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A Bayesian approach to parameter identification in gas networks

Soheil Hajian¹, Michael Hintermüller^{1,2}, Claudia Schillings³, Nikolai Strogies²

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¹ Humboldt-Universität zu Berlin
Unter den Linden 6
10099 Berlin
Germany
E-Mail: soheil.hajian@hu-berlin.de
hint@math.hu-berlin.de

² Weierstrass Institute
Mohrenstr. 39
10117 Berlin
Germany
E-Mail: michael.hintermueller@wias-berlin.de

³ University of Mannheim
68131 Mannheim
Germany
E-Mail: c.schillings@uni-mannheim.de

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Edited by
Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
10117 Berlin
Germany

Fax: +49 30 20372-303
E-Mail: preprint@wias-berlin.de
World Wide Web: <http://www.wias-berlin.de/>

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Abstract

The inverse problem of identifying the friction coefficient in an isothermal semilinear Euler system is considered. Adopting a Bayesian approach, the goal is to identify the distribution of the quantity of interest based on a finite number of noisy measurements of the pressure at the boundaries of the domain. First well-posedness of the underlying non-linear PDE system is shown using semigroup theory, and then Lipschitz continuity of the solution operator with respect to the friction coefficient is established. Based on the Lipschitz property, well-posedness of the resulting Bayesian inverse problem for the identification of the friction coefficient is inferred. Numerical tests for scalar and distributed parameters are performed to validate the theoretical results.

1 Introduction

In many countries, the turnaround in energy policy is one of the main focus areas of political decision making and public opinion in the energy sector. In particular, the shift away from nuclear energy supply will only be possible by exploring new sustainable resources. During the transition from the current energy portfolio to one which has an emphasis on renewable energies and other energy carriers such as hydrogen, it is widely believed that an optimized use of natural gas will play a key role. This is in particular plausible when considering the currently known available gas resources, the transportability of gas over long distances, its storage capacity, and the fact that it can be traded on markets which helps an efficient distribution.

The transport of natural gas is typically achieved through a complex system of pipelines emanating at production sites or storage facilities and ending at customer locations. Mathematically and generally speaking, the gas transport in pipes is described by the compressible Euler equations, a system of hyperbolic partial differential equations (PDEs). It provides the dynamics of the density, momentum and energy of the underlying gas. As in our target application the diameter of a pipe is much smaller than the length, the study of a one-dimensional version of the PDE model is sufficient. Moreover, since the flow in pipes is usually assumed to start at a stationary state and to evolve smoothly due to industry regulations (thus preventing shock formation), the one-dimensional Euler system simplifies to isothermal equations where the unknowns are density and momentum. Now, under the assumption that the speed of the gas is significantly smaller than the speed of sound, we arrive at the following semi-linear PDE system describing the gas dynamics in a single pipe:

$$\begin{aligned}\partial_t p(x, t) + c^2 \partial_x q(x, t) &= 0 && \text{in } \Omega \times (0, T), \\ \partial_t q(x, t) + \partial_x p(x, t) &= \lambda a(p(x, t), q(x, t)) && \text{in } \Omega \times (0, T),\end{aligned}\tag{1}$$

where Ω is the physical domain, which is—without loss of generality—assumed to be $\Omega := (0, 1)$, $T > 0$ is some finite time horizon, $p(x, t)$ is the pressure of the gas in the pipe at location $x \in \Omega$ and time $t \in [0, T]$, and $q(x, t)$ is the momentum density. The parameter $c > 0$ relates to the speed of sound. In (1), $a(\cdot, \cdot) : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ is the friction function and $\lambda \in L^\infty(\Omega)$ denotes the *friction coefficient*. Loosely speaking, λa describes the roughness of the interior walls of the pipes and influences

the transport in a decisive way. While a scalar value for λ is typically provided for newly produced pipes by manufacturers, its value and in particular its spatial distribution during operation (over time) is neither accessible to direct measurements nor known in general. For specific settings (see [DHLT17]), however, approximation formulas for scalar λ are known from the engineering literature. Under a regular operating mode and assuming usual manufacturing and quality conditions in the production of pipeline tubes, $a(\cdot, \cdot)$ can be assumed Lipschitz continuous with respect to each argument. According to the application in mind, system (1) is completed by the following initial and boundary conditions:

$$p(x, 0) = p_0(x), q(x, 0) = q_0(x) \quad \forall x \in \Omega, \quad (2a)$$

$$q(0, t) = g_L(t), q(1, t) = g_R(t) \quad \forall t > 0, \quad (2b)$$

where p_0, q_0, g_L , and g_R are given quantities. Combining (1) and (2) provides our overall model of gas flow. We refer to [DHLT17, LeV02] for more on this and further details on the model reduction process.

Motivated by the simulation or optimization of the aforementioned gas pipeline network, we are interested in the inverse problem of identifying the friction coefficient of a gas pipe from a finite set of noisy observations of the pressure drop at both ends of the pipe. Here, the pressure drop is given by

$$\delta p(t) := \left| \|p(\cdot, t)\|_{L^2(0, \epsilon)} - \|p(\cdot, t)\|_{L^2(1-\epsilon, 1)} \right| \quad \forall t \in [0, T],$$

for $0 < \epsilon \ll 1$, which accommodates the L^1 -regularity of p with the latter preventing the evaluation of the pressure precisely at the endpoints of the pipe. For a classical inverse problem for the conditional identification of a friction law for the isothermal Euler equations we refer to the work [EKS17] which relies on regularity of the solution and differentiability of the underlying solution operator.

Important questions in the optimization of gas networks are related to robust control of the system [ALS17] or the study of probabilistic constraints [GHH17], both involving the friction coefficient which, as highlighted above, is uncertain during operation. The pertinent mathematical formulations indeed depend on statistical properties of the associated uncertain quantities such as the mean value, standard deviation or even the entire distribution. As a consequence, this paper addresses the aforementioned inverse problem by employing a Bayesian approach [KS05, Stu, Tar05]. Here we consider both, a finite dimensional and an infinite dimensional friction coefficient, thus necessitating the application of the respectively associated version of Bayes' rule. Adapting the infinite dimensional approach (rather than considering discretized versions of the friction coefficient only) is beneficial as it provides us with algorithms which are robust with respect to discretization refinements.

