Data assimilation using 4D-Var and links to regularisation

Melina Freitag

Department of Mathematical Sciences
University of Bath

7th Bath/RAL NA Day
23rd September 2008

Outline

What is Data Assimilation?

Loose definition

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

What is Data Assimilation?

Loose definition

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

Some examples

- Navigation
- Geosciences
- 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

Data Assimilation in NWP

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

A priori information $\mathbf{x}^B$

- background state (usual previous forecast)

Observations $\mathbf{y}$

- Satellites
- Ships and buoys
- Surface stations
- Aeroplanes

Data Assimilation in NWP

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

A priori information $\mathbf{x}^B$

- background state (usual previous forecast)

Models

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

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

Observations $\mathbf{y}$

- Satellites
- Ships and buoys
- Surface stations
- Aeroplanes

Data Assimilation in NWP

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

A priori information $\mathbf{x}^B$

- background state (usual previous forecast)

Models

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

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

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

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

Observations $\mathbf{y}$

- Satellites
- Ships and buoys
- Surface stations
- Aeroplanes

Data Assimilation in NWP

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

A priori information $\mathbf{x}^B$

- background state (usual previous forecast)

Models

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

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

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

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

Observations $\mathbf{y}$

- Satellites
- Ships and buoys
- Surface stations
- Aeroplanes

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)

Data Assimilation in NWP

Underdeterminacy

- Size of the state vector $\mathbf{x}$: $432 \times 320 \times 50 \times 7 = \mathcal{O}(10^7)$
- Number of observations (size of $\mathbf{y}$): $\mathcal{O}(10^5 - 10^6)$

Schematics of DA

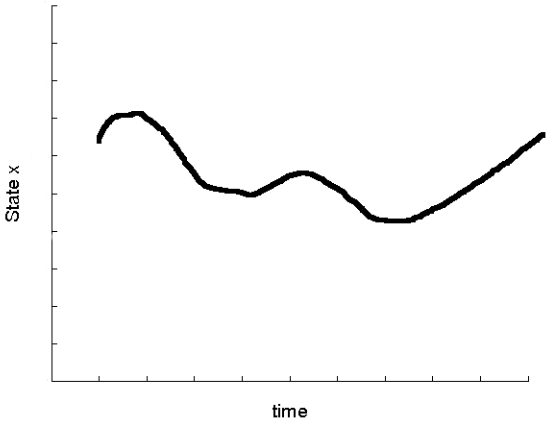


Figure: Background state $\mathbf{x}^B$

Schematics of DA

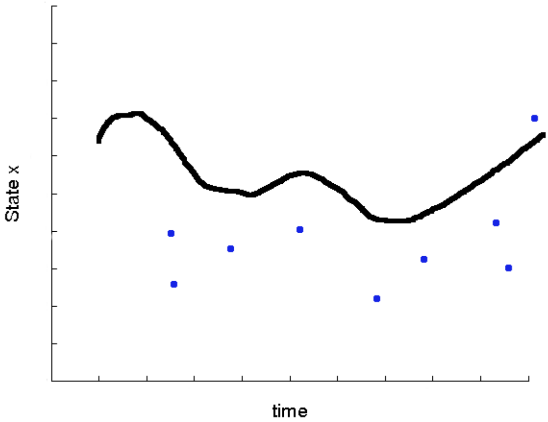


Figure: Observations $\mathbf{y}$

Schematics of DA

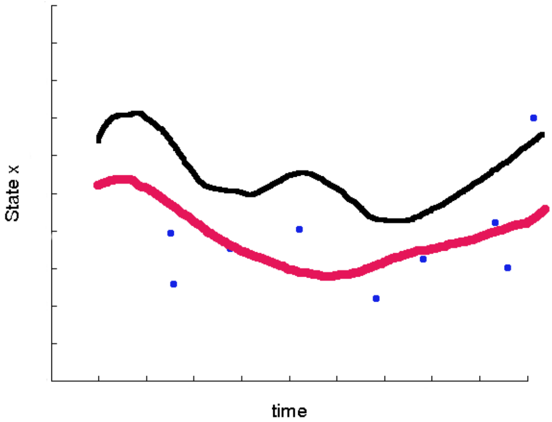


Figure: Analysis $\mathbf{x}^A$ (consistent with observations and model dynamics)

Outline

Introduction

Variational Data Assimilation

Tikhonov regularisation

Link between 4D-Var and Tikhonov regularisation

Work in progress

Optimal least-squares estimater

Cost function - 3D-VAR

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

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

Optimal least-squares estimater

Cost function - 3D-VAR

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

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

Interpolation equations - Optimal Interpolation

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

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

Four-dimensional variational assimilation (4D-VAR)

Minimise the cost function

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

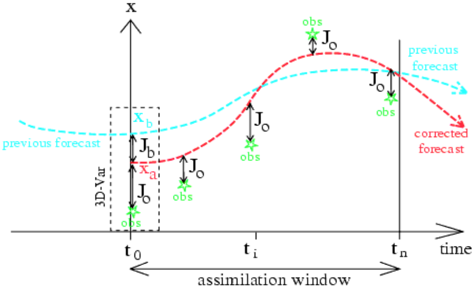
subject to model dynamics $\mathbf{x}_i = M_{0 \to i} \mathbf{x}_0$

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 $\mathbf{x}_i = M_{0\rightarrow i}\mathbf{x}_0$



4D-Var analysis

Model dynamics

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

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

nonlinear constraint optimisation problem (hard!)

