigma_{\mathrm{o}}^2$.
- Later will recognise that models are 'wrong'!

Look for simplifications:

Incremental 4DVar (linearized 4DVar)
3D-FGAT
3DVar

Complications:

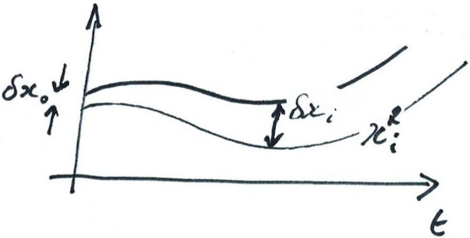
Weak constraint
(imperfect model)

Incremental 4DVar (1)

define reference trajectory: $\mathbf{x}^{\mathrm{R}}_{i+1} = \mathscr{M}_i\left(\mathbf{x}^{\mathrm{R}}_i\right)$

$$\mathbf{x}_i = \mathbf{x}^{\mathrm{R}}_i + \delta\mathbf{x}_i \qquad \mathbf{x}^{\mathrm{b}}_0 = \mathbf{x}^{\mathrm{R}}_0 + \delta\mathbf{x}^{\mathrm{b}}_0$$

$$\begin{aligned}
\mathbf{x}_{i+1} &= \mathscr{M}_i(\mathbf{x}_i) = \mathscr{M}_i\left(\mathbf{x}^{\mathrm{R}}_i + \delta\mathbf{x}_i\right) \\
\mathbf{x}^{\mathrm{R}}_{i+1} + \delta\mathbf{x}_{i+1} &\approx \mathscr{M}_i\left(\mathbf{x}^{\mathrm{R}}_i\right) + \mathbf{M}_i\delta\mathbf{x}_i \qquad \delta\mathbf{x}_{i+1} \approx \mathbf{M}_i\delta\mathbf{x}_i \\
\mathbf{y}^{\mathrm{m}}_i &= \mathscr{H}_i(\mathbf{x}_i) = \mathscr{H}_i\left(\mathbf{x}^{\mathrm{R}}_i + \delta\mathbf{x}_i\right) \\
\mathbf{y}^{\mathrm{mR}}_i + \delta\mathbf{y}^{\mathrm{m}}_i &\approx \mathscr{H}_i\left(\mathbf{x}^{\mathrm{R}}_i\right) + \mathbf{H}_i\delta\mathbf{x}_i \qquad \delta\mathbf{y}^{\mathrm{m}}_i \approx \mathbf{H}_i\delta\mathbf{x}_i
\end{aligned}$$

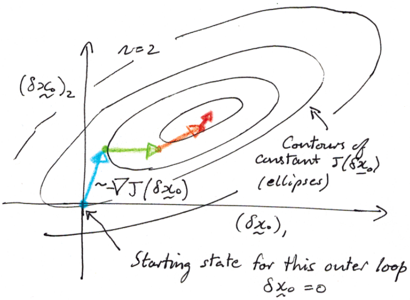


Incremental 4DVar (2)

$$
\begin{aligned}
J(\delta\mathbf{x}_0) &= \frac{1}{2}\left(\delta\mathbf{x}_0 - \delta\mathbf{x}_0^{\mathrm{b}}\right)^{\mathrm{T}} \mathbf{B}_0^{-1}(\bullet) + \\
&\quad \frac{1}{2}\sum_{i=0}^{T}\left(\mathbf{y}_i - \mathscr{H}_i(\mathbf{x}_i^{\mathrm{R}}) - \mathbf{H}_i\delta\mathbf{x}_i\right)^{\mathrm{T}} \mathbf{R}_i^{-1}(\bullet) \\
\delta\mathbf{x}_i &\approx \mathbf{M}_{i-1}\mathbf{M}_{i-2}\ldots\mathbf{M}_0\,\delta\mathbf{x}_0
\end{aligned}
$$

- Initially set reference to background, $\mathbf{x}_0^{\mathrm{R}} = \mathbf{x}_0^{\mathrm{b}}$.
- 'Inner loop': iterations to find $\delta\mathbf{x}_0^{\mathrm{a}} = \mathrm{argmin} J(\delta\mathbf{x}_0)$ (use adjoint method).
- 'Outer loop': iterate $\mathbf{x}_0^{\mathrm{R}} \to \mathbf{x}_0^{\mathrm{R}} + \delta\mathbf{x}_0^{\mathrm{a}}$
- Inner loop is exactly quadratic (e.g. has a unique minimum).
- Inner loop can be simplified (lower res., simplified physics).

Minimize $J(\delta \mathbf{x})$ iteratively



Use the gradient of J at each iteration:

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

The gradient of the cost function

$$\nabla J(\delta \mathbf{x}_0) = \begin{pmatrix} \partial J / \partial(\delta \mathbf{x}_0)_1 \\ \vdots \\ \partial J / \partial(\delta \mathbf{x}_0)_n \end{pmatrix}$$

$-\nabla J$ points in the direction of steepest descent.

