Synergy of inverse problems and data assimilation techniques

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Abstract. This review article aims to provide a theoretical framework for data assimilation, a specific type of an inverse problem arising for example in numerical weather prediction, hydrology and geology.

We consider the general mathematical theory for inverse problems and regularisation, before we consider Tikhonov regularisation as one of the most popular methods for solving inverse problems. We show that data assimilation techniques such as three-dimensional and four-dimensional variational data assimilation (3DVar and 4DVar) as well as the Kalman filter and Bayes' data assimilation are, in the linear case, a form of cycled Tikhonov regularisation. We give an introduction to key data assimilation methods as currently used in practice, link them and show their similarities. We also give an overview of ensemble methods. Furthermore, we provide an error analysis for the data assimilation process in general, show research problems and give numerical examples for simple data assimilation problems. An extensive list of references is given for further reading.

Keywords. Inverse problems, ill-posedness, regularisation theory, Tikhonov regularisation, error analysis, 3DVar, 4DVar, Bayesian perspective, Kalman filter, Kalman smoother, ensemble methods, advection diffusion equation, Lorenz-95 system.

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1 Introduction

Inverse problems appear in many applications and have received a great deal of attention from applied mathematicians, engineers and statisticians. They occur, for example, in geophysics, medical imaging (such as ultrasound, computerised tomography and electrical impedance tomography), computer vision, machine learning, statistical inference, geology, hydrology, atmospheric dynamics and many other important areas of physics and industrial mathematics.

This article aims to provide a theoretical framework for data assimilation, a specific inverse problem arising for example in numerical weather prediction (NWP) and hydrology [48, 57, 58, 70, 83]. A few introductory articles on data assimilation in the atmospheric and ocean sciences are available, mainly from the engineering and meteorological point of view, see, for example [20, 44, 48, 66, 51, 63, 71], however, a comprehensive mathematical analysis in the light of the theory of inverse problem is missing. This expository article aims to achieve this.

An inverse problem is a problem, which is posed in a way that is inverse to most direct problems. The so-called direct problem we have in mind is that of determining the effect f from given causes and conditions φ, when a definite physical or mathematical model H in form of a relation

$$H(\varphi) = f \tag{1.1}$$

is given. In general, the operator H is nonlinear and describes the governing equations that relate the model parameters to the observed data. Hence, in an inverse problem we are looking for φ, that is a special cause, state, parameter or condition of a mathematical model. The solution of an inverse problem can be described as the construction of φ from data f (see, for example [22, 49]). We now consider the specific inverse problem arising in data assimilation, which usually contains also a dynamic aspect.

Data assimilation is, loosely speaking, a method for combining observations of the state of a complex system with predictions from a computer model output of that same state, where both the observations and the model output data contain errors and (in case of the observations) are often incomplete. The task in data assimilation (and hence the inverse problem) is seeking the best state estimate with the available information about the physical model and observations.

Let X be the state space. For the remainder of this article we generally assume that X (and also Y) are Hilbert spaces unless otherwise stated. Let $\varphi \in X$, where φ is the state (of the atmosphere, for example), that is, a vector containing all state variables. Furthermore, let $\varphi_k \in X$ be the state at time t_k and $M_k : X \to X$ the (generally nonlinear) model operator at time t_k which describes the evolution of the states from time t_k to time t_{k+1}, that is $\varphi_{k+1} = M_k(\varphi_k)$. For the moment we consider a perfect model, that is, the true system dynamics are assumed to be known. We also use the notation

$$M_{k,\ell} = M_{k-1} M_{k-2} \cdots M_{\ell+1} M_\ell, \quad k > \ell \in \mathbb{N}_0, \tag{1.2}$$

to describe the evolution of the system dynamics from time t_ℓ to time t_k.

Let Y_k be the observation space at time t_k and $f_k \in Y_k$ be the observation vector, collecting all the observations at time t_k. Finally, let $H_k : X \to Y_k$ be the (generally nonlinear) observation operator at time t_k, mapping variables in the state space to variables in the observation space. The data assimilation problem can then be defined as follows.

Definition 1.1 (Data assimilation problem). Given observations $f_k \in Y_k$ at time t_k, determine the states $\varphi_k \in X$ from the operator equations

$$H_k(\varphi_k) = f_k, \quad k = 0, 1, 2, \ldots, \tag{1.3}$$

subject to the model dynamics $M_k : X \to X$ given by $\varphi_{k+1} = M_k(\varphi_k)$, where $k = 0, 1, 2, \ldots$.

In numerical weather prediction the operator M_k involves the solution of a time-dependent nonlinear partial differential equation. Usually the observation operator

H_k is dynamic, that is, it changes at every time step, but for simplicity we often let $H_k := H$. Both the operator H_k and the data f_k contain errors. Also, in practice, the dynamical model M_k involves errors, that is, M_k does not represent the true system dynamics because of model errors. For a detailed account on errors occurring in the data assimilation problem we refer to Section 4. Moreover, the model dynamics represented by the nonlinear operators M_k are usually chaotic. In the context of data assimilation, additional information might be given through known prior information (background information) about the state variable, denoted by $\varphi_k^{(b)} \in X$.

The operator equation (1.3) (see also (1.1)) is usually ill-posed, that is, at least one of the following well-posedness conditions according to Hadamard [33] is not satisfied.

Definition 1.2 (Well-Posedness [49, 82]). Let X, Y be normed spaces and $H : X \rightarrow Y$ be a nonlinear mapping. Then the operator equation $H(\varphi) = f$ from (1.1) is called well-posed if the following holds:

- Existence: For every $f \in Y$ there exists at least one $\varphi \in X$ such that $H(\varphi) = f$, that is, the operator H is surjective.
- Uniqueness: The solution φ from $H(\varphi) = f$ is unique, that is, the operator H is injective.
- Stability: The solution φ depends continuously on the data f, that is, it is stable with respect to perturbations in f.

Equation (1.1) is ill-posed if it is not well-posed.

Note that for a general nonlinear operator H both existence and uniqueness of the operator equation need not be satisfied. If the existence condition in Definition 1.2 is not satisfied then it is possible that $f \in \mathcal{R}(H)$ but for a perturbed right hand side f^δ we have $f^\delta \notin \mathcal{R}(H)$, where $\mathcal{R}(H) = \{f \in Y, f = H(\varphi), \varphi \in X\}$ is the range of H. Existence of a generalised solution can sometimes (for instance in the finite-dimensional case) be ensured by solving the minimisation problem

$$\min \|f - H(\varphi)\|_Y^2, \tag{1.4}$$

which is equivalent to (1.1) if $f \in \mathcal{R}(H)$. The norm $\|\cdot\|_Y$ is a generic norm in Y. The second condition in Definition 1.2 implies that an inverse operator $H^{-1} : \mathcal{R}(H) \subseteq Y \rightarrow X$ with $H^{-1}(f) = \varphi$ exists. If the uniqueness condition is not satisfied then it is possible to ensure uniqueness by looking for special solutions, for example solutions that are closest to a reference element $\varphi^* \in X$, or, solutions with a minimum norm. Hence, at least in the linear case, uniqueness can be ensured if

$$\|f - H(\varphi_{uni})\|_Y = \min_{\varphi \in X} \|f - H(\varphi)\|_Y, \tag{1.5}$$

where $\|\varphi_{uni} - \varphi^*\|_X = \min\{\|\varphi - \varphi^*\|_X, \varphi \in X, \varphi$ is a minimiser in (1.5)$\}$. The third condition in Definition 1.2 implies that the inverse operator $H^{-1} : \mathcal{R}(H) \subseteq Y \rightarrow X$

is continuous. Usually this problem is the most severe one as small perturbations in the right hand side $f \in Y$ lead to large errors in the solution $\varphi \in X$ and the problem needs to be regularised. We will look at this aspect in Section 2.

From the above discussion it follows that the operator equation (1.3) is well-posed if the operator H_k is bijective and has a well-defined inverse operator H_k^{-1} which is continuous. A least squares solution can be found by solving the minimisation problem

$$\min_{\varphi_k \in X} \|f_k - H_k(\varphi_k)\|_Y^2, \quad k = 0, 1, 2, \ldots. \tag{1.6}$$

We can solve (1.6) at every time step k, which is a sequential data assimilation problem. If we include the nonlinear model dynamics constraint $M_k : X \to X$ given by $\varphi_{k+1} = M_k(\varphi_k)$, over the time steps t_k, $k = 0, \ldots, K$, and take the sum of the least squares problem in every time step, the minimisation problem becomes

$$\min_{\varphi_k \in X} \sum_{k=0}^{K} \|f_k - H_k(\varphi_k)\|_Y^2 = \min_{\varphi_0 \in X} \sum_{k=0}^{K} \|f_k - H_k M_{k,0}(\varphi_0)\|_Y^2, \tag{1.7}$$

where $M_{k,0}$ denotes the evolution of the model operator from time t_0 to time t_k, that is, $M_{k,0} = M_{k-1} M_{k-2} \cdots M_0$, using the system dynamics (1.2), and $M_{k,k} = I$. Both the sequential data assimilation system (1.6) and the consecutive data assimilation system (1.7) can be written in the form

$$\min_{\varphi \in X} \|\bar{f} - \bar{H}(\varphi)\|_Y^2, \tag{1.8}$$

with an appropriate operator $\bar{H}$. Problem (1.8) is equivalent to $\bar{H}(\varphi) = \bar{f}$ (cf. (1.1)) if $\bar{f} \in \mathcal{R}(\bar{H})$. For the sequential assimilation system (1.6) we have $\bar{H} := H_k$, $\bar{f} := f_k$ and $\varphi := \varphi_k$ at every step $k = 0, 1, \ldots$. For the consecutive system (1.7) we have $\varphi := \varphi_0$,

$$\bar{H} := \begin{bmatrix} H_0 \\ H_1 M_{1,0} \\ H_2 M_{2,0} \\ \vdots \\ H_K M_{K,0} \end{bmatrix} \quad \text{and} \quad \bar{f} := \begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \\ f_K \end{bmatrix}.$$

In general $\bar{H}$ is a *nonlinear* operator, since both the model dynamics M_k and the observation operators H_k are nonlinear. If the equation $\bar{H}(\varphi) = \bar{f}$ is well-posed, then $\bar{H}$ has a well-defined continuous inverse operator $\bar{H}^{-1}$ and $\mathcal{R}(\bar{H}) = Y$.

Now, if $\bar{H}$ is a *linear* operator in Banach spaces, then well-posedness follows from the first two conditions in Definition 1.2, which are equivalent to $\mathcal{R}(\bar{H}) = Y$ and $\mathcal{N}(\bar{H}) = \{0\}$, where $\mathcal{N}(\bar{H})$ is the null space of $\bar{H}$. Moreover, if $\bar{H}$ is a *linear* operator on a finite dimensional Hilbert space (in particular, if $\mathcal{R}(\bar{H})$ is of finite dimension) then the stability condition in Definition 1.2 holds automatically and well-posedness

follows from either one of the first two conditions in 1.2. (The last condition in Definition 1.2 follows from the compactness of the unit ball in finite dimensions [49].) For linear $\bar{H}$ the uniqueness condition $\mathcal{N}(\bar{H}) = \{0\}$ is clearly satisfied if the *observability matrix* $\bar{H}$ has full row rank. In this case the system is observable, that is, it is possible to determine the behaviour of the entire system from the systems output, see [47, 73].

The remaining question is the stability of the (injective) operator equation $\bar{H}(\varphi) = \bar{f}$ (or $H\varphi = H(\varphi) = f$, a notation which we are going to use from now on) for a compact linear operator $H : X \to Y$ in infinite dimensions. As a compact linear operator is always ill-posed in an infinite dimensional space (as $\mathcal{R}(H)$ is not closed) we need some form of regularisation.

Note that the discretisation of an infinite dimensional unstable ill-posed problem naturally leads to a finite dimensional problem which is well-posed, according to Definition 1.2. However, the discrete problem will be ill-conditioned, that is, an error in the input data will still lead to large errors in the solution. Hence some form of regularisation is also needed for finite dimensional problems arising from infinite dimensional ill-posed operators.

In the following we consider compact linear operators H for which a singular value decomposition exists (see, for example [49]).

Lemma 1.3 (Singular system of compact linear operators). *Let $H : X \to Y$ be a compact linear operator. Then there exist sets of indices $J = \{1, \ldots, m\}$ for $dim(R(H)) = m$ and $J = \mathbb{N}$ for $dim(R(H)) = \infty$, orthonormal systems $\{u_j\}_{j \in J}$ in X and $\{v_j\}_{j \in J}$ in Y and a sequence $\{\sigma_j\}_{j \in J}$ of positive real numbers with the following properties:*

$$\{\sigma_j\}_{j \in J} \quad \text{is non-increasing and} \quad \lim_{j \to \infty} \sigma_j = 0 \quad \text{for} \quad J = \mathbb{N}, \tag{1.9}$$

$$Hu_j = \sigma_j v_j, \ (j \in J) \quad \text{and} \quad H^* v_j = \sigma_j u_j, \ (j \in J). \tag{1.10}$$

For all $\varphi \in X$ there exists an element $\varphi_0 \in \mathcal{N}(H)$ with

$$\varphi = \varphi_0 + \sum_{j \in J} \langle \varphi, u_j \rangle_X u_j \quad \text{and} \quad H\varphi = \sum_{j \in J} \sigma_j \langle \varphi, u_j \rangle_X v_j. \tag{1.11}$$

Furthermore

$$H^* f = \sum_{j \in J} \sigma_j \langle f, v_j \rangle_Y u_j. \tag{1.12}$$

holds for all $f \in Y$. The countable set of triples $\{\sigma_j, u_j, v_j\}_{j \in J}$ is called singular system, $\{\sigma_j\}_{j \in J}$ are called singular values, $\{u_j\}_{j \in J}$ are right singular vectors and form an orthonormal basis for $\mathcal{N}(H)^\perp$ and $\{v_j\}_{j \in J}$ are left singular vectors and form an orthonormal basis for $\overline{\mathcal{R}(H)}$.

In the following we mostly consider compact linear operators although the concept of ill-posedness can be extended to nonlinear operators [49, 82, 40, 23] by considering

linearisations of the nonlinear problem using, for example, the Fréchet derivative of the nonlinear operator. One can show that for compact nonlinear operators the Fréchet derivative is compact, too, leading to the concept of locally ill-posed problems for nonlinear operator equations. For solving nonlinear problems computationally usually some form of linearisation is required. Hence, most of our results for linear problems can be extended to the case of iterative solutions to nonlinear problems (where a linear problem needs to be solved at each iteration).

2 Regularisation theory

Problems of the form $H\varphi = f$ with a compact operator H are ill-posed in infinite dimensions since the inverse of H is not uniformly bounded and hence in order to solve $H\varphi = f$ (or, for $f \notin \mathcal{R}(H)$ its equivalent minimisation problem $\min \|H\varphi - f\|^2$), regularisation is needed.

Let $H : X \to Y$ and denote its adjoint operator by $H^* : Y \to X$. Furthermore let φ be the unique solution to the least squares minimisation problem $\min \|H\varphi - f\|^2$. Then the solution to the minimisation problem is equivalent to the solution of the normal equations

$$H^*H\varphi = H^*f. \tag{2.1}$$

Clearly, if $H : X \to Y$ is compact then H^*H is compact and the normal equations (2.1) remain ill-posed. However, if we replace (2.1) by

$$(\alpha I + H^*H)\varphi_\alpha = \alpha\varphi_\alpha + H^*H\varphi_\alpha = H^*f, \tag{2.2}$$

with $\alpha > 0$, then the operator $(\alpha I + H^*H)$ has a bounded inverse. The equation (2.2) is typically referred to as Tikhonov regularisation and α is a regularisation parameter. We have the following theorem (see for example [40, 17, 82, 78, 62]).

Theorem 2.1 (Tikhonov regularisation). *Let $H : X \to Y$ be a compact linear operator. Then the operator $(\alpha I + H^*H)$ has a bounded inverse and the problem (2.2) is well-posed for $\alpha > 0$ and $\varphi_\alpha = (\alpha I + H^*H)^{-1}H^*f$ is the Tikhonov approximation of a minimum-norm least squares solution φ of (2.1). Furthermore, the solution φ_α is equivalent to the unique solution of the minimisation problem*

$$\min_{\varphi \in X} T_\alpha(\varphi) := \min_{\varphi \in X}\{\|f - H\varphi\|_Y^2 + \alpha\|\varphi\|_X^2\}, \tag{2.3}$$

where $T_\alpha(\varphi)$ is the so-called Tikhonov functional.

In general, Tikhonov regularisation can be used with a known reference element $\varphi^{(b)}$, that is, the term $\|\varphi\|_X^2$ in (2.3) is replaced by $\|\varphi - \varphi^{(b)}\|_X^2$, and the problem is often refereed to as generalised Tikhonov regularisation. We consider this problem in Section 3.

We have the following definition for a general linear regularisation scheme.

Definition 2.2 (Regularisation scheme). A family of bounded linear operators $\{R_\alpha\}_{\alpha>0}$, $R_\alpha : Y \to X$ is a linear regularisation scheme for the compact bounded linear injective operator H if

$$\lim_{\alpha \to 0} R_\alpha H\varphi = \varphi \quad \forall \varphi \in X. \tag{2.4}$$

Clearly the family of approximate inverses $R_\alpha = (\alpha I + H^*H)^{-1}H^* : Y \to X$ is a linear regularisation scheme for H. If the range of H, $\mathcal{R}(H)$ is not closed then

$$\lim_{\alpha \to 0} \|R_\alpha\| = \infty. \tag{2.5}$$

If we apply the regularisation operator R_α to noisy data f^δ with noise level δ, that is, $\|f^\delta - f\|_Y \leq \delta$ we get regularised solutions

$$\varphi_\alpha^\delta = R_\alpha f^\delta.$$

Using the singular system of a compact operator from Lemma 1.3 we may also write the regularised solution arising from Tikhonov regularisation via the minimisation problem in (2.3) as

$$\varphi_\alpha^\delta = \sum_{j \in J} \frac{\sigma_j}{\sigma_j^2 + \alpha} \langle f^\delta, v_j \rangle_Y u_j. \tag{2.6}$$

We observe that, for $\alpha = 0$, the solution φ_α^δ amplifies the noise in f^δ as for compact operators we have $\lim_{j \to \infty} \sigma_j = 0$.

Furthermore, for the exact unique solution we have $\varphi = H^\dagger f$, where $H^\dagger : \mathcal{R}(H) + \mathcal{R}(H)^\perp \to X$ denotes the Moore-Penrose pseudo-inverse of H (see [82]) and it is continuous if $\mathcal{R}(H)$ is closed. Therefore we may estimate the total regularisation error

$$\|\varphi_\alpha^\delta - \varphi\|_X \leq \|R_\alpha\|\delta + \|R_\alpha f - H^\dagger f\|_X,$$

or, for $\mathcal{N}(H) = \{0\}$,

$$\|\varphi_\alpha^\delta - \varphi\|_X \leq \|R_\alpha\|\delta + \|R_\alpha H\varphi - \varphi\|_X, \tag{2.7}$$

Hence, the total regularisation error consists of a stability component $\|R_\alpha\|\delta$ which represents the influence of the data error δ and a component $\|R_\alpha H\varphi - \varphi\|_X$ which represents the approximation error of the regularisation scheme. For small α the second component will be small (see (2.4)), but the first component will be large (see (2.5)), whereas for large values of α the first term will be small and the second one large. We will see this in the examples in Section 9. Hence, finding a good value for the regularisation parameter α is important. Techniques for regularisation parameter estimation aim to find a reasonably good value for α (see, for example [82, 37, 38]). The most prominent ones are the L-curve method, generalised cross-validation and the discrepancy principle.