For setting up the Bayesian framework in our context, next we introduce the *uncertainty-to-observation operator* \mathcal{G} , which maps the underlying unknown (i.e., the friction coefficient) onto the data y . It is the composition of the solution operator of the forward problem (1) applied to the friction function λ and a data formation operator. Measuring δp at finitely many time instances $t_j \in [0, T]$, $j = 1, \dots, K$, we have here

$$\mathcal{G}(\lambda) = (\delta p(t_1), \dots, \delta p(t_K))^T.$$

As observations are inevitably noisy we arrive at

$$y = \mathcal{G}(\lambda) + \eta,$$

where $\eta \in \mathbb{R}^K$ represents Gaussian noise with mean zero and associated covariance matrix $\Gamma \in \mathbb{R}^{K \times K}$. The pertinent probability density function (PDF) is denoted by $\rho(\cdot)$.

Then, the probability of obtaining y for a given friction coefficient λ is $\mathbb{P}(y|\lambda) = \rho(y - \mathcal{G}(\lambda))$, which is the *likelihood* of the data. Moreover, using Bayes' theorem, we can incorporate our "prior" knowledge on λ and provide its probability given the data y by

$$\mathbb{P}(\lambda|y) \propto \mathbb{P}(y|\lambda)\mathbb{P}(\lambda). \quad (3)$$

Our knowledge on λ , i.e., $\mathbb{P}(\lambda)$, is called *prior* and the probability of the function λ given the data y , i.e., $\mathbb{P}(\lambda|y)$, is called *posterior*. In an infinite dimensional setting, e.g., when $\lambda \in L^\infty(\Omega)$, then there is no density with respect to the Lebesgue measure and Bayes' rule is understood as the Radon-Nikodym derivative of the posterior measure $\mu^y(d\lambda)$ with respect to the prior measure $\mu_0(d\lambda)$, i.e.,

$$\frac{d\mu^y}{d\mu_0}(\lambda) \propto \rho(y - \mathcal{G}(\lambda)). \quad (4)$$

For an overview on the Bayesian approach to statistics in finite dimensions we refer the reader to [BS94]. Bayesian inverse problems with an emphasis on modelling and computation are addressed in [KS05]. We also mention that the Bayesian inversion methods that will be used in this paper have been successfully applied to linear elliptic problems such as Darcy's flow in [DS11] and viscous incompressible flow on a two-dimensional torus in [CDRS09].

Uncertainty quantification for inverse problems has become a very active field of research over the recent years. Adopting, in this context, the Bayesian viewpoint leads to a complete characterisation of the uncertainty via the posterior distribution; see, e.g., [DS16, KS05, Stu]. In a general inverse problem setting, the goal is to recover unknown parameters from noisy measurements of system quantities. Bayesian inversion, however, interprets the unknown as a random variable and computes the conditional distribution of the unknown parameters given noisy measurements and prior distribution. It is known [Stu] that the latter approach is well defined in the infinite-dimensional setting. Thus, it is suitable for the identification of parameter functions belonging to some infinite dimensional Banach space.

Under certain regularity assumptions on the forward problem describing the underlying physics, well-posedness and stability results can be established for the Bayesian problem. In particular, robustness with respect to numerical approximations of the forward problem is of interest to ensure a stable inversion of the problem; see [DS16]. However, computational challenges arise due to the complex structure of probability measures in high or infinite dimensional settings. In order to circumvent the curse of dimensionality, there is substantial interest in the development of dimension independent methods, i.e., algorithms which are robust with respect to the dimension of the parameter space and thus, applicable to high-dimensional real-world problems; see, e.g., [CRSW13, DGGS16, EMM12, MZRL16, SST17, SS13].

In this paper, we will focus on Markov-Chain-Monte-Carlo (MCMC) methods formulated in function spaces. For our focus application, the identification of the friction coefficient in an isothermal Euler system, it represents a suitable choice due to the low requirements on the regularity of the forward problem. It is well known that, in general, solutions of hyperbolic systems develop discontinuities in finite time and therefore pose additional difficulties in the efficient treatment of uncertainties due to the lack of smoothness with respect to uncertain inputs.

As our forward (or state) system is hyperbolic, we mention that the uncertainty quantification for hyperbolic differential equations with random data has been a very active field of research over the recent past; see [AM17, BLMS13] and the references therein. In the data assimilation context, especially for weather forecasting applications, efficient methods for state estimation have received particular attention in recent years [AHSV07, HOT11, MH12]. However, the quantification of uncertainties in the inverse setting has been the subject of only a very small number of publications; compare [BPL14, CDRS09]. None of these is related to our work.

The rest of this paper is organized as follows. In section 2 the PDE system is studied with respect to existence and Lipschitz stability. Prior modelling and the Bayesian framework are the subjects of section 3. The numerical realisation of the forward problem is considered in section 4, and numerical

results are provided in section 5.

2 Properties of the underlying PDE system

In order to establish well-posedness of the Bayesian inverse problem, it is sufficient to show that the underlying PDE is well-posed and that the solution operator is Lipschitz continuous with respect to the friction coefficient.

