

Discretization error in dynamical inverse problems: one-dimensional model case

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Abstract. We examine nonstationary inverse problems in which the time evolution of the unknown quantity is modelled by a stochastic partial differential equation. We consider the problem as a state estimation problem. The time discrete state evolution equation is exact since the solution is given by an analytic semigroup. For the practical reasons the space discretization of the time discrete state estimation system must be performed. However, space discretization causes an error and inverse problems are known to be very intolerant to both measurement errors and errors in models. In this paper we analyse the discretization error so that the statistics of the discretization error can be taken into account in the estimation. We are interested in the related filtering problem. A suitable filtering method is presented. We also verify the method using numerical simulation.

1 Introduction

We are interested in the values of a quantity X in a domain along time. We are not able to perform direct measurements of X but a quantity Y can be observed at direct time instants. The interdependence between X and Y is assumed to be known and there is a measurement noise in the measured values of Y . The time evolution of X is presented by a known model with a source term representing possible modelling errors. The aim is to estimate the values of X based on the observed values of Y .

Nonstationary inverse problems are often treated as a state estimation problems, i.e., the quantity of interest X_k and the measurements Y_k at the measurement instants t_k are assumed to satisfy the evolution and observation equations

$$\begin{aligned} X_{k+1} &= f_{k+1}(X_k, W_{k+1}), & k &= 0, 1, \dots, \\ Y_k &= g_k(X_k, S_k), & k &= 1, 2, \dots \end{aligned} \tag{1}$$

where f_k and g_k are known mappings and W_k and S_k are noise processes. Model (1) is called a state estimation system or a state-space model. We want to calculate an estimator for X_k based on observed values of Y_1, \dots, Y_k for all $k \in \mathbb{N}$.

In many applications the exact modelling of a physical phenomenon may lead to a case in which the state of the system is an element in an infinite-dimensional space. For example, in several physical phenomena the state of a system is presented as a function which satisfies a partial differential equation, e.g., the thermal equation or the convection–diffusion equation. However, to treat the state estimation problem numerically, we need to represent the state by means of finitely many degrees of freedom and approximate the exact model with a finite-dimensional model, i.e., discretize the state estimation system (1). Discretization usually causes discrepancy between the solution given by the finite-dimensional model and the exact solution. Since inverse problems are often ill-posed, and hence solutions may be sensitive to errors, discretization errors may have a dramatic

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effect on the quality of the solution. To overcome this problem we can make the finite-dimensional model more accurate, i.e., increase the discretization level. However, that will also increase computational burden and memory consumption.

Approximation and modelling errors in stationary inverse problems have been researched in [5, 6]. In these references approximation and modelling errors are examined using statistical analysis. In addition, a method which takes an approximation error into account and allows a lower discretization level without weakening the quality of the solution to an estimation problem is introduced. The method is based on Bayesian inversion theory. The method has been applied to several applications, for example, image reconstruction [5], electrical impedance tomography [5] and optical tomography [2].

Discretization error in nonstationary inverse problems has been studied in [12, 13, 4]. In paper [4] discretization errors are approximated by the discrepancy between two different finite-dimensional models. In references [12, 13] the distribution of approximation errors are determined by using an infinite-dimensional model. This has such an advantage that the tenability of the distributions of discretization errors do not depend on any of our choices related to discretization. In addition, the use of an infinite-dimensional model gives us a straightforward way to determine the distributions of the initial state and the state noise. In finite-dimensional models the choice of the initial state and the state noise is usually somehow based on discretization or a mesh. Therefore if the discretization level is changed, the statistical properties of the initial state and the state noise are not necessarily reserved properly. This cannot occur when the distributions of the initial state and the state noise are determined based on an infinite-dimensional model and are discretized properly.

In this paper we carry out a further research of the study in [12, 13]. We examine the presented method using a numerical example. In addition, the estimation problem is solved using the filtering method presented in [4] which is more usable from the practical point of view than the method presented in [13].

For simplicity, the discussion in [12, 13] and here have been restricted to linear nonstationary inverse problems in which the time evolution of the state of system is modelled by a (stochastic) parabolic partial differential equation under certain assumptions. The temporal discretization of the continuous infinite-dimensional state estimation system is exact since the solution to the evolution equation is given by an analytic semigroup. Hence the space discretization is only analysed.

This paper is divided into the following sections. In section 2 we represent an infinite-dimensional state estimation system and its discretization. In section 3 we give a brief description of the estimation algorithm used in this paper. The one-dimensional model case with the numerical implementation is introduced in section 4. Discussion is given in section 5.

2 Discretized state estimation system

In this section we summarize results concerning the discretization of the linear state estimation system presented in paper [13]. We concentrate on the case where the state estimation equation is given by a second order stochastic partial differential equation.

Let $D \subset \mathbb{R}^d$ be a domain that corresponds to the object of interest. We denote by

$X = X(t, x)$, $x \in D$, the unknown distribution of the physical quantity we are interested in at time $t \geq 0$. We assume that $X(t, \cdot)$ belong to $L^2(D)$ for every $t \geq 0$.

Assumption 1. Let D be either \mathbb{R}^d or an open subset of \mathbb{R}^d with uniformly C^2 -smooth boundary ∂D . Let a_{ij} , b_i and c be bounded uniformly continuous functions from \bar{D} to \mathbb{R} and β_i and γ be bounded uniformly continuously differentiable functions from \bar{D} to \mathbb{R} for all $i, j = 1, \dots, d$. We assume that the matrix $[a_{ij}(x)]_{i,j=1}^d$ is symmetric for all $x \in \bar{D}$ and

$$\sum_{i,j=1}^d a_{ij}(x) \xi_i \xi_j \geq \delta |\xi|^2$$

for all $x \in \bar{D}$ and $\xi \in \mathbb{R}^d$ with some $\delta > 0$. If D is a proper subset of \mathbb{R}^d , we suppose that

$$\inf_{x \in \partial D} \left| \sum_{i=1}^d \beta_i(x) n_i(x) \right| > 0$$

where $n(x) = (n_1(x), \dots, n_d(x))$ is the exterior unit normal vector to ∂D at a point $x \in \partial D$.

Let assumption 1 be fulfilled. We define an elliptic second order differential operator A by

$$A : \mathcal{D}(A) \subset L^2(D) \rightarrow L^2(D), \quad f \mapsto \sum_{i,j=1}^d a_{ij} \partial_i \partial_j f + \sum_{i=1}^d b_i \partial_i f + c f$$

where

$$\mathcal{D}(A) = \left\{ f \in H^2(D) : \left(\sum_{i=1}^d \beta_i \partial_i f + \gamma f \right) \Big|_{\partial D} = 0 \right\}.$$

We would like to model the time evolution of the quantity X by the parabolic PDE

$$\frac{d}{dt} X(t, x) = AX(t, x) \tag{2}$$

for all $t > 0$ and $x \in D$. Since we cannot be sure that equation (2) is the correct evolution model for X , we suppose that instead of being a deterministic function X is a stochastic process $\{X(t)\}_{t \geq 0}$ with values in $L^2(D)$. The stochastic nature of X allows us to incorporate modelling uncertainties into the time evolution model.

Assumption 2. Let $x_0 \in L^2(D)$, Γ_0 and Q be positive self-adjoint trace class operators from $L^2(D)$ to itself with trivial null spaces, and $T > 0$.

When assumption 2 is valid, according to Kolmogorov's existence theorem [15, remark II.9.2] there exist a probability space $(\Omega, \mathcal{F}, \mathbb{P})$, a Q -Wiener process $W(t)$, $t \in [0, T]$, in $(\Omega, \mathcal{F}, \mathbb{P})$ with values in $L^2(D)$ and an $L^2(D)$ -valued random variable X_0 in $(\Omega, \mathcal{F}, \mathbb{P})$ such that X_0 and $W(t)$ are independent for all $t \in (0, T]$ and X_0 is Gaussian with mean x_0 and covariance Γ_0 [14, propositions 2.18 and 4.2]. The time evolution of the process X is modelled by the stochastic partial differential equation

$$dX(t) = AX(t)dt + dW(t) \tag{3}$$

for every $t > 0$ with the initial value

$$X(0) = X_0. \tag{4}$$

The term $dW(t)$ is a source term representing possible modelling errors in the time evolution model.

Let $Y = Y(t)$ denote the quantity that we are able to measure for all $t > 0$. Since in practical measurements only finite-dimensional elements can be observed, we suppose that the values of Y belongs to the space \mathbb{R}^L . We assume that the dependence of Y upon the state X is known up to an observation noise. The quantity Y is described by the stochastic process $\{Y(t)\}_{t \in (0, T]}$ with values in \mathbb{R}^L . The measurement process is modelled by the equation

$$Y(t) = C(t)X(t) + S(t)$$

for all $0 < t \leq T$ where $\{C(t)\}_{t \in (0, T]}$ is a family of bounded linear operators from $L^2(D)$ to \mathbb{R}^L and $S(t)$, $t \in [0, T]$, is an \mathbb{R}^L -valued stochastic process. The process S represents possible measurement errors.