Methods: steepest descent (inefficient), conjugate gradient (more efficient), ...

Simplification 1: 3D-FGAT

- Three dimensional variational data assimilation with first guess (i.e. $\mathbf{x}_i^{\mathrm{R}}$) is computed at the appropriate time.
- Simplification is that $\mathbf{M}_i \to \mathbf{I}$, i.e. $\delta\mathbf{x}_i = \mathbf{M}_{i-1} \ldots \mathbf{M}_0 \delta\mathbf{x}_0 \to \delta\mathbf{x}_0$.

$$
\begin{aligned}
J^{\mathrm{3DFGAT}}(\delta\mathbf{x}_0) \quad = \quad & \frac{1}{2}\left(\delta\mathbf{x}_0 - \delta\mathbf{x}_0^{\mathrm{b}}\right)^{\mathrm{T}} \mathbf{B}_0^{-1} (\bullet) + \\
& \frac{1}{2}\sum_{i=0}^{T}\left(\mathbf{y}_i - \mathscr{H}_i(\mathbf{x}_i^{\mathrm{R}}) - \mathbf{H}_i\delta\mathbf{x}_0\right)^{\mathrm{T}} \mathbf{R}_i^{-1} (\bullet)
\end{aligned}
$$

Simplification 2: 3DVar

- This has no time dependence within the assimilation window.
- Not used (these days "3DVar" really means 3D-FGAT).

$$
\begin{aligned}
J^{\text{3DVar}}(\delta\mathbf{x}_0) &= \frac{1}{2}\left(\delta\mathbf{x}_0 - \delta\mathbf{x}_0^{\text{b}}\right)^{\text{T}}\mathbf{B}_0^{-1}(\bullet) + \\
&\quad \frac{1}{2}\sum_{i=0}^{T}\left(\mathbf{y}_i - \mathscr{H}_i(\mathbf{x}_0^{\text{R}}) - \mathbf{H}_i\delta\mathbf{x}_0\right)^{\text{T}}\mathbf{R}_i^{-1}(\bullet)
\end{aligned}
$$

But note

3DVar is not an approx. if all obs. in this cycle are at $t = 0$. For $\mathbf{x}_0^{\text{R}} = \mathbf{x}_0^{\text{b}}$:

$$
\begin{aligned}
J^{\text{3DVar}}(\delta\mathbf{x}_0) &= \frac{1}{2}\delta\mathbf{x}_0^{\text{T}}\mathbf{B}_0^{-1}\delta\mathbf{x}_0 + \frac{1}{2}\left(\mathbf{y}_0 - \mathscr{H}_0(\mathbf{x}_0^{\text{b}}) - \mathbf{H}_0\delta\mathbf{x}_0\right)^{\text{T}}\mathbf{R}_0^{-1}(\bullet) \\
\text{Setting } \nabla J^{\text{3DVar}} &= \mathbf{B}_0^{-1}\delta\mathbf{x}_0 - \mathbf{H}_0^{\text{T}}\mathbf{R}_0^{-1}\left(\mathbf{y}_0 - \mathscr{H}_0(\mathbf{x}_0^{\text{b}}) - \mathbf{H}_0\delta\mathbf{x}_0\right) = 0 \\
\text{Gives } \mathbf{x}_0^{\text{a}} = \mathbf{x}_0^{\text{b}} + \delta\mathbf{x}_0 &= \mathbf{x}_0^{\text{b}} + \left(\mathbf{B}_0^{-1} + \mathbf{H}_0^{\text{T}}\mathbf{R}_0^{-1}\mathbf{H}_0\right)^{-1}\mathbf{H}_0^{\text{T}}\mathbf{R}_0^{-1}\left(\mathbf{y}_0 - \mathscr{H}_0(\mathbf{x}_0^{\text{b}})\right) \\
\text{As the Kalman Filter!} &= \mathbf{x}_0^{\text{b}} + \mathbf{B}_0\mathbf{H}_0^{\text{T}}\left(\mathbf{R}_0 + \mathbf{H}_0\mathbf{B}_0\mathbf{H}_0^{\text{T}}\right)^{-1}\left(\mathbf{y}_0 - \mathscr{H}_0(\mathbf{x}_0^{\text{b}})\right)
\end{aligned}
$$

Reminder: the Kalman Filter

$$\begin{aligned}
\mathbf{x}^{\mathrm{a}}_t &= \mathbf{x}^{\mathrm{f}}_t + \mathbf{K}_t\left(\mathbf{y_t} - \mathscr{H}_t(\mathbf{x}^{\mathrm{f}}_t)\right)\\
\mathbf{P}^{\mathrm{a}}_t &= \left(\mathbf{I} - \mathbf{K_t}\mathbf{H}_t\right)\mathbf{P}^{\mathrm{f}}_t\\
\mathbf{K}_t &= \mathbf{P}^{\mathrm{f}}_t\mathbf{H}^{\mathrm{T}}_t\left(\mathbf{R}_t + \mathbf{H}_t\mathbf{P}^{\mathrm{f}}_t\mathbf{H}^{\mathrm{T}}_t\right)^{-1} \longleftarrow
\end{aligned}$$

