Introduction to Data Assimilation with 4D-Var and its relation to Tikhonov regularisation

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Outline

What is Data Assimilation?

Loose definition

Estimation and prediction (analysis) of an unknown, true state by combining observations and system dynamics (model output).

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Some examples

- Navigation
- Medical imaging
- Numerical weather prediction

Data Assimilation in NWP

Estimate the state of the atmosphere $\mathbf{x}_i$.

Observations $\mathbf{y}$

- Satellites
- Ships and buoys
- Surface stations
- Aeroplanes

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- a model how the atmosphere evolves in time (imperfect)

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

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Assimilation algorithms

- used to find an (approximate) state of the atmosphere $\mathbf{x}_i$ at times i (usually $i = 0$)
- using this state a forecast for future states of the atmosphere can be obtained
- $\mathbf{x}^A$: Analysis (estimation of the true state after the DA)

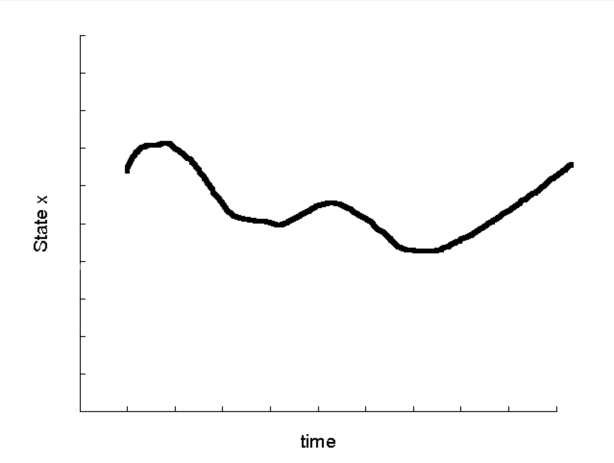

Figure: Background state $\mathbf{x}^B$

Schematics of DA

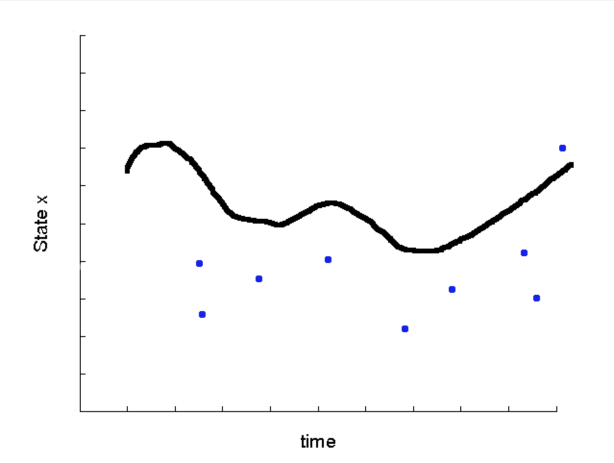

Figure: Observations $\mathbf{y}$

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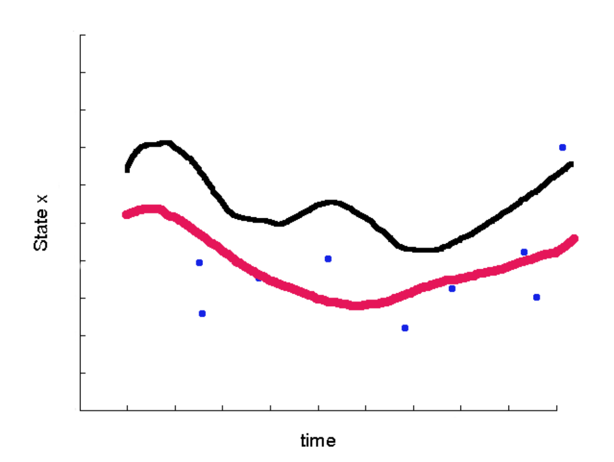

Figure: Analysis $\mathbf{x}^A$ (consistent with observations and model dynamics)

Underdeterminacy

- Size of the state vector $\mathbf{x}$: $432 \times 320 \times 50 \times 7 = \mathcal{O}(10^7)$

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- Number of observations (size of $\mathbf{y}$): $\mathcal{O}(10^5 - 10^6)$
- Operator H (nonlinear!) maps from state space into observations space: $\mathbf{y} = H(\mathbf{x})$

Any easy scheme

Cressman analysis

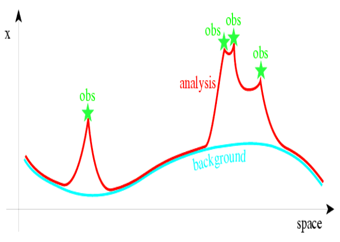

Figure: Copyright:ECMWF

At each time step i

$$\mathbf{x}^A(k) = \mathbf{x}^B(k) + \frac{\sum_{l=1}^{n} w(lk)(\mathbf{y}(l) - \mathbf{x}^B(l))}{\sum_{l=1}^{n} w(lk)}$$

$$w(lk) = \max\left(0, \frac{R^2 - d_{lk}^2}{R^2 + d_{lk}^2}\right)$$

d_{lk} measures the distance between points l and k.

