Data Assimilation for Parameter Estimation with Application to a Simple Morphodynamic Model

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on the second of these applications and describe a method for using data assimilation to deliver improved parameter estimates.

The dynamical system we wish to model depends on parameters whose exact values are not known, for example those that arise from parameterization of the sediment transport flux. Inaccurate representation of model parameters can lead to the growth of model error and therefore e□ect the ability of our model to accurately predict the true system state. A key question in model development is how to estimate these values a priori. Generally, parameters are determined theoretically or by calibration of the model against observations. Here we present an alternative approach using a variational data assimilation technique within a simplified 1D model of bedform propagation to develop a scheme that enables model parameters to be estimated alongside the model bathymetry as part of the assimilation process.

In section 2 we present the data assimilation problem for a general case and give an overview of the three dimensional variational assimilation algorithm used in this work. In section 3 we describe the technique employed for parameter estimation and reformulate the data assimilation problem for this special case. Our simple 1D model is introduced in section 4. In section 5 we discuss the roles of the observation and background error covariance matrices. Particular attention is given to the cross correlations between the background errors in the state and parameter estimates. The experimental design is described in section 6 followed by results in section 7. Finally, in section 8 we summarise the conclusions from this work and outline areas for further study.

2 Data assimilation for state estimation

In reality, a model cannot represent the behaviour of a morphodynamic system exactly. Over time the model bathymetry will diverge from the true bathymetry and errors will arise due to imperfect initial conditions and inaccuracies in physical equations, parameters and numerical implementation. Data assimilation can be used to compensate for the inadequacies of a model and help keep the model bathymetry on track. By periodically incorporating measured observations into the model, data assimilation nudges the model bathymetry back towards the true bathymetry, thus improving the ability of the model to predict future bathymetry.

In this report we consider the consider the discrete, linear, time-invariant system model

$$\mathbf{z}_{k+1} = M\mathbf{z}_k, \qquad k = 0, \ldots, N-1, \tag{2.1}$$

where the vector $\mathbf{z}_k \in \mathbb{R}^m$ represents the model state at time t_k and $M \in \mathbb{R}^{m\times m}$ is a constant, non-singular matrix describing the dynamic evolution of the state from time t_k to time t_{k+1}.

We have a set of r observations to assimilate and these are related to the model state by the equations

$$\mathbf{y}_k = \mathbf{h}(\mathbf{z}_k) + \varepsilon^o_k, \qquad k = 0, \ldots, N-1, \tag{2.2}$$

where $\mathbf{y}_k \in \mathbb{R}^r$ is a vector of r observations at time t_k, $\mathbf{h} : \mathbb{R}^m \rightarrow \mathbb{R}^r$ is a nonlinear observation operator that maps from model to observation space, and $\varepsilon^o_k \in \mathbb{R}^r$ is a random vector representing the observation errors. If we have direct observations, h is simply an interpolation operator for interpolating variables from the model grid to observation locations. Often, the model variables we wish to analyse cannot be observed directly and instead we have observations of another measurable quantity. In this case, h will also include transformations based on physical relationships that convert the model variables to the observations. We also assume that an a priori or background estimate $\mathbf{z}^b_0 \in \mathbb{R}^m$ of the initial system state $\mathbf{z}_0$ is known with error ε^b.

The aim of data assimilation is to combine the measured observations $\mathbf{y}$ with the model predictions $\mathbf{z}^{\mathbf{b}}$ to derive a model state $\mathbf{z}^{\mathbf{a}} \in \mathbb{R}^{\mathbf{m}}$

3.1 Augmented data assimilation problem

We augment the state vector z with a vector p containing the parameters we wish to estimate, this gives us the augmented state vector

$$\mathbf{w} = \begin{pmatrix} \mathbf{z} \\ \mathbf{p} \end{pmatrix}, \tag{3.1}$$

where $\mathbf{z} \in \mathbb{R}^{m}$, $\mathbf{p} \in \mathbb{R}^{q}$, and $\mathbf{w} \in \mathbb{R}^{m+q}$.

We assume that the vector p is constant; the parameters are not altered by the forecast model from one time step to the next and are only updated when a new 3D Var analysis is generated. We is our background state. Note that this vector must now also include prior estimates of the parameters $\mathbf{p}^b$. These could be, for example, the latest estimates obtained from a previous analysis.