A regularisation scheme is called convergent, if from the convergence of the data error to zero, it follows that the regularised solution converges to the exact solution.

One can show that a regularisation scheme $R_\alpha = (\alpha I + H^* H)^{-1} H^* : Y \to X$ arising in Tikhonov regularisation is a convergent regularisation if $\alpha(\delta) \to 0$ and $\frac{\delta^2}{\alpha(\delta)} \to 0$ as $\delta \to 0$ (see [22]). For Tikhonov regularisation one may choose $\alpha = \mathcal{O}(\delta)$ such that this holds [82].

Other regularisation schemes for inverse problems are also possible, some of the most well known ones are the truncated singular value decomposition (TSVD) and the Landweber iteration (see, for example, [22, 35, 34]). Moreover, it is possible to change the penalty term $\|\varphi\|_X^2$ in (2.3). Other penalty functionals can be used to incorporate a priori information about the solution φ. Prominent methods are Total Variation regularisation or the use of sparsity promoting norms (like the L_1-norm, for example) in the penalty functional. There is a fast growing literature on this topic, see, for example [82, 13, 7, 86, 1] and the articles by Burger et al. [10] and van den Doel et al. [81] in this book.

In the following we use the results from inverse problems and regularisation theory to develop a coherent mathematical framework for several data assimilation techniques used in practice.

3 Cycling, Tikhonov regularisation and 3DVar

Data assimilation aims to solve a dynamic inverse problem which includes measurement data $f_1, f_2, f_3, \ldots, f_k, \ldots$ at various times $t_1 < t_2 < t_3 < \ldots < t_k < \ldots$. At every time t_k the inversion problem is given by (1.3). However, usually the data f_k do not contain enough information to recover the state φ_k at time t_k completely. Thus, it is crucial to take the dynamical evolution of the states into account.

Assume that we are given some reconstruction $\varphi_k^{(a)}$ at time t_k for some $k \in \mathbb{N}$. Then, we expect that

$$\varphi_{k+1}^{(b)} := M_k(\varphi_k^{(a)}) \tag{3.1}$$

is a reasonable first guess for the system state at time t_{k+1}, where M_k describes the model dynamics and is given in Definition 1.1. In data assimilation, $\varphi^{(b)}$ is called the *background* or *first guess*. At time t_{k+1} we would like to assimilate the data f_{k+1} to calculate a reconstruction $\varphi_{k+1}^{(a)}$, which is also called the *analysis* in data assimilation. Then, the background $\varphi_{k+2}^{(b)}$ at time t_{k+2} can be calculated using (3.1) with k replaced by $k+1$ and another reconstruction can be carried out at time t_{k+2}. This approach is called *cycling* of reconstruction and dynamics.

Definition 3.1 (Cycling for data assimilation). Start with some initial state $\varphi_0^{(a)}$ at time t_0. For $k = 0, 1, 2, \ldots$ carry out the cycling steps:

(i) **Propagation Step.** Use the system dynamics M_k to calculate a *background* $\varphi_{k+1}^{(b)}$ at time t_{k+1} using (3.1).

(ii) **Analysis Step.** With the data f_{k+1} at time t_{k+1} (and the knowledge of the background $\varphi_{k+1}^{(b)}$) calculate a reconstruction or *analysis* $\varphi_{k+1}^{(a)}$.

Increase the index k to $k+1$ and go to Step i.

A key characteristic of a data assimilation system is its Analysis Step (ii). Here, for any step k, the task is to calculate a reconstruction $\varphi_k^{(a)}$ using the data f_k and the knowledge of the background $\varphi_k^{(b)}$. We need to choose or develop a reconstruction method which optimally combines the given information.

To carry out the analysis we will study two basic approaches, one coming from optimisation and *optimal control theory*, the other arising from *stochastics and probability theory*. In this section we focus on the *optimisation* approach, Section 5 will provide an introduction to the stochastic approach using Bayes' formula. The relationship between the two approaches will be discussed in detail in Section 5.

With a norm $||\cdot||_X$ in the state space X and a norm $||\cdot||_Y$ in the data (or observation) space Y we can combine the given information at step k, namely the observation data $f_k \in Y$ and the background $\varphi_k^{(b)} \in X$ by minimising the *inhomogeneous Tikhonov functional*

$$J_k(\varphi) := \alpha||\varphi - \varphi_k^{(b)}||_X^2 + ||f_k - H\varphi||_Y^2 \tag{3.2}$$

at time t_k. $H : X \to Y$ is the observation operator defined in Section 1. With $\tilde{\varphi}_k := \varphi - \varphi_k^{(b)}$ this is transformed into the Tikhonov functional (2.3) in the formula

$$\tilde{J}_k(\tilde{\varphi}_k) := \alpha||\tilde{\varphi}_k||_X^2 + ||(f_k - H\varphi_k^{(b)}) - H\tilde{\varphi}_k||_Y^2, \tag{3.3}$$

which according to Theorem 2.1 is minimised by

$$\tilde{\varphi}_k^{(a)} := (\alpha I + H^*H)^{-1}H^*(f_k - H\varphi_k^{(b)}), \tag{3.4}$$

leading to the minimiser

$$\varphi_k^{(a)} = \varphi_k^{(b)} + (\alpha I + H^*H)^{-1}H^*(f_k - H\varphi_k^{(b)}) \tag{3.5}$$

of the functional (3.2). We denote the cycling of Definition 3.1 with an analysis calculated by (3.5) as *cycled Tikhonov regularisation*.

Often, data assimilation works in spaces $X = \mathbb{R}^n$ and $Y = \mathbb{R}^m$ of dimensions $n \in \mathbb{N}$ and $m \in \mathbb{N}$. The norms in the spaces X and Y are given explicitly using the standard L^2-norms and some weighting matrices $B \in \mathbb{R}^{n \times n}$ and $R \in \mathbb{R}^{m \times m}$. In Section 5, these matrices will be chosen to coincide with the error covariance matrices of the state distributions in X and the error covariance matrices of the observation distributions in Y. For the moment we assume the matrices to be symmetric, positive definite and invertible. Then, we define a weighted scalar product in $X = \mathbb{R}^n$ by

$$\langle \varphi, \psi \rangle_{B^{-1}} := \varphi^T B^{-1} \psi, \quad \varphi, \psi \in X = \mathbb{R}^n, \tag{3.6}$$

and a weighted scalar product in $Y = \mathbb{R}^m$ by

$$\langle f, g \rangle_{R^{-1}} := f^T R^{-1} g, \quad f, g \in Y = \mathbb{R}^m. \tag{3.7}$$

With the corresponding norms $|| \cdot ||_{B^{-1}}$ in X and $|| \cdot ||_{R^{-1}}$ in Y we can rewrite the functional (3.2) into the form

$$J_k(\varphi) = \alpha(\varphi - \varphi_k^{(b)})^T B^{-1}(\varphi - \varphi_k^{(b)}) + (f_k - H\varphi)^T R^{-1}(f_k - H\varphi). \tag{3.8}$$

In the framework of the cycling given by Definition 3.1, this functional is known as the *three-dimensional variational data assimilation scheme* (3DVar), see, for example [20, 51]. Often, the notation x and $x^{(b)}$ for the state and the background, as well as y for the observations is used in the meteorological literature of data assimilation. Here, building a bridge to the functional analytic framework, we will use $\varphi \in X$ for the states and $f \in Y$ for the observations. x, y will be points in the physical space $\mathbb{R}^3$, respectively. This is also advantageous when we employ ensemble methods and analyse localisation techniques.

The functional (3.8) can easily be transformed into the general Tikhonov regularisation form. By H' we denote the adjoint operator of H with respect to the standard L^2 scalar products in $X = \mathbb{R}^n$ and $Y = \mathbb{R}^m$. The notation H^* is used for the adjoint operator with respect to the weighted scalar products $\langle \cdot, \cdot \rangle_{B^{-1}}$ and $\langle \cdot, \cdot \rangle_{R^{-1}}$. Then, we calculate

$$\begin{aligned}
\langle \varphi, H\psi \rangle_{R^{-1}} &= \langle \varphi, R^{-1} H\psi \rangle \\
&= \langle H'R^{-1}\varphi, \psi \rangle \\
&= \langle H'R^{-1}\varphi, BB^{-1}\psi \rangle \\
&= \langle BH'R^{-1}\varphi, B^{-1}\psi \rangle \\
&= \langle BH'R^{-1}\varphi, \psi \rangle_{B^{-1}} \\
&= \langle H^*\varphi, \psi \rangle_{B^{-1}},
\end{aligned}$$

leading to

$$H^* = BH'R^{-1}.$$

This means that the minimiser (3.5) of (3.2) with the norms based on the scalar products (3.6) and (3.7) is given by

$$\begin{aligned}
\varphi_k^{(a)} &= \varphi_k^{(b)} + (\alpha I + H^*H)^{-1} H^*(f_k - H\varphi_k^{(b)}) \\
&= \varphi_k^{(b)} + (\alpha I + BH'R^{-1}H)^{-1} BH'R^{-1}(f_k - H\varphi_k^{(b)}). \tag{3.9}
\end{aligned}$$

The operator $\alpha I + H^*H$ maps the state space X into itself. In large-scale data assimilation problems the dimension n of the state space is often much larger than the dimension m of the data space Y. In this case the inversion of $\alpha I + H^*H$ is not

feasible, and it is advantageous to derive a different form of the update formula, known as *measurement space inversion*. Using the invertibility of the operators $\alpha I + H^*H$ in X and $\alpha I + HH^*$ in Y we start from

$$(\alpha I + H^*H)H^* = H^*(\alpha I + HH^*).$$

We multiply with the inverse $(\alpha I + H^*H)^{-1}$ from the left and by $(\alpha I + HH^*)^{-1}$ from the right to obtain

$$H^*(\alpha I + HH^*)^{-1} = (\alpha I + H^*H)^{-1}H^*. \tag{3.10}$$

With the help of (3.10) we transform (3.9) into

$$\begin{aligned}
\varphi_k^{(a)} &= \varphi_k^{(b)} + H^*(\alpha I + HH^*)^{-1}(f_k - H\varphi_k^{(b)}) \\
&= \varphi_k^{(b)} + BH'R^{-1}(\alpha I + HBH'R^{-1})^{-1}(f_k - H\varphi_k^{(b)}). \\
&= \varphi_k^{(b)} + BH'(\alpha R + HBH')^{-1}(f_k - H\varphi_k^{(b)}). \tag{3.11}
\end{aligned}$$

Here, the inversion of $(\alpha I + HH^*)$ or $(\alpha R + HBH')$, respectively, takes place in the space $Y = \mathbb{R}^m$. The solution is then projected into the state space by the application of BH'. In the meteorological literature of data assimilation, the solution (3.9) is often referred to as the solution arising from Optimal Interpolation (OI) [68, 29]. It refers to a direct method being used to solve the 3DVar minimisation problem (3.8) rather than an iterative optimisation technique. In the linear case Optimal Interpolation and 3DVar are equivalent. Method (3.11) is often called PSAS (physical space statistical analysis) scheme in the literature on meteorology and oceanography [18, 16].

We summarise our results in the following theorem.

Theorem 3.2 (Equivalence of cycled Tikhonov regularisation and 3DVar). *3DVar or three-dimensional variational data assimilation (3.9) or (3.11) is equivalent to cycled Tikhonov regularisation (3.5) when the norms are arising from the weighted inner products (3.6) and (3.7).*

Theorem 3.2 shows that 3DVar is merely a cycled Tikhonov regularisation in an appropriately chosen norm.

4 Error analysis

In this part we investigate the error arising in data assimilation, that is, we consider the error between the true solution and the solution obtained from a data assimilation scheme. The solution obtained from solving a data assimilation problem is often referred to as "analysis" in the data assimilation literature. As a generic method we will study cycled Tikhonov regularisation, which according to Theorem 3.2 includes three-dimensional variational assimilation. We will later see that this also carries over

to cycled four-dimensional variational data assimilation, which we will discuss in Section 6.

We need to take into account errors which can arise when we cycle the update formula (3.5) according to Definition 3.1. Assume that $\varphi_k^{(true)}$ is the true state at time t_k, $k = 0, 1, 2, ...$ and $f_k^{(true)}$ are the true values of the data. The errors we need to take into account include

(i) **Measurement error:** Errors in the data f_k, that is, we measure f_k^δ with a *data error* $d_k^\delta := f_k^\delta - f_k^{(true)}$ of size $||d_k^\delta|| \leq \delta$. This error was discussed in Section 2 and arises through errors in the measurements and noisy data.

(ii) **Observation operator error:** Errors in the *measurement operator H*, that is, we use a measurement operator H which is different from the true mapping $H^{(true)}$ of the state φ to the data f.

(iii) **Reconstruction/approximation error:** Reconstruction errors by using the inverse $R_\alpha = (\alpha I + H^*H)^{-1}H^*$ as an approximation to the inverse H^{-1} of H. This error was discussed in Section 2.

(iv) **Model error:** The model operator which we defined in Section 1 is usually only an approximation M to the true system dynamics $M^{(true)}$. Model error arises as the dynamical model does not usually describe the system behaviour exactly. It incorporates numerical error arising from discretisation of the partial differential equations that need to be solved and includes inaccuracies in the physical parameters, forcing terms and as well as in the model itself which is usually merely a simplification of the reality.

(v) **Accumulated errors:** There will be *accumulated errors* in the background in the sense that the analysis error from the previous step leads to an error in the background of the next step in contrast to the background which would be arising from the true state $\varphi^{(true)}$.

In every analysis step of the assimilation, we obtain an error contribution by the measurement error, by the error in the observation operator H and by the regularisation operator R_α approximating the inversion of H. For the propagation step we obtain an error caused by the model M approximating the true dynamics $M^{(true)}$. Moreover the errors may accumulate over time.

Theorem 4.1. *The evolution of the analysis error $e_k := \varphi_k^{(a)} - \varphi_k^{(true)}$ for cycled Tikhonov regularisation and three-dimensional variational assimilation is given by*

$$e_{k+1} = \overbrace{(I - R_\alpha H)}^{reconstruction\ error} \overbrace{\left\{ M_k e_k + \left(M_k - M_k^{(true)} \right) \varphi_k^{(true)} \right\}}^{propagation\ of\ previous\ error\ and\ model\ error} \tag{4.1}$$

$$+ \overbrace{R_\alpha d_{k+1}^\delta}^{data\ error\ influence} + \overbrace{R_\alpha \left((H^{(true)} - H) \varphi_{k+1}^{(true)} \right)}^{observation\ operator\ error}$$

Proof. We know from Theorem 3.2 that 3DVar and Tikhonov regularisation are equivalent. We use the update formula (3.5) and the Tikhonov regularisation operator $R_\alpha := (\alpha I + H^* H)^{-1} H^*$. With (3.1) as well as

$$\varphi_{k+1}^{(true)} = M_k^{(true)} \varphi_k^{(true)} \quad \text{and} \quad f_k^{(true)} = H^{(true)} \varphi_k^{(true)},$$

and subtracting $\varphi_{k+1}^{(true)}$ from $\varphi_{k+1}^{(a)}$ we calculate

$$
\begin{aligned}
e_{k+1} \quad &:= \quad \varphi_{k+1}^{(a)} - \varphi_{k+1}^{(true)} \\
&= \quad \varphi_{k+1}^{(b)} - \varphi_{k+1}^{(true)} + R_\alpha \Big(f_{k+1} - f_{k+1}^{(true)} \Big) \\
&\qquad\qquad + R_\alpha \Big(f_{k+1}^{(true)} - H \varphi_{k+1}^{(b)} \Big) \qquad\qquad (4.2) \\
&= \quad M_k \varphi_k^{(a)} - M_k^{(true)} \varphi_k^{(true)} + R_\alpha d_{k+1}^\delta \\
&\qquad\qquad + R_\alpha \Big(H^{(true)} \varphi_{k+1}^{(true)} - H \varphi_{k+1}^{(b)} \Big) \\
&= \quad M_k \Big(\varphi_k^{(a)} - \varphi_k^{(true)} \Big) + \Big(M_k - M_k^{(true)} \Big) \varphi_k^{(true)} + R_\alpha d_{k+1}^\delta \\
&\qquad + R_\alpha \Big((H^{(true)} - H) \varphi_{k+1}^{(true)} + H \Big(\varphi_{k+1}^{(true)} - \varphi_{k+1}^{(b)} \Big) \Big). \qquad (4.3)
\end{aligned}
$$

We treat the last term in (4.3) similarly to the first term in (4.2). Then, collecting all parts, we derive (4.1). $\qquad\qquad\square$

If the model error and the error in the observation operator in Theorem 4.1 is excluded we obtain

$$e_{k+1} = R_\alpha d_{k+1}^\delta + (I - R_\alpha H) M_k e_k,$$

and, taking norms and using $||d_k^\delta|| \le \delta$, this is precisely the regularisation error arising in Tikhonov regularisation (2.7). If we select an appropriate value for α this error can be made very small.

However, in many (practical) cases the errors arising from the model and the observation operator are much bigger than the regularisation error. *Model error* in particular can be very large due to insufficient resolution and inaccuracies in the physical model dynamics. This is specifically the case for a chaotic behaviour of the system. The model error is a very important part of the total error and a very active area of current research (see, for example [52, 27, 80, 87, 14]).

We also notice that, even if there is no model error, no observation error and no data error, then $e_{k+1} = (I - R_\alpha H) M_k e_k$, and the errors can accumulate if α is chosen too large, in particular if $\|(I - R_\alpha H) M_k\| > 1$ (see also [67], [60]). Note that for any regularisation scheme condition (2.4) holds and therefore, α needs to be chosen small enough.

We have shown that within cycled data assimilation schemes various forms of errors occur and influence each other which is important to consider when applying data assimilation methods in practice.

We will see in Section 6 that cycled four-dimensional variational data assimilation can be covered by the same framework of error analysis since cycled 4DVar is a form of cycled nonlinear Tikhonov regularisation.

In the remainder of this article we assume that no model error is present, that is the model operator M_k represents the perfect model dynamics.

5 Bayesian approach to inverse problems

Probability theory provides a wide set of tools which can be used to solve inverse problems. In particular, the Bayesian theory has become quite popular as a generic approach which can be applied to inverse and ill-posed problems as well (see, for example [85, 5, 75, 12]).

Bayesian theory has the potential to provide a stochastic background for many ideas which might appear *ad-hoc* in the area of deterministic inverse problems and functional analysis. Also, Bayesian theory provides much more than just a solution to the inverse or data assimilation problem, but a full-grown theory to calculate estimates for the uncertainty as well.

However, we will see that all algorithms which can be formulated on a Bayesian background have their deterministic counterpart and, alternatively, can be studied purely within the framework of functional analysis and optimisation. In this section we apply Bayesian ideas to the observation and background errors.

Let us consider the equation

$$H(\varphi) = f, \tag{5.1}$$

as introduced in (1.1) as a starting point, where in this section we assume that $X = \mathbb{R}^n$ and $Y = \mathbb{R}^m$, $m, n \in \mathbb{N}$. The more general case with probability measures on infinite dimensional spaces can be done formally in a similar way, but involves some non-trivial technicalities.

In the stochastic framework the task of inverting equation (5.1) given some measurement f does not ask for *one* special solution. Since f is just one draw from some random distribution π_Y, any particular solution is of limited value and significance, but we want to know the *conditional probability distribution* of φ given some information about the error distribution of f. This conditional distribution can then be used either to calculate an *expectation value* for φ given f or to evaluate the *uncertainty* of this estimate measured for example by its *variance*.