4D-Var analysis

Model dynamics

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

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

nonlinear constraint optimisation problem (hard!)

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)

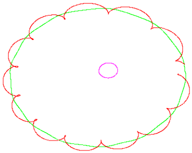
$$\mathbf{y}_i - H_i(\mathbf{x}_i) = \mathbf{y}_i - H_i(M_{0\to i}\mathbf{x}_0) = \mathbf{y}_i - H_i(M_{0\to i}\mathbf{x}_0^B) - \mathbf{H}_i\mathbf{M}_{0\to i}(\mathbf{x}_0 - \mathbf{x}_0^B)$$

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

- unconstrained quadratic optimisation problem (easier).

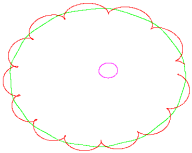
Example - Three-Body Problem

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



Example - Three-Body Problem

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



Equations of motion

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

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 previous forecast

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 previous forecast
- assimilation window is taken 300 time steps
- minimisation of cost function J using a Gauss-Newton method (neglecting all second derivatives)

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

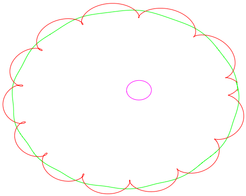
$$\nabla\nabla J(\mathbf{x}_0^j)\Delta\mathbf{x}_0^j = -\nabla J(\mathbf{x}_0^j), \quad \mathbf{x}_0^{j+1} = \mathbf{x}_0^j + \Delta\mathbf{x}_0^j$$

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

Changing the masses of the bodies

DA needs Model error!

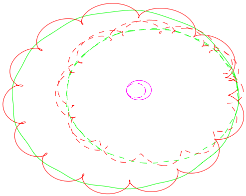
$$m_s = 1.0 \quad \rightarrow \quad m_s = 1.1$$
$$m_p = 0.1 \quad \rightarrow \quad m_p = 0.11$$
$$m_m = 0.01 \quad \rightarrow \quad m_m = 0.011$$



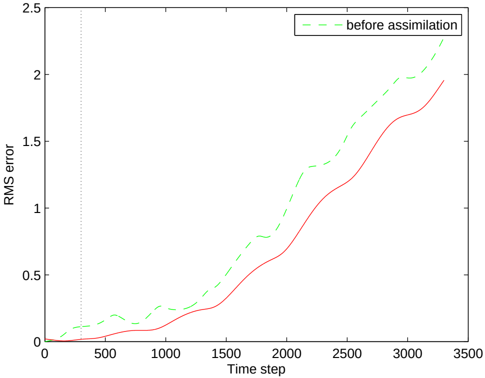
Changing the masses of the bodies

DA needs Model error!

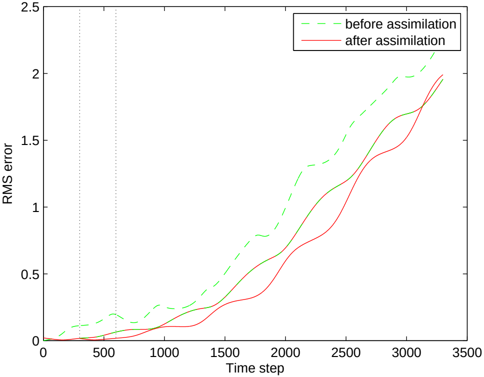
$$\begin{aligned} m_s = 1.0 \quad &\rightarrow \quad m_s = 1.1 \\ m_p = 0.1 \quad &\rightarrow \quad m_p = 0.11 \\ m_m = 0.01 \quad &\rightarrow \quad m_m = 0.011 \end{aligned}$$