The matrix $\tilde{\mathbf{B}} \in \mathbb{R}^{(m+q)\times(m+q)}$ is the background error covariance matrix for the augmented system, and can be written as

$$\tilde{\mathbf{B}} = \begin{pmatrix} \mathbf{B}_{zz} & \mathbf{B}_{zp} \\ \mathbf{B}_{zp}^T & \mathbf{B}_{pp} \end{pmatrix}. \tag{3.7}$$

$\mathbf{p}^b$ $\mathbf{B}_{pp}$

Here $\mathbf{B}_{zz} \in \mathbb{R}^{m\times m}$ is the covariance matrix of the background errors in the state estimate $\mathbf{z}^b$

z^a and p^a separately as

$$z^a = z^b + K_z(y - h(z^b)), \tag{3.13}$$
$$p^a = p^b + K_p(y - h(z^b)). \tag{3.14}$$

Equation (3.13) is identical to (2.6) derived in section 2.1 and [illegible] -.313314(i)-[()]0.313311()0

The idea is to explore the application of the state augmentation method within the framework of this simple model before moving on to a more complex model of morphodynamic evolution based background) statistics and studying differences in background fields using ensemble techniques. A review of current operational techniques is given in Fisher (2003).

Calculation of the background error covariance can be made considerably easier by specifying the error correlations as analytic functions. A number of correlation models have been proposed (see Daley (1991) for further discussion on this). One of the most simple ways of representing **B** is to assume that the background error covariances are homogeneous and isotropic. **B** is then equal to the estimated error variance times a correlation matrix defined using a prespecified correlation function. Although this method is somewhat crude it makes the data assimilation problem far more tractable.

5.2.1 The state vector

To characterise the background errors in the state vector **z** we use the correlation function [Rodgers (2000)]

$$b_{ij} = \sigma_b^2 \rho^{|i-j|}, \qquad i, j = 1, \dots, m. \tag{5.2}$$

$\rho = \exp(-\Delta x/L)$ where Δx is the model grid spacing and L is known as the background correlation length scale.

Element b_{ij} defines the covariance between components i and j of the error vector ε_b. The form (5.2) gives us a full symmetric error covariance matrix with variance σ_b^2 on the diagonal and non-zero off-diagonal elements. We can write this explicitly as

$$\mathbf{B}_{zz} = \sigma_b^2 \begin{pmatrix} 1 & \rho & \rho^2 & \cdots & \cdots & \rho^{m-1} \\ \rho & 1 & \rho & \rho^2 & \cdots & \rho^{m-2} \\ \rho^2 & \rho & 1 & \rho & \cdots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & \ddots & 1 & \rho \\ \rho^{m-1} & \cdots & \cdots & \rho^2 & \rho & 1 \end{pmatrix}. \tag{5.3}$$

The reason for choosing this covariance matrix is that its inverse can be calculated explicitly and has a particularly simple form (see appendix A)

$$\mathbf{B}_{zz}{}^{-1} = \sigma_b^{-2}$$

5.2.2 The parameter vector

For the augmented system we have the added difficulty of specifying the background error covariance matrices for the parameter vector, $\mathbf{B}_{\mathrm{pp}}$, and for the cross correlations between the state and parameter errors, $\mathbf{B}_{\mathrm{zp}}$. One possible method for calculating these covariance matrices is by averaging the statistics over the assimilation window, using our knowledge of the truth and background states. However, since in reality the true solution is not known, this is difficult to do in practice. For simplicity we would like these matrices to be of a functional form similar to that used for the state background error covariance matrix, $\mathbf{B}_{\mathrm{zz}}$. Successful parameter estimation relies upon these correlations being suitably specified, so it is important to ensure that the choice of function is appropriate to the particular model application.

For our linear advection model we have a single unknown parameter - the advection velocity. We approximate the true advection velocity a with $\tilde{a}$ where $\tilde{a} = a + \varepsilon_{\mathbf{A}}$. In this case, the parameter vector $\mathbf{p}^{\mathbf{b}}$ is a scalar with error $\varepsilon_{\mathbf{p}} = \varepsilon_{\mathbf{A}}$. The error covariance matrix $\mathbf{B}_{\mathrm{pp}}$ is then simply

$$E(\varepsilon_{\mathbf{A}}^2) = \mathrm{Var}(\varepsilon_{\mathbf{A}}) = \sigma_{\mathbf{A}}^2. \tag{5.5}$$

5.2.3 Cross covariances

To determine a suitable form for the cross covariance matrix $\mathbf{B}_{\mathrm{zp}}$ we first need to derive an expression for the background error $\varepsilon_{\mathbf{b}}$.