We need to formulate our setup in more detail and with well-defined spaces and operators. Stochastic theory assumes that the quantity φ is a *random variable* on some probability space (Ω, Σ, P) with values in X. Here, Σ denotes some σ-algebra and P is a probability measure, which maps any subset $A \subset \Omega$ for which $A \in \Sigma$ into a number $P(A) \in [0, 1]$. $P(A)$ is the probability of the set A. We then obtain a probability P_X of the values of φ to be in some set $C \subset X$ by

$$P_X(\varphi \in C) := P(\{\omega : \varphi(\omega) \in C\}). \tag{5.2}$$

We also assume that the measurement f is a random variable with some probability distribution P_Y on Y. This probability distribution will depend on the true value $f^{(true)}$ and is our model for measurement error during the process of measuring f. Here, we assume that the probability distribution (5.2) on X has a probability density $\pi_X : X \to [0,1]$, such that

$$P_X(C) = \int_C \pi_X(\varphi)d\varphi, \tag{5.3}$$

for every open subset $C \subset X$. In the same way we assume that P_Y has a probability density π_Y on Y such that

$$P_Y(U) = \int_U \pi_Y(f)df,$$

for every open subset $U \subset Y$. Usually for simplicity we drop the letters X and Y.

Clearly, since the conditional probability of some event $C \subset X$ given some event $\tilde{C} \subset X$ is defined by $P(C|\tilde{C}) := P(C \cap \tilde{C})/P(\tilde{C})$ we have that the conditional probability of event C given U is

$$P(C|U) = \frac{P(\{\omega : \varphi(\omega) \in C \text{ and } f(\omega) \in U\})}{P(\{\omega : f(\omega) \in U\})},$$

where $P(\{\omega : f(\omega) \in U\}) > 0$. In terms of the *probability density functions* (PDFs) conditional probability is formulated by

$$\pi(\varphi|f) = \frac{\pi(\varphi, f)}{\pi(f)}, \tag{5.4}$$

where $\pi(\varphi, f)$ is the joint probability density of φ and f living on the space $X \times Y$ and $\pi(f) \neq 0$ is the probability density of f in X. Equation (5.4) also holds with the role of φ and f exchanged, i.e. we have

$$\pi(f|\varphi) = \frac{\pi(\varphi, f)}{\pi(\varphi)}, \tag{5.5}$$

assuming that $\pi(\varphi) \neq 0$. Now, from equations (5.4) and (5.5) we get the famous *Bayes' formula* for conditional probability densities,

$$\pi(\varphi|f) = \frac{\pi(\varphi)\pi(f|\varphi)}{\pi(f)}. \tag{5.6}$$

Note that the value of $\pi(f)$ can be obtained by the knowledge that the integral of $\pi(\varphi|f)$ over the whole space X should be equal to one, i.e. it is not necessary to know $\pi(f)$ (it is merely a normalising constant).

Bayes' formula now provides a 'simple' solution to the stochastic inverse problem of inverting equation (5.1). Given a probability density $\pi(\varphi)$ on X and some error

density π on Y which can be used to calculate the density of the data distribution (often called the "measurement model" in statistics),

$$\pi(f|\varphi) = \pi(f - H(\varphi)). \tag{5.7}$$

We employ (5.6) to calculate the conditional probability density function $\pi(\varphi|f)$. This probability density is also known as *posterior density* or *analysis density function*. It is the density of the unobservable $\varphi \in X$ given the data $f \in Y$, that is, the probability of observing the data f as a function of φ. The density function $\pi(\varphi)$ on X is denoted as *prior* density. The posterior density is considered as the solution to the inverse problem.

Remark 5.1. Note that Bayes' formula seems to provide a very easy and stable approach to solving the inverse problem. The calculation of the posterior density $\pi(\varphi|f)$ is obtained by a *multiplication* of two given distributions $\pi(\varphi)$ and $\pi(f - H(\varphi))$. But the calculation of the mean of the posterior distribution involves the solution of an ill-posed equation. In general, the full ill-posedness of the task is implicitly involved in Bayes' data assimilation as it is in all other schemes as well.

We can now formulate a general approach to data assimilation based on Bayes' formula.

Definition 5.2 (Bayes' data assimilation). Bayes' data assimilation determines probability density functions $\pi_k^{(a)}$ at time t_k for the states $\varphi \in X$ given data $f_k \in Y$ at time t_k by cycling the following propagation and analysis steps:

(i) **Propagation Step.** Calculate the prior density $\pi_k^{(b)}(\varphi)$ at time t_k by propagating the analysis density $\pi_{k-1}^{(a)}$ from time t_{k-1} to t_k based on the (linear or nonlinear) model dynamics M_{k-1}.

(ii) **Analysis Step.** Calculate the posterior or *analysis density* $\pi_k^{(a)}(\varphi|f_k)$ at time t_k by Bayes' formula (5.6) using the measurement model (5.7).

An important special case of Bayes' formula is the setup where all densities are *normal* or *Gaussian* distributions. For the prior distribution we assume that it is a multivariate Gaussian distribution, that is, the probability density function is given by

$$\pi(\varphi) = \frac{1}{\sqrt{(2\pi)^n \det(B)}} e^{-\frac{1}{2}(\varphi-\mu)^T B^{-1}(\varphi-\mu)}, \quad \varphi \in \mathbb{R}^n, \tag{5.8}$$

around some state $\mu := \varphi^{(b)} \in X = \mathbb{R}^n$ with some symmetric positive define matrix B. Gaussian densities are completely determined by their mean value $\mu = \mathbb{E}(\varphi) \in \mathbb{R}^n$ and the matrix B, which is well-known to be the covariance matrix,

$$B = \mathbb{E}((\varphi - \mu)(\varphi - \mu)^T), \tag{5.9}$$

of the Gaussian distribution (5.8). We write $\varphi \sim \mathcal{N}(\mu, B)$. The normalisation is based on the integral formula

$$\int_{\mathbb{R}^n} e^{-\frac{1}{2}\varphi^T B^{-1}\varphi} d\varphi = \sqrt{\frac{(2\pi)^n}{\det(B^{-1})}} = \sqrt{(2\pi)^n \det(B)}.$$

Let us study the case where also the probability density $\pi(f|\varphi)$ of the measurements f is given by a Gaussian distribution with probability density function

$$\pi(f|\varphi) = \frac{1}{\sqrt{(2\pi)^m \det(R)}} e^{-\frac{1}{2}(f-H(\varphi))^T R^{-1}(f-H(\varphi))}, \quad f \in \mathbb{R}^m, \qquad (5.10)$$

around the values $H(\varphi) \in Y = \mathbb{R}^m$ with the symmetric positive definite covariance matrix $R \in \mathbb{R}^{m \times m}$ of the observation error. Then, according to Bayes' formula (5.6) we obtain

$$\pi(\varphi|f) \propto \exp\left\{ -\frac{1}{2}\Big((\varphi-\mu)^T B^{-1}(\varphi-\mu) + (f-H(\varphi))^T R^{-1}(f-H(\varphi)) \Big) \right\}$$

for the probability density function of the posterior distribution. If H is *linear*, this is again a normal distribution with probability density

$$\pi(\varphi|f) \propto \exp\left\{ -\frac{1}{2}(\varphi-\tilde{\mu})^T \tilde{B}^{-1}(\varphi-\tilde{\mu}) \right\}.$$

Using $\mu = \varphi^{(b)}$, its mean $\tilde{\mu}$ is given by

$$\tilde{\mu} = \varphi^{(b)} + BH^*(R+HBH^*)^{-1}(f-H\varphi^{(b)}) = \varphi^{(b)} + K(f-H\varphi^{(b)}), \quad (5.11)$$

and its covariance matrix $\tilde{B}$ is given by

$$\tilde{B} = (B^{-1} + H^* R^{-1} H)^{-1} = (I - KH)B, \qquad (5.12)$$

where $K = BH^*(R+HBH^*)^{-1}$ is called the (Kalman) gain. The proof of (5.11) and (5.12) will be worked out in detail in Section 7 on the Kalman filter, see equations (7.6) and (7.8). The equivalence of the two different expressions in (5.12) can also be obtained via the Sherman-Morrison-Woodbury formula (see, for example [31]), here it is worked out elementarily in Lemma 7.3. We summarise the above arguments in the following theorem.

Theorem 5.3 (Bayes' data assimilation for Gaussian probability densities). *In the case of a linear observation operator H assume that the prior distribution is Gaussian with probability density function $\pi(\varphi)$ and the same is true for the distribution of the measurements with probability density function $\pi(f|\varphi)$ as given in (5.10). Then the posterior distribution with density function $\pi(\varphi|f)$ is Gaussian as well. Its mean is calculated by the update formula (5.11), its covariance matrix is given by (5.12).*

Note that the update formula (5.11) for the mean of the posterior Gaussian distribution is the same as for the update vector (or reconstruction) $\varphi_k^{(a)}$ obtained from (cycled) Tikhonov regularisation (3.11), which is equivalent to 3DVar. In this respect we see that Bayes' data assimilation gives more information by calculating a whole probability distribution of a state estimate whereas Tikhonov regularisation/3DVar only provides the mean of the estimate.

Further, when the dynamics M of a dynamical system is *linear*, then it maps a Gaussian distribution into a Gaussian distribution. The covariance matrix B in (5.11) and (5.12) needs to be replaced by its transported version $B^{(b)}$ calculated from the matrix B at the previous assimilation step by $B^{(b)} := MBM^*$. The propagation $B^{(b)}$ arises from the definition of the covariance matrix (5.9) and the linearity of the expected value. In this case we can formulate the full cycling of the Bayesian approach explicitly.

Definition 5.4 (Gaussian Bayes' data assimilation for linear systems). For linear dynamical systems M_k and linear observation operators H_k we start with some prior distribution with probability density function $\pi_0^{(a)}(\varphi)$ given by its mean $\varphi_0^{(a)}$ and its covariance matrix $B_0^{(a)}$. Then, for $k = 1, 2, 3, ...$ we carry out Bayes' data assimilation by cycling the following propagation and analysis steps.

(i) **Propagation Step.** Calculate the mean state $\varphi_k^{(b)}$ and the covariance matrix $B_k^{(b)}$ of the prior density $\pi_k^{(b)}(\varphi)$ at time t_k by

$$\varphi_k^{(b)} = M_{k-1}\varphi_{k-1}^{(a)}, \quad B_k^{(b)} := M_{k-1}B_{k-1}^{(a)}M_{k-1}^*. \tag{5.13}$$

(ii) **Analysis Step.** Calculate the Gaussian posterior or *analysis density* $\pi_k^{(a)}(\varphi|f_k)$ at time t_k by its mean and covariance

$$\varphi_k^{(a)} \quad := \quad \varphi_k^{(b)} + B_k^{(b)}H_k^*(R + H_k B_k^{(b)} H_k^*)^{-1}(f_k - H_k\varphi_k^{(b)}), \tag{5.14}$$

$$(B_k^{(a)})^{-1} \quad := \quad (B_k^{(b)})^{-1} + H_k^* R^{-1} H_k. \tag{5.15}$$

The above calculations treat the case of linear systems. Of course, Bayes' formula also works for nonlinear dynamics and nonlinear observation operators, for which the numerics is much more difficult to carry out efficiently. A numerical method to approximately calculate the densities by *ensemble approaches* will be introduced in Section 8.

6 4DVar

A natural approach to the solution of a time-dependent state estimation problem is to put all available measurements into one big minimisation problem. Given measure-

ments $f_{k+1}, ..., f_{k+K} \in Y$ this leads to

$$J_k(\varphi) := ||\varphi - \varphi_k^{(b)}||_X^2 + \sum_{j=1}^{K} ||f_{k+j} - HM_{k+j,k}(\varphi)||_Y^2, \qquad (6.1)$$

where $M_{k+j,k}$ is defined in (1.2) and for simplicity we use a fixed (possibly nonlinear) observation operator H. Similar to the approach in Section 1 we can rewrite the problem (6.1) in a 3DVar type form like (3.2) by putting all the measurements $f_{k+1}, ..., f_{k+K}$ into one long vector and removing the sum and defining a new (possibly nonlinear) operator $\bar{H}_k$, that is,

$$J_k(\varphi) := ||\varphi - \varphi_k^{(b)}||_X^2 + ||\bar{f}_k - \bar{H}_k(\varphi)||_Y^2,$$

where

$$\bar{f}_k = \begin{bmatrix} f_{k+1} \\ f_{k+2} \\ \vdots \\ f_{k+K} \end{bmatrix} \quad \text{and} \quad \bar{H}_k = \begin{bmatrix} HM_{k+1,k} \\ HM_{k+2,k} \\ \vdots \\ HM_{k+K,k} \end{bmatrix}.$$

The minimisation of (6.1) corresponds to the fit of the full dynamic trajectory of the states to the given measurements f_{k+j}, $j = 1, \ldots, K$ over the time window between t_k and t_{k+K}. As in Section 3 we can transform the functional (6.1) into a (generally nonlinear) Tikhonov functional of the form (2.3), see, for example [45, 28]. Note that sometimes the observation f_k at time step t_k is included in the sum (here, in the functional (6.1) it is not included).

Denote the minimum of (6.1) by $\varphi_k^{(a)}$. A cycling of the assimilation is then obtained by using a new background at time t_{k+K} defined by

$$\varphi_{k+K}^{(b)} := M_{k+K,k}(\varphi_k^{(a)}), \qquad (6.2)$$

for $k = 0, K, 2K, 3K, \ldots$. The process of minimising the functional (6.1) and using the minimising ϕ as initial condition for the forecast is known as four-dimensional variational data assimilation (4DVar) [51, 50, 72, 19, 6]. The repeated minimisation of (6.1) combined with (6.2) is then a cycled 4DVar scheme. As we can write 4DVar in the form of 3DVar this is merely a form of (nonlinear) cycled Tikhonov regularisation as shown in Section 3.

Usually, the minimisation of (6.1) is carried out by a *gradient method*, that is, we calculate the gradient $\nabla_\varphi J_k(\varphi)|_{\varphi^{(\ell)}}$ at points $\varphi^{(\ell)}$ in the state space and update

$$\varphi^{(\ell+1)} := \varphi^{(\ell)} - h\nabla_\varphi J_k(\varphi)|_{\varphi^{(\ell)}} \qquad (6.3)$$

with some appropriately chosen step size $h > 0$ and starting guess $\varphi^{(0)}$ (often $\varphi^{(0)} := \varphi_k^{(b)}$ is used).

For simplicity we consider the case where $X = \mathbb{R}^n$ and $Y = \mathbb{R}^m$ and the scalar products are the l^2 scalar products. Let us study terms of the form

$$g(\varphi) := ||f - HM\varphi||_Y^2, \tag{6.4}$$

with $f \in Y$ and some linear operator $M : X \to X$. The gradient of $g(\varphi)$ with respect to φ is given by

$$\nabla_\varphi g(\varphi) \;\; = \;\; -2\Big(M^* H^* (f - HM\varphi)\Big). \tag{6.5}$$

If M is a nonlinear operator, then we obtain the nonlinear version

$$\nabla_\varphi g(\varphi) = -2\Big(\big(\frac{dM(\varphi)}{d\varphi}\big)^* H^* (f - HM(\varphi))\Big) \tag{6.6}$$

of (6.5), where $dM(\varphi)/d\varphi$ denotes the Fréchet derivative of $M(\varphi)$ with respect to φ. The derivative

$$\mathbf{M}(\varphi) := \frac{dM(\varphi)}{d\varphi} \tag{6.7}$$

is also known as the *tangent linear* model [26, 50].

For many applications, the dynamical model is given as a system of ordinary differential equations in the form

$$\dot{\varphi} = F(\varphi), \;\; \varphi(0) = \varphi_0. \tag{6.8}$$

Since the model dynamics is given by $\varphi(t) = M_{t,0}(\varphi(0)) = M_{t,0}(\varphi_0)$, this means that

$$F(\varphi) = \frac{d}{dt} M_{t,0}(\varphi_0). \tag{6.9}$$

We denote the derivative with respect to the initial state φ_0 by

$$\varphi'(t) := \frac{d\varphi}{d\varphi_0}. \tag{6.10}$$

Note that φ' is a linear mapping from X into X; when $X = \mathbb{R}^n$ it is the $n \times n$-matrix with elements $\partial\varphi_j/\partial\varphi_{0,i}$ for $i, j = 1, ..., n$.

We assume that the solution $\varphi = \varphi(t)$ is continuously differentiable with respect to the initial state φ_0 as well as with respect to the time t. In this case we can exchange the differentiation with respect to time t and the initial state φ_0 and, differentiating (6.8) with respect to φ_0, we obtain

$$\frac{d\dot{\varphi}}{d\varphi_0} = \frac{d}{d\varphi_0} \frac{d}{dt} M_{t,0}(\varphi_0) = \frac{d}{dt} \frac{d}{d\varphi_0} M_{t,0}(\varphi_0) = \frac{d}{dt} \varphi'(t). \tag{6.11}$$

This means that the time evolution of the derivative φ' is given by

$$\frac{d}{dt}\varphi'(t) = \frac{d}{d\varphi_0}F(\varphi(t)) = F'(\varphi(t))\frac{d\varphi(t)}{d\varphi_0}. \tag{6.12}$$

At time $t = 0$ this is equal to $F'(\varphi_0) = dF(\varphi)/d\varphi_0|_{\varphi=\varphi_0}$, that is,

$$\frac{d}{dt}\varphi'(t)|_{t=0} = F'(\varphi_0). \tag{6.13}$$

This means that the tangent linear model φ' can be calculated by solving the system

$$\frac{d}{dt}\varphi'(t) = F'(\varphi(t))\varphi'(t), \quad t \geq 0 \tag{6.14}$$

of ordinary differential equations with initial condition $\varphi'(0) = I$ and with the solution φ of the original system of equations (6.8). Using $\varphi(t) = M_{t,0}(\varphi_0)$ and $\varphi'(t) = dM_{t,0}(\varphi_0)/d\varphi_0$ as well as (6.7) we obtain

$$\varphi'(t) = \frac{dM_{t,0}(\varphi_0)}{d\varphi_0} =: \mathbf{M}_{t,0}(\varphi_0)$$

for the tangent linear model.

We remark that the tangent linear adjoint is an $n \times n$ matrix, which might be huge when n is large. Thus, efficient methods for its evaluation need to be set-up. To evaluate the adjoint in (6.5), we define a function $\psi(t) \in X$ on the interval $[t_{k+1}, t_k]$ by

$$\dot{\psi} = -F'(\varphi(t))^*\psi(t), \tag{6.15}$$

with *final condition*

$$\psi(t_{k+1}) = H^*(f_{k+1} - HM(\varphi_k)). \tag{6.16}$$

Lemma 6.1. *For $t \in [t_k, t_{k+1}]$, the inner product*

$$h(t) := \Big\langle \varphi'(t)(\delta\varphi_0), \psi(t) \Big\rangle$$

is constant over time for any $\delta\varphi_0 \in X$.