It is convenient to reformulate the PDE (1) such that the flux function $q(x, t)$ has vanishing traces. For this purpose, let us define $q = \tilde{q} + \hat{q}$ where $\tilde{q}(x, t) := xg_L(t) + (1 - x)g_R(t)$. Then, since $\hat{q}(0, t) = \hat{q}(1, t) = 0$, we can write the underlying PDE (1) in the following abstract form of a dynamical system:

$$\begin{aligned} \mathbf{u}'(t) + A\mathbf{u}(t) &= \mathbf{f}(\lambda, \mathbf{u}(t), t) \quad (t > 0), \\ \mathbf{u}(0) &= \mathbf{u}_0, \end{aligned} \quad (5)$$

where $\mathbf{u}(t) := (p(\cdot, t), \hat{q}(\cdot, t))^\top$ and $\mathbf{u}_0 := (p_0(\cdot), q_0(\cdot) - \tilde{q}(\cdot, 0))^\top$. Here, $A : V \rightarrow L$ is given by

$$A := \begin{bmatrix} 0 & c^2 \partial_x \\ \partial_x & 0 \end{bmatrix}, \quad (6)$$

where $V := \mathbf{H}^1(\Omega) \times \mathbf{H}_0^1(\Omega)$, $L := \mathbf{L}_w^2(\Omega) \times \mathbf{L}^2(\Omega)$ with the weighted \mathbf{L}^2 -space \mathbf{L}_w defined by

$$\mathbf{L}_w^2(\Omega) := \left\{ v : \Omega \rightarrow \mathbb{R} : \int_{\Omega} \frac{v^2(x)}{c^2} dx < \infty \right\}.$$

The right-hand side $\mathbf{f} : X \times L \times [0, T] \rightarrow L$, where $X := \mathbf{L}^\infty(\Omega)$, is given by

$$\mathbf{f}(\lambda, \mathbf{u}, t) := \begin{pmatrix} -c^2(g_L(t) - g_R(t)) \\ \lambda a(p, \hat{q} + \tilde{q}) - xg_L'(t) - (1 - x)g_R'(t) \end{pmatrix}. \quad (7)$$

Note that properties of boundary conditions as well as the friction function $a(\cdot, \cdot)$ have an impact on $\mathbf{f}(\cdot, \cdot, \cdot)$. In the following lemma we state continuity properties of \mathbf{f} .

Lemma 2.1. *Let $g_L(t), g_R(t) \in C^1([0, T])$, and suppose that $a(\cdot, \cdot) : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ is Lipschitz continuous with respect to its arguments. Then $\mathbf{f} : X \times L \times [0, T] \rightarrow L$ is continuous in time and Lipschitz continuous in L for a fixed $\lambda \in X$. Moreover, if g_L' and g_R' are Lipschitz continuous on $[0, T]$, then \mathbf{f} is Lipschitz continuous in both variables.*

Proof. We first prove Lipschitz continuity with respect to \mathbf{u} . Note that for a fixed time t and λ we have

$$\mathbf{f}(\lambda, \mathbf{u}_1, t) - \mathbf{f}(\lambda, \mathbf{u}_2, t) = \begin{pmatrix} 0 \\ \lambda[a(p_1, \hat{q}_1 + \tilde{q}) - a(p_2, \hat{q}_2 + \tilde{q})] \end{pmatrix},$$

for all $\mathbf{u}_1 = (p_1, \hat{q}_1) \in L$ and $\mathbf{u}_2 = (p_2, \hat{q}_2) \in L$. Therefore we get

$$\begin{aligned} \|\mathbf{f}(\lambda, \mathbf{u}_1, t) - \mathbf{f}(\lambda, \mathbf{u}_2, t)\|_L &= \|\lambda[a(p_1, \hat{q}_1 + \tilde{q}) - a(p_2, \hat{q}_2 + \tilde{q})]\|_{\mathbf{L}^2(\Omega)} \\ &\leq C_L \|\lambda\|_{\mathbf{L}^2(\Omega)} \|\mathbf{u}_1 - \mathbf{u}_2\|_L, \end{aligned}$$

where C_L is the Lipschitz constant of $a(\cdot, \cdot)$. Similarly, continuity in time follows from

$$\begin{aligned} \|\mathbf{f}(\lambda, \mathbf{u}, t_1) - \mathbf{f}(\lambda, \mathbf{u}, t_2)\|_L &\leq \max(1, C_L \|\lambda\|_{\mathbf{L}^2(\Omega)}) \left(|g_L(t_1) - g_L(t_2)| + |g_L'(t_1) - g_L'(t_2)| \right. \\ &\quad \left. + |g_R'(t_1) - g_R'(t_2)| + |g_R(t_1) - g_R(t_2)| \right), \end{aligned}$$

with $t_1, t_2 \in [0, T]$. Since g_L and g_R are continuously differentiable we conclude that \mathbf{f} is continuous in time. Finally, if both $g'_L(t)$ and $g'_R(t)$ are Lipschitz continuous, then we conclude that \mathbf{f} is Lipschitz continuous in both variables. \square

From the definition of the dynamical system in (5), it is natural to look for solutions $\mathbf{u} \in C^1([0, T]; L) \cap C^0([0, T]; V)$ which are called classical solutions in the context of semigroup theory; see [Paz83, Definition 4.2.1]. There are, however, two other notions of solution associated with (5): *strong solutions* ([Paz83, Definition 4.2.8]) and *mild solutions* ([Paz83, Definition 4.2.3]). We will work in this paper with strong solutions of (5):

Definition 2.2 (strong solutions). A function \mathbf{u} which is differentiable almost everywhere on $[0, T]$ such that $\mathbf{u}' \in L^1(0, T; L)$ is called a strong solution of the initial value problem (5) if $\mathbf{u}(0) = \mathbf{u}_0$ and $\mathbf{u}' + A\mathbf{u}(t) = \mathbf{f}(\lambda, \mathbf{u}(t), t)$ almost everywhere (a.e.) on $(0, T]$.

For the moment consider that the right-hand side is fixed, i.e.,

$$\begin{aligned} \mathbf{u}'(t) + A\mathbf{u}(t) &= \mathbf{f}(t) \quad (t > 0), \\ \mathbf{u}(0) &= \mathbf{u}_0, \end{aligned} \tag{8}$$

for a given $\mathbf{f}(t)$. We then seek $\mathbf{u}(t) \in C([0, T]; L) \cap L^1(0, T; V)$ with $\mathbf{u}' \in L^1(0, T; L)$ such that (8) is satisfied a.e. in $[0, T]$. Semigroup theory is used to establish existence and uniqueness of the solution as A is non-coercive. For this purpose, recall the following definition (see [EG04, Chapter 6.3]):

Definition 2.3 (Monotone and maximal operator). The operator $A : V \rightarrow L$ is said to be monotone if and only if for all $u \in V$, $(Au, u)_L \geq 0$. Moreover, A is said to be maximal if and only if for all $\hat{f} \in L$, there exists $u \in V$ such that $u + Au = \hat{f}$. If A is monotone, L is reflexive, and

$$\|Au\|_L \geq c_1\|u\|_V - c_2\|u\|_L \quad \forall u \in V, \tag{9}$$

for some $c_1, c_2 > 0$ then we can conclude that A is maximal.