We start by considering a single realisation. The background error $\varepsilon_{\mathbf{b}}(x,t)$, at a particlar point x and time t, will be a combination of error in the initial condition and error in the parameter estimate. We consider the following possiblitites:

1. known initial state $f(x)$, known advection velocity a;
2. unknown initial state $\tilde{f}(x)$, known advection velocity a;
3. known initial state $f(x)$, unknown advection velocity $\tilde{a}$;
4. unknown initial state $\tilde{f}(x)$, unknown advection velocity $\tilde{a}$.

By defining

$$\tilde{f}(x) = f(x) + \varepsilon_{\mathbf{b}}^0(x), \tag{5.6}$$

and

$$\tilde{a} = a + \varepsilon_{\mathbf{A}}, \tag{5.7}$$

we can derive expressions for the solution $\tilde{z}(x,t)$ and its error $\varepsilon_{\mathbf{b}}(x,t)$ in each of the above cases.

Case 1: The solution is the exact solution $z(x,t)$ given by (4.3).

Case 2: Here the solution is given by

$$\tilde{z}(x,t) = \tilde{f}(x - at), \qquad t \geq 0. \tag{5.8}$$

Using

$$\tilde{z}(x,t) = z(x,t) + \varepsilon_{\mathbf{b}}(x,t),$$

we have

$$\varepsilon_{\mathbf{b}}(x,t) = \tilde{z}(x,t) - z(x,t) = \tilde{f}(x-at) - f(x-at).$$

From (5.6)

$$\tilde{f}(x-at) = f(x-at) + \varepsilon_{\mathbf{b}}^{0}(x-at),$$

which gives us the following expression for the error

$$\varepsilon_{\mathbf{b}}(x,t) = \varepsilon_{\mathbf{b}}^{0}(x-at) = \varepsilon_{\mathbf{b}}^{0}(x_0). \tag{5.9}$$

In this case, the initial error profile propagates unchanged with velocity a (see figure 5.1).

Case 3: We have the solution

$$\tilde{z}(x,t) = f(x-\tilde{a}t). \tag{5.10}$$

The error at time $t \geq 0$ is

$$\begin{aligned}
\varepsilon_{\mathbf{b}}(x,t) &= f(x-\tilde{a}t) - f(x-at) \\
&= f(x-(a+\varepsilon_{\mathbf{A}})t) - f(x-at) \\
&= f(x-at-\varepsilon_{\mathbf{A}}t) - f(x-at).
\end{aligned}$$

Assuming that $f(x)$ is a continous, differentiable function we can expand in a Taylor series about $f(x-at)$ yielding,

$$\begin{aligned}
\varepsilon_{\mathbf{b}}(x,t) &= f(x-at-\varepsilon_{\mathbf{A}}t) - f(x-at) \\
&= \left(f(x-at) - \varepsilon_{\mathbf{A}}tf'(x-at) + \frac{\varepsilon_{\mathbf{A}}^2}{2!}t^2 f''(x-at) - \ldots \right) - f(x-at) \\
&= -\varepsilon_{\mathbf{A}}tf'(x-at) + O\left((\varepsilon_{\mathbf{A}}t)^2\right)
\end{aligned} \tag{5.11}$$

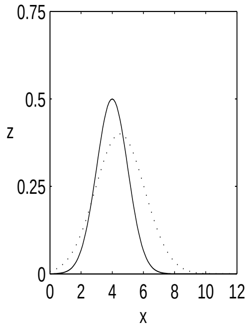
Solution (5.10) and its error (5.11) are illustrated in figure 5.2. Incorrect specification of the advection velocity introduces a phase error that grows with time. This error is similar in character to the derivative $f'(x)$ but increases in width and magnitude as t increases. Note that this Taylor expansion is only valid for small $\varepsilon_{\mathbf{A}}t$; the approximation (5.11) breaks down as t becomes large.

Case 4: The solution at time $t \geq 0$ is

$$\tilde{z}(x,t) = \tilde{f}(x-\tilde{a}t). \tag{5.12}$$

Using Taylor series, as above, we find that the error is given by

$$\begin{aligned}
\varepsilon_{\mathbf{b}}(x,t) &= \tilde{f}(x-\tilde{a}t) - f(x-at) \\
&= \tilde{f}(x-at-\varepsilon_{\mathbf{A}}t) - f(x-at) \\
&= \left(\tilde{f}(x-at) + \varepsilon_{\mathbf{A}}t\tilde{f}'(x-at) + \frac{\varepsilon_{\mathbf{A}}^2}{2!}t^2 \tilde{f}''(x-at) - \ldots \right) - f(x-at) \\
&= \varepsilon_{\mathbf{b}}^{0}(x-at) - \varepsilon_{\mathbf{A}}t\tilde{f}'(x-at) + O\left((\varepsilon_{\mathbf{A}}t)^2\right)
\end{aligned} \tag{5.13}$$