Proof. We differentiate $h(t)$ with respect to t and calculate

$$
\begin{aligned}
\frac{dh(t)}{dt} &= \frac{d}{dt}\Big\langle \varphi'(t)(\delta\varphi_0), \psi(t) \Big\rangle \tag{6.17}\\
&= \Big\langle \frac{d}{dt}\varphi'(t)(\delta\varphi_0), \psi(t) \Big\rangle + \Big\langle \varphi'(t)(\delta\varphi_0), \frac{d}{dt}\psi(t) \Big\rangle\\
&= \Big\langle F'(\varphi(t))\varphi'(t)(\delta\varphi_0), \psi(t) \Big\rangle + \Big\langle \varphi'(t)(\delta\varphi_0), -F'(\varphi(t))^*\psi(t) \Big\rangle\\
&= \Big\langle \varphi'(t)(\delta\varphi_0), F'(\varphi(t))^*\psi(t) \Big\rangle - \Big\langle \varphi'(t)(\delta\varphi_0), F'(\varphi(t))^*\psi(t) \Big\rangle\\
&= 0,
\end{aligned}
$$

where we have used (6.14) and (6.15). Since the derivative of $h(t)$ is zero by (6.17), we obtain the statement of the lemma. □

Let e_j, $j = 1, ..., n$ be the canonical basis of $\mathbb{R}^n$. We can now calculate the gradient ∇g of (6.5) by

$$
\begin{aligned}
\nabla g_j(\varphi_k) &= -2\Big\langle \varphi'(t_{k+1})e_j, H^*(f_{k+1} - HM(\varphi_k)) \Big\rangle \\
&= -2\Big\langle \varphi'(t_{k+1})e_j, \psi(t_{k+1}) \Big\rangle \\
&= -2\Big\langle \varphi'(t_k)e_j, \psi(t_k) \Big\rangle \\
&= -2\Big\langle e_j, \psi(t_k) \Big\rangle = -2\psi(t_k)_j \quad\quad (6.18)
\end{aligned}
$$

for $j = 1, ..., n$. Thus, the gradient is calculated by propagating the field forward in time by (6.8), then propagating the observation error back by (6.15), (6.16) and calculating the gradient using (6.18).

In general we consider the time step t_k as the initial time step or, subsequently, the intermediate time step, so that (6.8) becomes

$$
\dot{\varphi} = F(\varphi), \quad \varphi(0) = \varphi_k, \quad \text{where} \quad \varphi_k := \varphi(t_k), \quad\quad (6.19)
$$

and the derivative $'$ with respect to the initial state φ_k is given by $\varphi'(t) := \frac{d\varphi}{d\varphi_k}$. Hence, discretising (6.19) using, for example, a simple finite difference between time steps t_k and t_{k+1} leads to

$$
\frac{\varphi_{k+1} - \varphi_k}{\Delta t} = F(\varphi_k), \qu\quad\quad (6.20)
$$

and therefore the discretised model operator M_k from time step t_k to time step t_{k+1} is given by

$$
\varphi_{k+1} = \varphi_k + \Delta t F(\varphi_k) = M_k(\varphi_k) = M_{k+1,k}(\varphi_k).
$$

Moreover discretising (6.14) leads to

$$
\frac{\varphi'_{k+1} - \varphi'_k}{\Delta t} = F'(\varphi_k). \qu\quad\quad (6.21)
$$

Hence, using $\varphi'_k = d\varphi'_k/d\varphi'_k = I$ the (discretised) tangent linear model is given by

$$
\varphi'_{k+1} = I + \Delta t F'(\varphi_k) = \mathbf{M}_k(\varphi_k) = \mathbf{M}_{k+1,k}(\varphi_k) := \frac{dM_k}{d\varphi}\Big|_{\varphi_k} = \frac{dM_{k+1,k}}{d\varphi}\Big|_{\varphi_k},
$$

which can also be obtained by differentiating (6.20) with respect to φ_k. Note, that we can similarly find the (nonlinear) operators $M_{k+j,k}$ and their tangent linear models $\mathbf{M}_{k+j,k}(\varphi_k) := \frac{dM_{k+j,k}}{d\varphi}\Big|_{\varphi_k}$ for any $j = 1, \ldots, K$, and, by the chain rule applied to (1.2) it follows that

$$
\mathbf{M}_{k+j,k}(\varphi_k) = \mathbf{M}_{k+j,k+j-1} \cdots \mathbf{M}_{k+2,k+1}\mathbf{M}_{k+1,k}(\varphi_k).
$$

Studying the case $X = \mathbb{R}^n$ and $Y = \mathbb{R}^m$ and using the weighted scalar product (3.6) and (3.7) we may compute the gradient $\nabla_\varphi J_k(\varphi)$ of the full functional $J_k(\varphi)$ given in (6.1) by

$$\nabla_\varphi J_k(\varphi) := 2B^{-1}(\varphi - \varphi_k^{(b)}) - 2\sum_{j=1}^{K} (\mathbf{M}_{k+j,k}(\varphi)^* H^* R^{-1}(f_{k+j} - HM_{k+j,k}(\varphi)).$$

(6.22)

A gradient method like (6.3) can then be used to obtain a local minimiser for the functional $J_k(\varphi)$ in (6.1). Another method which may be used to find a local minimum of $J_k(\varphi)$ in (6.1) is the Gauß-Newton method [21]. We solve $\nabla_\varphi J_k(\varphi) = 0$ in order to find the minimum of (6.1) using Newton's method, that is,

$$\varphi^{(\ell+1)} := \varphi^{(\ell)} - \left(\nabla\nabla_\varphi J_k(\varphi)|_{\varphi^{(\ell)}}\right)^{-1} \nabla_\varphi J_k(\varphi)|_{\varphi^{(\ell)}},$$

with some starting guess $\varphi^{(0)}$, where $\nabla\nabla_\varphi J_k(\varphi)|_{\varphi^{(\ell)}}$ is the Jacobian of $\nabla_\varphi J_k(\varphi)$ at $\varphi^{(\ell)}$, that is, the Hessian. Usually the starting guess $\varphi^{(0)} = \varphi_k^{(b)}$ is taken. Often instead of the correct Hessian $\nabla\nabla_\varphi J_k(\varphi)|_{\varphi^{(\ell)}}$, an approximate version is used, neglecting terms involving the gradient of the tangent linear model, thereby leading to a quasi-Newton method. The gradient method usually only gives linear convergence. The Gauß-Newton method with approximate Hessian converges superlinearly for well-posed problems and a sufficiently close starting guess. For linear observation operators H and linear model dynamics M_k the Newton and Gauß-Newton method are the same and any local minimiser of (6.1) is clearly also a global minimiser (see, for example [32]) and the convergence speed to the global minimum is quadratic.

7 Kalman filter and Kalman smoother

The Kalman filter is a method to solve the data assimilation problem (1.3) similarly to the cycled Tikhonov regularisation, 3DVar or 4DVar. But in addition to calculating an analysis in every step, it also iteratively updates the norm of the state space to include the knowledge from previous assimilation cycles.

We can introduce the Kalman filter using deterministic and stochastic arguments. Here, we will start with a deterministic approach, which also proves equivalence of the Kalman filter and Kalman smoother to the four-dimensional variational data assimilation for linear model dynamics $M_k : X \to X$ and linear observation operators $H : X \to Y$. Then, we discuss a stochastic approach to the Kalman filter.

Let us study assimilation for a *linear* model dynamics M_k, a linear observation operator H and measurements f_1 and f_2 at times t_1 and t_2. Then, four-dimensional variational data assimilation with weighted norms as in Section 3 minimises the functional (see (6.1))

$$J_{4DVar}(\varphi) := ||\varphi - \varphi_0^{(b)}||^2_{B^{-1}} + ||f_1 - HM_0\varphi||^2_{R^{-1}} + ||f_2 - HM_1M_0\varphi||^2_{R^{-1}}, \quad (7.1)$$

with $B \in \mathbb{R}^{n \times n}$ and $R \in \mathbb{R}^{m \times m}$. Alternatively, we study the assimilation of the data f_1 in a first step by minimisation of

$$J_1(\varphi) := ||\varphi - \varphi_0^{(b)}||_{B^{-1}}^2 + ||f_1 - HM_0\varphi||_{R^{-1}}^2, \qquad (7.2)$$

with minimiser $\tilde{\varphi}^{(a)}$ and the assimilation of f_2 in a *second step* by minimising

$$J_2(\varphi) := ||\varphi - \tilde{\varphi}^{(a)}||_{\tilde{B}^{-1}}^2 + ||f_2 - HM_1M_0\varphi||_{R^{-1}}^2, \qquad (7.3)$$

with a weight matrix $\tilde{B}$. The key question here is to determine the new weight $\tilde{B}$ such that the minimiser of J_2 is equal to the minimiser of the full functional J_{4DVar} in (7.1). This is the case if we can choose $\tilde{B}$ such that $J_2(\varphi) = J_{4DVar}(\varphi) + c$ with some constant c, where J_1 is implicitly used via $\tilde{\varphi}^{(a)}$ in (7.3). The problem is solved if we can determine $\tilde{\varphi}^{(a)}$ and $\tilde{B}$ such that J_1 and the first term of J_2 are identical. Starting with J_1 we obtain

$$
\begin{aligned}
J_1(\varphi) &= \left\langle \varphi - \varphi_0^{(b)}, B^{-1}(\varphi - \varphi_0^{(b)}) \right\rangle \\
&\quad + \left\langle f_1 - HM_0\varphi, R^{-1}(f_1 - HM_0\varphi) \right\rangle \\
&= \left\langle \varphi, (B^{-1} + M_0^*H^*R^{-1}HM_0)\varphi \right\rangle \qquad (7.4) \\
&\quad - 2\left\langle \varphi, B^{-1}\varphi_0^{(b)} + M_0^*H^*R^{-1}f_1 \right\rangle + c,
\end{aligned}
$$

with some constant c independent of φ. The first term of J_2 is given by

$$||\varphi - \tilde{\varphi}^{(a)}||_{\tilde{B}^{-1}}^2 = \left\langle \varphi, \tilde{B}^{-1}\varphi \right\rangle - 2\left\langle \varphi, \tilde{B}^{-1}\tilde{\varphi}^{(a)} \right\rangle + \tilde{c}, \qquad (7.5)$$

with some constant $\tilde{c}$ not depending on φ. A comparison of the coefficients of the quadratic and linear terms in (7.4) and (7.5) immediately shows that with

$$\tilde{B}^{-1} := B^{-1} + M_0^*H^*R^{-1}HM_0 \qquad (7.6)$$

and

$$\tilde{B}^{-1}\tilde{\varphi}^{(a)} := B^{-1}\varphi_0^{(b)} + M_0^*H^*, R^{-1}f_1 \qquad (7.7)$$

the functional J_1 given by (7.4) and the first term of the functional J_2 given by (7.5) are the same up to some constant not depending on φ. Finally, from (7.7) using (7.6) we derive

$$
\begin{aligned}
\tilde{\varphi}^{(a)} &= \tilde{B}\left(B^{-1}\varphi_0^{(b)} + M_0^*H^*R^{-1}f_1\right) \\
&= (I + BM_0^*H^*R^{-1}HM_0)^{-1}\left(\varphi_0^{(b)} + BM_0^*H^*R^{-1}f_1\right). \qquad (7.8)
\end{aligned}
$$

After some algebraic manipulations inserting

$$I = (I + BM_0^*H^*R^{-1}HM_0) - BM_0^*H^*R^{-1}HM_0$$

we obtain

$$
\begin{aligned}
\tilde{\varphi}^{(a)} &= \varphi_0^{(b)} + (I + BM_0^*H^*R^{-1}HM_0)^{-1}BM_0^*H^*R^{-1}(f_1 - HM_0\varphi_0^{(b)}) \\
&= \varphi_0^{(b)} + BM_0^*H^*(R + HM_0BM_0^*H^*)^{-1}\left(f_1 - HM_0\varphi_0^{(b)}\right),
\end{aligned}
$$

which is the minimiser of J_1 as in (3.9) or (3.11) when the propagation M_0 from φ_0 at time t_0 to φ_1 at time t_1, that is, $\varphi_1 = M_0\varphi_0$ is used. The above approach can be carried out successively for the measurements f_1, f_2, f_3 etc. This sequential approach leads to the Kalman smoother (see, for example, [59, 53, 27]). We will see later in Theorem 7.5 that the Kalman smoother is equivalent to the Kalman filter at the final time.

Definition 7.1 (Kalman smoother (KS)). Let $H_k : X \rightarrow Y$ and $M_k : X \rightarrow X$, $k = 0, 1, 2, ...$ given in Definition 1.1 be linear and assume that measurements $f_1, f_2, ...$ at times $t_1, t_2, ...$ are given. Then, we calculate weight matrices

$$
\tilde{B}_k^{-1} := \tilde{B}_{k-1}^{-1} + M_{k,0}^*H_k^*R^{-1}H_kM_{k,0}, \quad k = 1, 2, ..., \tag{7.9}
$$

with $\tilde{B}_0 := B$, where $M_{k,0}$ is defined in (1.2), and analysis states $\tilde{\varphi}_k^{(a)}$ at time t_k defined by

$$
\begin{aligned}
\tilde{\varphi}_k^{(a)} &:= \tilde{\varphi}_{k-1}^{(a)} \tag{7.10} \\
&\quad + \tilde{B}_{k-1}M_{k,0}^*H_k^*(R + H_kM_{k,0}\tilde{B}_{k-1}M_{k,0}^*H_k^*)^{-1}\left(f_k - H_kM_{k,0}\tilde{\varphi}_{k-1}^{(a)}\right)
\end{aligned}
$$

for $k = 1, 2, ...$ with $\tilde{\varphi}_0^{(a)} := \varphi_0^{(b)}$.

From our derivation it is clear that the following theorem holds.

Theorem 7.2 (Equivalence of 4DVar and Kalman smoother). *Let H_k and M_k for $k = 0, 1, 2, ...$ be linear operators and data $f_1, f_2, ...$ be given. Then, 4DVar carried out with data $f_1, ..., f_k$ is equivalent to the Kalman smoother given in Definition 7.1 in the sense that the minimum of the 4DVar functional (6.1) is given by the analysis $\tilde{\varphi}_k^{(a)}$ for $k = 1, 2, ..., K$ according to (7.10).*

Proof. The proof for $k = 1$ is given in equations (7.1) to (7.8). The general case is directly obtained by iterating the arguments. $\square$

In Definition 7.1 we worked with states at time t_0. Usually, the states of the Kalman filter are calculated at times t_1, t_2 etc. We need to propagate the states $\tilde{\varphi}_k^{(a)}$ from time t_0 to t_k by

$$
\varphi_k^{(b)} = M_{k,0}\tilde{\varphi}_{k-1}^{(a)}, \quad \text{and} \quad \varphi_k^{(a)} = M_{k,0}\tilde{\varphi}_k^{(a)}, \tag{7.11}
$$

for $k = 1, 2, 3, ...$, which means that

$$
\varphi_k^{(b)} = M_{k-1}(\varphi_{k-1}^{(a)}) \tag{7.12}
$$

propagates the state from t_{k-1} to t_k (see also (3.1)). The matrices $\tilde{B}$ are propagated from t_0 to t_k by

$$B_k^{(b)} = M_{k,0}\tilde{B}_{k-1}M_{k,0}^*, \quad \text{and} \quad B_k^{(a)} = M_{k,0}\tilde{B}_k M_{k,0}^*, \tag{7.13}$$

for $k = 1, 2, 3, ...$, where the *background matrix* at time t_k is obtained by propagating the *analysis matrix* from time t_{k-1} to t_k by

$$B_k^{(b)} = M_{k-1}B_{k-1}^{(a)}M_{k-1}^*. \tag{7.14}$$

Note that the propagation of the state (7.12) and the propagation of the weight matrix (7.14) are equivalent to the propagation step in Bayes' data assimilation for Gaussian probability densities and linear systems, see (5.13).

Using (7.11) and (7.13) the iterative version of (7.10) is then given by

$$\varphi_k^{(a)} = \varphi_k^{(b)} + B_k^{(b)}H_k^*(R + H_k B_k^{(b)}H_k^*)^{-1}(f_k - H_k\varphi_k^{(b)}) \tag{7.15}$$

for $k \in \mathbb{N}$, often written in the form

$$\varphi_k^{(a)} = \varphi_k^{(b)} + K_k(f_k - H_k\varphi_k^{(b)}) \tag{7.16}$$

with the *Kalman gain matrix*

$$K_k := B_k^{(b)}H_k^*(R + H_k B_k^{(b)}H_k^*)^{-1}. \tag{7.17}$$

Note that the Kalman gain matrix is identical to the Tikhonov regularisation matrix (3.11). Using (7.14) and (7.9) we readily verify that the analysis matrix $B_k^{(a)}$ at time t_k is obtained from the *background matrix* $B_k^{(b)}$ at time t_k by

$$(B_k^{(a)})^{-1} = (B_k^{(b)})^{-1} + H_k^*R^{-1}H_k, \tag{7.18}$$

for $k \in \mathbb{N}$. Note that the analysis matrix $B_k^{(a)}$ in (7.18) and the analysis state $\varphi_k^{(a)}$ in (7.15) is equivalent to the updated covariance matrix and the updated state in the analysis step in Bayes' data assimilation for Gaussian probability densities and linear systems, see (5.14 and 5.15)).

Often, another version of (7.18) is used, where the matrices appear without their inverse (see also (5.12)).

Lemma 7.3. *For $k \in N$ and $B_k^{(a)}$ in (7.18) we have*

$$B_k^{(a)} = (I - K_k H_k)B_k^{(b)}, \tag{7.19}$$

where K_k is given by (7.17).

Proof. We start from (7.18) in the form

$$B_k^{(a)} = \left(I + B_k^{(b)} H_k^* R^{-1} H_k\right)^{-1} B_k^{(b)}. \tag{7.20}$$

We expand

$$
\begin{aligned}
T &:= \left(I + B_k^{(b)} H_k^* R^{-1} H_k\right)(I - K_k H_k) \\
&= \left(I + B_k^{(b)} H_k^* R^{-1} H_k\right)\left(I - B_k^{(b)} H_k^*(R + H_k B_k^{(b)} H_k^*)^{-1} H_k\right) \\
&= I + \underbrace{B_k^{(b)} H_k^* R^{-1} H_k}_{=:S} - \underbrace{B_k^{(b)} H_k^*(R + H_k B_k^{(b)} H_k^*)^{-1} H_k}_{=:S_1} \\
&\quad - \underbrace{B_k^{(b)} H_k^* R^{-1} H_k B_k^{(b)} H_k^*(R + H_k B_k^{(b)} H_k^*)^{-1} H_k}_{:=S_2}. \tag{7.21}
\end{aligned}
$$

and remark that

$$S = B_k^{(b)} H_k^* R^{-1}(R + H_k B_k^{(b)} H_k^*)(R + H_k B_k^{(b)} H_k^*)^{-1} H_k = S_1 + S_2,$$

which yields $T = I$. Thus

$$\left(I + B_k^{(b)} H_k^* R^{-1} H_k\right)^{-1} = (I - K_k H_k)$$

and the proof is complete. □

We are now ready to define the Kalman filter (see, for example [2, 53, 39]).

Definition 7.4 (Kalman filter). Starting with an initial state $\varphi_0^{(b)}$ and an initial weight matrix $B_0^{(a)} := B$, for $k \in \mathbb{N}$ the Kalman filter iteratively calculates an analysis $\varphi_k^{(a)}$ at time t_k for $k = 1, 2, \ldots$ by

(i) propagating the state $\varphi_{k-1}^{(a)}$ from t_{k-1} to t_k via (7.12):

$$\varphi_k^{(b)} = M_{k-1}(\varphi_{k-1}^{(a)}),$$

(ii) propagating $B_{k-1}^{(a)}$ from t_{k-1} to t_k following (7.14):

$$B_k^{(b)} = M_{k-1} B_{k-1}^{(a)} M_{k-1}^*,$$

(iii) calculate the Kalman gain by (7.17):

$$K_k = B_k^{(b)} H_k^*(R + H_k B_k^{(b)} H_k^*)^{-1},$$

(iv) calculating an analysis state by (7.15):

$$\varphi_k^{(a)} = \varphi_k^{(b)} + K_k(f_k - H_k\varphi_k^{(b)}),$$

(v) calculating an analysis weight by (7.19):

$$B_k^{(a)} = (I - K_kH_k)B_k^{(b)}.$$

The first two steps of the Kalman filter are often referred to as the *predictor steps* as they predict a state and a covariance estimate by propagating them forward via the model dynamics. The last two steps are called analysis steps to update the state and covariance estimate.