According to assumption 1 the operator A generates a strongly continuous analytic semigroup $\{U(t)\}_{t \geq 0}$ [9, chapters 2–3]. Therefore there exists the weak solution to the state evolution equation (3) with the initial value (4) [14, theorem 5.4]. We assume that the measurements are made in time instants $0 < t_1 < \dots < t_n \leq T$. We use the notation $t_0 := 0$ and $\Delta_{k+1} := t_{k+1} - t_k$ for all $k = 0, \dots, n-1$. Furthermore, we denote $C_k := C(t_k)$, $S_k := S(t_k)$, $X_k := X(t_k)$ and $Y_k := Y(t_k)$ for all $k = 1, \dots, n$. Then the time discrete state estimation system is

$$X_{k+1} = U(\Delta_{k+1})X_k + W_{k+1}, \quad k = 0, \dots, n-1, \quad (5)$$

$$Y_k = C_k X_k + S_k, \quad k = 1, \dots, n \quad (6)$$

where the state noise W_{k+1} is given by the formula

$$W_{k+1} = \int_{t_k}^{t_{k+1}} U(t_{k+1} - s) dW(s).$$

The time discrete estimation system (5)–(6) is exact since the state evolution equation (3) with the initial value (4) is solved by using the analytic semigroup $\{U(t)\}_{t \geq 0}$.

The realizations of the process X are in the space $L^2(D)$. We want to discretize in space the time discrete state estimation system (5)–(6). We choose a finite-dimensional subspace of $L^2(D)$ and assume that the realizations of the process X are in that subspace. Since we want that the projection of X to the chosen subspace is in some sense close to X , we choose the subspace from a sequence of appropriate discretization spaces. The family $\{V_m\}_{m=1}^\infty$ of finite-dimensional subspaces of $L^2(D)$ is called a sequence of appropriate discretization spaces in $L^2(D)$ if $V_m \subset V_{m+1}$ for all $m \in \mathbb{N}$ and $\overline{\cup V_m} = L^2(D)$. Then the projections to the subspaces converge pointwise to the identity operator. Hence $\|X_k(\omega) - P_m X_k(\omega)\|_{L^2(D)} \rightarrow 0$ as $m \rightarrow \infty$ for all $k = 0, \dots, n$ and $\omega \in \Omega$ where P_m is the projection from $L^2(D)$ to V_m for all $m \in \mathbb{N}$.

Let $\{V_m\}_{m=1}^\infty$ be a sequence of appropriate discretization spaces in $L^2(D)$ and $\{\psi_l^m\}_{l=1}^{N_m}$ be an orthonormal basis of V_m for all $m \in \mathbb{N}$. The projection of an $L^2(D)$ -valued random variable Z to the subspace V_m can be identified with the vector containing the coordinates in the basis $\{\psi_l^m\}_{l=1}^{N_m}$, i.e., $Z^m := ((Z, \psi_1^m), (Z, \psi_2^m), \dots, (Z, \psi_{N_m}^m))^T$ for all $m \in \mathbb{N}$. We view Z^m as a discretized version of the random variable Z at the discretization level m . If Z is a Gaussian random variable, Z^m is a normal \mathbb{R}^{N_m} -valued random variable [10, theorem A.5].

Let the discretization level m be fixed. We denote by (\cdot, \cdot) the inner product in $L^2(D)$. By using the time discrete state evolution equation (5) we obtain

$$\begin{aligned} (X_{k+1}^m)_i &= (U(\Delta_{k+1})X_k + W_{k+1}, \psi_i^m) \\ &= (U(\Delta_{k+1})P_m X_k, \psi_i^m) + (U(\Delta_{k+1})X_k - U(\Delta_{k+1})P_m X_k, \psi_i^m) + (W_{k+1}, \psi_i^m) \\ &= \sum_{j=1}^{N_m} (U(\Delta_{k+1})\psi_j^m, \psi_i^m)(X_k^m)_j + (\epsilon_{k+1}^m)_i + (W_{k+1}^m)_i \end{aligned}$$

for all $i = 1, \dots, N_m$ where the stochastic process

$$\epsilon_{k+1}^m = ((X_k, (I - P_m)U^*(\Delta_{k+1})\psi_1^m), \dots, (X_k, (I - P_m)U^*(\Delta_{k+1})\psi_{N_m}^m))^T$$

represents the discretization error in the evolution equation and

$$W_{k+1}^m = ((W_{k+1}, \psi_1^m), \dots, (W_{k+1}, \psi_{N_m}^m))^T$$

is the state noise vector for all $k = 0, \dots, n-1$. By the Riesz representation theorem there exist functions $\varphi_p^{(k)} \in L^2(D)$ such that $(C_k f)_p = (f, \varphi_p^{(k)})$ for all $f \in L^2(D)$, $k = 1, \dots, n$ and $p = 1, \dots, L$. Thus

$$\begin{aligned} (Y_k)_p &= (X_k, \varphi_p^{(k)}) + (S_k)_p = (P_m X_k, \varphi_p^{(k)}) + (X_k - P_m X_k, \varphi_p^{(k)}) + (S_k)_p \\ &= \sum_{j=1}^{N_m} (\psi_j^m, \varphi_p^{(k)}) (X_k^m)_j + (\nu_k^m)_p + (S_k)_p \end{aligned}$$

for all $p = 1, \dots, L$ where the process

$$\nu_k^m = \left((X_k, (I - P_m)\varphi_1^{(k)}), \dots, (X_k, (I - P_m)\varphi_L^{(k)}) \right)^T$$

represents the discretization error in the observation equation for all $k = 0, \dots, n-1$.

Let A_k^m and C_k^m be matrices given by

$$(A_k^m)_{ij} := (U(\Delta_k)\psi_j^m, \psi_i^m) \quad \text{and} \quad (C_k^m)_{pj} := (\psi_j^m, \varphi_p^{(k)})$$

for all $i, j = 1, \dots, N_m$, $k = 1, \dots, n$ and $p = 1, \dots, L$. Then the state estimation system for the finite-dimensional processes $\{X_k^m\}_{k=0}^n$ and $\{Y_k\}_{k=1}^n$ is

$$X_{k+1}^m = A_{k+1}^m X_k^m + \epsilon_{k+1}^m + W_{k+1}^m, \quad k = 0, \dots, n-1, \quad (7)$$

$$Y_k = C_k^m X_k^m + \nu_k^m + S_k, \quad k = 1, \dots, n. \quad (8)$$

Equations (7) and (8) form a state estimation system whose statistics conform to the time discrete state estimation system (5)–(6).

3 Solution to the discretized filtering problem

We denote the random variables which we are able to observe by $D_k := (Y_k^T, Y_{k-1}^T, \dots, Y_1^T)^T$ and the measured data, i.e., a realization of D_k by $d_k := (y_k^T, y_{k-1}^T, \dots, y_1^T)^T$ for all $k = 1, \dots, n$. We are interested in a real-time monitoring for the quantity X . Hence for all $k = 1, \dots, n$ we want to find an estimate for the state X_k^m based on the measurements up to the time instant t_k , i.e., based on $D_k = d_k$. From the statistical point of view

all available information about X_k^m provided by these measurements is contained in the conditional distribution of X_k^m given $D_k = d_k$ denoted by $\bar{\mu}_k$. The aim in this section is to determine $\bar{\mu}_k$ for all $k = 1, \dots, n$.

The state noise W_{k+1} is a Gaussian random variable for all $k = 0, \dots, n-1$ [13, p. 368]. Hence the state noise vectors are normal. Furthermore, W_{k+1}^m is independent of X_l^m and ϵ_{l+1}^m for all $l \leq k$ and $k = 0, \dots, n-1$, and the state noise vectors W_k^m and W_l^m are mutually independent for all $k \neq l$ [13, pp. 371–372]. For the observation noise we make the following assumption.

Assumption 3. *The observation noise vectors S_k are chosen such a way that they are normal random variables, the mean $\mathbb{E}S_k$ is zero and S_k is independent of X_0 for all $k = 1, \dots, n$. In addition, S_k and S_l are mutually independent for all $k \neq l$ and S_k and W_l^m are mutually independent for all $k, l = 1, \dots, n$.*

Let $k \in \{1, \dots, n\}$. With assumption 3 the joint distribution of X_k^m and D_k is normal [13, lemma 1]. Hence the conditional distribution of X_k^m given $D_k = d_k$ is also a normal distribution (e.g., see [5, theorem 3.5]) and is determined by the expectation and the covariance matrix. We could solve the expectation $\bar{\eta}_k$ and the covariance matrix $\bar{\Sigma}_k$ of $\bar{\mu}_k$ from the formulae (e.g., see [5, theorem 3.5])

$$\bar{\eta}_k = \mathbb{E}X_k^m + \text{cor}(X_k^m, D_k) \text{cov}(D_k)^{-1}(d_k - \mathbb{E}D_k), \quad (9)$$

$$\bar{\Sigma}_k = \text{cov} X_k^m - \text{cor}(X_k^m, D_k) \text{cov}(D_k)^{-1} \text{cor}(X_k^m, D_k)^T. \quad (10)$$

However, the dimension of the estimation problem increases over time, especially if the number of measurements is large. Hence, instead of using equations (9) and (10), the estimation problem is usually solved using recursive methods in which the task is reduced to determining $\bar{\mu}_{k+1}$ from $\bar{\mu}_k$ based on the state-space model and the information provided by the measurement y_{k+1} .