Outline

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Data Assimilation in NWP

Estimate the state of the atmosphere $\mathbf{x}_i$.

Apriori information $\mathbf{x}^B$

- background state (usual previous forecast) has errors!

Models

- a model how the atmosphere evolves in time (imperfect)

$$\mathbf{x}_{i+1} = M(\mathbf{x}_i) + \text{error}$$

- a function linking model space and observation space (imperfect)

$$\mathbf{y}_i = H(\mathbf{x}_i) + \text{error}$$

Observations $\mathbf{y}$ has errors!

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Error variables

Modelling the errors

- background error $\varepsilon^B = \mathbf{x}^B - \mathbf{x}^{\mathrm{Truth}}$ of average $\overline{\varepsilon}^B$ and covariance

$$\mathbf{B} = \overline{(\varepsilon^B - \overline{\varepsilon}^B)(\varepsilon^B - \overline{\varepsilon}^B)^T}$$

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- observation error $\varepsilon^O = \mathbf{y} - H(\mathbf{x}^{\text{Truth}})$ of average $\overline{\varepsilon}^O$ and covariance

$$\mathbf{R} = \overline{(\varepsilon^O - \overline{\varepsilon}^O)(\varepsilon^O - \overline{\varepsilon}^O)^T}$$

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- analysis error $\varepsilon^A = \mathbf{x}^A - \mathbf{x}^{\text{Truth}}$ of average $\overline{\varepsilon}^A$ and covariance

$$\mathbf{A} = \overline{(\varepsilon^A - \overline{\varepsilon}^A)(\varepsilon^A - \overline{\varepsilon}^A)^T}$$

- measure of the analysis error that we want to minimise

$$\text{tr}(\mathbf{A}) = \overline{\|\varepsilon^A - \overline{\varepsilon}^A\|^2}$$

Assumptions

- Linearised observation operator: $H(\mathbf{x}) - H(\mathbf{x}^B) = \mathbf{H}(\mathbf{x} - \mathbf{x}^B)$
- Nontrivial errors: $\mathbf{B}$, $\mathbf{R}$ are positive definite
- Unbiased errors: $\overline{\mathbf{x}^B - \mathbf{x}^{\text{Truth}}} = \overline{\mathbf{y} - H(\mathbf{x}^{\text{Truth}})} = 0$
- Uncorrelated errors: $\overline{(\mathbf{x}^B - \mathbf{x}^{\text{Truth}})(\mathbf{y} - H(\mathbf{x}^{\text{Truth}}))^T} = 0$

Optimal least-squares estimater

Cost function

Solution of the variational optimisation problem $\mathbf{x}^A = \arg\min J(\mathbf{x})$ where

$$\begin{aligned} J(\mathbf{x}) &= (\mathbf{x}-\mathbf{x}^B)^T\mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}^B) + (\mathbf{y}-H(\mathbf{x}))^T\mathbf{R}^{-1}(\mathbf{y}-H(\mathbf{x})) \\ &= J_B(\mathbf{x}) + J_O(\mathbf{x}) \end{aligned}$$

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Interpolation equations

$$\mathbf{x}^A = \mathbf{x}^B + \mathbf{K}(\mathbf{y} - H(\mathbf{x}^B)), \quad \text{where}$$

$$\mathbf{K} = \mathbf{B}\mathbf{H}^T(\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R})^{-1} \quad \mathbf{K} \ldots \text{gain matrix}$$

Conditional probabilities

Non-Gaussian PDF's (probability density function)

- $P(\mathbf{x})$ is a priori PDF (background)
- $P(\mathbf{y}|\mathbf{x})$ is the observation PDF (likelihood of the observations given background $\mathbf{x}$)

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- $P(\mathbf{x}|\mathbf{y})$ conditional probability of the model state given the observations, Bayes theorem:

$$\arg_x \max P(\mathbf{x}|\mathbf{y}) = \arg_x \max \frac{P(\mathbf{y}|\mathbf{x})P(\mathbf{x})}{P(\mathbf{y})}$$

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Gaussian PDF's

$$\begin{aligned} P(\mathbf{x}|\mathbf{y}) &= c_1 \exp\left(-(\mathbf{x}-\mathbf{x}^B)^T \mathbf{B}^{-1}(\mathbf{x}-\mathbf{x}^B)\right) \cdot \\ &\quad c_2 \exp\left(-(\mathbf{y}-H(\mathbf{x}))^T \mathbf{R}^{-1}(\mathbf{y}-H(\mathbf{x}))\right) \end{aligned}$$

$\mathbf{x}^A$ is the maximum a posteriori estimator of $\mathbf{x}^{\text{Truth}}$. Maximising $P(\mathbf{x}|\mathbf{y})$ equivalent to minimising $J(\mathbf{x})$

A simple scalar illustration

Room temperature

- T^O observation with standard deviation σ_O
- T^B background with standard deviation σ_B