The relationship between the Kalman filter, the Kalman smoother and 4DVar is summarised in the following theorem.

Theorem 7.5 (Equivalence of 4DVar, Kalman filter and Kalman smoother). *Let the operators $H_k : X \to Y$ for $k \in \mathbb{N}$ and $M_k : X \to X$ for $k \in \mathbb{N}_0$ be linear. Let $\varphi_k^{(a)}$ be the analysis of the Kalman filter at time t_k, $\tilde{\varphi}_k^{(a)}$ the analysis of the Kalman smoother with data $f_1, ..., f_k$ at time t_0, $\tilde{\varphi}_{4DVar,k}^{(a)}$ the minimiser of the 4DVar functional (6.1) at time t_0 and define*

$$\varphi_{4DVar,k}^{(a)} := M_{k,0}\tilde{\varphi}_{4DVar,k}^{(a)}, \quad k = 1, 2, 3, ... \tag{7.22}$$

Then 4DVar is equivalent to the Kalman filter and to the Kalman smoother in the sense that

$$\varphi_{4DVar,k}^{(a)} = \varphi_k^{(a)} = M_{k,0}\tilde{\varphi}_k^{(a)}, \tag{7.23}$$

if we start the iterations with the same initial background state $\varphi_0^{(b)}$ and the same initial error covariance matrix $B_0^{(a)} := B$.

Proof. The equivalence of the Kalman smoother with the Kalman filter is obtained by our reformulation based on (7.11) worked out in equations (7.14) to (7.19). The equivalence to 4DVar is then a consequence of Theorem 7.2. □

Theorem 7.5 states that the Kalman smoother is equivalent to the Kalman filter (and 4DVar) at the end of some time window for linear operators.

We finally consider the stochastic approach to the Kalman filter, which we formulate as a basic theorem. Observing that the formulas for Bayes' data assimilation with Gaussian densities as given in Definition 5.4 are identical to the update formulas for the Kalman filter according to Definition 7.4, the proof of this result is straightforward.

Theorem 7.6 (Equivalence of Kalman filter and Bayes' data assimilation). *For linear systems $M_k : X \to X$, linear observation operators $H_k : X \to Y$, and Gaussian probability densities, the* Kalman filter *as given in Definition 7.4 is identical to* Bayes' data assimilation *given by Definition 5.4.*

For nonlinear system dynamics $M_k : X \to X$, and nonlinear observation operators $H_k : X \to Y$ the above equivalences do not hold any more. However, we may still apply the Kalman filter if we linearise both the model M_k and the observation operator H_k about the considered state. This leads to the Extended Kalman filter (EKF) ([46, 2]. The linearisations of the model operator M_k and the observation operator H_k, which are used within the Kalman filter (7.4) are given by

$$\mathbf{M}_k(\varphi_k) := \frac{dM_k}{d\varphi}|_{\varphi_k} \quad \text{and} \quad \mathbf{M}_k(\varphi_k) := \frac{dH_k}{d\varphi}|_{\varphi_k},$$

where $\mathbf{M}_k$ is the tangent linear model (see (6.7)).

We have introduced several data assimilation methods and shown that, for linear systems, they are all essentially equivalent to cycled Tikhonov regularisation with a weighted norm. In the next section we consider ensemble methods, which provide a way of (approximately) updating probability distributions and covariance matrices within the assimilation schemes.

8 Ensemble methods

We have introduced several methods for data assimilation in the previous sections, including Tikhonov data assimilation, 3DVar, 4DVar, Bayes' data assimilation and the Kalman filter.

Evaluating the different approaches, we note that 3DVar or Tikhonov data assimilation work with fixed norms at every time-step and do not fully include all the dynamic information which is available from previous assimilations. Since 4DVar uses full trajectories over some time window, it implicitly includes such information and we can expect it to be superior to the simple 3DVar. However, Bayes' data assimilation or the Kalman filter are equivalent to 4DVar for linear systems and include all available information by updating the weight matrices and propagating them through time. This is essentially done implicitly in 4DVar. In general, we can expect them to yield results comparable to those of 4DVar.

The need to propagate some probability distribution is a characteristic feature of the Bayes' data assimilation and the Kalman filter. It is also their main challenge, since the matrices $B_k^{(a)}$ or $B_k^{(b)}$ have dimension $n \times n$, which for large n is usually not feasible in terms of computation time or storage, even when supercomputers are employed for the calculation as in most operational centres for atmospheric data assimilation. Thus, a key need for these methods is to formulate algorithms which give a reasonable approximation to the weight matrices $B_k^{(b)}$ with less computational costs than by the use of (7.14) and (7.18) or (7.19).

Often, the approach to ensemble methods is carried out via stochastic estimators. Here, we want to stay within the framework of the previous sections and study the ensemble approach from the viewpoint of applied mathematics. The stochastic view

will be discussed in a second step. One of the most popular ensemble filter techniques is the Ensemble Kalman filter (see [25, 41, 42, 84, 65, 3, 43, 77, 11, 24, 70]).

Definition 8.1 (Ensemble). An *ensemble* with N members is any finite set of vectors $\varphi^{(\ell)} \in X$ for $\ell = 1, ..., N$. We can propagate the ensemble through time by applying our model dynamics $M : X \to X$ or $M_k : X \to X$, respectively. Starting with an *initial ensemble* $\varphi_0^{(\ell)}$, $\ell = 1, ..., N$, this leads to ensemble members

$$\varphi_k^{(\ell)} = M_{k-1}\varphi_{k-1}^{(\ell)}, \quad k = 1, 2, 3, ... \tag{8.1}$$

for $\ell = 1, ..., N$.

We will start with the construction of a particular family of ensembles generated by the eigenvalue decomposition of the weight matrix $B := B^{(b)}$ defined in Section 7 with $X = \mathbb{R}^n$. B is a self-adjoint and positive definite matrix, hence, there is a complete set of eigenvectors of B, i.e. we have vectors $\psi^{(1)}, ..., \psi^{(n)} \in X$ and eigenvalues $\lambda^{(1)}, ..., \lambda^{(n)}$ such that

$$B\psi^{(\ell)} = \lambda^{(\ell)}\psi^{(\ell)}, \quad \ell = 1, ..., n. \tag{8.2}$$

The eigenvalues are real valued and positive and we will always assume that they are ordered according to their size $\lambda^{(1)} \geq \lambda^{(2)} \geq ... \geq \lambda^{(n)}$. With the matrix $\Lambda := \mathrm{diag}[\sqrt{\lambda^{(1)}}, ..., \sqrt{\lambda^{(n)}}]$ and the orthogonal matrix $U := [\psi^{(1)}, ..., \psi^{(n)}]$ we obtain

$$B = U\Lambda^2 U^* = (U\Lambda)(U\Lambda)^*, \tag{8.3}$$

where we note that $U^* = U^{-1}$. This representation corresponds to the well-known *principle component analysis* of the *quadratic form* defined by

$$E(\varphi, \psi) := \varphi^T B\psi, \quad \varphi, \psi \in X. \tag{8.4}$$

Geometrically, B defines a hypersurface of second order with positive eigenvalues, whose level curves form a family of $n - 1$-dimensional ellipses in X. The principal axis of this ellipse are given by the eigenvectors $\psi^{(l)}$, $\ell = 1, ..., n$.

The application of B to some vector $\varphi \in X$ according to (8.3) is carried out by a projection of φ onto the principle axis $\psi^{(\ell)}$ of B, followed by the multiplication with $\lambda^{(\ell)}$. This setup can be a basis for further insight to construct a low-dimensional approximation of B.

Before we continue the ensemble construction we first need to discuss the *metric* in which we want an approximation of the B-matrix. We remark that the role of B in the Kalman filter is mainly in the update formulas (7.14), (7.15) and (7.19). Here, to obtain a good approximation of the vector updates in L^2, we need B to be approximated in the operator norm based on L^2 on $X = \mathbb{R}^n$. That is what we will use as our basis for the following arguments.

Lemma 8.2. *We construct an ensemble of vectors by choosing the $N-1$ maximal eigenvalues of B and its corresponding eigenvectors $\psi^{(1)}, ..., \psi^{(N-1)}$. We define*

$$Q := [\sqrt{\lambda^{(1)}}\psi^{(1)}, ..., \sqrt{\lambda^{(N-1)}}\psi^{(N-1)}]. \qquad (8.5)$$

Then, we have the error estimate

$$||B - QQ^*|| = \sup_{j=N,...,n} |\lambda^{(j)}| = |\lambda^{(N)}| = \lambda^{(N)}. \qquad (8.6)$$

Proof. The proof is obtained from

$$B - QQ^* = U\tilde{\Lambda}^2 U^*, \qquad (8.7)$$

with $\tilde{\Lambda}^2 = \mathrm{diag}[0, ..., 0, \lambda^{(N)}, \lambda^{(N+1)}, ..., \lambda^{(n)}]$, where there are $N-1$ zeros on the diagonal of $\tilde{\Lambda}$. Since U is an orthogonal matrix, the norm estimate (8.6) is straightforward. $\qquad \square$

We are now going to use arbitrary ensembles $\varphi^{(1)}, ..., \varphi^{(N)}$ and construct approximate weight matrices. From the Courant Minimum-Maximum Principle we know that

$$\lambda^{(\ell)} = \min_{\dim U = \ell - 1} \max_{\varphi \in U^\perp, ||\varphi|| = 1} \langle \varphi, B\varphi \rangle . \qquad (8.8)$$

For an arbitrary ensemble $\varphi^{(1)}, ..., \varphi^{(N)}$ we use the mean

$$\mu = \frac{1}{N} \sum_{\ell=1}^{N} \varphi^{(\ell)} \qquad (8.9)$$

to define the *ensemble matrix*

$$Q := [\varphi^{(1)} - \mu, ..., \varphi^{(N)} - \mu], \qquad (8.10)$$

and we define the *ensemble subspace* U_Q by

$$U_Q = \mathrm{span}\{\varphi^{(1)} - \mu, ..., \varphi^{(N)} - \mu\}. \qquad (8.11)$$

We call the vectors $\varphi^{(\ell)} - \mu$, $\ell = 1, ..., N$ the *centered ensemble*. We remark that $\dim U_Q = N - 1$. Then, we have

$$
\begin{aligned}
||B - QQ^*|| &\geq \sup_{B\varphi \perp U_Q, ||\varphi||=1} ||(B - QQ^*)\varphi|| \\
&\geq \sup_{B\varphi \perp U_Q, ||\varphi||=1} ||B\varphi|| \\
&\geq \sup_{B\varphi \perp U_Q, ||\varphi||=1} \langle \varphi, B\varphi \rangle \\
&\geq \min_{\dim U = N-1} \sup_{\varphi \perp U, ||\varphi||=1} \langle \varphi, B\varphi \rangle \\
&= \lambda^{(N)}.
\end{aligned}
\qquad (8.12)
$$

The above results are summarised in the following theorem.

Theorem 8.3. *Let the eigenvalues $\lambda^{(1)} \geq \lambda^{(2)} \geq \cdots \geq \lambda^{(n)}$ of the self-adjoint weight matrix B be ordered according to its size and let $\varphi^{(1)}, ..., \varphi^{(N)}$ with $N \in \mathbb{N}$ be an arbitrary ensemble of states in X. Then, the error for the approximation of the weight matrix B by QQ^* with Q defined in (8.10) is estimated by*

$$||B - QQ^*||_2 \geq \lambda^{(N)} \tag{8.13}$$

Remark 8.4. The optimal error $\lambda^{(N)}$ can be achieved if the centred ensemble spans the space of the $N - 1$ eigenvectors $\psi^{(1)}, ..., \psi^{(N-1)}$ of B corresponding to the largest eigenvalues $\lambda^{(1)}, ..., \lambda^{(N-1)}$ with appropriate coefficients as in (8.5).

Ensembles can be used to approximate the weight matrix $B_{k+1}^{(b)}$ when the weight matrix $B_k^{(a)}$ is given (see (7.15)). If $B_k^{(a)}$ is approximated by the ensemble $\varphi_k^{(1)}, ..., \varphi_k^{(N)}$ in the form

$$B_k^{(a)} \approx Q_k^{(a)}(Q_k^{(a)})^*, \tag{8.14}$$

with $Q_k^{(a)} := [(\varphi^{(1)})^{(a)} - \mu^{(a)}, ..., (\varphi^{(N)})^{(a)} - \mu^{(a)}]$, then by (7.14) we derive an approximation for $B_{k+1}^{(b)}$ by

$$
\begin{aligned}
B_{k+1}^{(b)} &= M_k B_k^{(a)} M_k^* \\
&\approx M_k Q_k^{(a)}(Q_k^{(a)})^* M_k^* \\
&= M_k Q_k^{(a)}(M_k Q_k^{(a)})^* \\
&= Q_{k+1}^{(b)}(Q_{k+1}^{(b)})^*, \tag{8.15}
\end{aligned}
$$

where $Q_{k+1}^{(b)} = M_k Q_k^{(a)}$.

Lemma 8.5. *Consider the approximation of $B_k^{(a)}$ by an ensemble $\varphi_k^{(1)}, ..., \varphi_k^{(N)}$ with ensemble matrix $Q_k^{(a)}$. If the error satisfies*

$$||B_k^{(a)} - Q_k^{(a)}(Q_k^{(a)})^*|| \leq \epsilon, \tag{8.16}$$

for some $\epsilon > 0$ then, the error estimate for the propagated ensemble at time t_{k+1} is given by

$$||B_{k+1}^{(b)} - Q_{k+1}^{(b)}(Q_{k+1}^{(b)})^*|| \leq ||M_k|| ||M_k^*|| \epsilon. \tag{8.17}$$

Proof. Based on (8.15) the proof is straightforward. □

A key question of ensemble methods is how to update the ensemble in the data assimilation step. Given the data f_k at time t_k, how do we get an ensemble which approximates the analysis covariance matrix $B_k^{(a)}$ given an ensemble which approximates the background error covariance matrix $B_k^{(b)}$. We know that for the Kalman

filter the analysis covariance matrix $B_k^{(a)}$ is calculated from $B_k^{(b)}$ by (7.19). In terms of the ensemble approximations this means

$$Q_k^{(a)}(Q_k^{(a)})^* = (I - K_k H_k) Q_k^{(b)}(Q_k^{(b)})^* \tag{8.18}$$

with the *ensemble Kalman matrix*

$$K_k := Q_k^{(b)}(Q_k^{(b)})^* H_k^* (R + H_k Q_k^{(b)}(Q_k^{(b)})^* H_k^*)^{-1}, \tag{8.19}$$

leading to

$$Q_k^{(a)}(Q_k^{(a)})^* = Q_k^{(b)} \underbrace{\left\{ I - (Q_k^{(b)})^* H_k^* \left(R + H_k Q_k^{(b)}(Q_k^{(b)})^* H_k^* \right)^{-1} H_k Q_k^{(b)} \right\}}_{=:T} (Q_k^{(b)})^*.$$
$$\tag{8.20}$$

The matrix T in the curly brackets is self-adjoint and positive semi-definite, hence there exists a matrix L such that $T = LL^*$. This finally leads to

$$Q_k^{(a)} = Q_k^{(b)} L, \tag{8.21}$$

which we denote as *square root filter* [4, 8, 65, 79].

Lemma 8.6. *Assume that $\varphi_k^{(1)}, ..., \varphi_k^{(N)}$ is an ensemble which satisfies*

$$||B_k^{(b)} - Q_k^{(b)}(Q_k^{(b)})^*|| \le \epsilon, \tag{8.22}$$

with some $\epsilon < ||B_k^{(b)}||$. Then, for the analysis ensemble defined by (8.21) we have

$$||B_k^{(a)} - Q_k^{(a)}(Q_k^{(a)})^*|| \le C\epsilon, \tag{8.23}$$

with some constant C not depending on $Q_k^{(a)}$.

Proof. Using the notation $K_k^{(true)}$ for the Kalman gain matrix in the general case (see (7.17) and (7.19)), and $Q_k^{(a)}(Q_k^{(a)})^*$ from (8.18) we write

$$
\begin{aligned}
B_k^{(a)} - Q_k^{(a)}(Q_k^{(a)})^* &= (I - K_k^{(true)} H_k)(B_k^{(b)} - Q_k^{(b)}(Q_k^{(b)})^*) \\
&\quad + (K_k - K_k^{(true)}) H_k Q_k^{(b)}(Q_k^{(b)})^*,
\end{aligned}
\tag{8.24}
$$

with K_k defined by (8.19). We remark that due to its special structure the norm of the inverse $(R + H_k Q_k^{(b)}(Q_k^{(b)})^* H_k^*)^{-1}$ in (8.19) is bounded uniformly independent of $Q_k^{(b)}$. Furthermore, using $\epsilon < ||B_k^{(b)}||$, the norm

$$
\begin{aligned}
||Q_k^{(b)}(Q_k^{(b)})^*|| &= ||B_k^{(b)} + \left(Q_k^{(b)}(Q_k^{(b)})^* - B_k^{(b)} \right)|| \\
&\le ||B_k^{(b)}|| + \epsilon \\
&\le 2||B_k^{(b)}||
\end{aligned}
$$

is bounded uniformly, leading to

$$||K_k^{(true)} - K_k|| \leq c\epsilon, \tag{8.25}$$

with a constant c not depending on $Q_k^{(b)}$. Finally, a similar estimate applied to (8.24) yields the desired result (8.23), and the proof is complete. □

For further insight into ensemble methods we refer to the article [69] in this book.

9 Numerical examples

We examine data assimilation techniques discussed in this article, and their relation to inverse problem theory, for simple model problems. First we consider an advection-diffusion equation in Section 9.1 and then the Lorenz-95 system in Section 9.2.