A widely used recursive method to solve filtering problems concerning finite-dimensional state estimation systems is the Kalman filter (e.g., see [7, 1, 3]). In the Kalman filtering method it is assumed that the noise terms are independent of the state. In our case, the terms ϵ_{k+1}^m and ν_k^m representing the discretation errors depend on X_k^m for all k . Hence we cannot use the Kalman filtering method. In paper [4] a filtering method for the case where noise terms depend on the state is introduced. We use that method to solve the discretized filtering problem.

We calculate also the conditional distribution of X_{k+1}^m given $D_k = d_k$ denoted by $\tilde{\mu}_{k+1}$ for all $k = 0, \dots, n-1$. The distribution $\tilde{\mu}_{k+1}$ is normal [13, lemma 1] and [5, theorems 3.5 and 3.6]. For shortening the notation the expectation of $\tilde{\mu}_{k+1}$ is marked with $\tilde{\eta}_{k+1}$ and the covariance matrix with $\tilde{\Sigma}_{k+1}$. In future, for square-integrable random variables Z_1 and Z_2 we denote by $\mathbb{E}^{d_k}(Z_1)$ and $\text{cov}^{d_k}(Z_1)$ the conditional expectation and covariance of Z_1 given $D_k = d_k$, respectively, and by $\text{cor}^{d_k}(Z_1, Z_2)$ the conditional cross-correlation of Z_1 and Z_2 given $D_k = d_k$ for all $k = 1, \dots, n$. For $k = 0$ we set $\mathbb{E}^{d_0}(Z_1) = \mathbb{E}Z_1$, $\text{cor}^{d_0}(Z_1) = \text{cor}(Z_1)$ and $\text{cor}^{d_0}(Z_1, Z_2) = \text{cor}(Z_1, Z_2)$. The solution to the discretized filtering problem is given by the following theorem, which summarizes the results given in [4].

Theorem 4. *We suppose that assumptions 1, 2 and 3 are fulfilled. The expectations and*

the covariance matrices of the conditional distributions $\bar{\mu}_{k+1}$ and $\tilde{\mu}_{k+1}$ are given by

$$\tilde{\eta}_{k+1} = A_{k+1}^m \bar{\eta}_k + \mathbb{E}^{d_k}(\epsilon_{k+1}^m), \quad (11)$$

$$\begin{aligned} \tilde{\Sigma}_{k+1} &= A_{k+1}^m \bar{\Sigma}_k (A_{k+1}^m)^T + \text{cov}^{d_k}(\epsilon_{k+1}^m) + \text{cov}(W_{k+1}^m) \\ &\quad + A_{k+1}^m \text{cor}^{d_k}(X_k^m, \epsilon_{k+1}^m) + \text{cor}^{d_k}(\epsilon_{k+1}^m, X_k^m) (A_{k+1}^m)^T, \end{aligned} \quad (12)$$

$$\bar{\eta}_{k+1} = \tilde{\eta}_{k+1} + K_{k+1}^m \left(y_{k+1} - C_k^m \tilde{\eta}_{k+1} - \mathbb{E}^{d_k}(\nu_{k+1}^m) \right), \quad (13)$$

$$\bar{\Sigma}_{k+1} = \tilde{\Sigma}_{k+1} - K_{k+1}^m \left(C_k^m \tilde{\Sigma}_{k+1} + \text{cor}^{d_k}(\nu_{k+1}^m, X_{k+1}^m) \right) \quad (14)$$

for all $k = 0, \dots, n-1$ where the matrix K_{k+1}^m is

$$\begin{aligned} K_{k+1}^m &= \left(\tilde{\Sigma}_{k+1} (C_k^m)^T + \text{cor}^{d_k}(X_{k+1}^m, \nu_{k+1}^m) \right) \\ &\quad \times \left\{ C_k^m \tilde{\Sigma}_{k+1} (C_k^m)^T + \text{cov}^{d_k}(\nu_{k+1}^m) + \text{cov}(S_{k+1}) \right. \\ &\quad \left. + C_k^m \text{cor}^{d_k}(X_{k+1}^m, \nu_{k+1}^m) + \text{cor}^{d_k}(\nu_{k+1}^m, X_{k+1}^m) (C_k^m)^T \right\}^{-1}. \end{aligned} \quad (15)$$

Equations (11)–(15) can be used to solve the filtering problem recursively if the conditional expectations, the conditional covariance matrices and the conditional cross-correlation matrices related to ϵ_{k+1}^m and ν_k^m are known for all k .

3.1 The distributions of the error vectors ϵ_{k+1}^m , ν_k^m and W_k^m

To be able to solve the filtering problem concerning the discretized state estimation system (7)–(8) we need to determine the vectors $\mathbb{E}^{d_k}(\epsilon_{k+1}^m)$ and $\mathbb{E}^{d_k}(\nu_{k+1}^m)$ and the matrices $\text{cov}^{d_k}(\epsilon_{k+1}^m)$, $\text{cov}^{d_k}(\nu_{k+1}^m)$, $\text{cor}^{d_k}(X_k^m, \epsilon_{k+1}^m)$, $\text{cor}^{d_k}(X_{k+1}^m, \nu_{k+1}^m)$ and $\text{cov}(W_{k+1}^m)$ for all $k = 0, \dots, n-1$. Since the joint distribution of the discretization errors and the measurement is normal (proved similarly as [13, lemma 1]), we could solve, for example, the conditional distributions of ϵ_{k+1}^m given $D_k = d_k$ by using similar formulae as (9)–(10) for all $k = 0, \dots, n-1$ (e.g., see [5, theorem 3.5]). However, also in that case the dimension of the problem increases over time and that is what we wanted to avoid. Therefore we choose an another approach.

By the definition of ϵ_{k+1}^m ,

$$\begin{aligned} (\mathbb{E}^{d_k}(\epsilon_{k+1}^m))_i &= (\mathbb{E}^{d_k}(X_k), (I - P_m)U^*(\Delta_{k+1})\psi_i^m), \\ (\text{cov}^{d_k}(\epsilon_{k+1}^m))_{ij} &= (\text{cov}^{d_k}(X_k)(I - P_m)U^*(\Delta_{k+1})\psi_j^m, (I - P_m)U^*(\Delta_{k+1})\psi_i^m), \\ (\text{cor}^{d_k}(X_k^m, \epsilon_{k+1}^m))_{ij} &= (\text{cov}^{d_k}(X_k)(I - P_m)U^*(\Delta_{k+1})\psi_j^m, \psi_i^m) \end{aligned}$$

for all $i, j = 1, \dots, N_m$ and $k = 0, \dots, n-1$. Furthermore, for ν_{k+1}^m we have

$$\begin{aligned} (\mathbb{E}^{d_k}(\nu_{k+1}^m))_p &= \left(\mathbb{E}^{d_k}(X_{k+1}), (I - P_m)\varphi_p^{(k+1)} \right), \\ (\text{cov}^{d_k}(\nu_{k+1}^m))_{pq} &= \left(\text{cov}^{d_k}(X_{k+1})(I - P_m)\varphi_q^{(k+1)}, (I - P_m)\varphi_p^{(k+1)} \right), \\ (\text{cor}^{d_k}(X_{k+1}^m, \nu_{k+1}^m))_{ip} &= \left(\text{cov}^{d_k}(X_{k+1})(I - P_m)\varphi_p^{(k+1)}, \psi_i^m \right) \end{aligned}$$

for all $i = 1, \dots, N_m$, $k = 0, \dots, n-1$ and $p, q = 1, \dots, L$. There is no straightforward way to calculate the conditional expectations $\mathbb{E}^{d_k}(X_k)$ and $\mathbb{E}^{d_k}(X_{k+1})$ and the conditional

covariances $\text{cov}^{d_k}(X_k)$ and $\text{cov}^{d_k}(X_{k+1})$ for all $k = 0, \dots, n-1$. Hence we neglect the dependence of the measurements and approximate $\mathbb{E}^{d_k}(X_k) \approx \mathbb{E}X_k$, $\mathbb{E}^{d_k}(X_{k+1}) \approx \mathbb{E}X_{k+1}$, $\text{cov}^{d_k}(X_k) \approx \text{cov}(X_k)$ and $\text{cov}^{d_k}(X_{k+1}) \approx \text{cov}(X_{k+1})$ for all $k = 0, \dots, n-1$. By performing the approximation the conditional expectations, the conditional covariances and the conditional correlations of the discretization errors are replaced by the regular ones. For example, $\mathbb{E}^{d_k}(\epsilon_{k+1}^m)$ is replaced by $\mathbb{E}(\epsilon_{k+1}^m)$ for all $k = 0, \dots, n-1$. The error related to the replacement of the conditional expectations, the conditional covariances and the conditional correlations with the regular ones is not analysed in this paper.

