

L1-regularisation in 4DVar

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Introduction

Tikhonov regularisation

Link between 4DVar and Tikhonov regularisation

Motivation: Results from image processing

First results on L_1 -regularisation in 4DVar

Outline

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Four-dimensional variational assimilation (4DVar)

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

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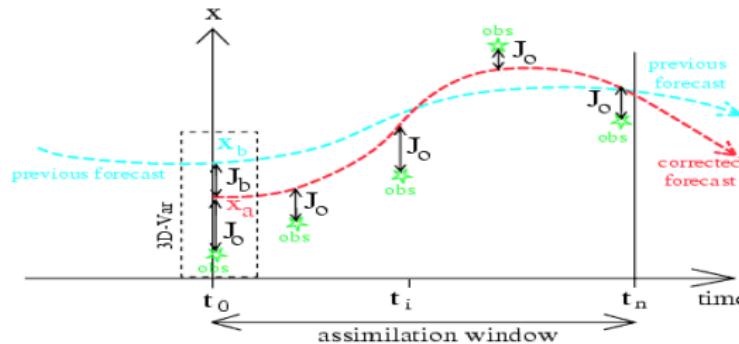


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Ill-posed problems

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

Linear, finite dimensional case

Finite dimensions

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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**
- \mathbf{A}^{-1} is unstable!

A way out of this - Tikhonov regularisation

Solution to the minimisation problem

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

where α is called the regularisation parameter.

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

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 &= \mathbf{V} \text{diag} \left(\frac{s_i^2}{s_i^2 + \alpha} \frac{1}{s_i} \right) \mathbf{U}^T \mathbf{b} \\
 \mathbf{x}_\alpha &= \sum_{i=1}^n \frac{s_i^2}{s_i^2 + \alpha} \frac{\mathbf{u}_i^T \mathbf{b}}{s_i} \mathbf{v}_i
 \end{aligned}$$

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 estimator 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

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

and Tikhonov cost functional is

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

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4DVar minimises

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

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

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

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

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

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

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is given by

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

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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 $\hat{\mathbf{H}}$

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

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 4DVar and Tikhonov regularisation

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

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Variable transformations

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

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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 **Tikhonov regularisation!**

$$J(\mathbf{x}) = \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 + \alpha \|\mathbf{x}\|_2^2$$

Example

Burger's equation

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

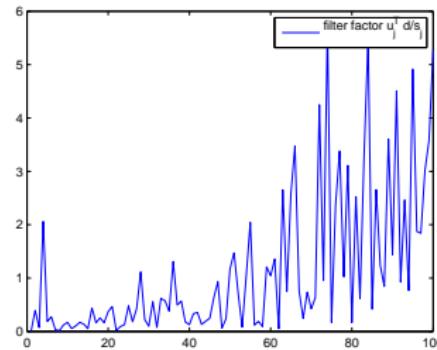
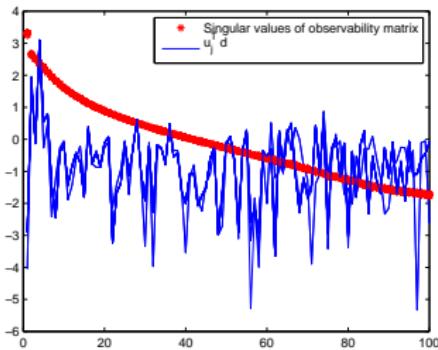
Optimal solution (4DVar)

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

Singular value analysis - observations everywhere

Optimal solution (4DVar)

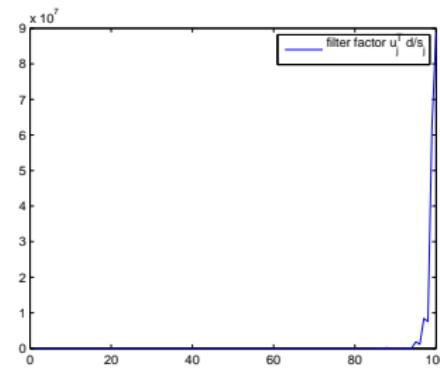
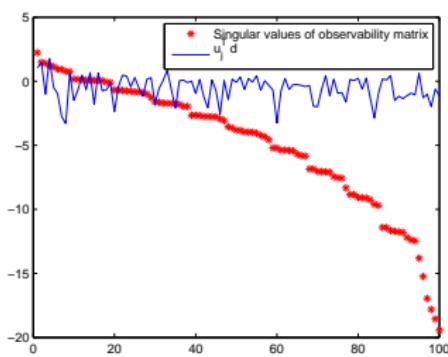
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Singular value analysis - observations every 10 points

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Blurred and exact images

The blurring process as a linear model

- ▶ Let \mathbf{X} be the exact image
- ▶ Let \mathbf{B} be the blurred image

$$\mathbf{x} = \text{vec}(\mathbf{X}) = \begin{bmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_N \end{bmatrix} \in \mathbb{R}^N, \quad \mathbf{b} = \text{vec}(\mathbf{B}) = \begin{bmatrix} \mathbf{b}_1 \\ \vdots \\ \mathbf{b}_N \end{bmatrix} \in \mathbb{R}^N$$

$N = m * n$ are related by the linear model

$$\mathbf{Ax} = \mathbf{b}$$

where \mathbf{A} is the discretisation of a point spread function.