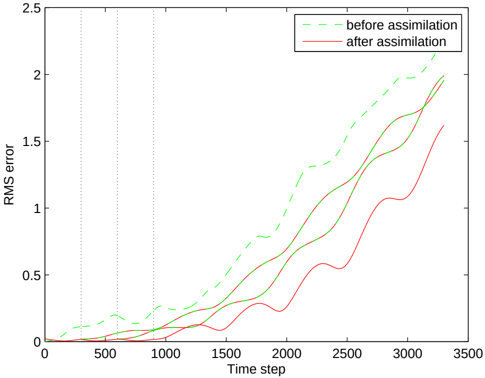
Changing the masses of the bodies



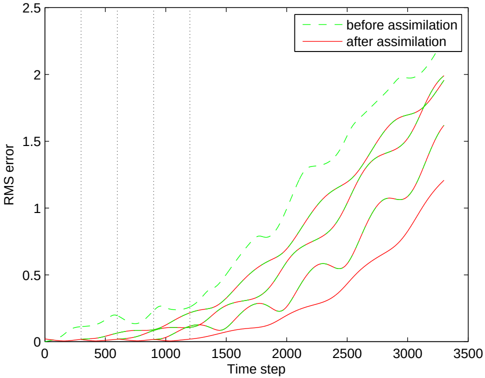
Changing the masses of the bodies



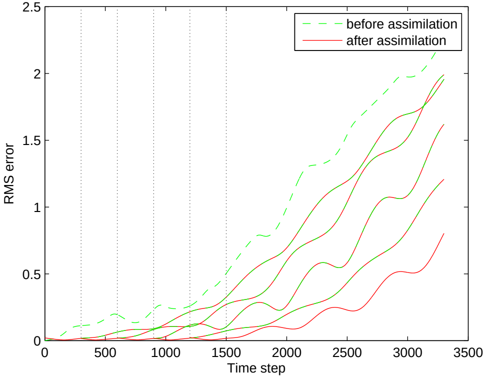
Changing the masses of the bodies



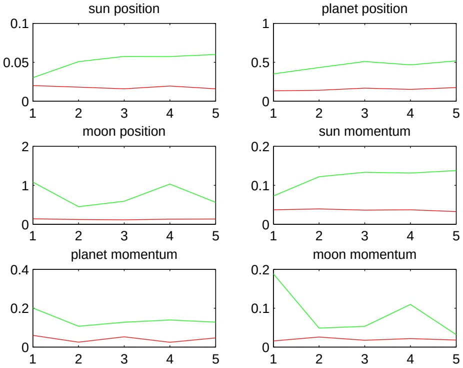
Changing the masses of the bodies



Changing the masses of the bodies

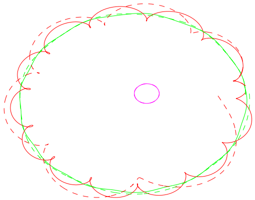


Root mean square error over whole assimilation window

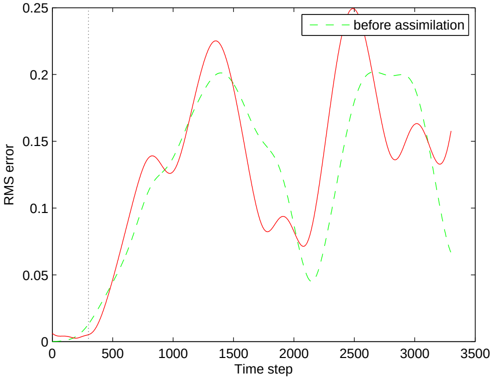


Changing numerical method

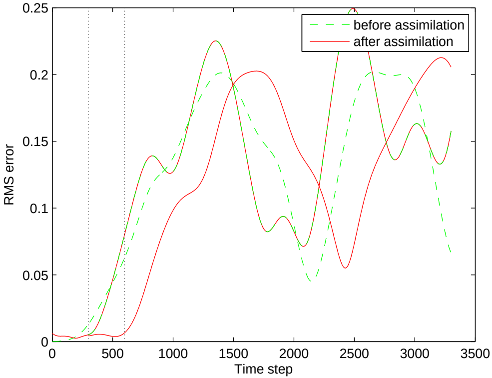
- Truth trajectory: 4th order Runge-Kutta method with local truncation error $\mathcal{O}(\Delta t^5)$
- Model trajectory: Explicit Euler method with local truncation error $\mathcal{O}(\Delta t^2)$



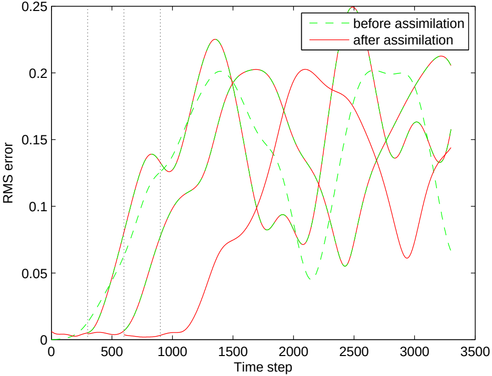
Changing numerical method



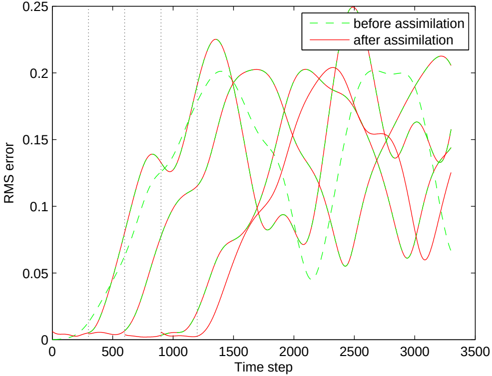
Changing numerical method



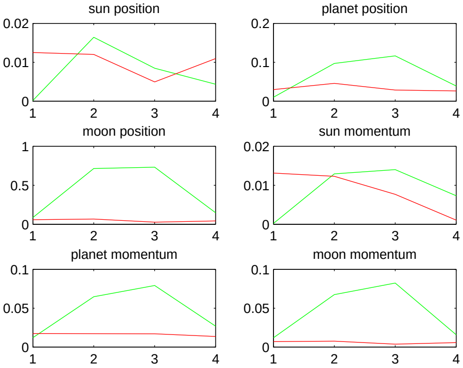
Changing numerical method



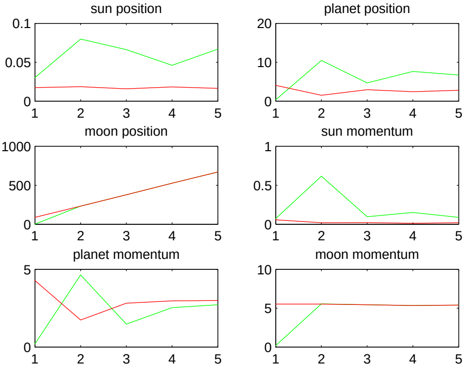
Changing numerical method



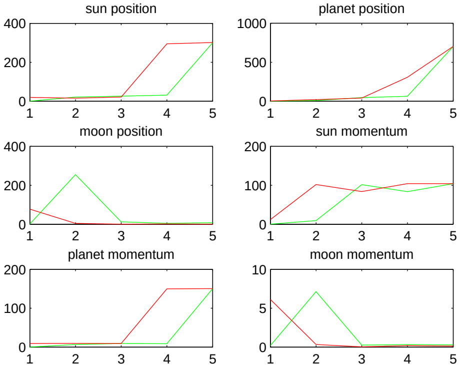
Root mean square error over whole assimilation window