The preceding approximations yield the following formulae (see [13] for details). The expectations of the discretation errors are

$$\mathbb{E}(\epsilon_{k+1}^m) = [(U(t_{k+1})x_0, \psi_i^m)]_{i=1}^{N_m} - A_{k+1}^m [(U(t_k)x_0, \psi_i^m)]_{i=1}^{N_m} \quad (16)$$

and

$$\mathbb{E}(\nu_{k+1}^m) = \left[(U(t_{k+1})x_0, \varphi_p^{(k+1)}) \right]_{p=1}^L - C_{k+1}^m [(U(t_{k+1})x_0, \psi_i^m)]_{i=1}^{N_m} \quad (17)$$

for all $k = 0, \dots, n-1$. For shortening the notation we denote

$$\begin{aligned} (\Gamma_{k,l}^\psi)_{ij} &:= (U(t_k)\Gamma_0 U^*(t_l)\psi_i^m, \psi_j^m), \\ (\Gamma_{k,l}^{\psi,\varphi})_{ip} &:= (U(t_k)\Gamma_0 U^*(t_l)\psi_i^m, \varphi_p^{(k)}), \\ (\Gamma_{k,l}^\varphi)_{pq} &:= (U(t_k)\Gamma_0 U^*(t_l)\varphi_p^{(l)}, \varphi_q^{(k)}), \\ (Q_{k,l}^\psi(s))_{ij} &:= (U(t_k-s)QU^*(t_l-s)\psi_i^m, \psi_j^m), \\ (Q_{k,l}^{\psi,\varphi}(s))_{ip} &:= (U(t_k-s)QU^*(t_l-s)\psi_i^m, \varphi_p^{(k)}), \\ (Q_{k,l}^\varphi(s))_{pq} &:= (U(t_k-s)QU^*(t_l-s)\varphi_p^{(l)}, \varphi_q^{(k)}) \end{aligned}$$

for all $i, j = 1, \dots, N_m$, $k, l = 0, \dots, n$, $p, q = 1, \dots, L$ and $s \in [0, t_k \wedge t_l]$. Then the covariance matrices of the discretization errors are

$$\begin{aligned} \text{cov}(\epsilon_{k+1}^m) &= \Gamma_{k+1,k+1}^\psi - \Gamma_{k,k+1}^\psi (A_{k+1}^m)^T - A_{k+1}^m \Gamma_{k+1,k}^\psi + A_{k+1}^m \Gamma_{k,k}^\psi (A_{k+1}^m)^T \\ &\quad + \int_0^{t_k} \left[Q_{k+1,k+1}^\psi(s) - Q_{k,k+1}^\psi(s) (A_{k+1}^m)^T \right] ds \\ &\quad - \int_0^{t_k} \left[A_{k+1}^m Q_{k+1,k}^\psi(s) - A_{k+1}^m Q_{k,k}^\psi(s) (A_{k+1}^m)^T \right] ds \end{aligned} \quad (18)$$

and

$$\begin{aligned} \text{cov}(\nu_{k+1}^m) &= \Gamma_{k+1,k+1}^\varphi - C_{k+1}^m \Gamma_{k+1,k+1}^{\psi,\varphi} - (C_{k+1}^m \Gamma_{k+1,k+1}^{\psi,\varphi})^T + C_{k+1}^m \Gamma_{k+1,k+1}^\psi (C_{k+1}^m)^T \\ &\quad + \int_0^{t_{k+1}} \left[Q_{k+1,k+1}^\varphi(s) - C_{k+1}^m Q_{k+1,k+1}^{\psi,\varphi}(s) \right] ds \\ &\quad - \int_0^{t_{k+1}} \left[Q_{k+1,k+1}^{\psi,\varphi}(s)^T (C_{k+1}^m)^T - C_{k+1}^m Q_{k+1,k+1}^\psi(s) (C_{k+1}^m)^T \right] ds \end{aligned} \quad (19)$$

for all $k = 0, \dots, n-1$. The correlation of the process X_k^m and discretization errors are

$$\text{cor}(X_k^m, \epsilon_{k+1}^m) = \Gamma_{k+1,k}^\psi - \Gamma_{k,k}^\psi (A_{k+1}^m)^T + \int_0^{t_k} \left[Q_{k+1,k}^\psi(s) - Q_{k,k}^\psi(s) (A_{k+1}^m)^T \right] ds \quad (20)$$

and

$$\begin{aligned} \text{cor}(X_{k+1}^m, \nu_{k+1}^m) &= \Gamma_{k+1,k+1}^{\psi,\varphi} - \Gamma_{k+1,k+1}^{\psi} (C_{k+1}^m)^T \\ &\quad + \int_0^{t_{k+1}} \left[Q_{k+1,k+1}^{\psi,\varphi}(s) - Q_{k+1,k+1}^{\psi}(s) (C_{k+1}^m)^T \right] ds \end{aligned} \quad (21)$$

for all $k = 0, \dots, n-1$.

With the same notation the covariance matrix of the state noise vector is (see [13] for details)

$$\text{cov}(W_{k+1}^m) = \int_{t_k}^{t_{k+1}} Q_{k+1,k+1}^{\psi}(s) ds \quad (22)$$

for all $k = 0, \dots, n-1$.

4 One-dimensional model case

As an example of nonstationary inverse problems we examine a one-dimensional model for process tomography. We are interested in the real-time monitoring of the concentration distribution of a given substance in a fluid moving in a pipeline. We assume that the concentration distribution is rotationally symmetrical. Then we can use a one-dimensional model. Since we do not want to use inexact boundary conditions in the input and output end of the pipe, we suppose that the pipeline is infinitely long. The time evolution of the concentration distribution is modelled by the stochastic convection–diffusion equation. Measurements are obtained by observing point values of the concentration distribution through a blurring kernel and an additive noise. We view the problem as a state estimation problem and use the methods of the previous section to solve the corresponding discretized filtering problem. This problem is partly presented in doctoral thesis [12]. The numerical implementation of the problem was not included to the dissertation.

Let $x_0 \in L^2(\mathbb{R})$, Γ_0 and Q be positive self-adjoint trace class operators from $L^2(\mathbb{R})$ to itself with trivial null spaces, and $T > 0$. There exist a probability space $(\Omega, \mathcal{F}, \mathbb{P})$, an $L^2(\mathbb{R})$ -valued Q -Wiener process $\{W(t)\}_{t \in [0, T]}$, and an $L^2(\mathbb{R})$ -valued Gaussian random variable X_0 with mean x_0 and covariance Γ_0 such that X_0 and $W(t)$ are independent for all $t \in (0, T]$. The time evolution of the concentration distribution X is modelled by the stochastic initial value problem

$$\begin{cases} dX(t) = AX(t)dt + dW(t), & t > 0, \\ X(0) = X_0 \end{cases} \quad (23)$$

where the operator A is defined by

$$A : H^2(\mathbb{R}) \rightarrow L^2(\mathbb{R}), \quad f \mapsto \frac{d}{dx} \left(\kappa(x) \frac{d}{dx} f \right) - v(x) \frac{d}{dx} f. \quad (24)$$

For simplicity we assume that the diffusion coefficient and the velocity of the flow do not depend on the space variable, i.e., $\kappa(x) = \kappa > 0$ and $v(x) = v > 0$ for all $x \in \mathbb{R}$. Measurements are made in time instants $0 < t_1 < \dots < t_n \leq T$ and are described by the observation equation

$$Y_k = CX_k + S_k \quad (25)$$

for all $k = 1, \dots, n$. The operator $C : L^2(\mathbb{R}) \rightarrow \mathbb{R}^L$ is defined by

$$(Cf)_p = \int_{-\infty}^{\infty} f(x) \varphi_p(x) dx = (f, \varphi_p)$$

for all $p = 1, \dots, L$ with

$$\varphi_p(x) = \frac{1}{2w_p} \exp\left(-\frac{|x - x_p|}{w_p}\right) \quad (26)$$

for all $x \in \mathbb{R}$ where $x_p \in \mathbb{R}$ is a measurement position and $0 < w_p < 1$. The normal \mathbb{R}^L -valued process $\{S_k\}_{k=1}^n$ represents possible measurement errors.

To be able to solve numerically the filtering problem related to the state estimation system (23) and (25) we need to define the strongly continuous analytic semigroup generated by the operator A , the covariance operator Q of the Wiener process, the mean x_0 and the covariance operator Γ_0 of the initial value, and a sequence of appropriate discretization spaces $\{V_m\}_{m=1}^\infty$ in $L^2(\mathbb{R})$.