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Noise $\mathbf{b} = \mathbf{b}_{\text{exact}} + \mathbf{e}$

$$\mathbf{x}_{\text{Naive}} = \mathbf{A}^{-1}\mathbf{b} = \mathbf{A}^{-1}\mathbf{b}_{\text{exact}} + \mathbf{A}^{-1}\mathbf{e} = \mathbf{x} + \mathbf{A}^{-1}\mathbf{e}$$

Need regularisation techniques!

Standard technique: Tikhonov regularisation

$$\min \{ \|\mathbf{Ax} - \mathbf{b}\|_2^2 + \alpha \|\mathbf{x}\|_2^2 \}$$

equivalent to

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

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L1 regularisation

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

$$\min \{ \| \mathbf{A}\mathbf{x} - \mathbf{b} \|_2^2 + \alpha \| \mathbf{x} \|_1 \}$$

Results from image deblurring: L1 regularisation

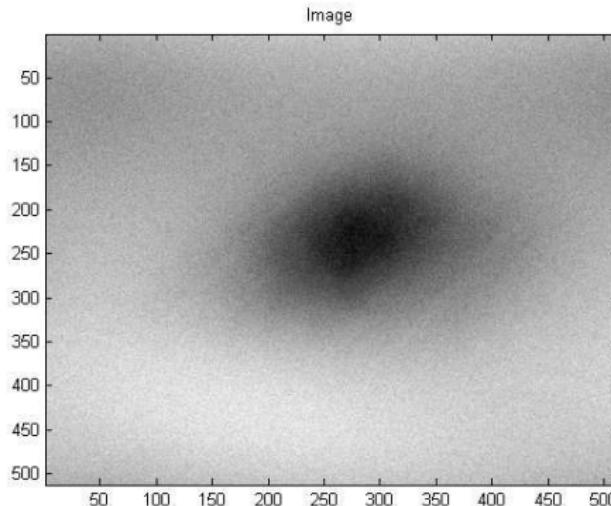


Figure: Blurred picture

Results from image deblurring: L1 regularisation

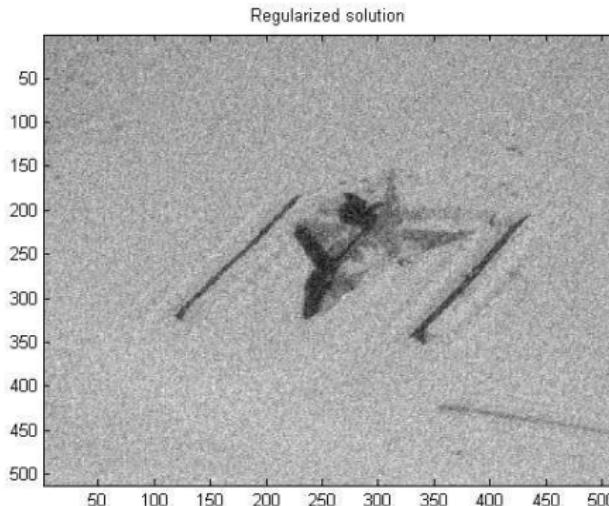


Figure: Tikhonov regularisation $\min \{ \| \mathbf{A}\mathbf{x} - \mathbf{b} \|_2^2 + \alpha \|\mathbf{x}\|_2^2 \}$

Results from image deblurring: L_1 regularisation



Figure: L_1 -norm regularisation $\min \{ \| \mathbf{A}\mathbf{x} - \mathbf{b} \|_2^2 + \alpha \|\mathbf{x}\|_1 \}$

L1 regularisation

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

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

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Inviscid Burger's equation

Inviscid Burger's equation

$$u_t + uu_x = 0$$

Inviscid Burger's equation

Inviscid Burger's equation

$$u_t + uu_x = 0$$

Conservative first order upwind method

$$U_j^{n+1} = U_j^n - \frac{\Delta t}{\Delta x} (F_{j+\frac{1}{2}}^n - F_{j-\frac{1}{2}}^n),$$

where

$$F_{j+\frac{1}{2}} = \begin{cases} \frac{1}{2} U_j^2 & v_{j+\frac{1}{2}} > 0 \\ \frac{1}{2} U_{j+1}^2 & v_{j+\frac{1}{2}} < 0 \end{cases}$$

$$v_{j+\frac{1}{2}} = \begin{cases} \frac{1}{2}(U_j + U_{j+1}) & U_j \neq U_{j+1} \\ U_j & U_j = U_{j+1}. \end{cases}$$

Initial conditions

Initial conditions for the **true solution** are

$$x(j) = 10(j - 1/2)\Delta x; \quad U^0(x(j)) = \begin{cases} 2 & 0 \leq x(j) < 2.5 \\ 0.5 & 2.5 \leq x(j) \leq 10. \end{cases}$$

with $\Delta x = \frac{1}{100}$ and $j = 1, \dots, N$

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with $\Delta x = \frac{1}{100}$ and $j = 1, \dots, N$ and for the **background solution** they are

$$U_B^0(x(j)) = \begin{cases} 2.1 & 0 \leq x(j) < 3.5 \\ 0.6 & 3.5 \leq x(j) \leq 10. \end{cases}$$