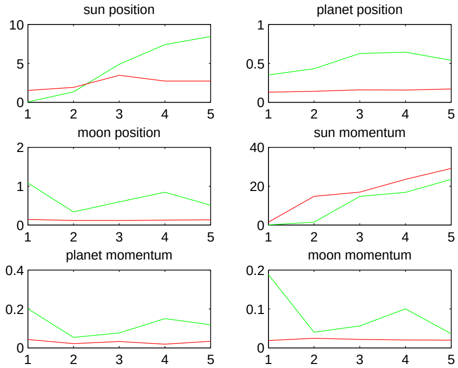
Less observations - observations in sun only



Less observations - observations in moon only



Less observations - observations in planet and moon only



Observations in all timescales necessary!

N-dimensional (chaotic) Lorenz system (Lorenz95)

The system is given by

$$\frac{dx_i}{dt} = -x_{i-2}x_{i-1} + x_{i-1}x_{i+1} - x_i + F, \quad i = 1, \ldots, N,$$

cyclic boundary conditions $x_0 = x_N$, $x_{-1} = x_{N+1}$, $x_{N+1} = x_1$.

- $F = 8$, $N = 40$ (13 positive Lyapunov exponents). Model error introduced by parameter change $F_{mod} = 10$.
- solver: Runge-Kutta method with time step $h = 0.001$

N-dimensional (chaotic) Lorenz system (Lorenz95)

The system is given by

$$\frac{dx_i}{dt} = -x_{i-2}x_{i-1} + x_{i-1}x_{i+1} - x_i + F, \quad i = 1, \ldots, N,$$

cyclic boundary conditions $x_0 = x_N$, $x_{-1} = x_{N+1}$, $x_{N+1} = x_1$.

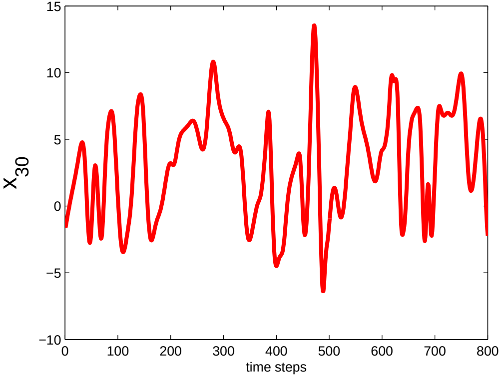
- $F = 8$, $N = 40$ (13 positive Lyapunov exponents). Model error introduced by parameter change $F_{mod} = 10$.
- solver: Runge-Kutta method with time step $h = 0.001$
- observations are taken as noise from the truth trajectory
- assimilation window: 1000 time steps
- subsequent forecast: 5000 time steps

Lorenz95 dynamics

The system is given by

$$\frac{dx_i}{dt} = -x_{i-2}x_{i-1} + x_{i-1}x_{i+1} - x_i + F, \quad i = 1, \ldots, N,$$

cyclic boundary conditions $x_0 = x_N$, $x_{-1} = x_{N+1}$, $x_{N+1} = x_1$. $F = 8$, $N = 40$ (13 positive Lyapunov exponents).

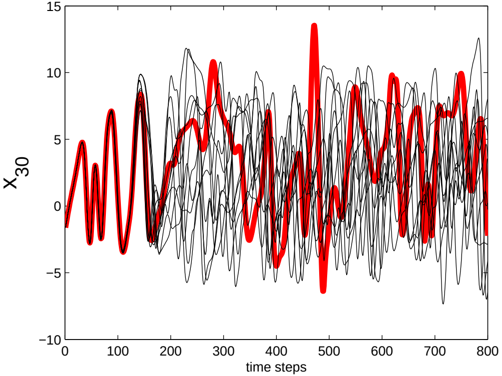


Lorenz95 dynamics

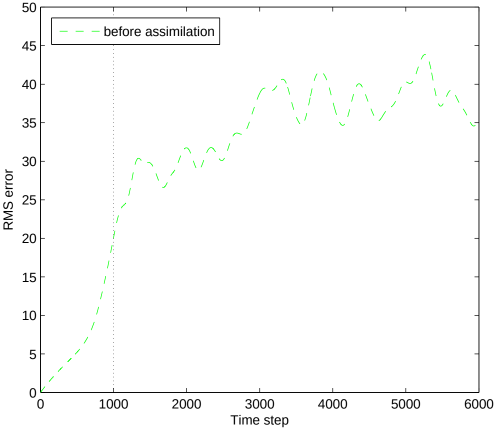
The system is given by

$$\frac{dx_i}{dt} = -x_{i-2}x_{i-1} + x_{i-1}x_{i+1} - x_i + F, \quad i = 1, \dots, N,$$

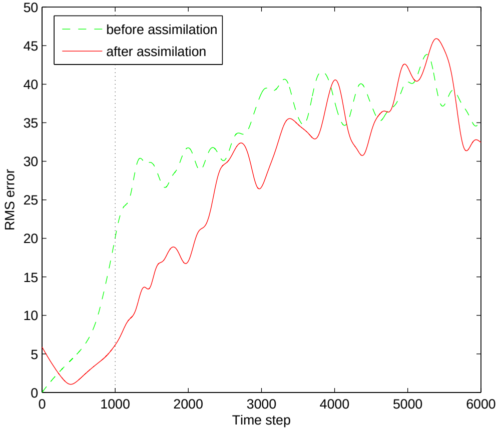
cyclic boundary conditions $x_0 = x_N$, $x_{-1} = x_{N+1}$, $x_{N+1} = x_1$. $F = 8$, $N = 40$ (13 positive Lyapunov exponents).