4.1 Analytic semigroup

The convection–diffusion operator A defined by (24) where $\kappa, v > 0$ generates an analytic semigroup [12, theorem 6.5]. Furthermore, the semigroup is strongly continuous. In general, the analytic semigroup is defined by using the spectral properties of the infinitesimal generator. However, the solution to the initial value problem

$$\begin{cases} \frac{\partial}{\partial t} f(t, x) = \kappa \frac{\partial^2}{\partial x^2} f(t, x) - v \frac{\partial}{\partial x} f(t, x), & t > 0, \\ f(0, x) = f_0(x), \end{cases} \quad (27)$$

where $f_0 \in L^2(\mathbb{R})$, is given by the analytic semigroup generated by the convection–diffusion operator A [11, corollary 4.1.5]. By solving the initial value problem (27) using other techniques we are able to find the analytic semigroup generated by the convection–diffusion operator. We use an Itô diffusion [10, definition 7.1.1] to solve the initial value problem (27) when $f_0 \in C_0^2(\mathbb{R})$ and then generalize the form of the solution to the initial values $f_0 \in L^2(\mathbb{R})$.

Let $B(t)$ be a one-dimensional Brownian motion for all $t \geq 0$. The generator of the Itô diffusion

$$\begin{cases} dZ(t) = -vdt + \sqrt{2\kappa}dB(t), \\ Z(0) = x \end{cases}$$

is the convection–diffusion operator A and $C_0^2(\mathbb{R}) \subset \mathcal{D}(A)$ [10, theorem 7.3.3]. Thus the solution to the initial value problem (27) where $f_0 \in C_0^2(\mathbb{R})$ is

$$f(t, x) = \mathbb{E}^x[f_0(Z(t))]$$

for all $t > 0$ and $x \in \mathbb{R}$ [10, theorem 8.1.1] where \mathbb{E}^x is the expectation with respect to the distribution of the Itô diffusion Z assuming that $Z(0) = x$. But $Z^x(t) = x - vt + \sqrt{2\kappa}B(t)$ for all $t > 0$. Thus $Z^x(t) \sim \mathcal{N}(x - vt, 2\kappa t)$ for all $t > 0$ and the probability density of $Z^x(t)$ is

$$\pi_{Z^x}(y) = \frac{1}{2\sqrt{\pi\kappa t}} \exp\left(-\frac{(x - y - vt)^2}{4\kappa t}\right)$$

for all $y \in \mathbb{R}$. Hence

$$f(t, x) = \mathbb{E}[f_0(x - vt + \sqrt{2\kappa}B(t))] = \frac{1}{2\sqrt{\pi\kappa t}} \int_{-\infty}^{\infty} f_0(y) e^{-\frac{(x - y - vt)^2}{4\kappa t}} dy$$

for all $t > 0$ and $x \in \mathbb{R}$. Let us denote

$$\Phi(t, x) = \frac{1}{2\sqrt{\pi\kappa t}} \exp\left(-\frac{(x - vt)^2}{4\kappa t}\right)$$

for all $t > 0$ and $x \in \mathbb{R}$. Then the solution to the initial value problem (27) is the convolution of the initial value f_0 with the probability density Φ , i.e., $f(t, x) = (\Phi(t, \cdot) * f_0)(x)$ for all $t > 0$ and $x \in \mathbb{R}$ if $f_0 \in C_0^2(\mathbb{R})$. We want to generalize this result to $L^2(\mathbb{R})$ -initial values.

We define the operator family $\{U(t)\}_{t \geq 0}$ by

$$\begin{cases} U(0)f = f, \\ (U(t)f)(x) = (\Phi(t, \cdot) * f)(x), \quad t > 0, \end{cases}$$

for all $f \in L^2(\mathbb{R})$. Then $U(t)$ is a bounded linear operator from $L^2(\mathbb{R})$ to itself for all $t \geq 0$. Furthermore, $\{U(t)\}_{t \geq 0}$ is a semigroup. Let $f_0 \in L^2(\mathbb{R})$. The solution to the initial value problem (27) is $f(t, x) = U(t)f_0(x)$ for all $t \geq 0$ and $x \in \mathbb{R}$ because $f(0, x) = U(0)f_0(x) = f_0(x)$ and

$$\left(\frac{\partial}{\partial t} - \kappa \frac{\partial^2}{\partial x^2} + v \frac{\partial}{\partial x} \right) f(t, x) = \left(\left(\frac{\partial}{\partial t} - \kappa \frac{\partial^2}{\partial x^2} + v \frac{\partial}{\partial x} \right) \Phi(t, \cdot) \right) * f_0(x) = 0.$$

Hence the semigroup $\{U(t)\}_{t \geq 0}$ is the strongly continuous analytic semigroup generated by the convection–diffusion operator [11, corollary 4.1.5].

4.2 Wiener process and the initial value

Our prior knowledge of the application we are interested in is coded into the choice of the initial value and the covariance operator of the Wiener process. In this model case our prior assumption is that the concentration distribution is almost uniform because in some real life applications that may be expected. Hence the mean of the initial value could be a constant function. Since the mean of an $L^2(\mathbb{R})$ -valued Gaussian random variable should belong to $L^2(\mathbb{R})$ [12, proposition 4.17], we have to do a cutting. Our measurements are related to a finite numbers of points in the real line, i.e., x_p , $p = 1, \dots, L$. Hence our knowledge of the concentration distribution outside the so called measurement region is slight. Therefore we may assume that the mean is a constant in the measurement region $|x| \leq M$ where M is such that $|x_p| < M$ for all $p = 1, \dots, L$ and decays exponentially outside of it, i.e.,

$$x_0(x) = \begin{cases} x_0 & \text{if } |x| \leq M, \\ x_0 e^{-(|x|-M)} & \text{if } |x| > M \end{cases} \quad (28)$$

where x_0 is a positive constant.

We need to choose an appropriate covariance operator for the initial value X_0 . If the stochastic initial value problem (23) has the strong solution, the solution belongs to the domain of the convection–diffusion operator, i.e., $X(t, \omega) \in H^2(\mathbb{R})$ for almost all $(t, \omega) \in [0, T] \times \Omega$ [12, definition 4.44]. Thus we may expect that the initial value has some sort of smoothness properties.

We would like to have an $H^2(\mathbb{R})$ -valued Gaussian random variable Z such that

$$\eta := \left(1 - \frac{d^2}{dx^2} \right) Z$$

is the white noise process in $L^2(\mathbb{R})$. Then $\mathbb{E}[(f, \eta)(g, \eta)] = (f, g)$ for all $f, g \in L^2(\mathbb{R})$. Thus

for all $f, g \in C_0^\infty(\mathbb{R})$

$$\begin{aligned} (f, g) &= \mathbb{E} \left[\left(\left(1 - \frac{d^2}{dx^2} \right) f, Z \right) \left(\left(1 - \frac{d^2}{dx^2} \right) g, Z \right) \right] \\ &= \left(\Gamma \left(1 - \frac{d^2}{dx^2} \right) f, \left(1 - \frac{d^2}{dx^2} \right) g \right) \end{aligned}$$

where Γ is the covariance operator of Z . We assume that Γ is a convolution operator, i.e., $\Gamma f = \gamma * f$ for some $\gamma \in L^2(\mathbb{R})$. Then by the Parseval formula,

$$(f, g) = (2\pi)^{-1} \left(\hat{\gamma}(1 + \xi^2) \hat{f}, (1 + \xi^2) \hat{g} \right) = (2\pi)^{-1} \left(\hat{\gamma}(1 + \xi^2)^2 \hat{f}, \hat{g} \right)$$

for all $f, g \in C_0^\infty(\mathbb{R})$ where \hat{h} denotes the Fourier transformation of $h \in L^2(\mathbb{R})$. Hence we have $\hat{\gamma}(\xi) = (1 + \xi^2)^{-2}$ for all $\xi \in \mathbb{R}$. Thus by the calculus of residues,

$$\gamma(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{e^{ix\xi}}{(1 + \xi^2)^2} d\xi = \frac{1}{4} (1 + |x|) e^{-|x|}$$

for all $x \in \mathbb{R}$. Unfortunately, Γ defined as an integral operator having the integral kernel $\gamma(x - y)$ is not a trace class operator and hence cannot be a covariance operator of a Gaussian random variable [14, proposition 2.15]. We have to do some sort of modification. We define an integral operator $\tilde{\Gamma}$ with the integral kernel $\tilde{\gamma}(x, y) = w(x)\gamma(x - y)w(y)$ where

$$w(x) = \begin{cases} 1 & \text{if } |x| < N, \\ e^{-(|x| - N)} & \text{if } |x| \geq N, \end{cases} \quad (29)$$

with some $N > 0$. Then $\tilde{\Gamma}$ is a positive self-adjoint operator with a trivial kernel. The operator $\tilde{\Gamma}$ is a composition of three operators, $\tilde{\Gamma} = M_w m_{\hat{\gamma}} M_w$ where

$$M_w : L^2(\mathbb{R}) \rightarrow L^2(\mathbb{R}), \quad f \mapsto wf$$

is a multiplier and

$$m_{\hat{\gamma}} : L^2(\mathbb{R}) \rightarrow L^2(\mathbb{R}), \quad f \mapsto \mathcal{F}^{-1}(\hat{\gamma} \hat{f})$$