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Room temperature

- T^O observation with standard deviation σ_O
- T^B background with standard deviation σ_B
- $T^A = T^B + k(T^O - T^B)$ with error variance $\sigma_A^2 = (1-k)^2\sigma_B^2 + k^2\sigma_O^2$
- optimal k which minimises error variance

$$k = \frac{\sigma_B^2}{\sigma_B^2 + \sigma_O^2}$$

- equivalent to minimising

$$J(T) = \frac{(T - T^B)^2}{\sigma_B^2} + \frac{(T - T^O)^2}{\sigma_O^2}$$

and then $\dfrac{1}{\sigma_A^2} = \dfrac{1}{\sigma_B^2} + \dfrac{1}{\sigma_O^2}$

Optimal interpolation

Optimal interpolation

Computation of

$$\mathbf{x}^A = \mathbf{x}^B + \mathbf{K}(\mathbf{y} - H(\mathbf{x}^B))$$

$$\mathbf{K} = \mathbf{B}\mathbf{H}^T(\mathbf{H}\mathbf{B}\mathbf{H}^T + \mathbf{R})^{-1} \quad \mathbf{K}\ldots \text{gain matrix}$$

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- expensive!

Three-dimensional variational assimilation (3D-Var)

3D-Var

Minimisation of

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- avoids computation of $\mathbf{K}$ by using a descent algorithm s

Four-dimensional variational assimilation (4D-Var)

Minimise the cost function

$$J(\mathbf{x}_0) = (\mathbf{x}_0 - \mathbf{x}_0^B)^T \mathbf{B}^{-1} (\mathbf{x}_0 - \mathbf{x}_0^B) + \sum_{i=0}^{n} (\mathbf{y}_i - H_i(\mathbf{x}_i))^T \mathbf{R}_i^{-1} (\mathbf{y}_i - H_i(\mathbf{x}_i))$$

subject to model dynamics $\mathbf{x}_i = M_{0 \to i} \mathbf{x}_0$

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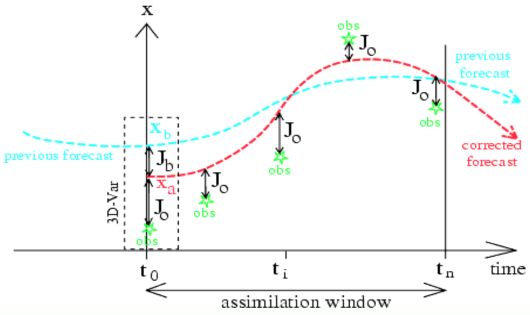

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4D-Var analysis

Model dynamics

Strong constraint: model states $\mathbf{x}_i$ are subject to

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nonlinear constraint optimisation problem (hard!)

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Simplifications

- Causality (forecast expressed as product of intermediate forecast steps)

$$\mathbf{x}_i = M_{i,i-1}M_{i-1,i-2}\dots M_{1,0}\mathbf{x}_0$$

- Tangent linear hypothesis (H and M can be linearised)

$$\mathbf{y}_i - H_i(\mathbf{x}_i) = \mathbf{y}_i - H_i(M_{0\to i}\mathbf{x}_0) = \mathbf{y}_i - H_i(M_{0\to i}\mathbf{x}_0^B) - \mathbf{H}_i\mathbf{M}_{0\to i}(\mathbf{x}_0 - \mathbf{x}_0^B)$$

$\mathbf{M}$ is the tangent linear model.

4D-Var analysis

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  $\mathbf{M}$ is the tangent linear model.

- unconstrained quadratic optimisation problem (easier).

Minimisation of the 4D-Var cost function

Efficient implementation of J and ∇J:

- forecast state $\mathbf{x}_i = M_{i,i-1} M_{i-1,i-2} \dots M_{1,0} \mathbf{x}_0$

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- ∇J is calculated by

$$
\begin{aligned}
-\frac{1}{2}\nabla J_O &= -\frac{1}{2}\sum_{i=0}^{n} \nabla J_{Oi} \\
&= \sum_{i=0}^{n} \mathbf{M}_{1,0}^T \ldots \mathbf{M}_{i,i-1}^T \mathbf{H}_i^T \mathbf{d}_i \\
&= \mathbf{H}_0^T \mathbf{d}_0 + \mathbf{M}_{1,0}^T [\mathbf{H}_1^T \mathbf{d}_1 + \mathbf{M}_{2,1} [\mathbf{H}_2^T \mathbf{d}_2 + \ldots + \mathbf{M}_{n,n-1}^T \mathbf{H}_n^T \mathbf{d}_n] \ldots]
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Minimisation of the 4D-Var cost function

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\end{aligned}$$

- initialise adjoint variable $\tilde{\mathbf{x}}_n = \mathbf{0}$ and then $\tilde{\mathbf{x}}_{i-1} = \mathbf{M}_{i,i-1}^T (\tilde{\mathbf{x}}_i + \mathbf{H}_i^T \mathbf{d}_i)$ etc., $\ldots \tilde{\mathbf{x}}_0 = -\frac{1}{2}\nabla J_O$

Minimisation of the 4D-Var cost function

Efficient implementation of J and ∇J:

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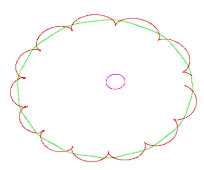
Further simplifications