9.1 Data assimilation for an advection-diffusion system

Consider the following linear (one-dimensional) advection-diffusion problem (see, for example [15]). The system dynamics are described by

$$\frac{\partial}{\partial t}\varphi(x,t) = \nu\frac{\partial^2}{\partial x^2}\varphi(x,t) - a\frac{\partial}{\partial x}\varphi(x,t), \tag{9.1}$$

for $x \in (0,1)$ and $t \in (0,T)$. As boundary and initial conditions we have

$$\begin{aligned}
\varphi(0,t) &= 0, \quad t \in (0,T), \\
\varphi(1,t) &= 0, \quad t \in (0,T), \\
\varphi(x,0) &= \varphi_0(x), \quad x \in (0,1).
\end{aligned}$$

Here $\nu > 0$ is the diffusion coefficient and a is the advection parameter. We want to determine the initial condition φ_0 from the measurements of the solution $\varphi(x,t)$ at certain points in space and time. Let $0 = x_0 < x_1... < x_n = 1$ and $x_i = ih$, $i = 0,\ldots,n+1$ and $h = \frac{1}{n+1}$. With the discretisations of the spatial derivatives

$$\frac{\partial^2}{\partial x^2}\varphi \approx \frac{\varphi^{i+1} - 2\varphi^i + \varphi^{i-1}}{h^2}, \quad \text{and} \quad \frac{\partial}{\partial x}\varphi \approx \frac{\varphi^i - \varphi^{i-1}}{h},$$

for $i = 0,\ldots,n$, we obtain a system of ordinary differential equations of the form

$$\dot{\varphi}(t) = F(\varphi), \quad t \in (0,T], \quad \varphi(0) = \varphi_0, \tag{9.2}$$

where, in this case $F(\varphi) = K\varphi(t)$, that is, F is linear, with

$$
K = \begin{bmatrix}
-2\frac{\nu}{h^2} - \frac{a}{h} & \frac{\nu}{h^2} & & & & \\
\frac{\nu}{h^2} + \frac{a}{h} & -2\frac{\nu}{h^2} - \frac{a}{h} & \frac{\nu}{h^2} & & & \\
& \frac{\nu}{h^2} + \frac{a}{h} & -2\frac{\nu}{h^2} - \frac{a}{h} & \frac{\nu}{h^2} & & \\
& \ddots & \ddots & \ddots & & \\
& & \frac{\nu}{h^2} + \frac{a}{h} & -2\frac{\nu}{h^2} - \frac{a}{h} & \frac{\nu}{h^2} \\
& & & \frac{\nu}{h^2} + \frac{a}{h} & -2\frac{\nu}{h^2} - \frac{a}{h}
\end{bmatrix} \in \mathbb{R}^{n+2 \times n+2},
$$

and $\varphi(t) = [\varphi^0(t), \ldots, \varphi^{n+1}(t)]^T \in \mathbb{R}^{n+2}$. To satisfy the boundary conditions we set $\varphi^0(t) = \varphi^{n+1}(t) = 0$ throughout. As initial condition we choose $\varphi^i(0) = \varphi_0(x_i)$, $i = 0 \ldots, n$. The solution to the linear system of ordinary differential equations with
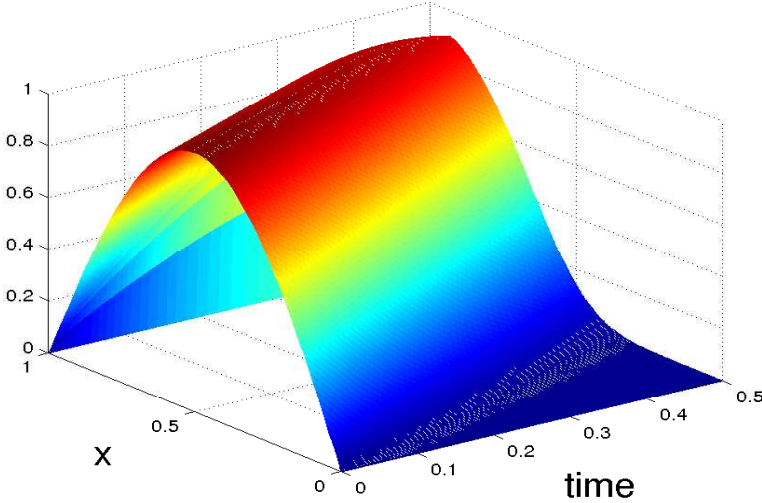
Figure 1: Solution of $\varphi(t) = (\exp Kt)\varphi_0$, $t \in [0, 0.5]$ (discretised advection-diffusion equation (9.1)) for initial condition $\varphi_0(x) = \sin(\pi x)$.

constant coefficients (9.2) is given by

$$
\varphi(t) = (\exp Kt)\varphi_0, \quad t \in [0, T], \tag{9.3}
$$

where $\exp Kt \in \mathbb{R}^{n+2 \times n+2}$, or, using an explicit first order Euler scheme we obtain the discrete linear model

$$
\varphi_{k+1} = \varphi_k + \Delta t K \varphi_k, \quad k = 0, \ldots, \frac{T}{\Delta t}, \tag{9.4}
$$

where $\varphi_k = [\varphi_k^0, \ldots, \varphi_k^{n+1}]^T \in \mathbb{R}^{n+2}$ and $\varphi_k^0 = \varphi_k^{n+1} = 0$ throughout. Note that we use a lower index to describe the time steps and an upper index to describe points in space/components of φ_k. The approach (9.4) is a more practical implementation as the analytical solution (9.3) would only be available for certain problems. We solve the advection-diffusion problem (9.1) (using the Forward Euler method) with $a = 1$, $\nu = 0.01$, $n = 100$, final time $T = 0.5$, time step $\Delta t = 0.001$ and initial condition $\varphi_0(x_i) = \sin(\pi x_i)$. The solution is shown in Figure 1.

For the inverse problem (data assimilation problem), we suppose we do not know the initial condition $\varphi_0(x)$. We want to estimate $\varphi_0(x)$ from measurements of r components $\varphi^{\frac{n}{r}}(t), \varphi^{2\frac{n}{r}}(t), \ldots, \varphi^n(t)$ of the solution $\varphi(t)$ at times $t_1 = 0.002, t_2 = 0.004, \ldots, t_m = 0.5$. For our experiment we use $r = 5$, hence, we observe 5 out of $n = 100$ components. Take noisy measurements of $H\varphi(t_1), H\varphi(t_2), \ldots, H\varphi(t_m)$, where $H \in \mathbb{R}^{r \times n+2}$ is the observation operator matrix (which is linear in this case) given by $H_{ij} = 1$ if $j = \frac{n}{r}i$ and $H_{ij} = 0$ otherwise. We obtain the (linear) least squares problem

$$\min_{\varphi_0 \in \mathbb{R}^{n+2}} \|\bar{H}\varphi_0 - f\|_2^2, \tag{9.5}$$

with $\bar{H}$ and f for the forward Euler method and observations every second time step given by

$$\bar{H} = \begin{bmatrix} H(I + 2\Delta tK) \\ H(I + 2\Delta tK)^2 \\ \vdots \\ H(I + 2\Delta tK)^m \end{bmatrix} \in \mathbb{R}^{rm \times n+2} \quad \text{and} \quad f = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_m \end{bmatrix} \in \mathbb{R}^{rm}.$$

The observations are obtained using the output from the exact initial condition and the measurements usually contain noise (see Section 4 for detailed description of the errors), that is $f = f^\delta = f^{(true)} + d^\delta$, where the noise is usually normally distributed, that is $d^\delta \sim \mathcal{N}(0, \rho^2 I)$, where ρ is the standard deviation. If we solve the problem using a naive approach with a standard least squares implementation [74] we obtain the result in Figure 2a.

Using the singular value decomposition given in Lemma 1.3 we have $\bar{H} = V\Sigma U^*$ and, with $f = f^{(true)} + d^\delta$ we obtain

$$\varphi_0^\delta = \sum_{j=1}^{n+2} \frac{\langle f^\delta, v_j \rangle_Y}{\sigma_j} u_j = \sum_{j=1}^{n+2} \left(\frac{v_j^T f^{(true)}}{\sigma_j} + \frac{v_j^T d^\delta}{\sigma_j} \right) u_j,$$

and clearly for small singular values σ_j the noise is magnified, hence the naive solution in Figure 2a. Figure 2b shows what happens for this particular example. The singular values σ_j decay rapidly and only the coefficients $|v_j^T f| = |v_j^T f^\delta|$ above the noise level (here we chose $d^\delta \sim \mathcal{N}(0, \rho^2 I)$ with $\rho = 0.1$) are useful and carry clear information about the data.

(a) Exact initial condition φ_0 and naive solution to the least squares problem.

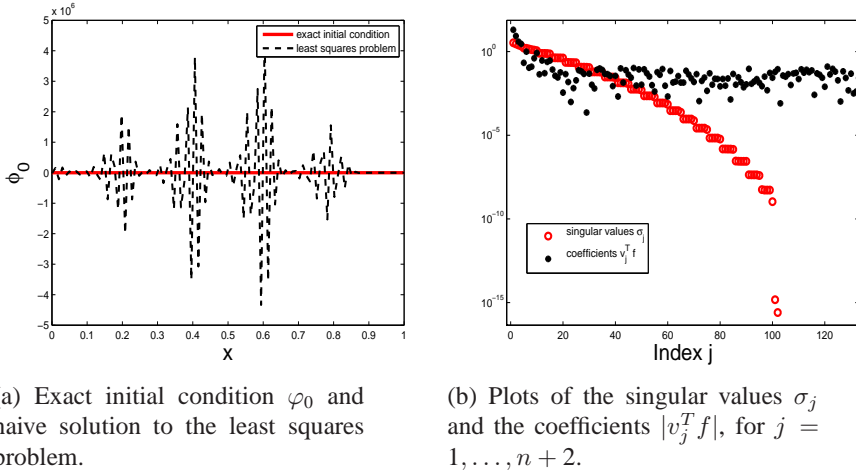(b) Plots of the singular values σ_j and the coefficients $|v_j^T f|$, for $j = 1, \ldots, n + 2$.

Figure 2: Naive solution to the least squares problem (9.5) and singular values of $\bar{H}$.

In order to compute a better solution φ_0 for the initial condition than the one given in Figure 2a we apply Tikhonov regularisation. From (3.11) the Tikhonov regularised solution is given by

$$\varphi_0^{(a)} = \varphi_0^{(b)} + B\bar{H}^*(\alpha R + \bar{H}B\bar{H}^*)^{-1}(f - \bar{H}^*\varphi_0^{(b)}).$$

For our problem we use the observation error covariance matrix $R = 0.01I$ (in line with the noise on the observations). For this particular problem we we chose $\varphi_0^{(b)} = 1 - 0.5\pi^2(x - 0.5)^2$ for the background estimate, which is the truncated Taylor series expansion of the true initial condition φ_0. For the background error covariance ma-
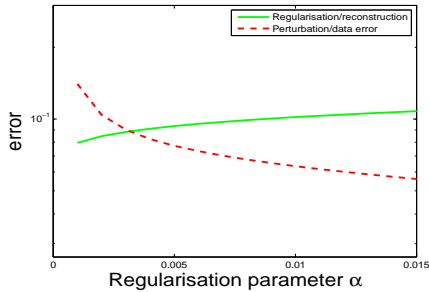
Figure 3: Regularisation/reconstruction and data/measurement error for different values of α between 0 and 0.015. The optimal α in this case is found to be $\alpha = 0.00359$.

trix we take B with entries $B_{ij} = 0.01 \exp\left(\frac{-|i-j|}{50}\right)$ and for α we choose the value $\alpha = 0.00359$ which minimises both the total error consisting of perturbation error

$\|R_\alpha d^\delta\|$ where $R_\alpha = B\bar{H}^*(\alpha R + \bar{H}B\bar{H}^*)^{-1}$ and regularisation error $\|R_\alpha \bar{H}\varphi_0 - \varphi_0\|$, see (2.7). The plots in Figure 3 show both the regularisation and perturbation error for this problem. For the value $\alpha = 0.00359$ the reconstruction of the initial condition is plotted in Figure 4a and the initial condition error is displayed in Figure 4b. Note
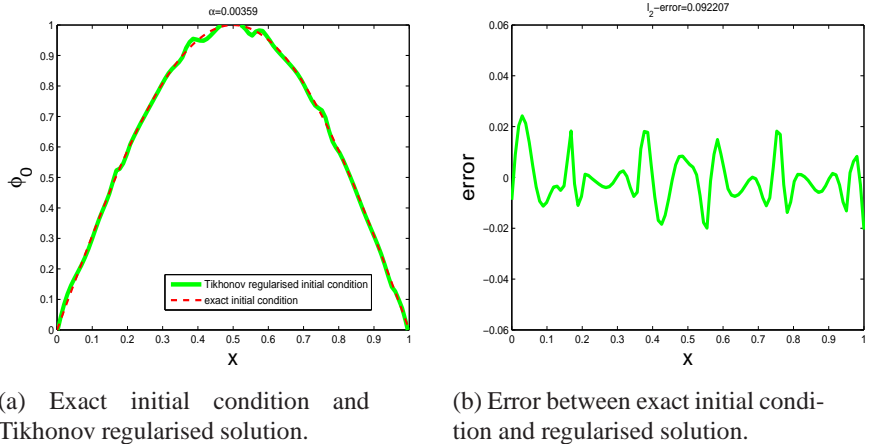

(a) Exact initial condition and Tikhonov regularised solution.

(b) Error between exact initial condition and regularised solution.

Figure 4: Exact initial condition and regularised solution for the regularisation parameter $\alpha = 0.00359$ and the l_2-norm error between exact and regularised solution for the linear advection equation (9.1).

that similar computations can be done using no background $\varphi_0^{(b)}$, the standard situation in Tikhonov regularisation, different background estimates, as well as different choices for the background error covariance matrices B. For the choice of α which corresponds to the choice of Tikhonov regularisation parameter several heuristics are available, such as the L-curve criterion [36], generalised cross-validation [30] and the discrepancy principle [61], where the latter is most appropriate for large scale computations.

We have essentially solved a 4DVar data assimilation problem, as we have shown in Section 6 that 4DVar can be written in the form of 3DVar which is merely a Tikhonov regularisation, discussed in Section 3.

The situation described above was an ideal situation. In reality models are nonlinear and imperfect, that is, they include model error. We give examples for these situations. First, consider a nonlinear problem. Instead of (9.1) consider

$$\frac{\partial}{\partial t}\varphi(x,t) = \nu\frac{\partial^2}{\partial x^2}\varphi(x,t) - a\frac{\partial}{\partial x}\varphi(x,t) + \varphi(x,t)^3,$$

and the discrete nonlinear problem becomes

$$\varphi_{k+1} = \varphi_k + \Delta t K\varphi_k + \varphi_k^3 = M_k(\varphi_k), \quad k = 0,\ldots,\frac{T}{\Delta t}. \tag{9.6}$$
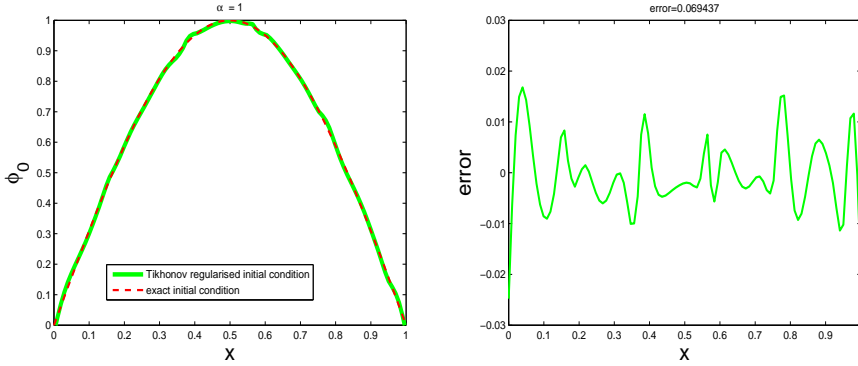
(a) Exact initial condition and Tikhonov regularised solution.

(b) Error between exact initial condition and regularised solution.

Figure 5: Exact initial condition and regularised solution for the regularisation parameter $\alpha = 1$ and the l_2-norm error between exact and regularised solution for the nonlinear advection equation.

We set up the nonlinear least squares problem

$$\min_{\varphi_0 \in \mathbb{R}^{n+2}} \|\bar{H}(\varphi_0) - f\|_2^2,$$

where here $\bar{H}$ is a nonlinear operator. The minimisation problem can be solved using the Gauss-Newton method [21, 64]. The results for the reconstructed initial condition for the same data as for the linear problem are displayed in Figure 5a and the initial condition error is displayed in Figure 5b.

Finally, consider the case where some model error is present. To this end, we assume the observations are created by the true model for the nonlinear advection-diffusion equation (9.1) with $a = 1$, $\nu = 0.01$. The model used in the data assimilation process uses perturbed parameters $a^{\text{pert}} = 1.1$, $\nu^{\text{pert}} = 0.009$. The results for the reconstructed initial condition are shown in Figure 6a and the initial condition error is displayed in Figure 6b. As the model contains an error we are trying to fit an initial condition for the wrong model and hence the error for this problem is rather large as seen in Figures 6b and 6b.

However, in Figures 7a and 7b we see that this relatively large error in the initial condition does not lead to large errors in the solution. Figure 7a shows the solution to the nonlinear advection equation with exact initial condition and Figure 7b shows the solution with the perturbed initial condition obtained after solving the inverse (data assimilation) problem. We see that, as the solution is propagated forward in time, the error in the initial condition is smoothed. The reason is the smoothing property of the forward operator. We have $\varphi_{k+1} = M_k(\varphi_k)$ where M_k is a linear (that is, $I + \Delta t K$) or a nonlinear (see (9.6)) operator. If the initial condition is perturbed by ζ_k, then we
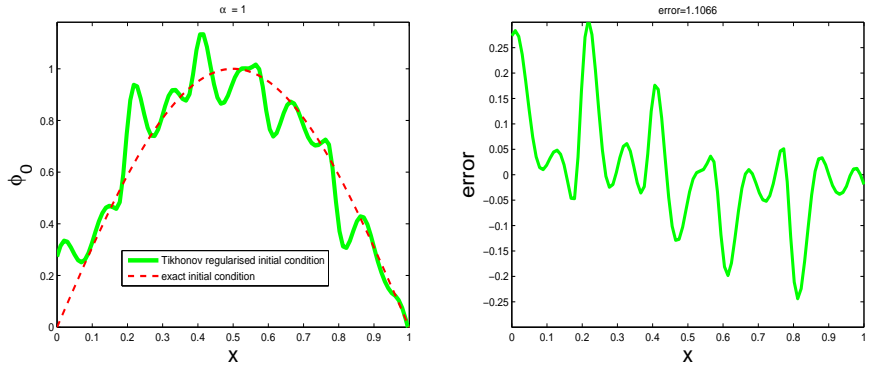
(a) Exact initial condition and Tikhonov regularised solution.

(b) Error between exact initial condition and regularised solution.

Figure 6: Exact initial condition and regularised solution for the regularisation parameter $\alpha = 1$ and the l_2-norm error between exact and regularised solution for the nonlinear advection equation when a model error is present.
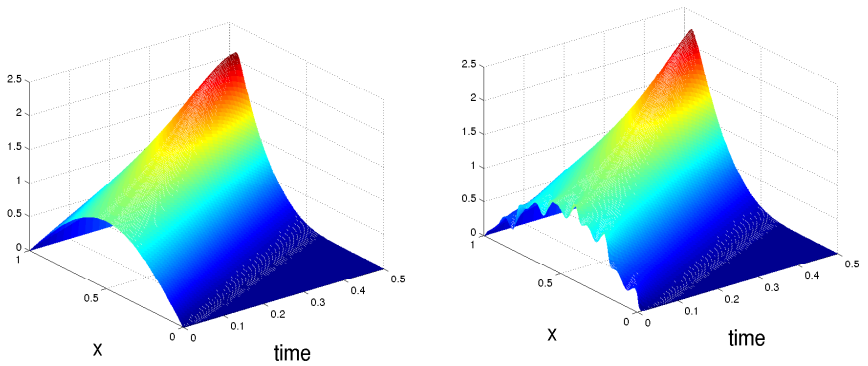
(a) Solution to nonlinear discretised advection-diffusion equation for initial condition $\varphi_0(x) = \sin(\pi x)$.

(b) Solution to nonlinear discretised advection-diffusion equation for perturbed initial condition computed from data assimilation problem.

Figure 7: Solution to nonlinear advection-diffusion problem with exact and perturbed initial condition.

have $\varphi_{k+1} + \zeta_{k+1} = M_k(\varphi_k + \zeta_k)$, and to leading order

$$\zeta_{k+1} = \mathbf{M}_k(\varphi_k)\zeta_k,$$

where $\mathbf{M}_k$ is the discretised tangent linear model. Assuming that $\mathbf{M}_k(\varphi_k) = \mathbf{M}$ (which holds for our linear example), then in the limit we have $\zeta_k = \mathbf{M}^k\zeta_0$. From

basic linear algebra (see [31]) we have that $\zeta_k \to 0$ if $\rho(\mathbf{M}) < 1$, where $\rho(\mathbf{M}) = \max\{|\lambda|, \lambda \in \Lambda(\mathbf{M})\}$ is the spectral radius. In our example, both for the linear and linearised nonlinear model dynamics the eigenvalues of $\mathbf{M}_k(\varphi_k)$ are within the unit circle, explaining the smoothing of the error in the initial condition as the solution propagates in time.