Root means square error before assimilation



Root means square error after assimilation



4D-Var and the Kalman Filter

- 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

4D-Var and the Kalman Filter

- 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

State and error covariance forecast

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

4D-Var and the Kalman Filter

- 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

State and error covariance forecast

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

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.

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.

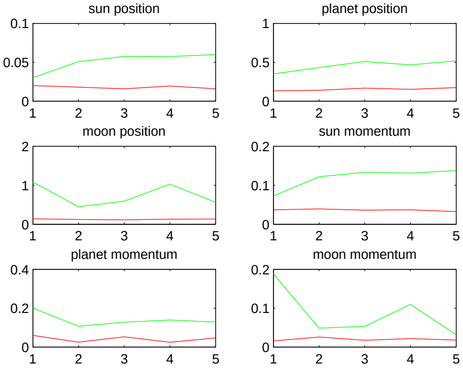
Equivalence 4D-Var Kalman Filter

Assume

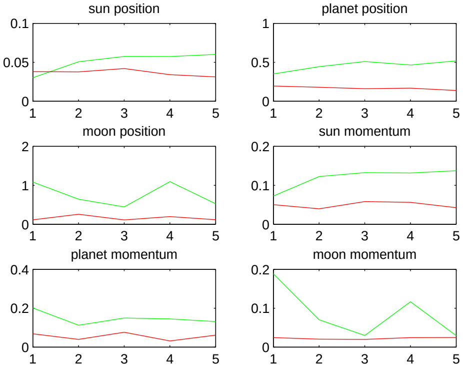
- $\mathbf{Q}_i = 0, \forall i$ (no model error)
- both 4D-Var and the Kalman filter use the same initial input data
- H and M are linear,

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



RMS error over whole assimilation window - using Kalman Filter



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
- minimisation of cost function J using a Gauss-Newton method (neglecting all second derivatives)
- application of 4D-Var

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
- minimisation of cost function J using a Gauss-Newton method (neglecting all second derivatives)
- application of 4D-Var
- 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))

Example - Three-Body Problem

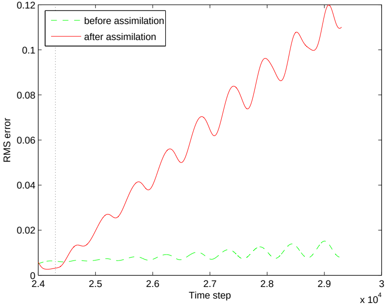


Figure: 4D-Var with $\mathbf{B} = \mathbf{I}$

Example - Three-Body Problem

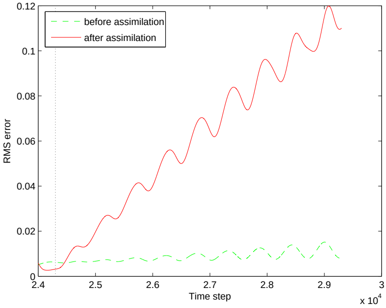


Figure: 4D-Var with $\mathbf{B} = \mathbf{I}$

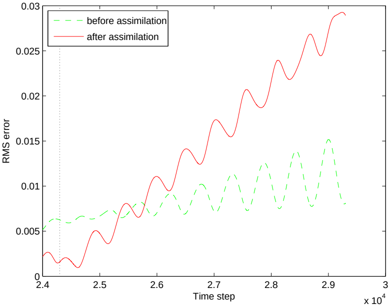


Figure: 4D-Var with $\mathbf{B} = \mathbf{P}^A$

Outline

Ill-posed problems

Given an operator $\mathbf{A}$ we wish to solve

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

it is well-posed if

- solution exits

Ill-posed problems

Given an operator $\mathbf{A}$ we wish to solve

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

it is well-posed if

- solution exits
- solution is unique

Ill-posed problems

Given an operator $\mathbf{A}$ we wish to solve

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

it is well-posed if

- solution exits
- solution is unique
- is stable ($\mathbf{A}^{-1}$ continuous)

Ill-posed problems

Given an operator $\mathbf{A}$ we wish to solve

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

it is well-posed if

- solution exits
- solution is unique
- is stable ($\mathbf{A}^{-1}$ continuous)

Equation is ill-posed if it is not well-posed.

Linear, finite dimensional case

Finite dimensions

- $\mathbf{A} : \mathbb{R}^n \to \mathbb{R}^n$, then $\mathbf{Ax} = \mathbf{b}$ is well-posed if $\mathbf{A}^{-1}$ exists.