- preconditioning with $\mathbf{B} = \mathbf{L}\mathbf{L}^T$ (transform into control variable space) so that $\hat{\mathbf{x}} = \mathbf{L}^{-1}\mathbf{x}$
- Incremental 4D-Var

Example - Three-Body Problem

Motion of three bodies in a plane, two position ($\mathbf{q}$) and two momentum ($\mathbf{p}$) coordinates for each body $\alpha = 1, 2, 3$



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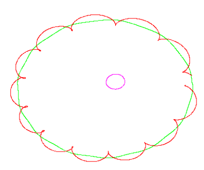

Equations of motion

$$
\begin{aligned}
H(\mathbf{q}, \mathbf{p}) &= \frac{1}{2} \sum_{\alpha} \frac{|\mathbf{p}_\alpha|^2}{m_\alpha} - \sum \sum_{\alpha<\beta} \frac{m_\alpha m_\beta}{|\mathbf{q}_\alpha - \mathbf{q}_\beta|} \\
\frac{d\mathbf{q}_\alpha}{dt} &= \frac{\partial H}{\partial \mathbf{p}_\alpha} \\
\frac{d\mathbf{p}_\alpha}{dt} &= -\frac{\partial H}{\partial \mathbf{q}_\alpha}
\end{aligned}
$$

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Example - Three-Body problem

- solver: partitioned Runge-Kutta scheme with time step $h = 0.001$
- observations are taken as noise from the truth trajectory
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- solver: partitioned Runge-Kutta scheme with time step $h = 0.001$
- observations are taken as noise from the truth trajectory
- background is given from a previous forecast
- assimilation window is taken 300 time steps
- minimisation of cost function J using a Gauss-Newton method (neglecting all second derivatives)

$$\nabla J(\mathbf{x}_0) = 0$$

$$\nabla\nabla J(\mathbf{x}_0^j)\Delta\mathbf{x}_0^j = -\nabla J(\mathbf{x}_0^j), \quad \mathbf{x}_0^{j+1} = \mathbf{x}_0^j + \Delta\mathbf{x}_0^j$$

- subsequent forecast is take 3000 time steps
- R is diagonal with variances between 10^{-3} and 10^{-5}

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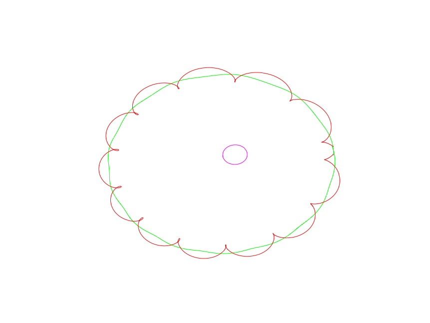
Changing the masses of the bodies

DA needs Model error!

$$\begin{aligned} m_s &= 1.0 \quad \longrightarrow \quad m_s = 1.1 \\ m_p &= 0.1 \quad \longrightarrow \quad m_p = 0.11 \\ m_m &= 0.01 \quad \longrightarrow \quad m_m = 0.011 \end{aligned}$$



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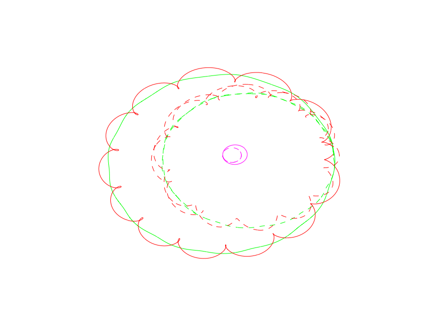

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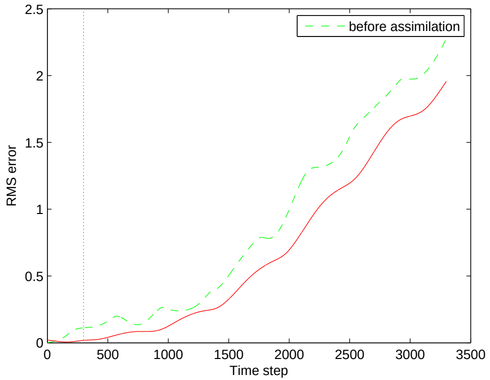

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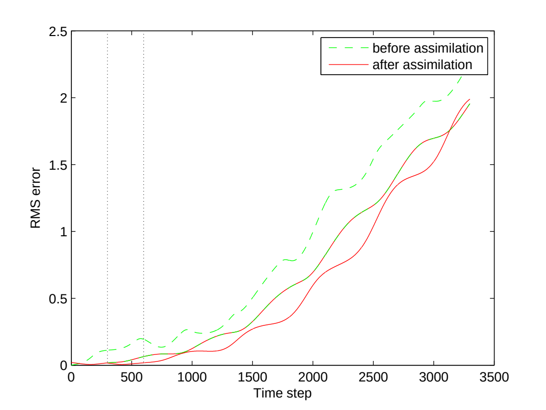
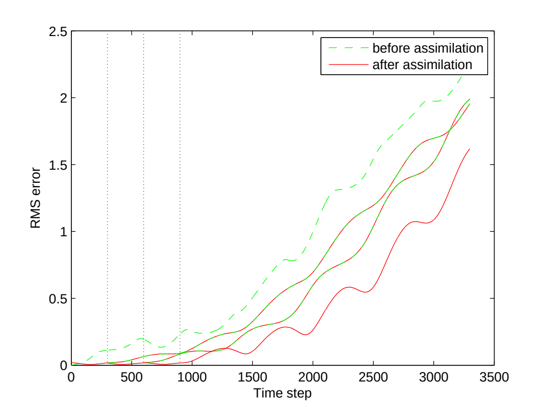