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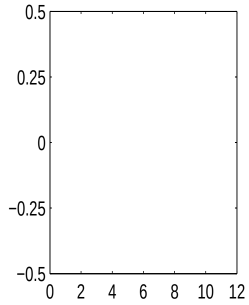

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Method A: The above analysis has shown that when the advection velocity a is unknown, the background error at the point x at time t is approximately proportional to $f'(x - at)t$, the value of the derivative of the initial state at the starting point x_0 multiplied by time. Conventional 3D Var schemes assume that the background error covariances are stationary and hold the matrix B fixed. Since we have already made this assumption for the state background error covariance matrix $\mathbf{B_{zz}}$

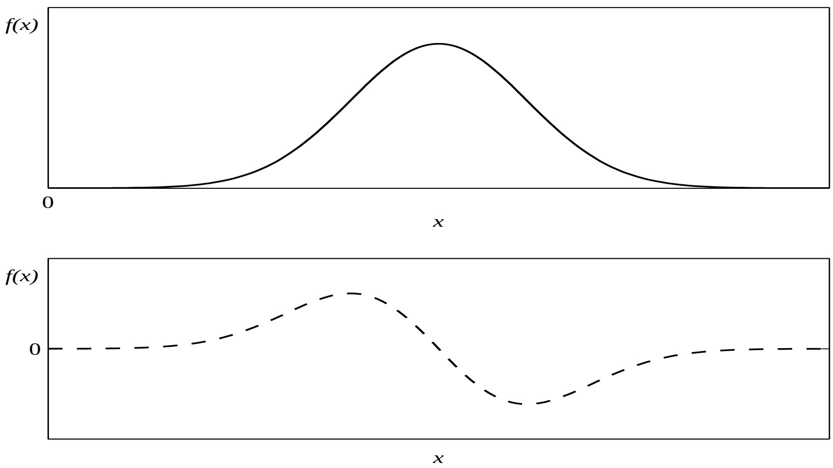


Figure 6.1: initial data (solid line) and its derivative (dashed line).

$\hat{\gamma}$

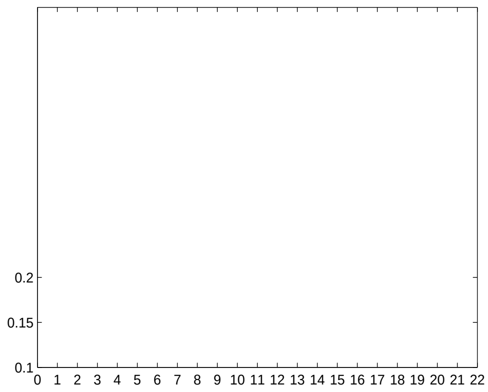
where y_i is an observation of the true bathymetry z_i^t given by (4.3) at the grid point x_i. The observation operator $\mathbf{h}$ is linear and $\mathbf{h} = \mathbf{H}$. The matrix $\mathbf{H} \in \mathbb{R}^{r \times m}$ takes a very simple form; it consists almost entirely of zeros except at positions corresponding to an observation location which take a value of one. The observation locations are determined at the start of the assimilation and remain fixed throughout. Since the observations are drawn from the truth we weight in their favour, setting the observation and background error variances to be $\sigma_o^2 = 0.1$ and $\sigma_b^2 = 1.0$ respectively.

The observation error covariance matrix $\mathbf{R}$ and sub-matrices $\mathbf{B}_{zz}$, $\mathbf{B}_{pp}$ of the augmented background error covariance matrix $\tilde{\mathbf{B}}$ were defined using (5.1), (5.3) and (5.5) respectively. Experiments were run using both method A (5.19) and B (5.20) to approximate the cross covariance matrix $\mathbf{B}_{zp}$. Results are presented in the following section.

7 Results

Figures 7.2 and 7.3 show the analysis produced for method A with initial parameter estimates (a) $\tilde{a} = 0.25$ and (b) $\tilde{a} = 0.75$. Results are given for times $t = 0$ to 20 with time step $\Delta t = 0.1$. Observations were taken at $20\Delta x$ intervals and assimilated every 20 time steps (2 time units). The dotted line represents the true bathymetry $\mathbf{z}^t$. Observations $\mathbf{y}$ are given by circles, the background $\mathbf{z}^b$ by the dashed line and the analysis $\mathbf{z}^a$ by the solid line. We found that although qualitatively the analysis is close to the truth (the main differences being small phase and amplitude errors), the scheme was unable to recover the true value of a. The parameter updates are shown in figure 7.1; the estimates do converge but to incorrect values of 0.379 and 0.799 respectively. In both cases we reach a point at around $t = 10$ after which the assimilation of new observations has no effect. We conclude that the representatation of the cross covariances used in method A is inadequate.