Linear, finite dimensional case

Finite dimensions

- $\mathbf{A} : \mathbb{R}^n \to \mathbb{R}^n$, then $\mathbf{Ax} = \mathbf{b}$ is well-posed if $\mathbf{A}^{-1}$ exists.
- Existence imposed by considering least squares solutions

$$\mathbf{x}_{LS} = \arg\min \|\mathbf{Ax} - \mathbf{b}\|^2$$

Linear, finite dimensional case

Finite dimensions

- $\mathbf{A} : \mathbb{R}^n \to \mathbb{R}^n$, then $\mathbf{Ax} = \mathbf{b}$ is well-posed if $\mathbf{A}^{-1}$ exists.
- Existence imposed by considering least squares solutions

$$\mathbf{x}_{LS} = \arg\min \|\mathbf{Ax} - \mathbf{b}\|^2$$

- Uniqueness imposed by taking minimum norm least squares solution

$$\mathbf{x}_{MNLS} = \arg\min \|\mathbf{x}_{LS}\|^2 = \mathbf{A}^{\dagger}\mathbf{b}.$$

Linear, finite dimensional case

Finite dimensions

- $\mathbf{A} : \mathbb{R}^n \to \mathbb{R}^n$, then $\mathbf{A}\mathbf{x} = \mathbf{b}$ is well-posed if $\mathbf{A}^{-1}$ exists.
- Existence imposed by considering least squares solutions

$$\mathbf{x}_{LS} = \arg\min \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2$$

- Uniqueness imposed by taking minimum norm least squares solution

$$\mathbf{x}_{MNLS} = \arg\min \|\mathbf{x}_{LS}\|^2 = \mathbf{A}^\dagger \mathbf{b}.$$

but ..

In the finite dimensional case one can replace $\mathbf{A}^{-1}$ by its pseudo-inverse $\mathbf{A}^\dagger$, but

- discrete problem of underlying ill-posed problem becomes ill-conditioned
- singular values of $\mathbf{A}$ decay to zero

A way out of this - Tikhonov regularisation

Solution to the minimisation problem

$$\begin{aligned}\mathbf{x}_\alpha &= \arg\min\left\{\|\mathbf{A}\mathbf{x}-\mathbf{b}\|^2+\alpha\|\mathbf{x}\|^2\right\}\\ &= (\mathbf{A}^T\mathbf{A}+\alpha\mathbf{I})^{-1}\mathbf{A}^T\mathbf{b}\end{aligned}$$

where α is called the regularisation parameter.

Bayesian Interpretation

Assuming X, B are random variables then

$$\pi(\mathbf{x}|\mathbf{b}) = \pi(\mathbf{b}|\mathbf{x})\pi(\mathbf{x})/\pi(\mathbf{b}),$$

Maximum a posteriori estimater is maximum of a posteriori pdf, hence minimise w.r.t. $\mathbf{x}$

$$-\log(\pi(\mathbf{x}|\mathbf{b})) = -\log(\pi(\mathbf{b}|\mathbf{x})) - \log(\pi(\mathbf{x}))$$

Bayesian Interpretation

Assuming X, B are random variables then

$$\pi(\mathbf{x}|\mathbf{b}) = \pi(\mathbf{b}|\mathbf{x})\pi(\mathbf{x})/\pi(\mathbf{b}),$$

Maximum a posteriori estimater is maximum of a posteriori pdf, hence minimise w.r.t. $\mathbf{x}$

$$-\log(\pi(\mathbf{x}|\mathbf{b})) = -\log(\pi(\mathbf{b}|\mathbf{x})) - \log(\pi(\mathbf{x}))$$

Example

If X and $\eta = B - AX$ are normally distributed then

$$\pi(\mathbf{x}) = C_1 \exp(-\frac{\|\mathbf{x}\|^2}{2\sigma_x}) \quad \text{and} \quad \pi(\mathbf{x}|\mathbf{b}) = C_2 \exp(-\frac{\|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2}{2\sigma_\eta^2})$$

and Tikhonov cost functional is

$$J(\mathbf{x}) = \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 + \alpha\|\mathbf{x}\|^2$$

Tikhonov regularisation using Singular Value Decomposition

Using the SVD of $\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T$ the regularised solution in Tikhonov regularisation is given by

$$\mathbf{x}_\alpha = (\mathbf{A}^T\mathbf{A} + \alpha\mathbf{I})^{-1}\mathbf{A}^T\mathbf{b}$$

Tikhonov regularisation using Singular Value Decomposition

Using the SVD of $\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T$ the regularised solution in Tikhonov regularisation is given by

$$\begin{aligned} \mathbf{x}_\alpha &= (\mathbf{A}^T\mathbf{A} + \alpha\mathbf{I})^{-1}\mathbf{A}^T\mathbf{b} \\ &= (\mathbf{V}\boldsymbol{\Sigma}^T\mathbf{U}^T\mathbf{U}\Sigma\mathbf{V}^T + \alpha\mathbf{V}\mathbf{V}^T)^{-1}\mathbf{V}\boldsymbol{\Sigma}^T\mathbf{U}^T\mathbf{b} \end{aligned}$$

Tikhonov regularisation using Singular Value Decomposition

Using the SVD of $\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T$ the regularised solution in Tikhonov regularisation is given by

$$\begin{aligned} \mathbf{x}_\alpha &= (\mathbf{A}^T\mathbf{A} + \alpha\mathbf{I})^{-1}\mathbf{A}^T\mathbf{b} \\ &= (\mathbf{V}\boldsymbol{\Sigma}^T\mathbf{U}^T\mathbf{U}\Sigma\mathbf{V}^T + \alpha\mathbf{V}\mathbf{V}^T)^{-1}\mathbf{V}\boldsymbol{\Sigma}^T\mathbf{U}^T\mathbf{b} \\ &= \mathbf{V}\mathrm{diag}\left(\frac{s_i^2}{s_i^2+\alpha}\frac{1}{s_i}\right)\mathbf{U}^T\mathbf{b} \end{aligned}$$