Changing the masses of the bodies



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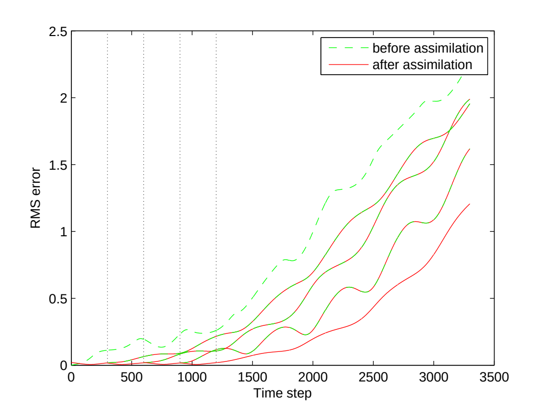

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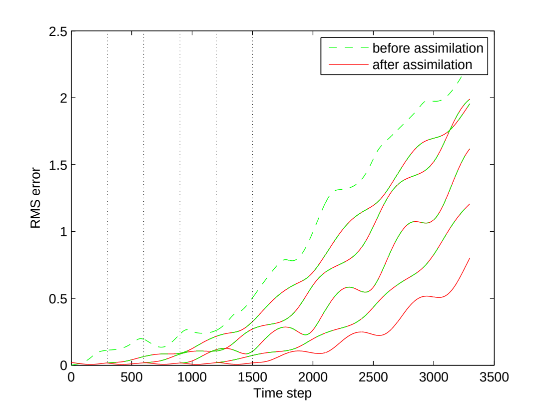
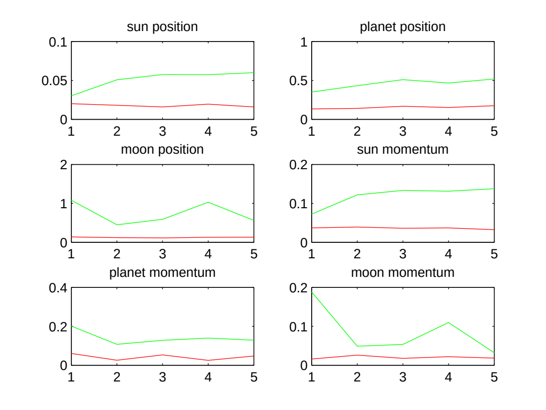
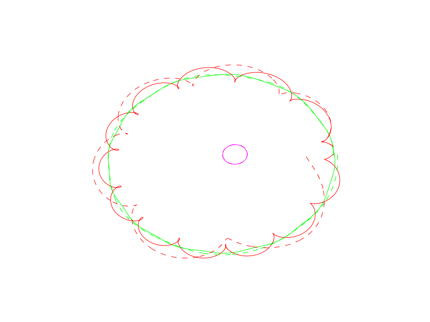


Root mean square error over whole assimilation window



Changing numerical method

- Truth trajectory: 4th order Runge-Kutta method with local truncation error $\mathcal{O}(\Delta t^5)$
- Model trajectory: Explicit Euler method with local truncation error $\mathcal{O}(\Delta t^2)$



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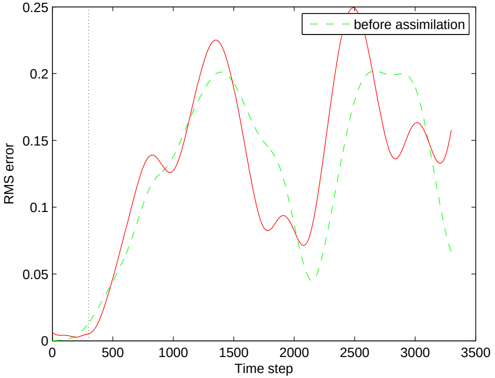

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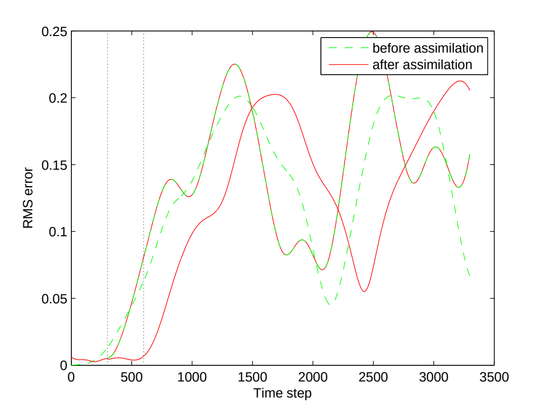