Truth and Background trajectory

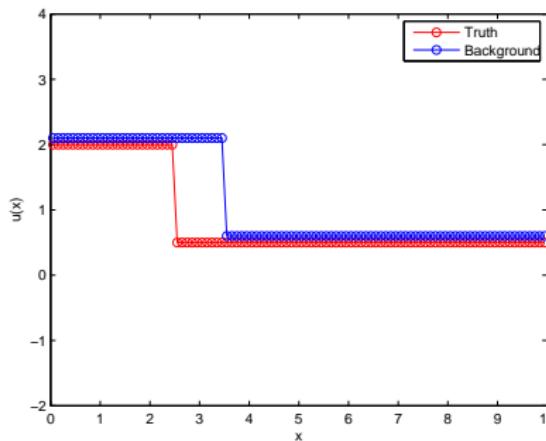


Figure: Initial conditions for Truth and Background, $t = 0$

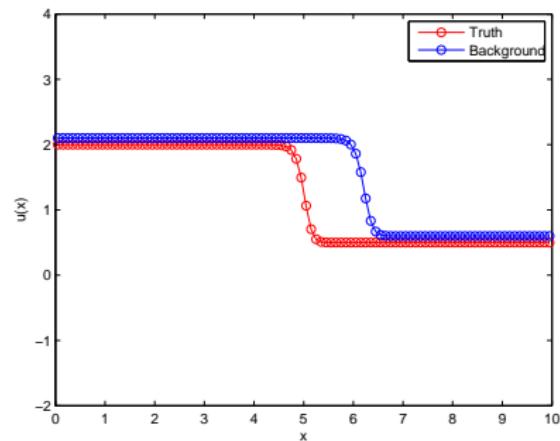


Figure: Truth and Background after 2000 time steps

Setup

- ▶ $\Delta t = 0.0001$

Setup

- ▶ $\Delta t = 0.0001$
- ▶ use "L1.1-regularisation" i.e.

$$\min \left\{ \|\mathbf{Ax} - \mathbf{b}\|_2^2 + \alpha \|\mathbf{x}\|_{1.1}^{1.1} \right\}$$

leading to a differentiable function and avoiding quadratic programming problem for the moment

Setup

- ▶ $\Delta t = 0.0001$
- ▶ use "L1.1-regularisation" i.e.

$$\min \left\{ \|\mathbf{Ax} - \mathbf{b}\|_2^2 + \alpha \|\mathbf{x}\|_{1.1}^{1.1} \right\}$$

leading to a differentiable function and avoiding quadratic programming problem for the moment

- ▶ length of the assimilation window: 1000 time steps

Setup

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leading to a differentiable function and avoiding quadratic programming problem for the moment

- ▶ length of the assimilation window: 1000 time steps
- ▶ perfect and noisy observations

Setup

Perfect observations

4DVar

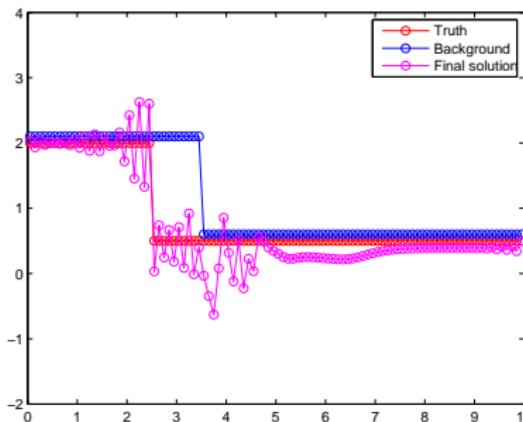


Figure: Truth and Background and final solution at time $t = 0$ (beginning of the assimilation window) using 4DVar

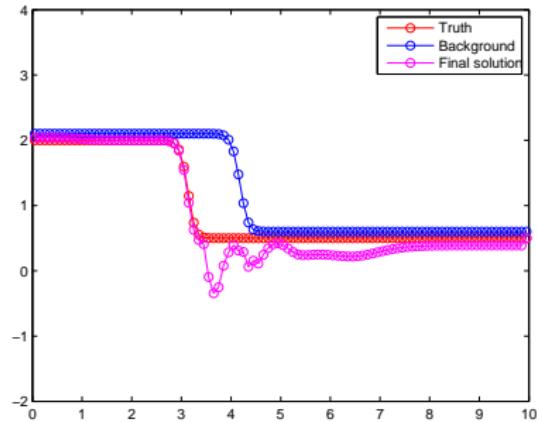


Figure: Truth and Background and final solution after 500 time steps (middle of the assimilation window) using 4DVar

4DVar

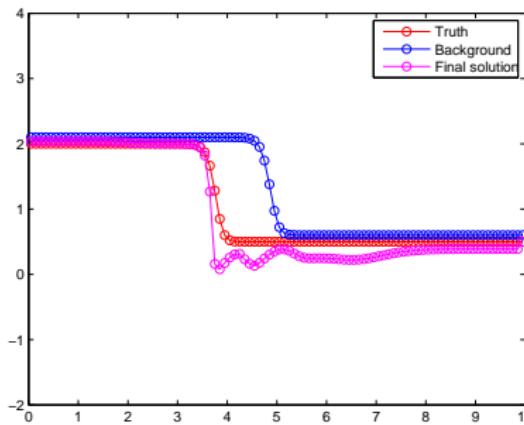


Figure: Truth and Background and final solution after 1000 time steps (which is the end of the assimilation window) using 4DVar