$$\begin{aligned}
\mathbf{x}^{\mathrm{f}}_{t+1} &= \mathscr{M}_t(\mathbf{x}^{\mathrm{a}}_t)\\
\mathbf{P}^{\mathrm{f}}_{t+1} &= \mathbf{M}_t\mathbf{P}^{\mathrm{a}}_t\mathbf{M}^{\mathrm{T}}_t
\end{aligned}$$

$$\left(\mathbf{B}^{-1} + \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{H}\right)\mathbf{B}\mathbf{H}^{\mathrm{T}}$$

$$= \mathbf{H}^{\mathrm{T}}\mathbf{R}^{-1}\left(\mathbf{R} + \mathbf{H}\mathbf{B}\mathbf{H}^{\mathrm{T}}\right)$$

$$\begin{aligned}
\mathbf{H}_t &= \left.\frac{\partial\left(\mathscr{H}_t(\mathbf{x})\right)}{\mathbf{x}}\right|_{\mathbf{x}=\mathbf{x}^{\mathrm{f}}_t}\\
\mathbf{M}_t &= \left.\frac{\partial\left(\mathscr{M}_t(\mathbf{x})\right)}{\mathbf{x}}\right|_{\mathbf{x}=\mathbf{x}^{\mathrm{a}}_t}
\end{aligned}$$

Properties of 4DVar

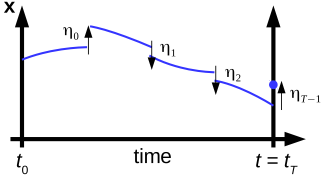
- Observations are treated at the correct time.
- Use of dynamics means that more information can be obtained from observations.
- Covariance $\mathbf{B}_0$ is implicitly evolved, $\mathbf{B}_i = (\mathbf{M}_{i-1} \dots \mathbf{M}_0)\,\mathbf{B}_0\,(\mathbf{M}_{i-1} \dots \mathbf{M}_0)^{\mathrm{T}}$.
- In practice development of linear and adjoint models is complex.
    - $\mathscr{M}_i$, $\mathscr{H}_i$, $\mathbf{M}_i$, $\mathbf{H}_i$, $\mathbf{M}_i^{\mathrm{T}}$, and $\mathbf{H}_i^{\mathrm{T}}$ are subroutines, and so 'matrices' are usually not in explicit matrix form.

But note

- Standard 4DVar assumes the model is perfect.
- This can lead to sub-optimalities.
- Weak-constraint 4DVar relaxes this assumption.

Modify evolution equation:

$$\begin{aligned} \mathbf{x}_{i+1} &= \mathcal{M}_i(\mathbf{x}_i) + \eta_i \\ \text{where } \eta_i &\sim N(0, \mathbf{Q}_i) \end{aligned}$$



'State formulation' of WC4DVar

$$J^{\mathrm{wc}}_{\mathrm{state}}(\mathbf{x}_0, \ldots, \mathbf{x}_T) = J^{\mathrm{b}} + J^{\mathrm{o}} + \frac{1}{2}\sum_{i=0}^{T-1} (\mathbf{x}_{i+1} - \mathcal{M}_i(\mathbf{x}_i))^{\mathrm{T}} \mathbf{Q}_i^{-1} (\bullet)$$

'Error formulation' of WC4DVar

$$J^{\mathrm{wc}}_{\mathrm{error}}(\mathbf{x}_0, \eta_0 \ldots, \eta_{T-1}) = J^{\mathrm{b}} + J^{\mathrm{o}} + \frac{1}{2}\sum_{i=0}^{T-1} \eta_i^{\mathrm{T}} \mathbf{Q}_i^{-1} \eta_i$$

Implementation of weak constraint 4DVar

- Vector to be determined ('control vector') increases from n in 4DVar to $n + n(T - 1)$ in WC4DVar.
- The model error covariance matrices, $\mathbf{Q}_i$, need to be estimated. How?
- The 'state' formulation (determine $\mathbf{x}_0, \ldots, \mathbf{x}_T$) and the 'error' formulation (determine $\mathbf{x}_0, \eta_0 \ldots, \eta_{T-1}$) are mathematically equivalent, but can behave differently in practice.
- There is an incremental form of WC4DVar.

Summary of 4DVar

- The variational method forms the basis of many operational weather and ocean forecasting systems, including at ECMWF, the Met Office, Météo-France, etc.
- It allows complicated observation operators to be used (e.g. for assimilation of satellite data).
- It has been very successful.
- Incremental (quasi-linear) versions are usually implemented.
- It requires specification of $\mathbf{B}_0$, the background error cov. matrix, and $\mathbf{R}_i$, the observation error cov. matrix.
- 4DVar requires the development of linear and adjoint models – not a simple task!
- Weak constraint formulations require the additional specification of $\mathbf{Q}_i$.

Selected References

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