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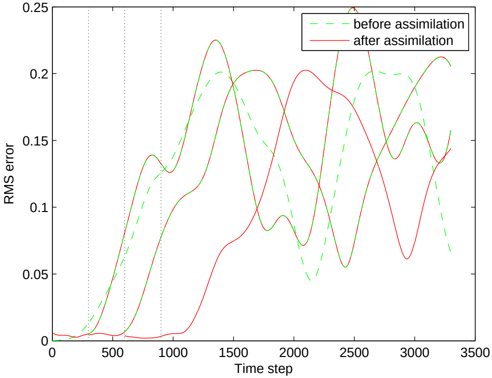

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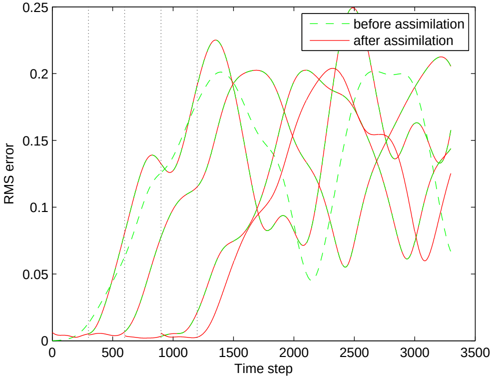

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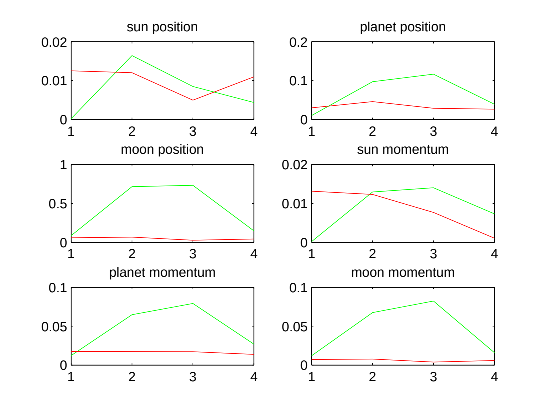
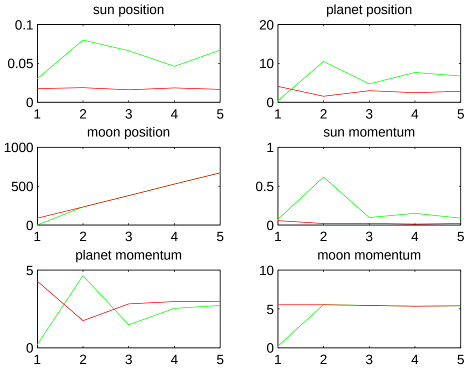
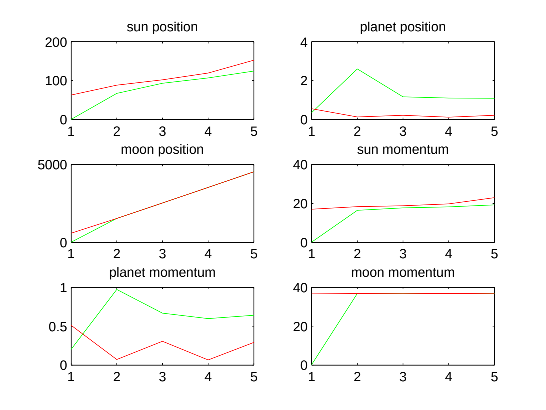


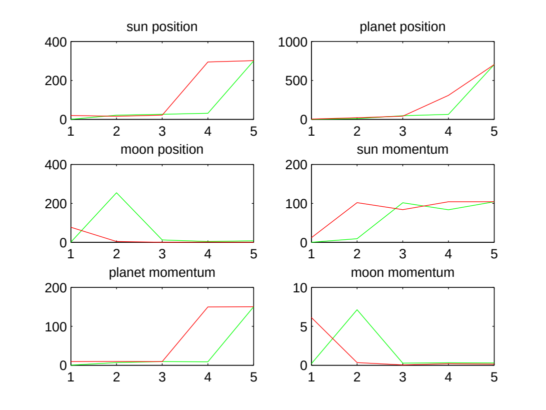
Less observations - observations in sun only



Less observations - observations in planet only



Less observations - observations in moon only



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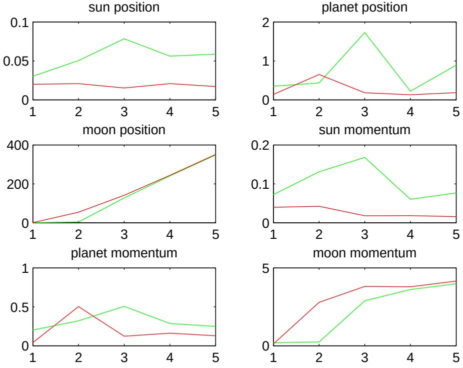
Less observations - observations in sun and planet only