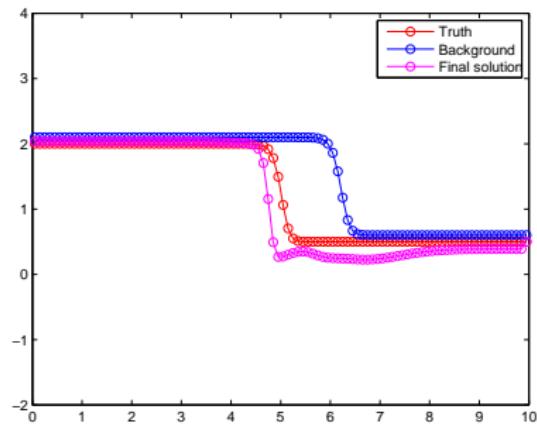


Figure: Truth and Background and final solution after 2000 time steps (assimilation window plus 1000 further steps forecast) using 4DVar

4DVar

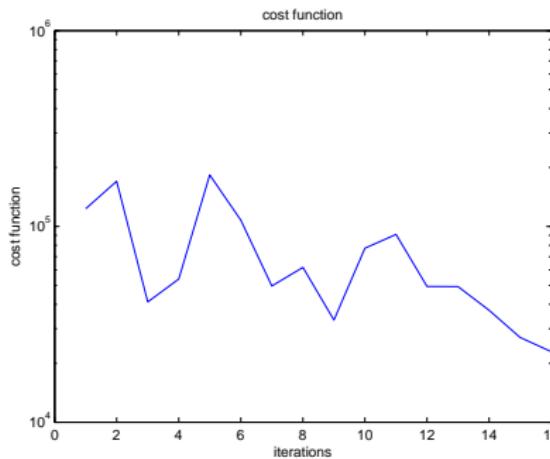


Figure: Cost function

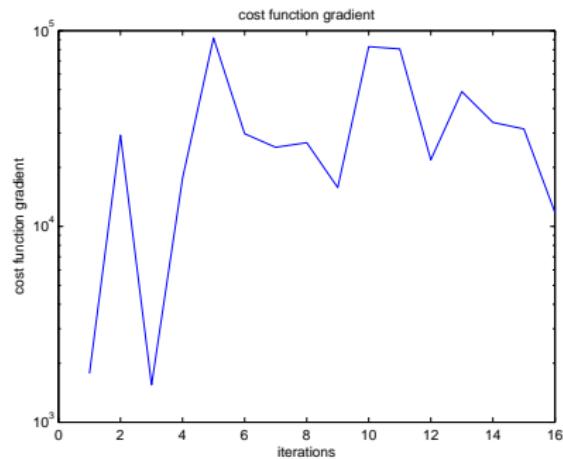


Figure: Cost function gradient

L1.1 Regularisation

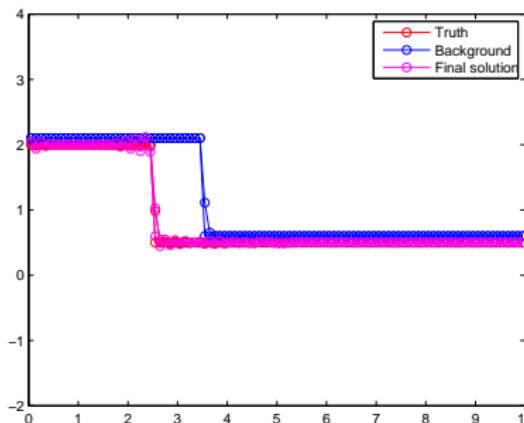


Figure: Truth and Background and final solution at time $t = 0$ (beginning of the assimilation window) using L1.1

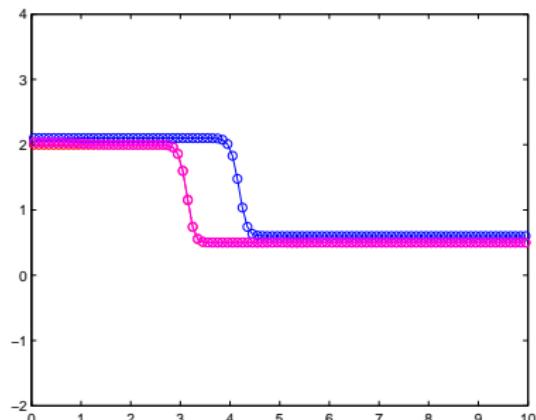


Figure: Truth and Background and final solution after 500 time steps (middle of the assimilation window) using L1.1

L1.1 Regularisation

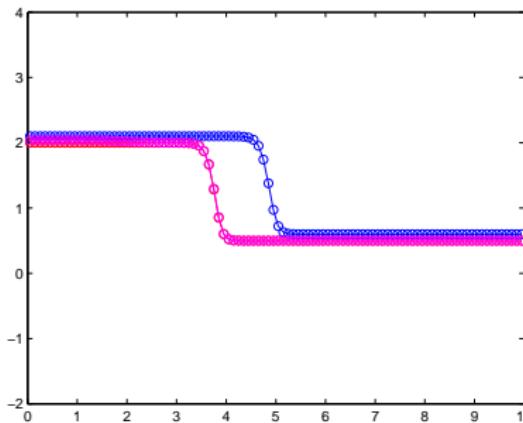


Figure: Truth and Background and final solution after 1000 time steps (which is the end of the assimilation window) using L1.1