The evolution of the parameter estimates using method B is shown in figures 7.5 to 7.8 for observations taken at (a) $10\Delta x$ (b) $20\Delta x$ and (c) $40\Delta x$ intervals and assimilated every 10 and 20 time steps. The accuracy of the estimated advection velocity increases with time as the assimilation cycle is repeated and more observations are processed. The scheme converges in all cases, managing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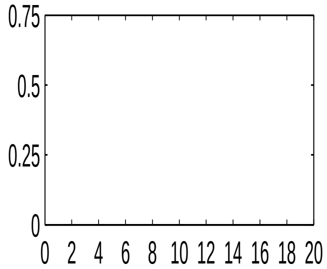
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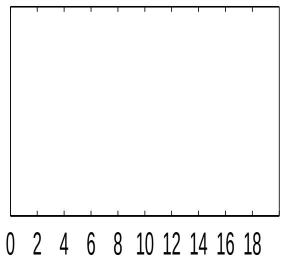
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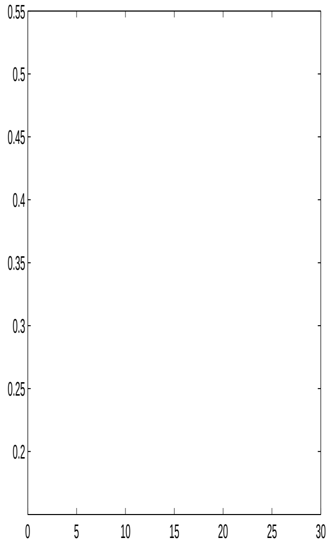
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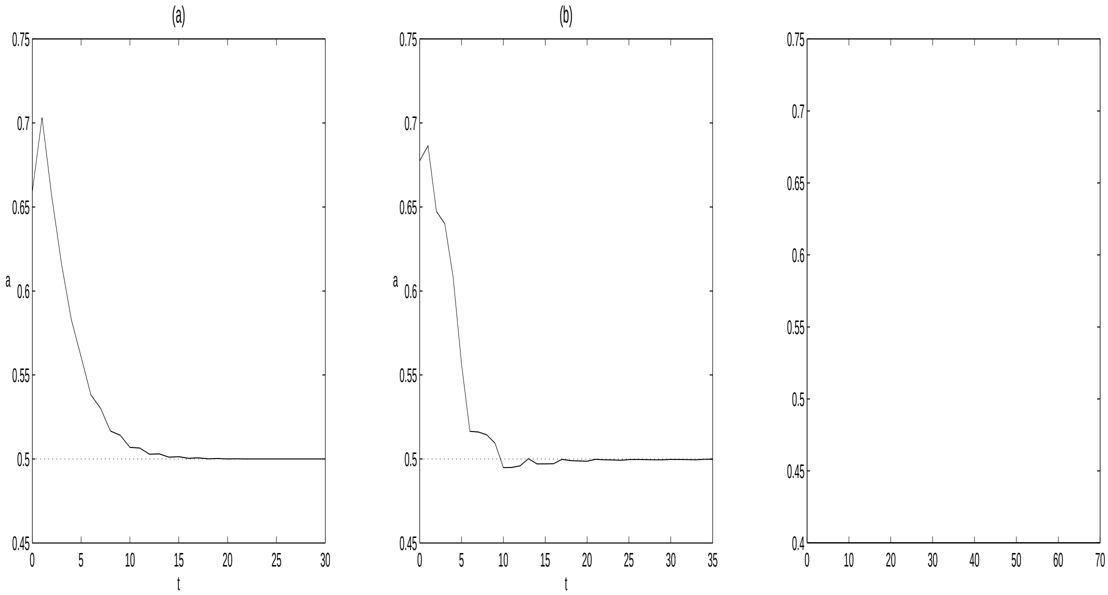
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70

$$\mathbf{B}^{-1} = \frac{\sigma_{\mathbf{b}}^{-2}}{1-\rho^2} \left[\begin{array}{cccccc} 1 & -\rho & 0 & \cdots & \cdots & 0 \\ -\rho & 1+\rho^2 & -\rho & 0 & & \vdots \\ 0 & -\rho & 1+\rho^2 & -\rho & & \\ & & & & & \end{array} \right.$$

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