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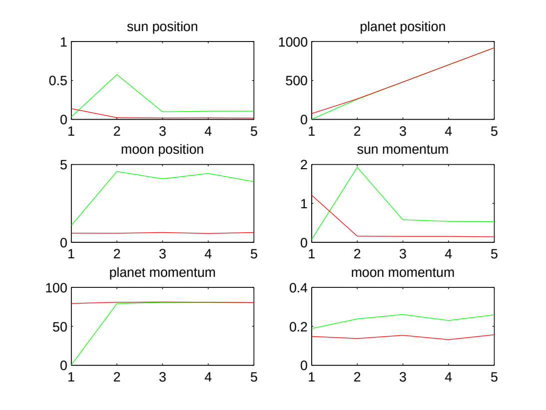

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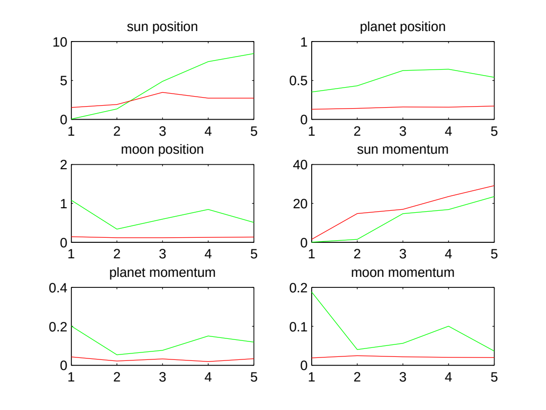

The Kalman Filter Algorithm

- Sequential data assimilation, background is provided by the forecast that starts from the previous analysis
- covariance matrices $\mathbf{B}^F$, $\mathbf{B}^A$
- forecast/model error $\mathbf{x}_{i+1}^{\text{Truth}} = \mathbf{M}_{i+1,i}\mathbf{x}_i^{\text{Truth}} + \eta_i$ where $\eta_i \sim \mathcal{N}(0, \mathbf{Q}_i)$, assumed to be uncorrelated to analysis error of previous forecast

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State and error covariance forecast

$$
\begin{aligned}
\text{State forecast} \quad \mathbf{x}_{i+1}^F &= \mathbf{M}_{i+1,i}\mathbf{x}_i^A \\
\text{Error covariance forecast} \quad \mathbf{B}_{i+1}^F &= \mathbf{M}_{i+1,i}\mathbf{B}_i^A\mathbf{M}_{i+1,i}^T + \mathbf{Q}_i
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State and error covariance analysis

$$\begin{aligned} \text{Kalman gain} \quad \mathbf{K}_i &= \mathbf{B}_i^F\mathbf{H}_i^T(\mathbf{H}_i\mathbf{B}_i^F\mathbf{H}_i^T + \mathbf{R}_i)^{-1} \\ \text{State analysis} \quad \mathbf{x}_i^A &= \mathbf{x}_i^F + \mathbf{K}_i(\mathbf{y}_i - \mathbf{H}_i\mathbf{x}_i^F) \\ \text{Error covariance of analysis} \quad \mathbf{B}_i^A &= (\mathbf{I} - \mathbf{K}_i\mathbf{H}_i)\mathbf{B}_i^F \end{aligned}$$

The Kalman Filter Algorithm

Extended Kalman Filter

Extension of the Kalman Filter Algorithm to nonlinear observation operators H and nonlinear model dynamics M, where both H and M are linearised.

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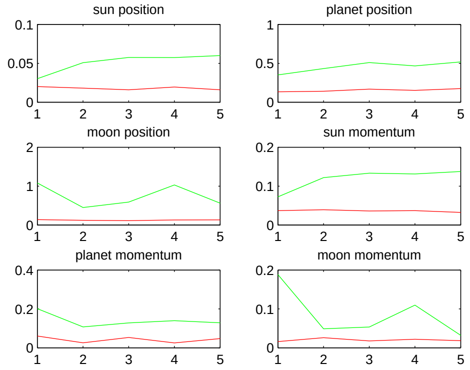
Equivalence 4D-Var Kalman Filter

Assume

- $\mathbf{Q}_i = 0$, $\forall i$ (no model error)
- both 4D-Var and the Kalman filter use the same initial input data
- H and M are linear,

then 4D-Var and the Kalman Filter produce the same state estimate $\mathbf{x}^A$ at the end of the assimilation window.

RMS error over whole assimilation window - using 4D-Var



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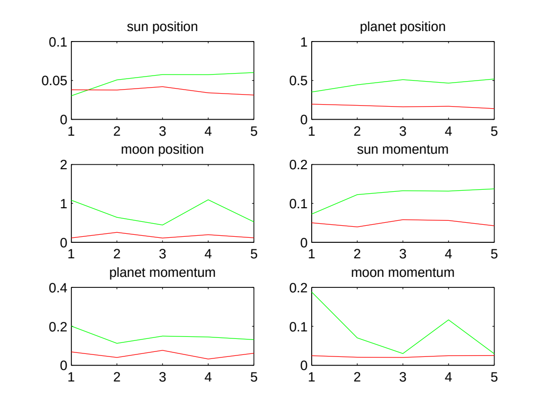