Tikhonov regularisation using Singular Value Decomposition

Using the SVD of $\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T$ the regularised solution in Tikhonov regularisation is given by

$$\begin{aligned} \mathbf{x}_\alpha &= (\mathbf{A}^T\mathbf{A} + \alpha\mathbf{I})^{-1}\mathbf{A}^T\mathbf{b} \\ &= (\mathbf{V}\mathbf{\Sigma}^T\mathbf{U}^T\mathbf{U}\Sigma\mathbf{V}^T + \alpha\mathbf{V}\mathbf{V}^T)^{-1}\mathbf{V}\mathbf{\Sigma}^T\mathbf{U}^T\mathbf{b} \\ &= \mathbf{V}\mathrm{diag}\left(\frac{s_i^2}{s_i^2+\alpha}\frac{1}{s_i}\right)\mathbf{U}^T\mathbf{b} \end{aligned}$$

$$\mathbf{x}_\alpha = \sum_{i=1}^{n} \frac{s_i^2}{s_i^2+\alpha}\frac{u_i^T\mathbf{b}}{s_i}\mathbf{v}_i$$

Outline

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

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

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

Linearise about $\mathbf{x}_0$ then the solution to the optimisation problem

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

is given by

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

Relation between 4D-Var and Tikhonov regularisation

Solution to the optimisation problem

Linearise about $\mathbf{x}_0$ then the solution to the optimisation problem

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

is given by

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

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 $\hat{\mathbf{H}}$

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

Then the optimal analysis can be written as

$$\mathbf{x}_0 = \mathbf{x}_0^B + \sum_j \frac{s_j^2}{\mu^2 + s_j^2} \frac{\mathbf{u}_j^T \hat{\mathbf{d}}}{s_j} \mathbf{v}_j, \quad \text{where} \quad \mu^2 = \frac{\sigma_O^2}{\sigma_B^2}.$$

Relation between 4D-Var and Tikhonov regularisation

If $\mathbf{B}$ and $\hat{\mathbf{R}}$ are not multiples of the identity

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

Relation between 4D-Var and Tikhonov regularisation

If $\mathbf{B}$ and $\hat{\mathbf{R}}$ are not multiples of the identity

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

Variable transformations

$\mathbf{B} = \sigma_B^2 \mathbf{F}_B$ and $\hat{\mathbf{R}} = \sigma_O^2 \mathbf{F}_R$ and

Relation between 4D-Var and Tikhonov regularisation

If $\mathbf{B}$ and $\hat{\mathbf{R}}$ are not multiples of the identity

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

Variable transformations

$\mathbf{B} = \sigma_B^2 \mathbf{F}_B$ and $\hat{\mathbf{R}} = \sigma_O^2 \mathbf{F}_R$ and define new variable $\mathbf{z} := \mathbf{F}_B^{-1/2}(\mathbf{x}_0 - \mathbf{x}_0^B)$

Relation between 4D-Var and Tikhonov regularisation

If $\mathbf{B}$ and $\hat{\mathbf{R}}$ are not multiples of the identity

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

Variable transformations

$\mathbf{B} = \sigma_B^2 \mathbf{F}_B$ and $\hat{\mathbf{R}} = \sigma_O^2 \mathbf{F}_R$ and define new variable $\mathbf{z} := \mathbf{F}_B^{-1/2}(\mathbf{x}_0 - \mathbf{x}_0^B)$

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

μ^2 can be interpreted as a regularisation parameter.

Relation between 4D-Var and Tikhonov regularisation

If $\mathbf{B}$ and $\hat{\mathbf{R}}$ are not multiples of the identity

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

Variable transformations

$\mathbf{B} = \sigma_B^2 \mathbf{F}_B$ and $\hat{\mathbf{R}} = \sigma_O^2 \mathbf{F}_R$ and define new variable $\mathbf{z} := \mathbf{F}_B^{-1/2}(\mathbf{x}_0 - \mathbf{x}_0^B)$

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

μ^2 can be interpreted as a regularisation parameter.
This is Tikhonov regularisation!

Example

Burger's equation

$$u_t + u\frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}$$

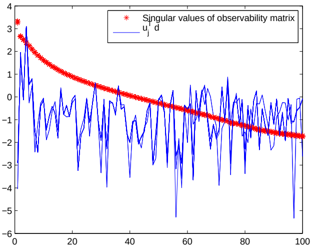
Optimal solution (4D-Var)

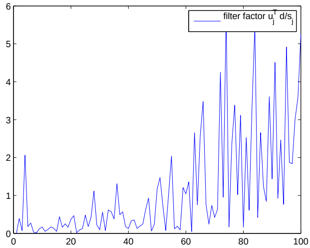
$$\mathbf{u}_0 = \mathbf{u}_0^B + \sum_j \frac{s_j^2}{\mu^2 + s_j^2} \frac{\mathbf{u}_j^T \hat{\mathbf{d}}}{s_j} \mathbf{v}_j, \quad \text{where} \quad \mu^2 = \frac{\sigma_O^2}{\sigma_B^2}.$$

Singular value analysis - observations everywhere

Optimal solution (4D-Var)

$$\mathbf{u}_0 = \mathbf{u}_0^B + \sum_j \frac{s_j^2}{\mu^2 + s_j^2} \frac{\mathbf{u}_j^T \hat{\mathbf{d}}}{s_j} \mathbf{v}_j, \quad \text{where} \quad \mu^2 = \frac{\sigma_O^2}{\sigma_B^2}.$$