In the next example we consider problems which are more sensitive to the initial conditions, that is systems that exhibit chaotic dynamics (and hence more accurately represent the effects in, say, weather forecasting). One such system is the Lorenz-95 model. In reality we would expect a mix of situations arising from chaotic and smoothing systems.

9.2 Data assimilation for the Lorenz-95 system

As a second example consider the Lorenz-95 system (see [55, 56]), a generalisation of the well-known three-dimensional Lorenz-63 System [54]. The model is given by a system of N coupled nonlinear ordinary differential equations whose solution φ with components $\varphi = [\varphi^1, \ldots, \varphi^N]$ satisfies

$$\frac{d\varphi^i}{dt} = -\varphi^{i-2}\varphi^{i-1} + \varphi^{i-1}\varphi^{i+1} - \varphi^i + f, \quad t \in (0, T] \quad \varphi^i(0) = \varphi_0^i, \qquad (9.7)$$

where $i = 0, \ldots, N$, with cyclic boundary conditions $\varphi^0 = \varphi^N$, $\varphi^{-1} = \varphi^{N-1}$, $\varphi^{N+1} = \varphi^1$ and f is a forcing term. For a forcing term $f = 8$ the system is chaotic (i.e. it has positive Lyapunov exponents, see [76]). For $N = 40$ the system has 13 positive Lyapunov exponents. Lorenz [55] observed that this system has a similar error growth characteristic as an operational numerical weather prediction system if a time $T = 1$ is associated with 5 days.

We solve (9.7) using the classical 4th order explicit Runge-Kutta scheme, which gives

$$\varphi_{k+1} = M_k(\varphi_k), \quad \text{where} \quad \varphi_k = [\varphi_k^1, \ldots, \varphi_k^N]^T, \qquad (9.8)$$

and M_k is the nonlinear model operator which propagates φ_k to φ_{k+1}. The solution trajectory of two components of φ computed with the Runge-Kutta method and $\Delta t = 0.01$ and $T = 21$ is displayed in Figure 8. In order to illustrate the chaotic dynamics of the Lorenz-95 model we run it with slightly perturbed initial conditions. Perturbing the initial condition randomly with an error of about 10% gives the ensemble of forecasts in Figure 9a, using a perturbation of about 0.1% gives the forecast ensemble in Figure 9b. We only show the trajectory of site 20. The figures show an unperturbed solution trajectory and an ensemble where the initial conditions have been slightly perturbed. It is easy to see that the larger the perturbation in the initial condition the more the error in the forecast grows. For this problem the eigenvalues of the matrix $\mathbf{M}_k(\varphi_k)$ from the linearisation of (9.8) are not necessarily within the unit disk.
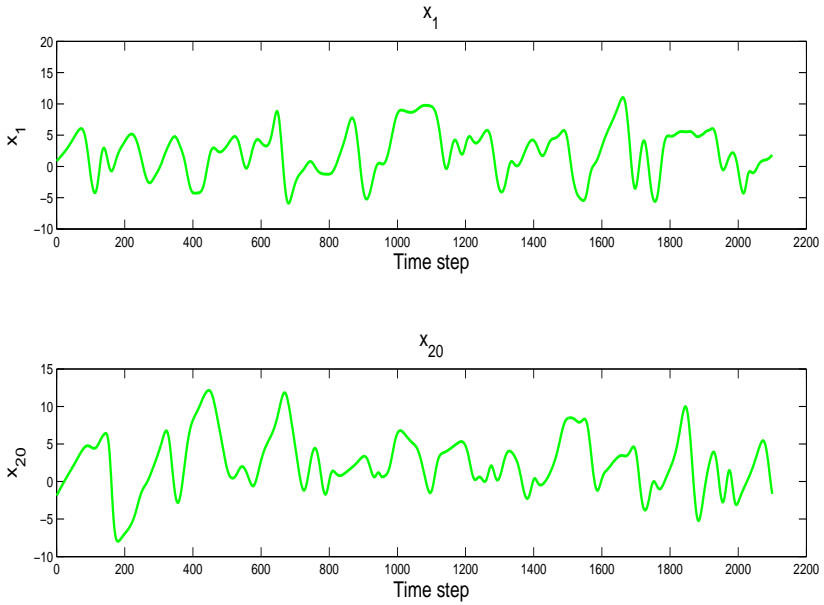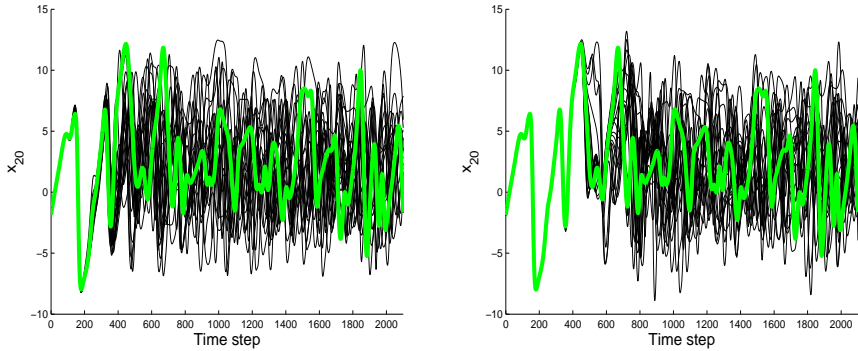
Figure 8: Components 1 and 20 of the solution to (9.7).

(a) Forecast ensemble for an initial condition error of 10%.

(b) Forecast ensemble for an initial condition error of 0.1%.

Figure 9: Trajectory of site 20 of Lorenz-95 system of size 40. Green thick line: unperturbed forecast. Black lines: Ensemble of 20 perturbed forecasts.

We carry out some data assimilation experiments with this problem. First, consider

the 4DVar minimisation problem (6.1). We need to minimise

$$J(\varphi_0) := (\varphi_0 - \varphi_0^{(b)})^T B^{-1}(\varphi_0 - \varphi_0^{(b)}) + \sum_{j=1}^{K}(f_j - H(\varphi_j))^T R^{-1}(f_j - H(\varphi_j)), \quad (9.9)$$

where $\varphi_j = M_{j-1}(\varphi_{j-1})$ is given by (9.8). We have

$$\nabla_{\varphi_0} J(\varphi_0) = 2B^{-1}(\varphi_0 - \varphi_0^{(b)}) - 2\sum_{j=1}^{K}(\mathbf{M}_{j,0}(\varphi_0))^T H^T R^{-1}(f_j - HM_{j,0}(\varphi_0)),$$

where $M_{j,0}$ is given by (1.2) and $\mathbf{M}_{j,0}$ is the tangent linear model. In order to minimise the cost function we need $\nabla_{\varphi_0} J(\varphi_0)$ and in order to solve this problem we apply Newton's method. The Hessian (or the Jacobian for Newton's method) is given by

$$\nabla\nabla_{\varphi_0} J(\varphi_0) = 2B^{-1} + 2\sum_{j=1}^{K}(\mathbf{M}_{j,0}(\varphi_0))^T H^T R^{-1} H\mathbf{M}_{j,0}(\varphi_0)) + Q(\varphi_0),$$

where $Q(\varphi_0)$ involves terms including second derivatives of the system dynamics. These are usually neglected as for large problems they are inefficient, impracticable and often infeasible to calculate. Hence we solve

$$\begin{aligned} \nabla\nabla_{\varphi_0} J(\varphi_0)\Delta\varphi_0^{(\ell)} &= -\nabla_{\varphi_0} J(\varphi_0^{(\ell)}), \\ \varphi_0^{(\ell+1)} &= \varphi_0^{(\ell)} + \Delta\varphi_0^{(\ell)}, \end{aligned}$$

for $\ell = 0, 1, \ldots$, where $\varphi_0^{(\ell)}$ is the ℓth iterate of Newton's method. As initial condition usually the background state is chosen, that is, $\varphi_0^{(0)} = \varphi_0^{(b)}$. We perform data assimilation for a single assimilation window of length 100 time steps, followed by a forecast of 2000 time steps. First we carry out an experiment with perfect observations. For the background estimate we choose a perturbed initial condition and $B = 0.01I$. Checking the singular values of the observability matrix for this problem we obtain that the singular values lie between 4 and 30 and the problem is not ill-conditioned. This is in contrast to the problem in Section 9.1, where the forward operator has very small singular values, which, however led to a smoothing property of the forecast. The problem here lies in the fact that the forecast error grows severely. The inverse problem is not actually ill-conditioned as such but the forward problem exhibits severe error growth for small perturbations! Figure 10 shows the 1st and 20th component of φ before and after the data assimilation process. The error between the true solution and the trajectory before and after the 4DVar data assimilation process is shown in Figure 11. We observe that the error in the analysis (thick line) is reduced significantly (compared to the background) in the first 600 time steps (where the assimilation window is of length 100 time steps). After that we see that the effect of the chaotic dynamics
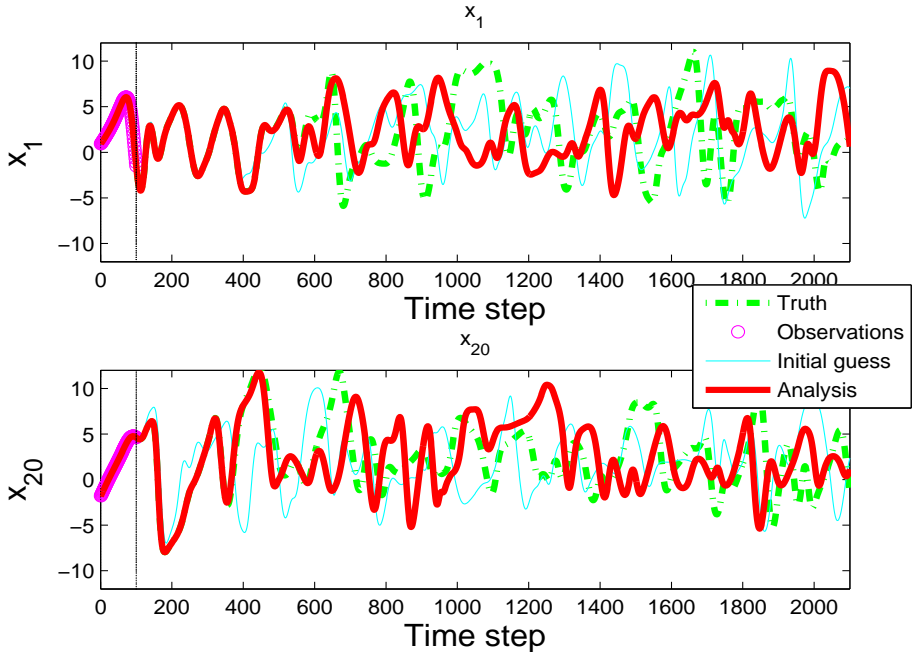
Figure 10: Components 1 and 20 of the solution to (9.7) for full and perfect observations. The plot shows the observations, the assimilation window, the exact trajectory, the background trajectory and the final solution (analysis) after 4DVar.

emerges and the error grows since the initial condition of the analysis vector is perturbed from the true initial condition. The initial condition error is of order $\mathcal{O}(10^{-3})$ at each of the sites and from Figure 9b we cannot anticipate a better performance of the forecast. We expect the results to be best for perfect and full observations. Next, we carry out an experiment with noisy observations. The observations are generated from the truth with an error of mean zero and covariance $R = 0.01I$. Moreover we only take observations every 5 time steps and we only observe 8 of the 40 variables (precisely, we observe every 5th component). For the background state we use a perturbed initial condition but this time with background error covariance matrix B with entries $B_{ij} = 0.01 \exp(\frac{-|i-j|}{50})$. We observe that the singular values of the observability matrix for this problem lie between 0.02 and 7 and not surprisingly the problem is slightly worse conditioned than the one for full observations.

Figure 12 shows the error between the true solution and the trajectory before and after the 4DVar data assimilation process. We observe that the error in both components is not reduced as much as the error in Figure 11 (for perfect and full observations) which is to be expected as we observe fewer components and moreover the observations are noisy. Note that with our setup the 1st component is an "observed site",
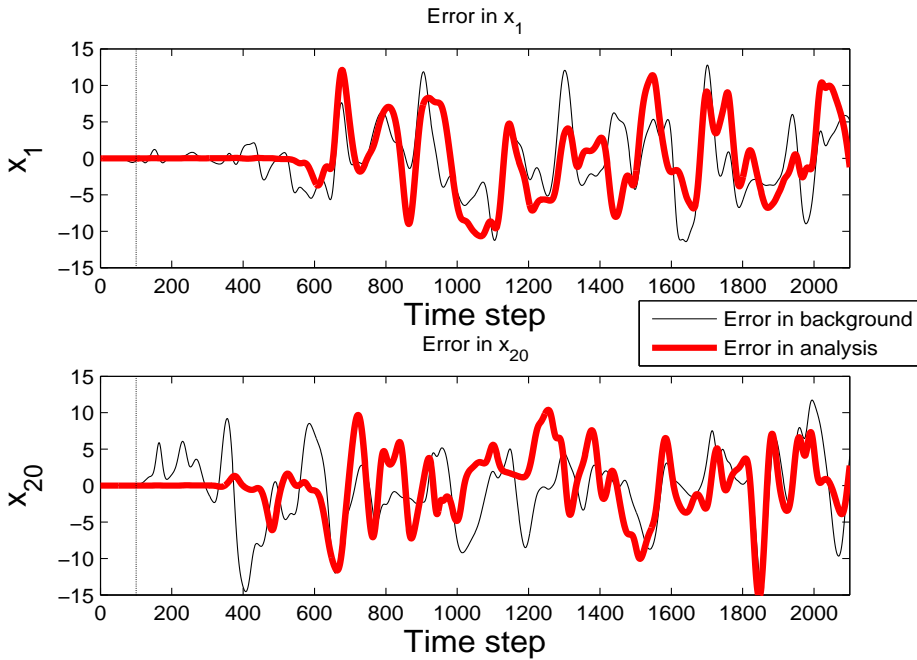
Figure 11: Error of components 1 and 20 of the solution to (9.7) for full and perfect observations. The plot shows the error in the background trajectory and the error in the final solution (analysis) after 4DVar.

where the 20th component is unobserved. We can therefore explain the slightly worse assimilation results of the trajectory of the 20th component compared to the trajectory of the 1st component in Figure 12.

To explore this relation further, Figure 13 shows the absolute value of the error in the initial condition for this problem including the sites of the observations. Clearly, at the observation sites the analysis error is generally smaller than at the unobserved sites. However, this is not always true as information about the true state from the observations is spread to the unobserved sites through the coupling of the problem and via the background error covariance matrix B.

We carried out tests with other data assimilation algorithms such as 3DVar and the Extended Kalman filter. We do not report the results for 3DVar here but mention that for full perfect observations, 3DVar produces very small errors at the end of the assimilation window as we have perfect observations which are sequentially assimilated into the trajectory. Then the forecast is run from a very small error at the end of the assimilation window. With fewer and noisy observations, 3DVar gives worse results than 4DVar (as in 4DVar the missing information is assimilated via the system dynamics). Also, if a model error is included in the system dynamics (that is the observations
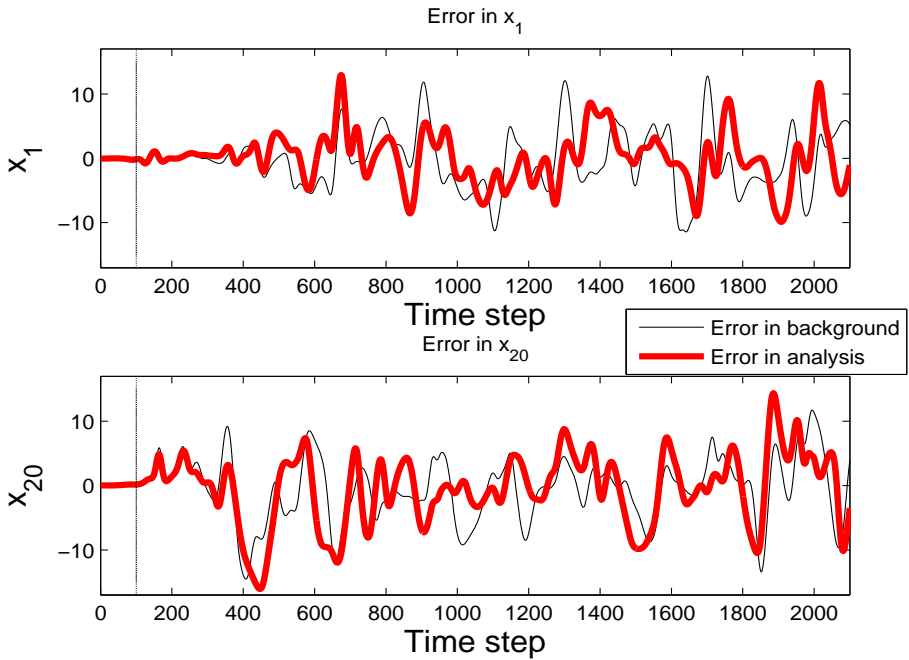
Figure 12: Error of components 1 and 20 of the solution to (9.7) for partial and noisy observations. The plot shows the error in the background trajectory and the error in the final solution (analysis) after 4DVar.
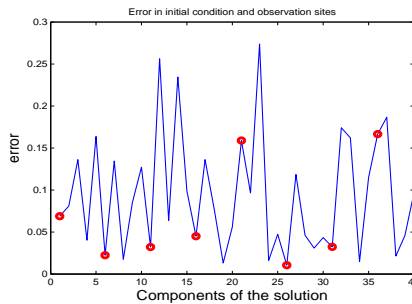

Figure 13: Error in the initial condition and observed sites for the solution to (9.7) after 4DVar for partial and noisy observations.

are created from the true trajectory whereas in the data assimilation process we use a different, perturbed model, replicating the practical situation) we obtain worse results than for the perfect model, as would be expected (see Section 9.1).

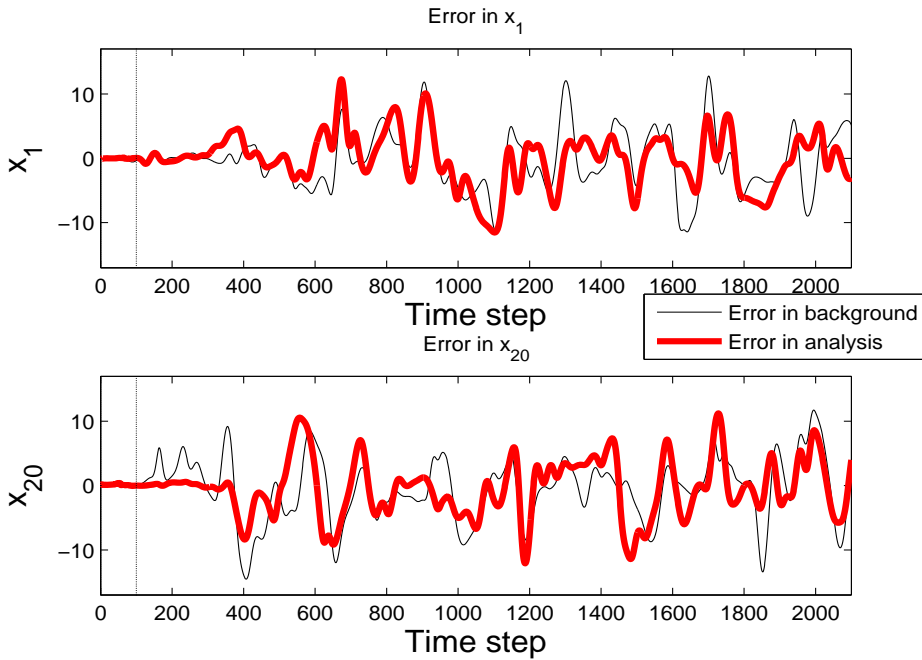Finally, we apply the Extended Kalman filter (EKF) to the Lorenz-95 problem. If

Figure 14: Error of components 1 and 20 of the solution to (9.7) for partial and noisy observations. The plot shows the error in the background trajectory and the error in the final solution (analysis) after applying the EKF.

we use the same background error covariance matrix and the same initial condition as for 4DVar we obtain essentially the same results as for 4DVar (as would be expected from Theorem 7.5). The results here are only approximately equivalent as Theorem 7.5 only holds for the Kalman filter applied to linear system dynamics. However, when plotting the error we hardly observe any difference.