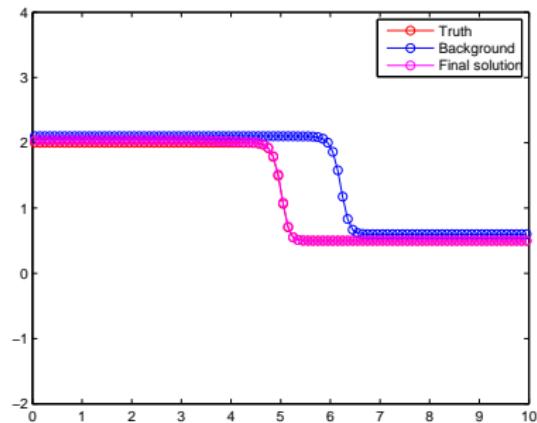


Figure: Truth and Background and final solution after 2000 time steps (assimilation window plus 1000 further steps forecast) using L1.1

L1.1 Regularisation

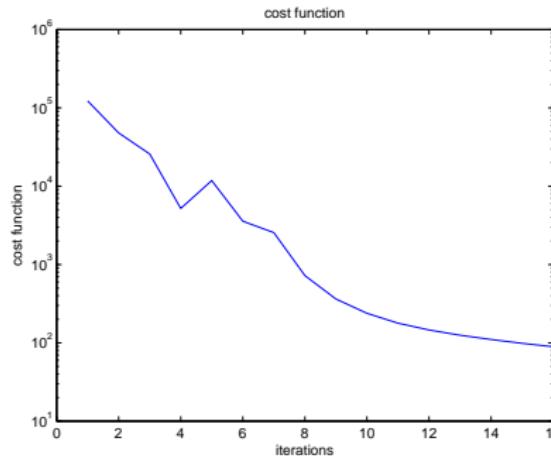


Figure: Cost function

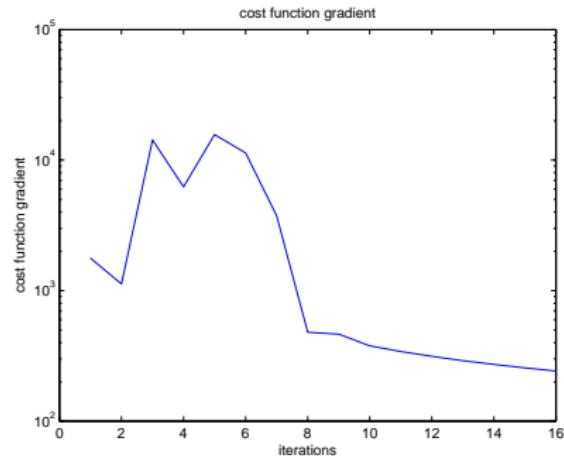


Figure: Cost function gradient

Comparison 4DVar and L1.1 Regularisation

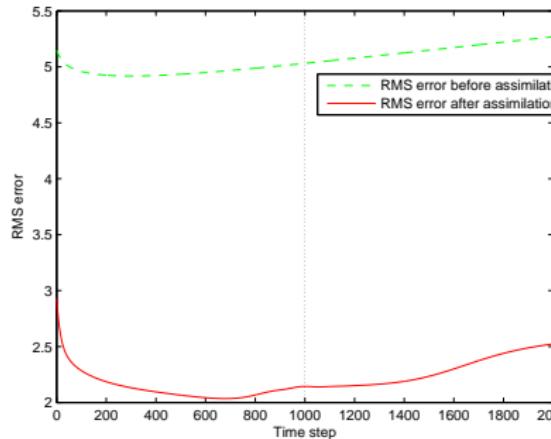


Figure: Root mean square error using 4DVar.

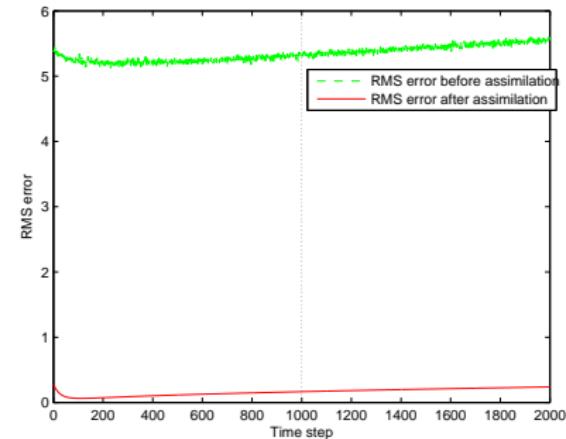


Figure: Root mean square error using L1.1.