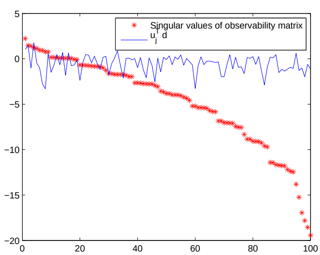


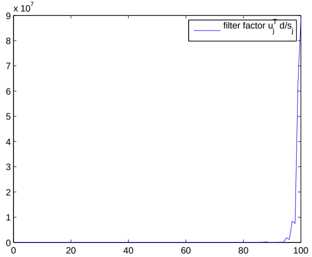


Singular value analysis - observations every 10 points

Optimal solution (4D-Var)

$$\mathbf{u}_0 = \mathbf{u}_0^B + \sum_j \frac{s_j^2}{\mu^2 + s_j^2} \frac{\mathbf{u}_j^T \hat{\mathbf{d}}}{s_j} \mathbf{v}_j, \quad \text{where} \quad \mu^2 = \frac{\sigma_O^2}{\sigma_B^2}.$$





Outline

Introduction

Variational Data Assimilation

Tikhonov regularisation

Link between 4D-Var and Tikhonov regularisation

Work in progress

L1 regularisation (with N. Nichols, University of Reading)

In image processing, L_1-norm regularisation provides edge preserving image deblurring!

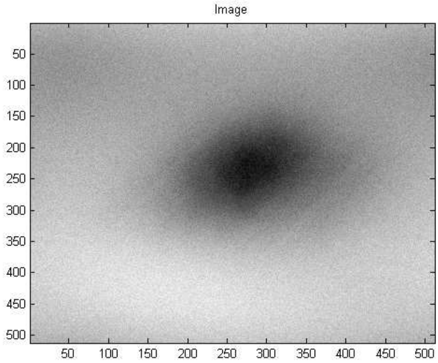


Figure: Blurred picture

L1 regularisation

In image processing, L_1-norm regularisation provides edge preserving image deblurring!

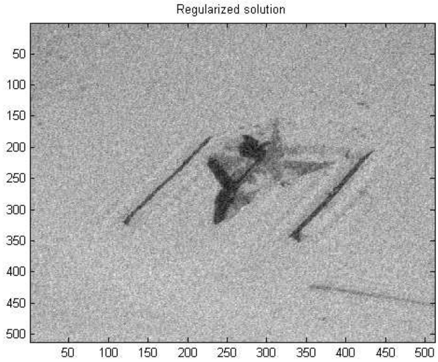


Figure: Tikhonov regularisation $\min\left\{\|\mathbf{Ax}-\mathbf{b}\|^2+\alpha\|\mathbf{x}\|^2\right\}$

L1 regularisation

In image processing, L_1-norm regularisation provides edge preserving image deblurring!

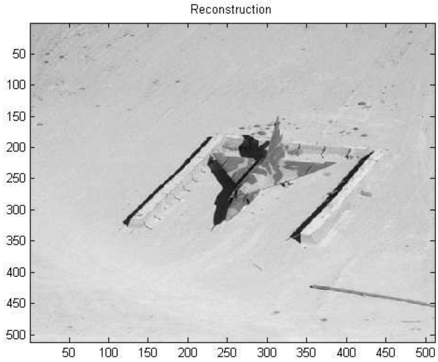


Figure: L1-norm regularisation $\min \left\{ \|\mathbf{Ax} - \mathbf{b}\|^2 + \alpha \|\mathbf{x}\|_1 \right\}$

L1 regularisation

In image processing, L_1-norm regularisation provides edge preserving image deblurring!

- L1 regularisation might be also beneficial in Data Assimilation
- 4D Var smears out sharp fronts

L1 regularisation

In image processing, L_1-norm regularisation provides edge preserving image deblurring!

- L1 regularisation might be also beneficial in Data Assimilation
- 4D Var smears out sharp fronts
- L1 regularisation has the potential to overcome this problem

Model error identification

Blind Deconvolution

Instead of the (linear) model

$$\mathbf{b} = \mathbf{A}\mathbf{x} + \mathbf{e}$$

use

$$\mathbf{b} = (\mathbf{A} + \mathbf{E})\mathbf{x} + \mathbf{e}$$

where both $\mathbf{e}$ and $\mathbf{E}$ are unknown.

Model error identification

Blind Deconvolution

Instead of the (linear) model

$$\mathbf{b} = \mathbf{A}\mathbf{x} + \mathbf{e}$$

use

$$\mathbf{b} = (\mathbf{A} + \mathbf{E})\mathbf{x} + \mathbf{e}$$

where both $\mathbf{e}$ and $\mathbf{E}$ are unknown. Instead of solving

$$\min \left\{ \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 + \alpha \|\mathbf{x}\|^2 \right\}$$

solve

$$\min \left\{ \|(\mathbf{A} + \mathbf{E})\mathbf{x} - \mathbf{b}\|^2 + \|\mathbf{E}\|_F^2 + \alpha \|\mathbf{x}\|^2 \right\}$$

over all choices of $\mathbf{e}$ and $\mathbf{E}$ (regularised total least squares).

Model error identification

Blind Deconvolution

Instead of the (linear) model

$$\mathbf{b} = \mathbf{A}\mathbf{x} + \mathbf{e}$$

use

$$\mathbf{b} = (\mathbf{A} + \mathbf{E})\mathbf{x} + \mathbf{e}$$

where both **e** and **E** are unknown. Instead of solving

$$\min \left\{ \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 + \alpha \|\mathbf{x}\|^2 \right\}$$

solve

$$\min \left\{ \|(\mathbf{A} + \mathbf{E})\mathbf{x} - \mathbf{b}\|^2 + \|\mathbf{E}\|_F^2 + \alpha \|\mathbf{x}\|^2 \right\}$$

over all choices of **e** and **E** (regularised total least squares).

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