Note that from the definition of A , as well as the spaces L and V , we have

$$(Av, v)_L = \int_{\Omega} p \partial_x q + q \partial_x p = (pq)|_{\partial\Omega} = 0.$$

Since A is monotone, L is reflexive and (9) holds trivially due to the definition of L and V , we conclude that A is also maximal. For what follows, let $D(A)$ denote the domain of A . Note that $D(A)$ is a linear subspace of L . Now, if the operator $A : D(A) \subset L \rightarrow L$ is maximal and monotone then it holds that

- 1 $D(A)$ is dense in L ;
- 2 the graph of A is closed;
- 3 $\forall \eta > 0, I + \eta A \in \mathcal{L}(D(A); L)$ is bijective and $\|(I + \eta A)^{-1}\|_{\mathcal{L}(L; L)} \leq 1$;

see [EG04, Lemma 6.51] and the references therein. The properties 1.-3. enable us to apply the Hille-Yosida theorem to show that A generates a C_0 -semigroup of contractions $\mathbb{T}(t)$, for $t > 0$. Then the function $\mathbf{u} \in C([0, T]; L)$ is a *mild solution* of (5) for $\mathbf{u}_0 \in L$ and $\mathbf{f}(\lambda, \mathbf{u}(t), t) \in L^1((0, T); L)$ if it satisfies

$$\mathbf{u}(t) = \mathbb{T}(t)\mathbf{u}_0 + \int_0^t \mathbb{T}(t-s)\mathbf{f}(\lambda, \mathbf{u}(s), s)ds \quad \forall t \in [0, T]. \tag{10}$$

The following theorem states existence and uniqueness of a mild solution which will be used later on to establish the analogous result for strong solutions. See [Paz83, Theorem 1.2, Chapter 6] for a proof.

Theorem 2.4. Let $\mathbf{f} : X \times L \times [0, T] \rightarrow L$ be continuous in t on $[0, T]$ and uniformly Lipschitz continuous on L . Then, for every $\mathbf{u}_0 \in L$ there exists a unique mild solution $\mathbf{u} \in C([0, T]; L)$ satisfying (10).

We now establish uniqueness and existence of a strong solution to (5) as well as boundedness and Lipschitz continuity of the solution with respect to the friction coefficient.

Theorem 2.5. Let $\mathbf{f} : X \times L \times [0, T] \rightarrow L$ be uniformly Lipschitz continuous in time, and on L for a given $\lambda \in X$, i.e., for some $C > 0$ depending on λ we have

$$\|\mathbf{f}(\lambda, \mathbf{v}_1, t_1) - \mathbf{f}(\lambda, \mathbf{v}_2, t_2)\|_L \leq C(\|\lambda\|_X)(|t_1 - t_2| + \|\mathbf{v}_1 - \mathbf{v}_2\|_L) \quad \forall t_1, t_2 \in [0, T],$$

for all $\mathbf{v}_1, \mathbf{v}_2 \in L$. Then, for $\mathbf{u}_0 \in D(A)$ there exists a unique strong solution $\mathbf{u} \in L^1(0, T; V) \cap C([0, T]; L)$ and $\mathbf{u}' \in L^1(0, T; L)$ satisfying (5) a.e. in time and

$$\|\mathbf{u}(t)\|_L \leq C(T, \mathbf{u}_0, \lambda) \quad \forall t \in [0, T]. \quad (11)$$

Moreover, if $\|\lambda\|_X \leq c$ for $\lambda \in X$ and \mathbf{f} is (locally) Lipschitz continuous with respect to λ , then we have

$$\|p_1(t) - p_2(t)\|_{L^2(\Omega)} \leq C\|\lambda_1 - \lambda_2\|_X \quad \forall t \in [0, T]. \quad (12)$$

Proof. Let $\mathbf{u} \in C([0, T]; L)$ be a mild solution of (5), $\|\mathbb{T}(t)\|_L \leq M$ and $\|\mathbf{f}(\lambda, \mathbf{u}(t), t)\|_L \leq N$ for $t \in [0, T]$. For $h \in [0, t]$ we obtain

$$\begin{aligned} \mathbf{u}(t+h) - \mathbf{u}(t) &= \mathbb{T}(t+h)\mathbf{u}_0 - \mathbb{T}(t)\mathbf{u}_0 \\ &\quad + \int_0^t \mathbb{T}(t-s)[\mathbf{f}(\lambda, \mathbf{u}(s+h), s+h) - \mathbf{f}(\lambda, \mathbf{u}(s), s)]ds \\ &\quad + \int_0^h \mathbb{T}(t+h-s)\mathbf{f}(\lambda, \mathbf{u}(s), s)ds. \end{aligned}$$

Taking norms on both sides, applying the triangle inequality and estimating yield

$$\begin{aligned} \|\mathbf{u}(t+h) - \mathbf{u}(t)\|_L &\leq hM\|A\mathbf{u}_0\|_L + MC \int_0^t \|\mathbf{u}(s+h) - \mathbf{u}(s)\|_L ds + hMN \\ &\leq C'h + MC \int_0^t \|\mathbf{u}(s+h) - \mathbf{u}(s)\|_L ds, \end{aligned}$$

where we have used that $\mathbb{T}(t+h)\mathbf{u}_0 - \mathbb{T}(t)\mathbf{u}_0 = \int_t^{t+h} \mathbb{T}(s)A\mathbf{u}_0 ds$ (see [Paz83, Theorem 1.2.4]). Then Grönwall's inequality implies

$$\|\mathbf{u}(t+h) - \mathbf{u}(t)\|_L \leq C'' \exp(TMC) h,$$

which shows that $\mathbf{u}(t)$ is Lipschitz continuous (and it also proves (11)). This, combined with Lipschitz continuity of \mathbf{f} , implies that $t \mapsto \mathbf{f}(\lambda, \mathbf{u}(t), t)$ is Lipschitz continuous on $[0, T]$. Since L is reflexive, $\mathbf{u}_0 \in D(A)$, and $\mathbf{f}(\lambda, \mathbf{u}(t), t)$ is Lipschitz continuous, [Paz83, Corollary 4.2.11] implies the existence of a unique strong solution on $[0, T]$ for the following problem

$$\begin{aligned} \mathbf{v}'(t) + A\mathbf{v}(t) &= \mathbf{f}(\lambda, \mathbf{u}(t), t) \quad (t \geq 0), \\ \mathbf{v}(0) &= \mathbf{u}_0. \end{aligned}$$