A better result as for 4DVar is obtained for the EKF if a better background error covariance matrix is chosen. To this end we use the covariance matrix produced by the EKF (after one data assimilation cycle at time step 100) as the initial background error covariance matrix for a new EKF experiment applied to the data assimilation problem we consider. This should give a better (flow-dependent) background error covariance matrix. This is indeed true as seen in Figure 14 compared to Figure 12. The new (flow-dependent) background covariance matrix can also be used for 4DVar, resulting in a hybrid method [9].

10 Concluding remarks

Inverse problems are an area of research dealing with the reconstruction of functions or parameter distributions from measurements. It has evolved over nearly 100 years in many applications, for example in electromagnetics and acoustics, in medical imaging and elastography. Today, a growing community of researchers employs both a large set of well-established methods for linear and nonlinear inverse problems as well as a large variety of specific new methods for reconstructions and imaging.

Data assimilation has evolved as a very important and popular research area from specific applications such as weather prediction or hydrology. Using measurement data to control the evolution of dynamical systems shares many of the features which are integral parts of inverse problems. Since World War II data assimilation has focussed on the state estimation problem, that is, the reconstruction of the state $\varphi \in X$ of the dynamical system under consideration, where X denotes the particular state space. Often, parameter functions are also involved and lead to an extended state space which includes unknown parameter functions as well. The algorithms which have been introduced here can easily be applied to this most general situation.

Historically, the communities of *inverse problems* and *data assimilation* have evolved independently, with particular notation and approaches which are similar in content, but have been expressed in different type of notation or terminology. One main goal of this article has been to describe key approaches to data assimilation in an *inverse problems terminology*, such that the *dynamic inverse problems* can be easily identified by the inverse problems community. At the same time, we provide an introduction into a functional analytic view for the data assimilation community, which is too often second priority by those working on important applications.

Today, the *convergence* of *inverse problems* and *data assimilation* is driven by the evolution of modern remote sensing measurement technologies. For example, there is an increasing set of satellite infra-red and microwave sounders, such that their assimilation into atmospheric models involves the use of ill-posed measurement operators. New radar machines measure not only Doppler shift and reflectivity of atmospheric meteors, but also polarisation. Ground-based LIDaRs involve further highly ill-posed measurement operators. Further techniques, such as GPS/GNSS slant delay measurements, lead to ill-posed tomographic problems, which become integral parts of operational data assimilation. We believe that the framework which we presented provides an adequate approach to the further development of these systems.

There is a *need for convergence* also on the level of *assimilation algorithms*. Clearly, methods like 3DVar or 4DVar are basically a version of Tikhonov regularisation. But also modern ensemble or particle methods increase the need for mathematical analysis with tools from functional analysis and approximation theory, since for typical applications only a very limited number of ensembles or particles can be used and we are in the range of low-dimensional approximation theory rather than in the stochastic limit of an infinite ensemble.

Our article has aimed to contribute to the convergence by presenting a concise introduction into key algorithms and results in a functional analytic language which has the potential to be understood by a large range of mathematicians and build a basis for further research and developments. We have included both the viewpoint of deterministic mathematics, numerical analysis and functional analysis as well as stochastics and Bayesian reasoning. Understanding important state-of-the-art algorithms within a uniform framework is a key step today to further develop the tools which are known to have the highest impact on society with respect to such crucial areas as high-impact weather, logistics, travel and energy supply by renewable energy resources.

Bibliography

[1] R. Acar and C. R. Vogel, Analysis of bounded variation penalty methods for ill-posed problems, *Inverse Problems* 10 (1999), 1217.

[2] B. D. O. Anderson and J. B. Moore, *Optimal filtering*, Prentice-Hall Englewood Cliffs, NJ, 1979.

[3] J. L. Anderson, An ensemble adjustment Kalman filter for data assimilation, *Monthly weather review* 129 (2001), 2884–2903.

[4] A. Andrews, A square root formulation of the Kalman covariance equations, *AIAA Journal* 6 (1968), 1165–1166.

[5] A. Apte, C. K. R. T. Jones, A. M. Stuart and J. Voss, Data assimilation: Mathematical and statistical perspectives, *International Journal for Numerical Methods in Fluids* 56 (2008), 1033–1046.

[6] R. N. Bannister, *Elementary 4D-Var*, University of Reading, DARC Technical Report no. 2, 2001.

[7] A. Beck and M. Teboulle, A fast iterative shrinkage-thresholding algorithm for linear inverse problems, *SIAM Journal on Imaging Sciences* 2 (2009), 183–202.

[8] G. J. Bierman, Factorization methods for discrete sequential estimation, *Mathematics in science and engineering* 128 (1977).

[9] M. Buehner, Ensemble-derived stationary and flow-dependent background-error covariances: Evaluation in a quasi-operational NWP setting, *Quarterly Journal of the Royal Meteorological Society* 131 (2005), 1013–1043.

[10] M. Burger, H. Dirks and J. Müller, *Inverse problems in imaging*, Large Scale Inverse Problems. Computational Methods and Applications in the Earth Sciences (M. Cullen, Freitag M. A., S. Kindermann and R. Scheichl, eds.), Radon Ser. Comput. Appl. Math. 13, Walter de Gruyter, Berlin, 2013, pp. 1–51.

[11] G. Burgers, P. J. Van Leeuwen and G. Evensen, Analysis scheme in the ensemble Kalman filter, *Monthly weather review* 126 (1998), 1719–1724.

[12] D. Calvetti and E. Somersalo, *Introduction to Bayesian scientific computing*, Surveys and Tutorials in the Applied Mathematical Sciences 2, Springer, New York, 2007.

[13] E. J. Candes, M. B. Wakin and S. P. Boyd, Enhancing sparsity by reweighted l_1 minimization, *Journal of Fourier Analysis and Applications* 14 (2008), 877–905.

[14] A. Carrassi and S. Vannitsem, Accounting for model error in variational data assimilation: A deterministic formulation, *Monthly Weather Review* 138 (2010), 3369–3386.

[15] T. F. Chan, Stability analysis of finite difference schemes for the advection-diffusion equation, *SIAM J. Numer. Anal.* 21 (1984), 272–284.

[16] S. E. Cohn, A. da Silva, J. Guo, M. Sienkiewicz and D. Lamich, Assessing the Effects of Data Selection with the DAO Physical-Space Statistical Analysis System, *Monthly Weather Review* 126 (1998), 2913–2926.

[17] D. L. Colton and R. Kress, *Inverse acoustic and electromagnetic scattering theory*, Springer Verlag, 1998.

[18] P. Courtier, Dual formulation of four-dimensional variational assimilation, *Quarterly Journal of the Royal Meteorological Society* 123 (1997), 2449–2461.

[19] P. Courtier, J.-N. Thépaut and A. Hollingsworth, A strategy for operational implementation of 4D-Var, using an incremental approach, *Quarterly Journal of the Royal Meteorological Society* 120 (1994), 1367–1387.

[20] R. Daley, *Atmospheric data analysis*, Cambridge: Cambridge University Press, 1991.

[21] J. E. Dennis and R. B. Schnabel, *Numerical Methods for Unconstrained Optimization and Nonlinear Equations*, Classics in Applied Mathematics 16, SIAM, Philadelphia, PA, 1996.

[22] H. W. Engl, M. Hanke and A. Neubauer, *Regularization of inverse problems*, Kluwer, Dortrecht, 1996.

[23] H. W. Engl, K. Kunisch and A. Neubauer, Convergence rates for Tikhonov regularisation of non-linear ill-posed problems, *Inverse Problems* 5 (1989), 523.

[24] G. Evensen, Sequential data assimilation with a nonlinear quasi-geostrophic model using Monte Carlo methods to forecast error statistics, *Journal of Geophysical Research* 99 (1994), 10143–10162.

[25] ———, The ensemble Kalman filter: Theoretical formulation and practical implementation, *Ocean dynamics* 53 (2003), 343–367.

[26] ———, *Data assimilation: the ensemble Kalman filter*, Springer, Berlin, 2009.

[27] M. Fisher, M. Leutbecher and G. A. Kelly, On the equivalence between Kalman smoothing and weak-constraint four-dimensional variational data assimilation, *Quarterly Journal of the Royal Meteorological Society* 131 (2006), 3235–3246.

[28] M. A. Freitag, N. K. Nichols and C. J. Budd, Resolution of sharp fronts in the presence of model error in variational data assimilation, *Quarterly Journal of the Royal Meteorological Society* (2012), doi: 10.1002/qj.2002.

[29] M. Ghil and P. Malanotte-Rizzoli, Data assimilation in meteorology and oceanography, *Adv. Geophys* 33 (1991), 141–266.

[30] G. H. Golub, M. Heath and G. Wahba, Generalized cross-validation as a method for choosing a good ridge parameter, *Technometrics* 21 (1979), 215–223.

[31] G. H. Golub and C. F. Van Loan, *Matrix Computations*, 3rd ed, John Hopkins University Press, Baltimore, 1996.

[32] S. Gratton, A. S. Lawless and N. K. Nichols, Approximate Gauss-Newton methods for nonlinear least squares problems, *SIAM Journal on Optimization* 18 (2007), 106–132.

[33] J. Hadamard, *Lectures on Cauchy's problem in linear partial differential equations*, Yale University Press, New Haven, 1923.

[34] M. Hanke, A. Neubauer and O. Scherzer, A convergence analysis of the Landweber iteration for nonlinear ill-posed problems, *Numerische Mathematik* 72 (1995), 21–37.

[35] P. C. Hansen, The truncated SVD as a method for regularization, *BIT* 27 (1987), 534–553.

[36] _____, Analysis of discrete ill-posed problems by means of the L-curve, *SIAM Rev.* 34 (1992), 561–580.

[37] _____, *Rank-deficient and discrete ill-posed problems*, SIAM Monographs on Mathematical Modeling and Computation, SIAM, Philadelphia, PA, 1998.

[38] P. C. Hansen, J. G. Nagy and D. P. O'Leary, *Deblurring images*, Fundamentals of Algorithms 3, SIAM, Philadelphia, PA, 2006.

[39] A. C. Harvey, *Forecasting, structural time series models and the Kalman filter*, Cambridge University Press, Cambridge.

[40] B. Hofmann, *Regularization for applied inverse and ill-posed problems*, Teubner Texts in Mathematics 85, Teubner, Leipzig, 1986.

[41] P. L. Houtekamer and H. L. Mitchell, Data assimilation using an ensemble Kalman filter technique, *Monthly Weather Review* 126 (1998), 796–811.

[42] _____, A sequential ensemble Kalman filter for atmospheric data assimilation, *Monthly Weather Review* 129 (2001), 123–137.

[43] B. R. Hunt, E. J. Kostelich and I. Szunyogh, Efficient data assimilation for spatiotemporal chaos: A local ensemble transform Kalman filter, *Physica D: Nonlinear Phenomena* 230 (2007), 112–126.

[44] K. Ide, P. Courtier, M. Ghil and A. C. Lorenc, Uni ed notation for data assimilation: operational, sequential and variational, *Practice* 75 (1997), 181–189.

[45] C. Johnson, B. J. Hoskins and N. K. Nichols, A singular vector perspective of 4D-Var: Filtering and interpolation, *Quarterly Journal of the Royal Meteorological Society* 131 (2006), 1–19.

[46] R. E. Kalman, A new approach to linear filtering and prediction problems, *Journal of Basic Engineering* 82 (1960), 35–45.

[47] _____, Mathematical description of linear dynamical systems, *Journal of the Society for Industrial & Applied Mathematics, Series A: Control* 1 (1963), 152–192.

[48] E. Kalnay, *Atmospheric modeling, data assimilation, and predictability*, Cambridge University Press, Cambridge, 2002.

[49] A. Kirsch, *An introduction to the mathematical theory of inverse problems*, Springer Verlag, 2011.

[50] F. X. Le Dimet and O. Talagrand, Variational algorithms for analysis and assimilation of meteorological observations: theoretical aspects, *Tellus. Series A, Dynamic meteorology and oceanography* 38 (1986), 97–110.

[51] J. M. Lewis, S. Lakshmivarahan and S. Dhall, *Dynamic data assimilation*, Encyclopedia of Mathematics and its Applications 104, Cambridge University Press, Cambridge, 2006.

[52] H. Li, E. Kalnay, T. Miyoshi and C. M. Danforth, Accounting for model errors in ensemble data assimilation, *Monthly Weather Review* 137 (2009), 3407–3419.

[53] Z. Li and I. M. Navon, Optimality of variational data assimilation and its relationship with the Kalman filter and smoother, *Quarterly Journal of the Royal Meteorological Society* 127 (2006), 661–683.

[54] E. N. Lorenz, Deterministic nonperiodic flow, *Journal of the Atmospheric Sciences* 20 (1963), 130–141.

[55] _____, Predictability: A problem partly solved, in: *Proc. Seminar on Predictability*, 1, 1996.

[56] _____, Designing chaotic models, *Journal of the Atmospheric Sciences* 62 (2005), 1574–1587.

[57] D. McLaughlin, Recent developments in hydrologic data assimilation, *Rev. Geophys* 33 (1995), 977–984.

[58] _____, An integrated approach to hydrologic data assimilation: interpolation, smoothing, and filtering, *Advances in Water Resources* 25 (2002), 1275–1286.

[59] R. Ménard and R. Daley, The application of Kalman smoother theory to the estimation of 4DVAR error statistics, *Tellus A* 48 (1996), 221–237.

[60] A. J. F. Moodey, A. S. Lawless, R. W. E. Potthast and P. J. van Leeuwen, *Nonlinear error dynamics for cycled data assimilation*, Report no. MPS-2012-06, 2013.

[61] V. A. Morozov, *On the solution of functional equations by the method of regularization*, Soviet Math. Dokl, 7, 1966, pp. 414–417.

[62] A. Neumaier, Solving ill-conditioned and singular linear systems: A tutorial on regularization, *Siam Rev.* 40 (1998), 636–666.

[63] N. K. Nichols, *Mathematical Concepts of Data Assimilation*, Data Assimilation: Making Sense of Observations (William Lahoz, Boris Khattatov and Richard Menard, eds.), Springer, 2010, pp. 13–39.

[64] J. M. Ortega and W. C. Rheinboldt, *Iterative solution of nonlinear equations in several variables*, Classics in Applied Mathematics 30, SIAM, Philadelphia, PA, 2000.

[65] E. Ott, B. R. Hunt, I. Szunyogh, A. V. Zimin, E. J. Kostelich, M. Corazza, E. Kalnay, D. J. Patil and J. A. Yorke, A local ensemble Kalman filter for atmospheric data assimilation, *Tellus A* 56 (2004), 415–428.

[66] S. K. Park and L. Xu, *Data assimilation for atmospheric, oceanic and hydrologic applications*, Springer, 2009.

[67] R. W. E. Potthast, A. J. F. Moodey, A. S. Lawless and P. J. van Leeuwen, *On error dynamics and instability in data assimilation*, University of Reading, Preprint, Report no. MPS-2012-06, 2012.

[68] F. Rabier, P. Courtier, J. Pailleux, O. Talagrand and D. Vasiljevic, A comparison between four-dimensional variational assimilation and simplified sequential assimilation relying on three-dimensional variational analysis, *Quarterly Journal of the Royal Meteorological Society* 119 (1993), 845–880.

[69] S. Reich and C. J. Cotter, *Ensemble filter techniques for intermittent data assimilation*, Large Scale Inverse Problems. Computational Methods and Applications in the Earth Sciences (M. Cullen, Freitag M. A., S. Kindermann and R. Scheichl, eds.), Radon Ser. Comput. Appl. Math. 13, Walter de Gruyter, Berlin, 2013, pp. 1–46.

[70] R. H. Reichle, D. B. McLaughlin and D. Entekhabi, Hydrologic data assimilation with the ensemble Kalman filter, *Monthly Weather Review* 130 (2002), 103–114.

[71] A. R. Robinson and P. F. J. Lermusiaux, Overview of data assimilation, *Harvard Reports in Physical/Interdisciplinary (Ocean Sciences)* 62 (2000), Cambridge, Massachusetts, USA.

[72] Y. Sasaki, Some basic formalisms in numerical variational analysis, *Monthly Weather Review* 98 (1970), 875–883.

[73] E. D. Sontag, *Mathematical control theory: deterministic finite dimensional systems*, Springer, 1998.

[74] G. Strang and K. Aarikka, *Introduction to applied mathematics*, Wellesley-Cambridge Press, Wellesley, MA, 1986.

[75] A. M. Stuart, Inverse problems: a Bayesian perspective, *Acta Numerica* 19 (2010), 451–559.

[76] A. M. Stuart and A. R. Humphries, *Dynamical systems and numerical analysis*, Cambridge University Press, Cambridge, 1998.

[77] I. Szunyogh, E. J. Kostelich, G. Gyarmati, E. Kalnay, B. R. Hunt, E. Ott, E. Satterfield and J. A. Yorke, A local ensemble transform Kalman filter data assimilation system for the NCEP global model, *Tellus A* 60 (2008), 113–130.

[78] A. N. Tikhonov and V. Y. Arsenin, *Solutions of ill-posed problems*, John Wiley & Sons, New York, 1977.

[79] M. K. Tippett, J. L. Anderson, C. H. Bishop, T. M. Hamill and J. S. Whitaker, Ensemble square root filters, *Monthly Weather Review* 131 (2003), 1485–1490.

[80] Y. Trémolet, Accounting for an imperfect model in 4D-Var, *Quarterly Journal of the Royal Meteorological Society* 132 (2006), 2483–2504.

[81] K. van den Doel, U. Ascher and E. Haber, *The lost honour of l_2-based regularization*, Large Scale Inverse Problems. Computational Methods and Applications in the Earth Sciences (M. Cullen, Freitag M. A., S. Kindermann and R. Scheichl, eds.), Radon Ser. Comput. Appl. Math. 13, Walter de Gruyter, Berlin, 2013, pp. 1–25.

[82] C. R. Vogel, *Computational methods for inverse problems*, SIAM, Philadelphia, PA, 1987.

[83] T. T. Warner, *Numerical weather and climate prediction*, Cambridge University Press, Cambridge, 2010.

[84] J. S. Whitaker and T. M. Hamill, Ensemble data assimilation without perturbed observations, *Monthly Weather Review* 130 (2002), 1913–1924.

[85] C. K. Wikle and L. M. Berliner, A Bayesian tutorial for data assimilation, *Physica D: Nonlinear Phenomena* 230 (2007), 1–16.

[86] X. X. Zhu and R. Bamler, Tomographic SAR Inversion by L1 Norm Regularization–The Compressive Sensing Approach, *IEEE transactions on Geoscience and Remote Sensing* 48 (2010), 3839–3846.

[87] D. Zupanski, A general weak constraint applicable to operational 4DVAR data assimilation systems, *Monthly Weather Review* 125 (1997), 2274–2292.

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