Setup

Noisy observations

Comparison 4DVar and L1.1 Regularisation

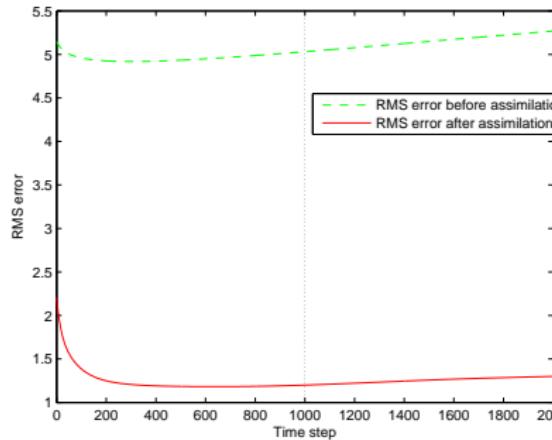


Figure: Root mean square error using 4DVar.

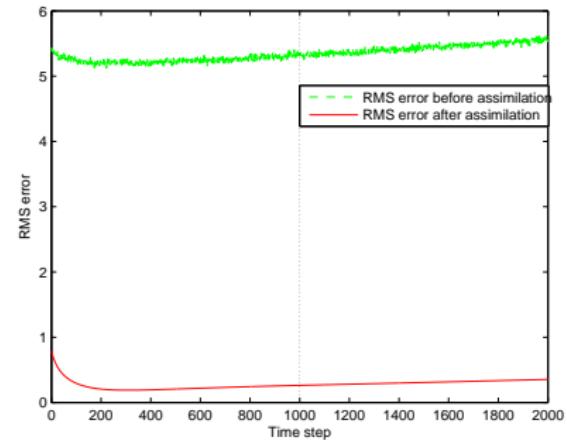


Figure: Root mean square error using L1.1.

4DVar - tridiagonal B

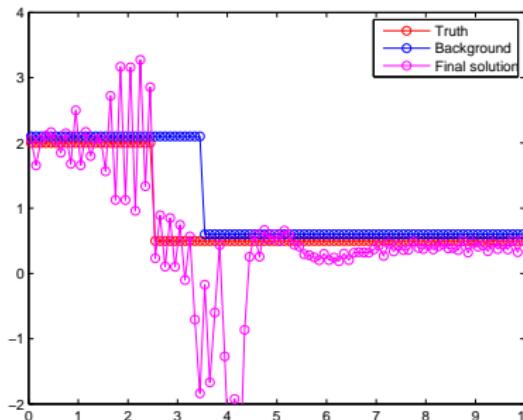


Figure: Truth and Background and final solution at time $t = 0$ (beginning of the assimilation window) using 4DVar

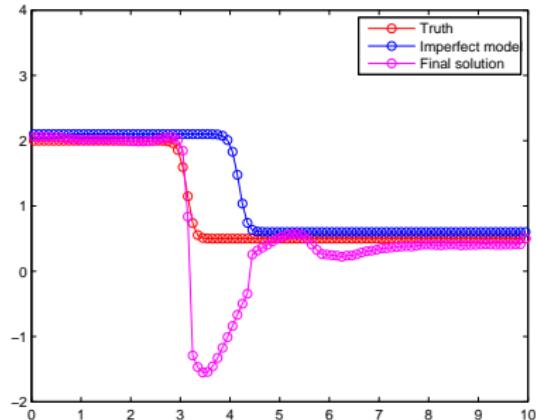


Figure: Truth and Background and final solution after 500 time steps (middle of the assimilation window) using 4DVar

4DVar - tridiagonal B

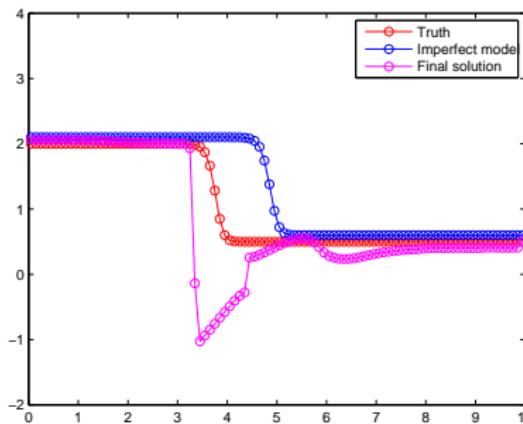


Figure: Truth and Background and final solution after 1000 time steps (which is the end of the assimilation window) using 4DVar

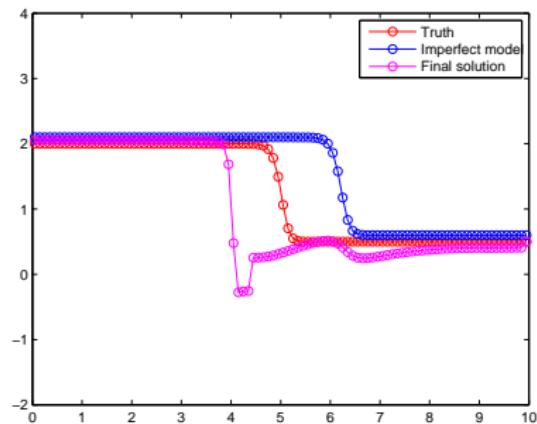


Figure: Truth and Background and final solution after 2000 time steps (assimilation window plus 1000 further steps forecast) using 4DVar