is a Fourier multiplier. Furthermore, $m_{\hat{\gamma}} = m_{\hat{\gamma}^{1/2}}^2$. So

$$\tilde{\Gamma} = M_w m_{\hat{\gamma}^{1/2}}^2 M_w = \left(M_w m_{\hat{\gamma}^{1/2}} \right) \left(m_{\hat{\gamma}^{1/2}} M_w \right) = K^* K$$

where

$$Kf := m_{\hat{\gamma}^{1/2}} M_w f = \mathcal{F}^{-1} \left(\hat{\gamma}^{1/2} \widehat{wf} \right) = \mathcal{F}^{-1} \left(\hat{\gamma}^{1/2} \right) * (wf)$$

for all $f \in L^2(\mathbb{R})$. Thus K is an integral operator with the integral kernel

$$k(x, y) = \mathcal{F}^{-1} \left(\hat{\gamma}^{1/2} \right) (x - y) w(y) = \frac{w(y)}{2\pi} \int_{-\infty}^{\infty} \frac{e^{i(x-y)\xi}}{1 + \xi^2} d\xi = \frac{1}{2} e^{-|x-y|} w(y)$$

for all $x, y \in \mathbb{R}$. Since k is square integrable in \mathbb{R}^2 , the operator K is a Hilbert-Schmidt operator [8, example I.1.3]. Hence the operator $\tilde{\Gamma}$ is nuclear [8, theorems I.1.2 and I.1.6]. Therefore $\tilde{\Gamma}$ is an appropriate covariance operator for a Gaussian random variable. Furthermore, $\tilde{\Gamma}$ is a smoothing operator.

We assume that the covariance operator of the initial value is $\Gamma_0 = \sigma_0^2 \tilde{\Gamma}$ with $\sigma_0 > 0$. In this model case we assume that our model for the flow is rather accurate. Hence we use the same covariance operator for the Wiener process as for the initial value with a different scaling factor, i.e., $Q = \sigma^2 \tilde{\Gamma}$ with $\sigma > 0$.

4.3 Discretization space

We need a family $\{V_m\}_{m=1}^\infty$ of finite-dimensional subspaces of $L^2(\mathbb{R})$ forming a sequence of appropriate discretization spaces in $L^2(\mathbb{R})$. Let us choose

$$V_m := \text{span} \left\{ \sqrt{m} \chi_{\left[\frac{i-1}{m}-m, \frac{i}{m}-m\right]}, i = 1, \dots, 2m^2 \right\}$$

for all $m \in \mathbb{N}$. Then $V_m \subset V_{m+1}$ and $\dim V_m = 2m^2$ for all $m \in \mathbb{N}$. Furthermore, $\overline{\cup V_m} = L^2(\mathbb{R})$ [12, lemma 6.11]. Hence the family $\{V_m\}_{m=1}^\infty$ is a sequence of appropriate discretization spaces in $L^2(\mathbb{R})$. We denote

$$\psi_i^m := \sqrt{m} \chi_{\left[\frac{i-1}{m}-m, \frac{i}{m}-m\right]}$$

for all $i = 1, \dots, 2m^2$ and $m \in \mathbb{N}$. The family $\{\psi_i^m\}_{i=1}^{2m^2}$ is an orthonormal basis of V_m for all $m \in \mathbb{N}$. We define the orthogonal projections $P_m : L^2(\mathbb{R}) \rightarrow V_m$ by

$$P_m f = \sum_{i=1}^{2m^2} (f, \psi_i^m) \psi_i^m = \sum_{i=-m^2+1}^{m^2} m \int_{\frac{i-1}{m}}^{\frac{i}{m}} f dx \chi_{\left[\frac{i-1}{m}, \frac{i}{m}\right]}$$

for all $f \in L^2(\mathbb{R})$. The basis functions of V_m are the simplest one, constant functions with finite supports. The choice of the discretization level m depends on how accurate and how fast computation we want to have. The support of a function in V_m belongs to the interval $[-m, m]$ for all $m \in \mathbb{N}$. Since we know that the measurements give information only from a part of the pipe, the discretization level need not to be bigger than half of the width of the measurement region.

4.4 Discretized filtering problem

Let the discretization level be m . Then the discretized state estimation system is

$$\begin{aligned} X_{k+1}^m &= A_{k+1}^m X_k^m + \epsilon_{k+1}^m + W_{k+1}^m, & k = 0, \dots, n-1, \\ Y_k &= C^m X_k^m + \nu_k^m + S_k, & k = 1, \dots, n \end{aligned}$$

where the matrix A_{k+1}^m is defined by

$$(A_{k+1}^m)_{ij} := (U(\Delta_{k+1})\psi_j^m, \psi_i^m)$$

and the matrix C^m by

$$(C^m)_{pj} := (\psi_j^m, \varphi_p)$$

for all $i, j = 1, \dots, 2m^2$ and $p = 1, \dots, L$. The observation noise vectors S_k are chosen such a way that S_k is normal with the mean $\mathbb{E}S_k = 0$ and the covariance matrix $\text{cov}(S_k) = \sigma_S^2 I$ for all $k = 1, \dots, n$ where $\sigma_S > 0$ and $I \in \mathbb{R}^{L \times L}$ is the identity matrix. In addition, S_k is independent of X_0 for all $k = 1, \dots, n$, S_k and S_l are mutually independent for all $k \neq l$, and S_k and W_l^m are mutually independent for all $k, l = 1, \dots, n$.

We solve the discretized filtering problem using the filtering method given by equations (11)–(15). The expectations $\mathbb{E}^{d_k}(\epsilon_{k+1}^m)$ and $\mathbb{E}^{d_k}(\nu_{k+1}^m)$ and the matrices $\text{cov}^{d_k}(\epsilon_{k+1}^m)$, $\text{cov}^{d_k}(\nu_{k+1}^m)$, $\text{cor}^{d_k}(X_k^m, \epsilon_{k+1}^m)$, $\text{cor}^{d_k}(X_{k+1}^m, \nu_{k+1}^m)$ and $\text{cov}(W_{k+1}^m)$ are computed using formulae (16)–(22) as described in section 3.1. Since we have chosen $\Gamma_0 = \sigma_0^2 \tilde{\Gamma}$ and $Q = \sigma^2 \tilde{\Gamma}$, for the computation of these matrices we need to calculate the inner products

$$(U(t)\psi_j^m, \psi_i^m), (\psi_i^m, \varphi_p), (U(t)x_0, \psi_i^m), (U(t)x_0, \varphi_p), \quad (30)$$

$$(U(t)\tilde{\Gamma}U^*(s)\psi_i^m, \psi_j^m), (U(t)\tilde{\Gamma}U^*(s)\psi_i^m, \varphi_p), (U(t)\tilde{\Gamma}U^*(s)\varphi_p, \varphi_q) \quad (31)$$

and the integrals

$$\int_u^r (U(t-\tau)\tilde{\Gamma}U^*(s-\tau)\psi_i^m, \psi_j^m) d\tau, \int_0^r (U(t-\tau)\tilde{\Gamma}U^*(s-\tau)\psi_i^m, \varphi_p) d\tau, \quad (32)$$

$$\int_0^r (U(t-\tau)\tilde{\Gamma}U^*(s-\tau)\varphi_p, \varphi_q) d\tau \quad (33)$$

for all $i, j = 1, \dots, 2m^2$, $p, q = 1, \dots, L$ and $0 \leq u \leq r \leq s, t \leq T$.

The inner products on line (30) can be presented in a closed form (see [12]). The covariance operator $\tilde{\Gamma}$ is the integral operator with the integral kernel $w(x)\gamma(x-y)w(y)$ where $\hat{\gamma}(\xi) = (1 + \xi^2)^{-2}$ for all $\xi \in \mathbb{R}$ and w is defined by (29). We are not able to calculate the inner product on line (31) in a closed form. Let f and g are either ψ_i^m or φ_p for some $i = 1, \dots, 2m^2$ or $p = 1, \dots, L$. By using the Parseval formula we notice that

$$(U(t)\tilde{\Gamma}U^*(s)f, g) = (\gamma * (wU^*(s)f), wU^*(t)g) = (2\pi)^{-1}(\hat{\gamma}\mathcal{F}(wU^*(s)f), \mathcal{F}(wU^*(t)g))$$

for all $t \geq 0$. The Fourier transform of γ is known. The Hilbert adjoint $U^*(t)$ is a convolution operator with the kernel

$$\Phi^*(t, x) := \frac{1}{2\sqrt{\pi\kappa t}} \exp\left(-\frac{(x+vt)^2}{4\kappa t}\right)$$

for all $t > 0$ and $x \in \mathbb{R}$ [12, pp. 127–128]. Hence $U^*(t)f$ can be calculated in a closed form for all $t > 0$. The Fourier transformation of $wU^*(t)f$ is not known but the Fourier transformation of $U^*(t)f$ can be calculated in a closed form for all $t > 0$. When N is chosen to be large, the Fourier transformations of $wU^*(t)f$ and $U^*(t)f$ are approximately equal for all $t > 0$. Hence we can approximate

$$(U(t)\tilde{\Gamma}U^*(s)f, g) \approx (2\pi)^{-1}(\hat{\gamma}\mathcal{F}(U^*(s)f), \mathcal{F}(U^*(t)g)).$$

The inner product on left is computed numerically by using the trapezoidal rule. In addition, the integrals on lines (32)–(33) are computed numerically.