Since a strong solution is a mild solution, we have

$$\mathbf{v}(t) = \mathbb{T}(t)\mathbf{u}_0 + \int_0^t \mathbb{T}(t-s)\mathbf{f}(\lambda, \mathbf{u}(s), s)ds = \mathbf{u}(t),$$

and, thus, $\mathbf{u}(t)$ is a strong solution to (5). Then by [Paz83, Theorem 4.2.9], we have $\mathbf{u} \in L^1(0, T; V)$ and $\mathbf{u}' \in L^1(0, T; L)$.

Suppose \mathbf{u}_1 and \mathbf{u}_2 are solutions obtained from two friction coefficients, λ_1 and λ_2 , respectively. Then, using the definition of mild solutions, we have for their difference

$$\begin{aligned} \|\mathbf{u}_1(t) - \mathbf{u}_2(t)\|_L &\leq M \int_0^t \|\mathbf{f}(\lambda_1, \mathbf{u}_1(s), s) - \mathbf{f}(\lambda_2, \mathbf{u}_2(s), s)\|_L ds \\ &\leq M \|\lambda_1 - \lambda_2\|_X C(\mathbf{u}_1(t)) + \|\lambda_2\|_X \int_0^t \|\mathbf{u}_1(s) - \mathbf{u}_2(s)\|_L ds \\ &\leq c_1 \|\lambda_1 - \lambda_2\|_X + c_2 \int_0^t \|\mathbf{u}_1(s) - \mathbf{u}_2(s)\|_L ds. \end{aligned}$$

An application of Grönwall inequality yields Lipschitz continuity of the pressure difference with respect to the friction coefficient, i.e.,

$$\|p_1(t) - p_2(t)\|_{L^2(\Omega)} \leq \|\mathbf{u}_1(t) - \mathbf{u}_2(t)\|_L \leq c_3 \|\lambda_1 - \lambda_2\|_X,$$

which completes the proof. \square

From the definition of \mathbf{f} in (7), Lemma 2.1 and Theorem 2.5, we obtain the following sufficient conditions on the boundary data g_L, g_R and the friction function such that the PDE in (1) admits a unique strong solution and the Lipschitz continuity result.

Corollary 2.6. *Let $g_L(t), g_R(t) \in C^1([0, T])$ and g'_L, g'_R be Lipschitz continuous on $[0, T]$. Moreover, suppose that $a(\cdot, \cdot)$ is uniformly Lipschitz continuous with respect to its arguments. Then, for every $(p_0, q_0) \in V$, there exists a unique strong solution $(p, q) \in C([0, T]; L) \cap L^1(0, T; V)$ with $(p', q') \in L^1(0, T; L)$ to (1). Further, we have*

$$\|(p(t), q(t))\|_L \leq C(T) \quad \forall t \in [0, T],$$

and if $\|\lambda\|_X \leq C'$ uniformly, then it holds that

$$\|p_1(t) - p_2(t)\|_{L^2(\Omega)} \leq C \|\lambda_1 - \lambda_2\|_X \quad \forall t \in [0, T].$$

3 Prior modelling and Bayesian inverse problem

Next we construct probability measures on a function space. It is natural to use separable Banach spaces to define random functions using a countable infinite sequence in a Banach space. For this purpose, let $\{\phi_j\}_{j=1}^\infty$ denote an infinite sequence in a Banach space X with the norm $\|\cdot\|_X$ associated with a bounded domain $\Omega \subset \mathbb{R}$. The functions are assumed to be normalized, i.e., $\|\phi_j\|_X = 1$. We then define the randomized function

$$\lambda = m_0 + \sum_{j=1}^{\infty} \lambda_j \phi_j, \tag{13}$$

where $m_0 \in X$ (not necessarily normalized) and $\{\lambda_j\}_{j=1}^\infty$ are random numbers defined by $\lambda_j = \gamma_j \xi_j$. Here $\{\gamma_j\}_{j=1}^\infty$ is a deterministic sequence, $\{\xi_j\}_{j=1}^\infty$ is an independent and identically distributed (i.i.d.) random sequence, and we assume that ξ_j has mean zero for all $j \in \mathbb{N}$. For $N \in \mathbb{N}$, we also define the truncated series

$$\lambda^N = m_0 + \sum_{j=1}^N \lambda_j \phi_j. \tag{14}$$

As before, we choose $X = L^\infty(\Omega)$, $\gamma = \{\gamma_j\}_{j=1}^\infty \in \ell^1$, and $\xi_j \sim U([-1, 1])$ for all $j \in \mathbb{N}$. Moreover, we assume that there exist positive constants $m_{\min} \leq m_{\max}$ and $\delta > 0$ such that

$$\operatorname{ess\,inf}_{x \in \Omega} m_0(x) \geq m_{\min}, \quad \operatorname{ess\,sup}_{x \in \Omega} m_0(x) \leq m_{\max}, \quad \|\gamma\|_{\ell^1} = \frac{\delta}{1+\delta} m_{\min}.$$

Since X is not separable, we work with the closure of the linear span of functions $(m_0, \{\phi_j\}_{j=1}^\infty)$ with respect to $\|\cdot\|_X$. The resulting space is denoted by \mathcal{X} in what follows. The next result, taken from [DS16, Theorem 2.1], states that $(\mathcal{X}, \|\cdot\|_X)$ is a Banach space.