L1.1 Regularisation - tridiagonal B

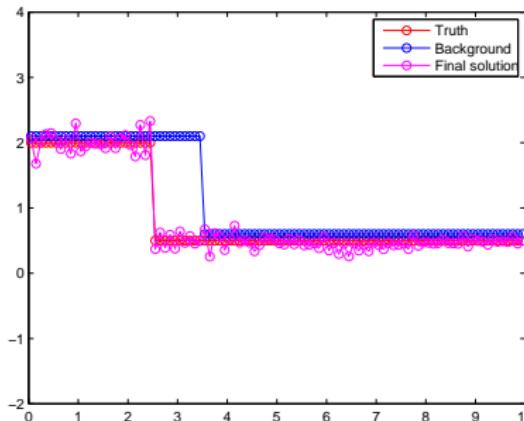


Figure: Truth and Background and final solution at time $t = 0$ (beginning of the assimilation window) using L1.1

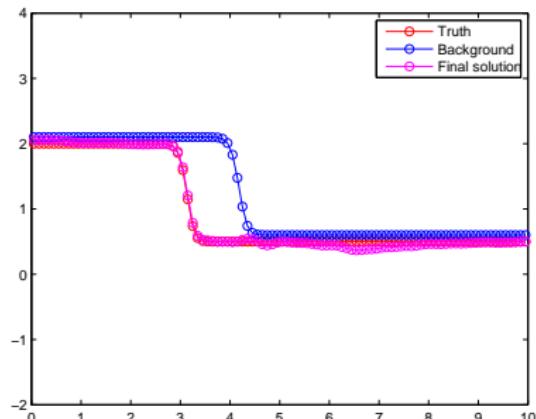


Figure: Truth and Background and final solution after 500 time steps (middle of the assimilation window) using L1.1

L1.1 Regularisation - tridiagonal B

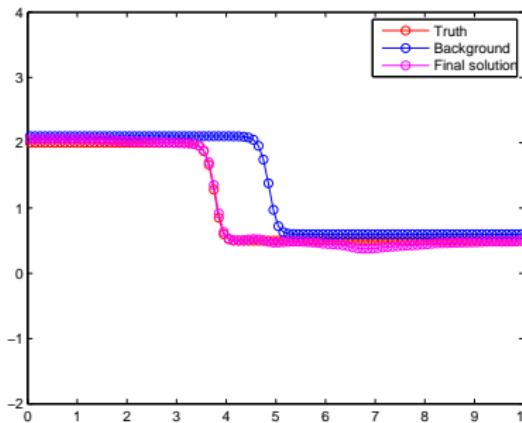


Figure: Truth and Background and final solution after 1000 time steps (which is the end of the assimilation window) using L1.1

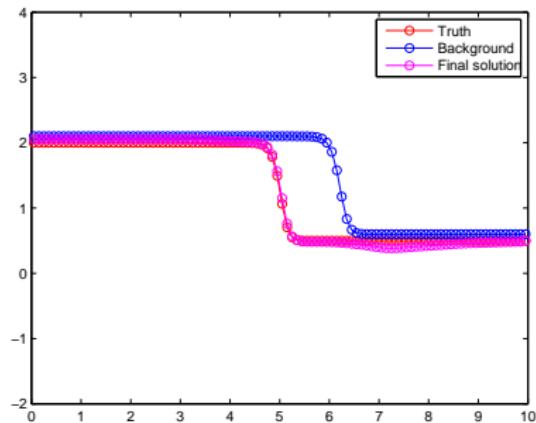


Figure: Truth and Background and final solution after 2000 time steps (assimilation window plus 1000 further steps forecast) using L1.1

4DVar - Gaussian exponential function in B , $b_{ij} = \sigma_b \exp(-r_{ij})$

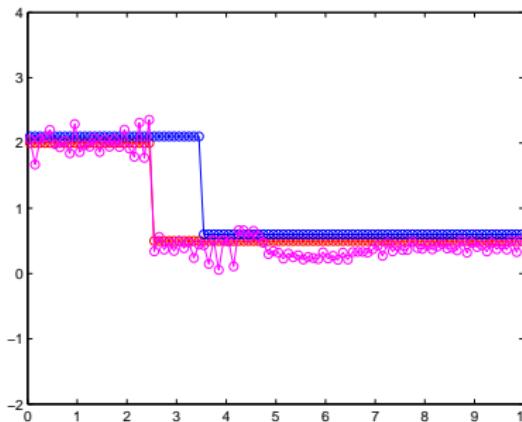


Figure: Truth and Background and final solution at time $t = 0$ (beginning of the assimilation window) using 4DVar

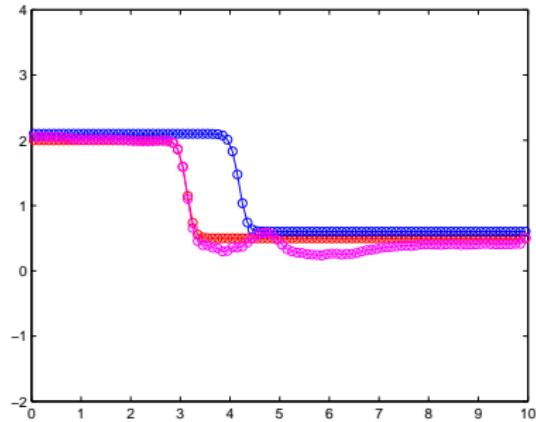


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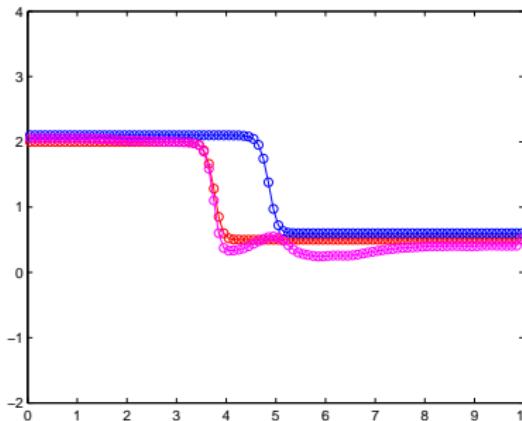