4.5 Computation of exact solution and data

For numerical simulations we need to produce an exact solution and data corresponding to it. The following lemma gives the joint distribution of X_1^m, \dots, X_n^m and Y_1, \dots, Y_n .

Lemma 5. *The joint probability distribution of X_1^m, \dots, X_n^m and Y_1, \dots, Y_n is normal. Furthermore, the mean and the cross-correlation matrix of the joint distribution can be calculated by the following formulae. The mean of the joint distribution is given by*

$$\mathbb{E}X_k^m = [(U(t_k)x_0, \psi_i^m)]_{i=1}^{N_m}, \quad (34)$$

$$\mathbb{E}Y_k = [(U(t_k)x_0, \varphi_p)]_{p=1}^L \quad (35)$$

and the covariance of the joint distribution is determined by the correlation matrices

$$\text{cor}(X_k^m, X_l^m) = \Gamma_{k,l}^\psi + \int_0^{t_k \wedge t_l} Q_{k,l}^\psi(s) ds, \quad (36)$$

$$\text{cor}(Y_k, Y_l) = \Gamma_{k,l}^\varphi + \int_0^{t_k \wedge t_l} Q_{k,l}^\varphi(s) ds + \delta_l^k \text{cov}(S_k), \quad (37)$$

$$\text{cor}(X_k^m, Y_l) = \Gamma_{k,l}^{\psi,\varphi} + \int_0^{t_k \wedge t_l} Q_{k,l}^{\psi,\varphi}(s) ds \quad (38)$$

for all $k, l = 1, \dots, n$ where δ_l^k is the Kronecker delta.

Table 1: Parameter values.

Coefficient	Value	Related to/Description
κ	1	model (23)
v	0.5	model (23)
x_0	1	the initial state, equation (28)
M	2	the initial state, equation (28)
σ_0	0.1	the covariance Γ_0 of the initial state
σ	0.04	the covariance Q of the Wiener process
σ_S	0.1	the covariance $\text{cov}(S_k)$
m	3	the discretation level
T	10	the overall time

Proof. The normality of the joint distribution is proved similarly as lemma 1 in [13]. The mean and the covariance matrix are calculated in the same way as in [13, pp. 375–376]. \square

Since we are able to compute the inner product on lines (30)–(31) and the integrals on lines (32)–(33), expectations (34)–(35) and correlation matrices (36)–(38) can be calculated. Hence the joint distribution of X_1^m, \dots, X_n^m and Y_1, \dots, Y_n is known. Therefore we can draw a sample from the joint distribution and get a real value and measurements simultaneously.

4.6 Numerical results

The parameter values are specified in table 1. The number of measurements is $L = 10$ and the data points are

$$x_p = -2 + 4 \frac{p-1}{L-1}$$

for all $p = 1, \dots, L$. The parameter w_p in the kernel φ_p is set to be 0.25 for each $p = 1, \dots, L$. The time instants of the measurements are chosen to be $t_k = k\Delta$ for all $k = 1, \dots, n$ where $\Delta = 2$. Thus the number of the measurement instants is $n = 5$.

Let f and g are either ψ_i^m or φ_p for some $i = 1, \dots, 2m^2$ or $p = 1, \dots, L$. The inner products on line (31) are computed by the trapezoidal rule using the values of $\mathcal{F}(U^*(s)f)$ at the points

$$\xi_k = -10 + \frac{k-1}{100}$$

for all $k = 1, \dots, 2000$. The integrals on lines (32)–(33) are computed using the trapezoidal rule from the values $(U(t - \tau_k)\Gamma U^*(s - \tau_k)f, g)$ where the time instants τ_k are

$$\tau_k = u + \tilde{\Delta}k$$

for all $k = 0, \dots, (r - u)/\tilde{\Delta}$ with $\tilde{\Delta} := \Delta/500$.

The norms of the expectations and the square-roots of the trace of the covariance matrices of the error terms ϵ_k^m , ν_k^m and W_k^m are shown in figure 1. The time average of $\|\mathbb{E}(\epsilon_k^m)\|^2 + \text{Tr cov}(\epsilon_k^m)$ is 0.0310 which should be compared to $\text{Tr cov}(W_k^m) = 0.0030$. This shows that the energy of the discretization error in the discretized state evolution equation is

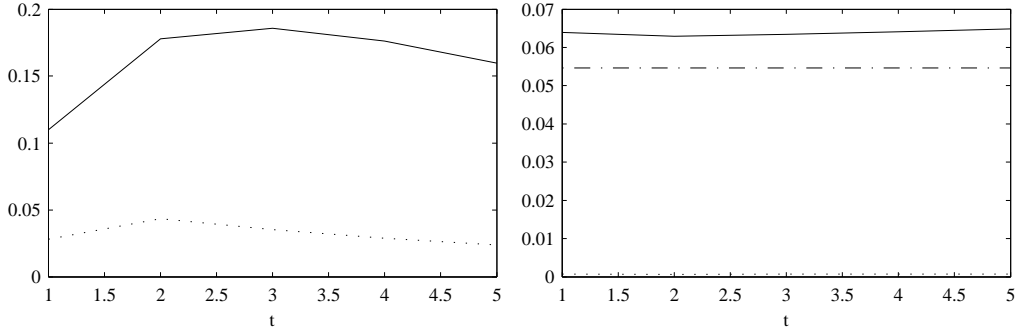


Figure 1: Left: The norm of the expectation of ϵ_k^m (—) and ν_k^m (··). Right: The square-root of the trace of the covariance of ϵ_k^m (—), ν_k^m (··) and W_k^m (-·).

clearly higher than the energy of the state noise vector. However, the time average of $\|\mathbb{E}(\nu_k^m)\|^2 + \text{Tr cov}(\nu_k^m)$ is 0.0011 and $\text{Tr cov}(S_k) = 0.1000$. So the measurement error dominates in the case of the observation equation.

We have computed three different estimates. The first estimate was calculated using the algorithm described in section 3 and the second when the error terms ϵ_k^m and ν_k^m in the discretized state estimation system (7)–(8) are set to zero (corresponds to the conventional Kalman filter estimate). The last estimate was the conditional distribution given by equations (9)–(10) which can be computed in this case due to the relatively low dimension of the state X_k^m and the small number of measurements. The vectors $\mathbb{E}X_k^m$ and $\mathbb{E}D_k$ and the matrices $\text{cov}(X_k^m)$, $\text{cov}(D_k)$ and $\text{cor}(X_k^m, D_k)$ for the conditional distribution are obtained from the expectation and the covariance of the joint distribution of X_1^m, \dots, X_n^m and Y_1, \dots, Y_n , which were already computed for the data generation (see section 4.5).

As results of the numerical computation we present the mean values of the distributions received by the methods above. The means and the absolute errors are shown in figure 2. The results show that the accuracy of the estimates computed using the presented method is almost as good as the accuracy of the conditional expectation. However, the accuracy of the conventional Kalman filter estimate is worse. It should be noted that the mean of the conditional distribution can be treated, in the statistical point of view, as the best point estimate for the state based on the given data, and the point estimate given by equations (11)–(15) differs from the conditional expectation only due to the approximations made in section 3.1.

Since the estimates given by the used estimation methods are distribution instead of just point estimates, these methods provides us also information about the error of point estimates. The computed point estimates and the confidence intervals for the final state $t = 10$ are shown in figure 3. The confidence intervals are the square roots of the diagonal elements of the covariance matrices and corresponds to the standard deviation of the estimation error. Figure 3 shows that the confidence intervals for the Kalman filter estimate corresponds poorly to the actual error. However, the error estimates computed using the presented method gives a rather good assessment of the errors.