Example - Three-Body Problem

- solver: partitioned Runge-Kutta scheme with time step $h = 0.001$
- observations are taken as noise from the truth trajectory
- background is given from a perturbed initial condition
- assimilation window is taken 300 time steps
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- Compare using $\mathbf{B} = \mathbf{I}$ with using a flow-dependent matrix $\mathbf{B}$ which was generated by a Kalman Filter before the assimilation starts (see G. Inverarity (2007))

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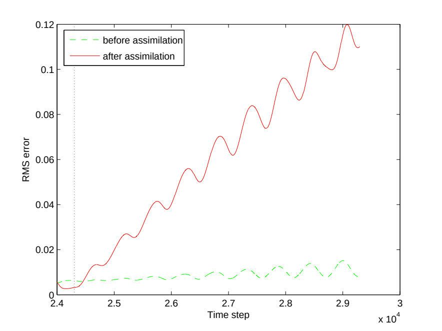

Figure: 4D-Var with $\mathbf{B} = \mathbf{I}$

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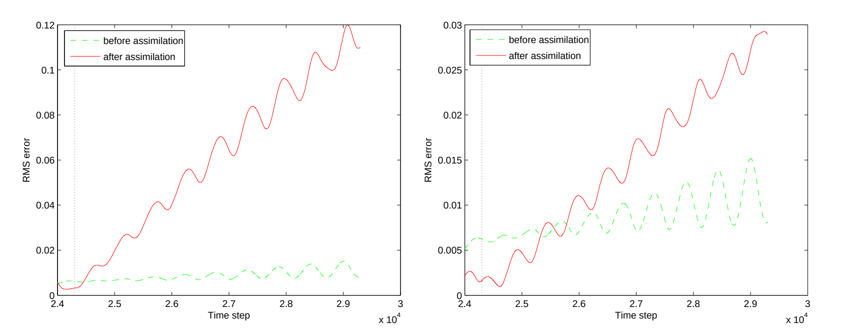

Figure: 4D-Var with $\mathbf{B} = \mathbf{I}$

Figure: 4D-Var with $\mathbf{B} = \mathbf{P}^A$

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  - in operational DA **B** is about $10^7 \times 10^7$
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- model error not included

Outline

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Relation between 4D-Var and Tikhonov regularisation

4D-Var minimises

$$J(\mathbf{x}_0) = (\mathbf{x}_0 - \mathbf{x}_0^B)^T \mathbf{B}^{-1} (\mathbf{x}_0 - \mathbf{x}_0^B) + \sum_{i=0}^{n} (\mathbf{y}_i - H_i(\mathbf{x}_i))^T \mathbf{R}_i^{-1} (\mathbf{y}_i - H_i(\mathbf{x}_i))$$

subject to model dynamics $\mathbf{x}_i = M_{0\to i}\mathbf{x}_0$

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or

$$J(\mathbf{x}_0) = (\mathbf{x}_0 - \mathbf{x}_0^B)^T \mathbf{B}^{-1} (\mathbf{x}_0 - \mathbf{x}_0^B) + (\hat{\mathbf{y}} - \hat{\mathbf{H}}(\mathbf{x}_0))^T \hat{\mathbf{R}}^{-1} (\hat{\mathbf{y}} - \hat{\mathbf{H}}(\mathbf{x}_0))$$

where

$$\hat{\mathbf{H}} = [H_0^T, (H_1 M(t_1, t_0))^T, \ldots (H_n M(t_n, t_0))^T]^T$$

$$\hat{\mathbf{y}} = [\mathbf{y}_0^T, \ldots, \mathbf{y}_n^T]$$

and $\hat{\mathbf{R}}$ is block diagonal with $\mathbf{R}_i$ on diagonal.

Relation between 4D-Var and Tikhonov regularisation

Solution to the optimisation problem

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is given by

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Singular value decomposition

Assume $\mathbf{B} = \sigma_B^2 \mathbf{I}$ and $\hat{\mathbf{R}} = \sigma_O^2 \mathbf{I}$ and define the SVD of the observability matrix $\hat{\mathbf{H}}$

$$\hat{\mathbf{H}} = \mathbf{U} \boldsymbol{\Lambda} \mathbf{V}^T$$

Then the optimal analysis can be written as

$$\mathbf{x}_0 = \mathbf{x}_0^B + \sum_j \frac{\lambda_j^2}{\mu^2 + \lambda_j^2} \frac{\mathbf{u}_j^T \hat{\mathbf{d}}}{\lambda_j} \mathbf{v}_j$$

where $\mu^2 = \dfrac{\sigma_O^2}{\sigma_B^2}$.

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$$\hat{J}(\mathbf{z}) = \mu^2 \|\mathbf{z}\|_2^2 + \|\mathbf{F}_R^{-1/2} \hat{\mathbf{d}} - \mathbf{F}_R^{-1/2} \hat{\mathbf{H}} \mathbf{F}_B^{-1/2} \mathbf{z}\|_2^2$$

μ^2 can be interpreted as a regularisation parameter.

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This is the well-known Tikhonov regularisation!

Outline

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Met Office research and plans

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- identify and **analyse model error** and analyse influence of this model error onto the DA scheme