Figure: Truth and Background and final solution after 1000 time steps (which is the end of the assimilation window) using 4DVar

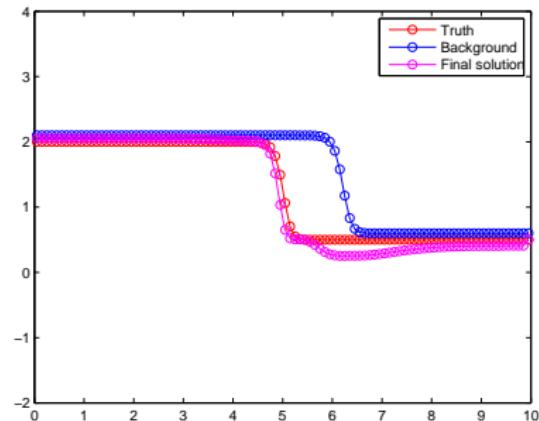


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L1.1 Regularisation - Gaussian exponential function in B , $b_{ij} = \sigma_b \exp(-r_{ij})$

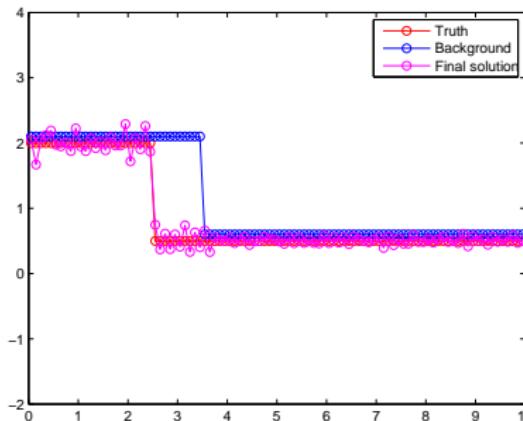


Figure: Truth and Background and final solution at time $t = 0$ (beginning of the assimilation window) using L1.1

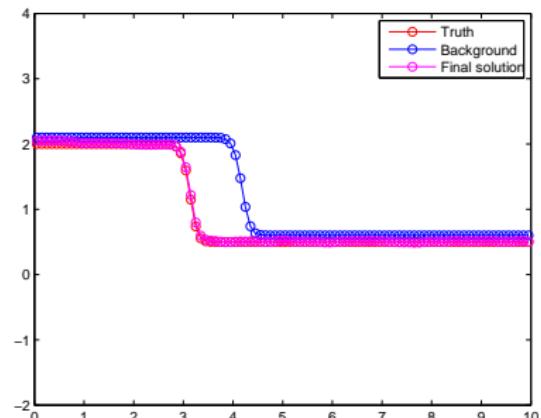


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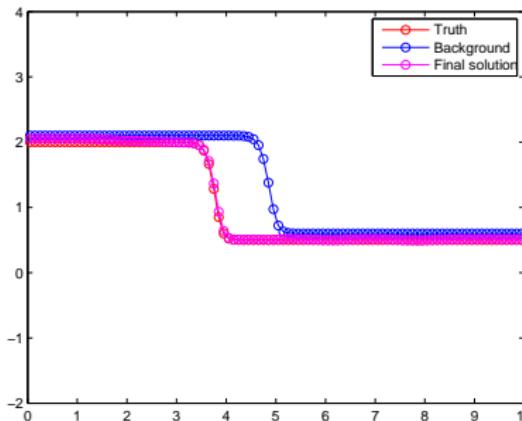


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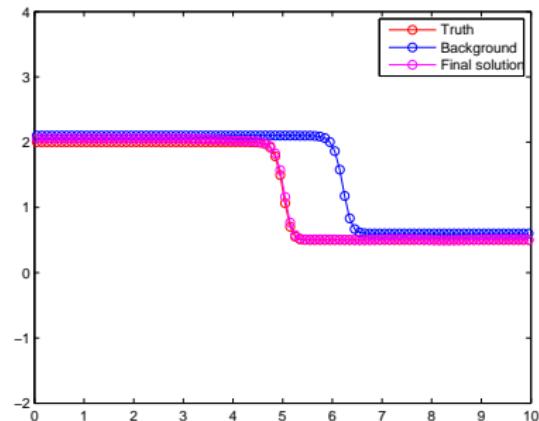


Figure: Truth and Background and final solution after 2000 time steps (assimilation window plus 1000 further steps forecast) using L1.1

Conclusions, questions and further work

- ▶ **L_1 -norm regularisation recovers discontinuity better than 4DVar**
- ▶ L_1 -minimisation gives smaller increments than 4DVar?
- ▶ Breakdown with fewer observations
- ▶ Implementation using quadratic/linear programming tools