Theorem 3.1. *The following holds \mathbb{P} -almost surely: The sequence of functions $\{\lambda^N\}_{N=1}^\infty$ given by (14) is Cauchy in \mathcal{X} and the limiting function λ given by (13) satisfies*

$$\frac{1}{1+\delta} m_{\min} \leq \lambda(x) \leq m_{\max} + \frac{\delta}{1+\delta} m_{\min} \quad \text{for almost every } x \in \Omega.$$

3.1 Bayesian inverse problem

According to our assumptions we have noisy observations of the pressure drop at our disposition, here denoted by $y = \{y_j\}_{j=1}^K \in \mathbb{R}^K$, for $K \in \mathbb{N}$, at times $t_j \in (0, T]$ for $j = 1, \dots, K$. Now, let $\mathcal{Y} := \mathbb{R}^K$, with norm $|\cdot|$, and \mathcal{X} from above. Then the uncertainty-to-observation operator \mathcal{G} is defined by

$$\mathcal{G} : \mathcal{X} \rightarrow \mathcal{Y}, \quad \mathcal{G}(\lambda) := (\delta p(t_1), \dots, \delta p(t_K))^\top. \quad (15)$$

Note that Corollary 2.6 implies that

$$|\mathcal{G}(\lambda_1) - \mathcal{G}(\lambda_2)| \leq C \|\lambda_1 - \lambda_2\|_{L^\infty(\Omega)}. \quad (16)$$

Moreover, Theorem 2.5 and Theorem 3.1 provide a constant $C' > 0$ such that

$$|\mathcal{G}(\lambda)| \leq C' K^{1/2}. \quad (17)$$

We use an additive linear noise model in our observations, i.e.,

$$y = \mathcal{G}(\lambda) + \eta,$$

where $\eta = \{\eta_j\}_{j=1}^K$ is Gaussian observation noise with mean zero and positive definite covariance matrix $\Gamma \in \mathbb{R}^{K \times K}$. In general, the observation operator is a map $\mathcal{G} : \mathbb{X} \rightarrow \mathcal{Y}$, where we consider \mathbb{X} either finite-dimensional ($\mathbb{X} = \mathbb{R}^M$, $M \in \mathbb{N}$) or infinite dimensional ($\mathbb{X} = \mathcal{X}$), and $\mathcal{Y} = \mathbb{R}^K$. In the case where \mathbb{X} is finite dimensional, the posterior distribution is obtained from (3). For infinite-dimensional \mathbb{X} the relation (4) between the posterior measure and the prior measure based on the Radon-Nikodym derivative yields

$$\frac{d\mu^y}{d\mu_0}(\lambda) = \frac{1}{Z} \exp(-\Phi(\lambda, y)), \quad (18a)$$

$$Z(y) = \int_{\mathbb{X}} \exp(-\Phi(\lambda, y)) d\mu_0(\lambda), \quad (18b)$$

where $Z = Z(y)$ is a normalization constant, $\Phi(\lambda, y) := \frac{1}{2} |\Gamma^{-1/2}(y - \mathcal{G}(\lambda))|^2$, and $|\cdot|$ is the usual Euclidean norm.

The following, rather general conditions on a function Ψ and the prior μ_0 are sufficient to guarantee that μ^y is a well-defined probability measure on \mathbb{X} if Ψ replaces Φ in (18). The conditions furthermore guarantee well-posedness of the posterior distribution with respect to perturbations of the data. We first state the conditions and then check whether they are satisfied by our Φ .

Assumption 3.2. Let Λ and Y be Banach spaces. The function $\Psi : \Lambda \times Y \rightarrow \mathbb{R}$ satisfies the following conditions.

- (i) For every $\epsilon > 0$ and $r > 0$ there is $\mathfrak{M} = \mathfrak{M}(\epsilon, r) \in \mathbb{R}$, such that for all $\lambda \in \Lambda$, and for all $y \in Y$ with $\|y\|_Y < r$, it holds that

$$\Psi(\lambda, y) \geq \mathfrak{M} - \epsilon \|\lambda\|_\Lambda^2.$$

- (ii) For every $r > 0$ there exists $\mathfrak{K} = \mathfrak{K}(r) > 0$ such that for all $\lambda \in \Lambda$, $y \in Y$ with $\max\{\|\lambda\|_\Lambda, \|y\|_Y\} < r$

$$\Psi(\lambda, y) \leq \mathfrak{K}.$$

- (iii) For every $r > 0$ there exists $\mathfrak{R} = \mathfrak{R}(r) > 0$ such that for all $\lambda_1, \lambda_2 \in \Lambda$ and $y \in Y$ with $\max\{\|\lambda_1\|_\Lambda, \|\lambda_2\|_\Lambda, \|y\|_Y\} < r$

$$|\Psi(\lambda_1, y) - \Psi(\lambda_2, y)| \leq \mathfrak{R} \|\lambda_1 - \lambda_2\|_\Lambda.$$

- (iv) For every $\epsilon > 0$ and $r > 0$, there is $\mathfrak{C} = \mathfrak{C}(\epsilon, r) \in \mathbb{R}$ such that for all $y_1, y_2 \in Y$ with $\max\{\|y_1\|_Y, \|y_2\|_Y\} < r$ and for every $\lambda \in \Lambda$

$$|\Psi(\lambda, y_1) - \Psi(\lambda, y_2)| \leq \exp(\epsilon \|\lambda\|_\Lambda^2 + \mathfrak{C}) \|y_1 - y_2\|_Y.$$

Using Corollary 2.6, we show in the following proposition that

$$\Phi : \mathbb{X} \times \mathcal{Y} \rightarrow \mathbb{R}, \quad \text{with} \quad \Phi(\lambda, y) = \frac{1}{2} |\Gamma^{-1/2}(y - \mathcal{G}(\lambda))|^2 \quad (19)$$

indeed satisfies Assumption 3.2.

Proposition 3.3. Let $u = (p, q)$ be the strong solution of (5), given $u_0 \in V$ and $\lambda \in \mathbb{X}$ such that $\|\lambda\|_X \leq C$ for some $C > 0$. Moreover, let the observation operator \mathcal{G} be defined as in (15). Then the likelihood function Φ as defined in (19) satisfies Assumption 3.2.