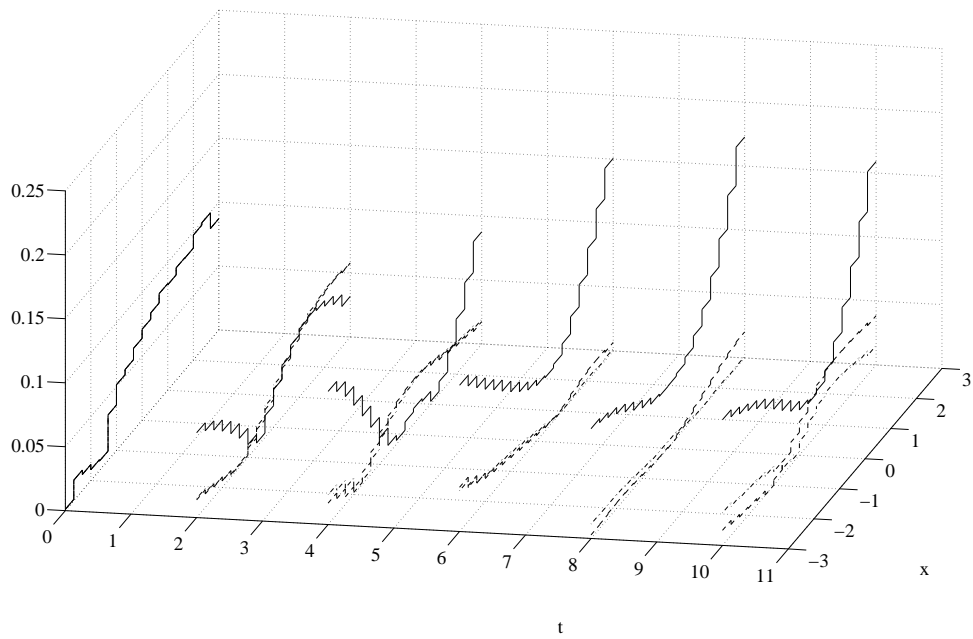
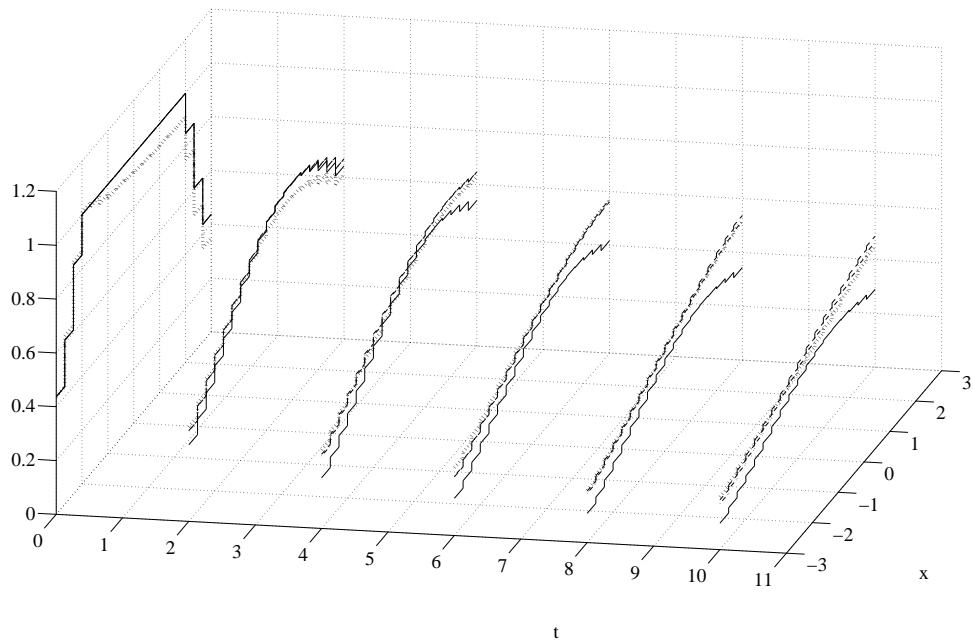


Figure 2: Computed point estimates (top) and absolute errors (bottom). The point estimates shown are the real conditional expectation (\cdots), the original Kalman filter estimate ($-$) and the point estimate computed using the presented method ($-\cdot-$). The real solution is also shown in the figure on top ($\cdot\cdot$).

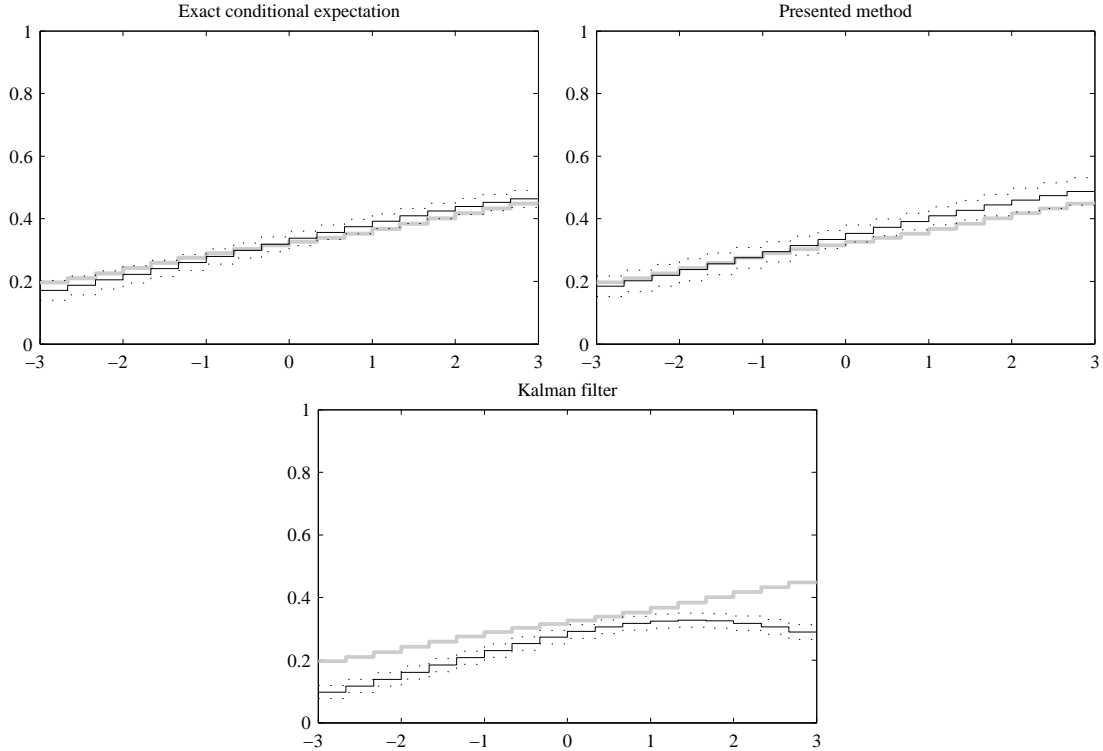


Figure 3: The computed point estimates for the final state $t = 10$ (black lines) with the S.D. error intervals ($\cdot\cdot$). A gray line corresponds to the exact solution.

5 Conclusions

This article discusses the use of continuous infinite-dimensional state-space models in the case of linear nonstationary inverse problems related to partial differential equations. We analyse the error caused by the discretization of the state-space model by using statistical approach. In addition, we describe a filtering method taking into account the statistical information about the discretization error. The method makes possible to control the discretization error when solving large-scale state estimation problems in which the computational cost is too high without significant mesh coarsening or model reduction.

The filtering method is demonstrated by a numerical example based on the one-dimensional convection–diffusion equation. The results show that the accuracy of the point estimate computed using the method is nearly as good as the conditional expectation computed using the infinite-dimensional model. The accuracy of the computed point estimates without discretization error were instead significantly worse. Therefore it seems that the method can control discretization errors without remarkable error in computed estimates.

The method is usable only in the linear Gaussian case. The assumption of Gaussianity seemed to be natural for the linear nonstationary inverse problems in which possible modelling errors in the time evolution model are described by a Wiener process. The solution to the infinite-dimensional state evolution equation is a Gaussian process if the initial value is assumed be Gaussian. Despite of the initial value the state noise is always a Gaussian process. Nonetheless, in some application non-Gaussian initial values and state noises may be reasonable. Because the Gaussianity is maintained by the linearity, for nonlinear nonstationary inverse problems other methods need to be developed.

A disadvantage of the method is that the closed form of an analytic semigroup is often unknown. In general, the analytic semigroup is defined by using the spectral properties of the infinitesimal generator. In some cases the analytic semigroup can be calculated, similarly as in the one-dimensional model case, e.g., by using the Feynman–Kac formula [10, section 8.2]. Possible boundary conditions in multidimensional cases may be handled by stopping times. If the analytic semigroup is unknown, we may approximate it by a suitable known semigroup. The effect of the approximation error is a subject of further studies.

In solving the filtering problem using the method (11)–(15) the conditional expectations, the conditional covariances and the conditional correlations are replaced by the regular expectations, the regular covariances and the regular correlations. The corresponding approximation errors is not examined in this article. In further studies the distance of the received distribution from the exact conditional distribution should be measured using an appropriate metric.

A more realistic example of linear nonstationary inverse problems would be the two-dimensional process tomography problem where the time evolution is modelled by the stochastic convection–diffusion equation and measurements are done by limited angle x-ray tomography. The related filtering problem can be solved using the filtering method presented in this paper.

Acknowledgments. The first author has been supported by Academy of Finland project 13666 and TEKES/MASI project 28118 (National Technology Agency of Finland). The second author has been supported by the Vilho, Yrjö and Kalle Väisälä Foundation of the Finnish Academy of Science and Letters, the Finnish Graduate School of Inverse Problems and the Austrian National Science Foundation FWF through the project SFB F1308.

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