Proof. In view of Assumption 3.2 we set $\Lambda := \mathbb{X}$, $Y := \mathcal{Y}$, and $\Psi \equiv \Phi$. Assumption (i) is satisfied trivially since $\Phi(\lambda, y) \geq 0$. For assumption (ii), using (17), we have

$$\Phi(\lambda, y) \leq \frac{1}{2} \|\Gamma^{-1}\|_{\mathcal{L}(\mathcal{Y}; \mathcal{Y})} (\|y\|_{\mathcal{Y}} + \|\mathcal{G}(\lambda)\|_{\mathcal{Y}})^2 \leq C.$$

for all $y \in \mathcal{Y}$ and $\lambda \in \mathbb{X}$ satisfying $\max\{\|y\|_{\mathcal{Y}}, \|\lambda\|_{\mathbb{X}}\} \leq \mathfrak{R}$. Assumption (iii) is fulfilled by the Lipschitz continuity of the pressure drop, i.e.,

$$\begin{aligned} |\Phi(\lambda_1, y) - \Phi(\lambda_2, y)| &= \left| \langle \mathcal{G}(\lambda_1) - \mathcal{G}(\lambda_2), 2y + \mathcal{G}(\lambda_1) + \mathcal{G}(\lambda_2) \rangle_{\Gamma^{-1}} \right| \\ &\leq \|\Gamma^{-1}\|_{\mathcal{L}(\mathcal{Y}; \mathcal{Y})} \|\mathcal{G}(\lambda_1) - \mathcal{G}(\lambda_2)\|_{\mathcal{Y}} \|2y + \mathcal{G}(\lambda_1) + \mathcal{G}(\lambda_2)\|_{\mathcal{Y}} \\ &\leq C \|\Gamma^{-1}\|_{\mathcal{L}(\mathcal{Y}; \mathcal{Y})} \|\mathcal{G}(\lambda_1) - \mathcal{G}(\lambda_2)\|_{\mathcal{Y}} \\ &\leq C' \|\Gamma^{-1}\|_{\mathcal{L}(\mathcal{Y}; \mathcal{Y})} \|\lambda_1 - \lambda_2\|_{\mathbb{X}}. \end{aligned}$$

where $\langle \cdot, \cdot \rangle_{\Gamma^{-1}}$ is the Euclidean inner product induced by matrix Γ^{-1} . The proof of assumption (iv) is similar to the one of assumption (iii). \square

We remark that in the uniform setting, boundedness of the potential follows directly from the model (13) and the properties of the forward problem. The existence and well-posedness results presented in this section are not limited to the uniform case and can be shown for rather general prior distributions provided that the conditions in Assumption 3.2 are satisfied. The following theorem asserts well-posedness of the posterior measure in our setting. It rests on the results in [DS16, Sul15].

Theorem 3.4. *Let $\mathbf{u} = (p, q)$ be the strong solution of (5), given $\mathbf{u}_0 \in V$ and the prior measure μ_0 according to (13). The uncertainty-to-observation map \mathcal{G} is as in (15). Then, the posterior measure μ^y satisfying (18) with (19) is a well-defined probability measure on \mathbb{X} for each observation $y \in \mathcal{Y} = \mathbb{R}^K$. Furthermore, the inference is well-posed with respect to perturbations in the data, i.e., there exists a constant $C \geq 0$ such that*

$$d_H(\mu^y, \mu^{\tilde{y}}) \leq C|y - \tilde{y}|, \quad \forall y, \tilde{y} \in \mathcal{Y},$$

where

$$d_H(\mu^y, \mu^{\tilde{y}}) = \left[\int_{\mathbb{X}} \left(\sqrt{\frac{d\mu^y}{d\mu_0}}(\lambda) - \sqrt{\frac{d\mu^{\tilde{y}}}{d\mu_0}}(\lambda) \right)^2 d\mu_0(\lambda) \right]^{1/2}$$

denotes the Hellinger distance of the measures $\mu^y, \mu^{\tilde{y}}$.

Proof. By Proposition 3.3, the likelihood function Φ satisfies Assumption 3.2. The local Lipschitz continuity of the potential implies the measurability of Φ with respect to the product measure $\nu_0(dy, d\lambda) = \rho(dy)\mu_0(d\lambda)$, where $\rho = \mathcal{N}(0, \Gamma)$, i.e., $\eta \sim \rho$. The boundedness of Φ further implies that $Z(y) > 0$. By [DS16, Theorem 3.4], the posterior μ^y is well-defined and fulfills (18). The boundedness of the potential implies $\exp(-M + \epsilon\|\lambda\|_{\mathbb{X}}^2)(1 + \exp(\epsilon\|\lambda\|_{\mathbb{X}}^2 + C)^2) \in L^1_{\mu_0}(\mathbb{X}, \mathbb{R})$ for every $r, \epsilon > 0$, with constants M, C given in Assumption 3.2. Here, $L^1_{\mu_0}(\mathbb{X}, \mathbb{R})$ denotes the Bochner space of all measurable functions $f : \mathbb{X} \rightarrow \mathbb{R}$ with $\int_{\mathbb{X}} |f(\lambda)| d\mu_0(\lambda) < \infty$. By [DS16, Theorem 4.5], the Lipschitz continuity of the posterior follows. \square

4 Discretization of the forward problem and sampling

The statistical inverse problem posed in Section 1 is now solved by using a discretization of the forward problem and the MCMC algorithm. More specifically, our goal is to reconstruct the friction coefficient $\lambda(x)$ from noisy observations of the pressure drop.

As motivated above, we model the truncated friction coefficient according to (14) yielding

$$\lambda^N(x) = m_0(x) + \sum_{k=-N}^N \lambda_k \phi_k(x),$$

where $m_0 \in L^\infty(\Omega)$ and $\phi_k(x)$ are scaled Fourier coefficients, i.e.,

$$\phi_k(x) = a_k \exp(ikx) \quad \text{for all } k \in \mathbb{Z},$$

$\{\lambda_k\}$ are complex coefficients that satisfy $\lambda_k^* = \lambda_{-k}$ and $\{a_k\}$ are real coefficients. Here and below λ_k^* denotes the complex conjugate of λ_k . In order to ensure that $\lambda^N(x) \geq \nu > 0$ for all $x \in \Omega$, we choose a_k with

$$\sum_{k \in \mathbb{Z}} |a_k| < \infty, \quad \sum_{k \in \mathbb{Z}, |k| > j} |a_k| < C j^{-\nu}, \quad (20)$$

for some $C > 0$ and $\nu > 0$; see [HSS13, SS12]. In particular, we use $a_k := \bar{a}|k|^2$ in order to ensure that (20) is satisfied. Then the mean function $m_0(x)$ can be chosen to ensure positivity of λ^N .

For the convenience of implementation, we reformulate the prior model as

$$\lambda^N(x) = m_0(x) + \sum_{k=0}^N a_k \left(\alpha_k \sin(2\pi kx) + \beta_k \cos(2\pi kx) \right), \quad (21)$$

where we have the following relation between $\{\lambda_k\}$ and $\{\alpha_k, \beta_k\}$

$$\lambda_k = \begin{cases} \frac{1}{2}(\beta_k - i\alpha_k) & \text{for } k > 0, \\ \beta_0 & \text{for } k = 0, \\ \lambda_{-k}^* & \text{for } k < 0. \end{cases}$$

The truncation λ^N converges towards $\lambda \in \mathbb{X}$ at rate ν , i.e. there exists $C > 0$ such that for all N and every $\lambda \in \mathbb{X}$, there holds

$$\|\lambda - \lambda^N\|_{\mathbb{X}} \leq CN^{-\nu}.$$

The Lipschitz continuity of the forward operator then leads to the estimate

$$|\mathcal{G}(\lambda) - \mathcal{G}(\lambda^N)| \leq CN^{-\nu}$$

with a possibly different constant $C > 0$. Instead of a fixed N -term truncation, random truncation leads to a variable dimension formulation. We refer to [CRSW13] for more details. By choosing a sufficiently large, but finite number N of terms, the truncated friction coefficient can be represented by using its degrees of freedoms (DOFs), i.e., we replace $\lambda^N(x)$ by

$$\boldsymbol{\lambda}^N = (\beta_0, \alpha_1, \beta_1, \dots, \alpha_N, \beta_N)^\top \in \mathbb{X}.$$

where in our finite dimensional setting, \mathbb{X} is defined by $\mathbb{X} = \{\boldsymbol{\lambda} \in \mathbb{R}^{2N+1} : \|\boldsymbol{\lambda}\|_\infty \leq C\}$ for a uniform positive constant C .

We seek an algorithm that finds the statistical properties of the components of $\boldsymbol{\lambda}^N$. In other words, providing a prior distribution for $\boldsymbol{\lambda}^N$ (for a fixed N) and a finite number of observations on the pressure drop, the MCMC algorithm aims to find a posterior probability distribution for the components of $\boldsymbol{\lambda}^N$. The method requires to solve the forward problem (1)–(2) frequently.

In order to discretize the forward problem, we first partition the domain Ω into N_h elements of non-overlapping intervals $I_j := (x_{j-1/2}, x_{j+1/2}]$, where $x_{j-1/2} < x_{j+1/2}$ for $j = 1, \dots, N_h$. Denoting the semi-discrete approximation of $p(x, t)$ and $q(x, t)$ at time t by

$$\mathbf{p}(t) := (p_1(t), p_2(t), \dots, p_{N_h}(t)), \quad \mathbf{q}(t) := (q_1(t), q_2(t), \dots, q_{N_h}(t)),$$

respectively, where

$$p_j(t) \approx \frac{1}{h_j} \int_{x_{j-1/2}}^{x_{j+1/2}} p(x, t) dx, \quad q_j(t) \approx \frac{1}{h_j} \int_{x_{j-1/2}}^{x_{j+1/2}} q(x, t) dx \quad \forall j = 1, \dots, N_h,$$

with $h_j = x_{j+1/2} - x_{j-1/2}$, we utilize the following semi-discrete scheme for the forward problem (1):

$$\begin{aligned} \frac{d}{dt} p_j(t) - \frac{1}{2\Delta t} (p_{j+1}(t) - 2p_j(t) + p_{j-1}(t)) + \frac{1}{c^2 h_j} (q_{j+1}(t) - q_{j-1}(t)) \\ = \frac{1}{2c^2} (\lambda_{j-1} a(p_{j-1}(t), q_{j-1}(t)) - \lambda_{j-1} a(p_{j+1}(t), q_{j+1}(t))), \\ \frac{d}{dt} q_j(t) - \frac{1}{2\Delta t} (q_{j+1}(t) - 2q_j(t) + q_{j-1}(t)) + \frac{c^2}{h_j} (p_{j+1}(t) - p_{j-1}(t)) \\ = \frac{1}{2} (\lambda_{j-1} a(p_{j-1}(t), q_{j-1}(t)) + \lambda_{j-1} a(p_{j+1}(t), q_{j+1}(t))), \end{aligned} \quad (22)$$

for all $j = 1, \dots, N_h$. In order to discretize in time and obtain the full discrete scheme, we partition the time direction into time slabs t_n for $n \in \mathbb{Z}_+$, where $t_n < t_{n+1}$. For simplicity we assume a uniform time-step, i.e., $t_{n+1} - t_n = \Delta t$ for all $n \in \mathbb{Z}_+$ and similarly a uniform mesh-size, i.e., $h_j = h$ for all $j \in \mathbb{Z}$. Then the time derivatives are approximated by

$$\frac{d}{dt} p_j(t_n) \approx \frac{1}{\Delta t} [p_j^{n+1} - p_j^n], \quad (23)$$

and analogously for q . In fact, substituting (23) into (22) provides the well known Lax-Friedrichs scheme for nonlinear conservation laws (see, e.g., [HHU17, HS17a]) combined with a special handling of the source term that in particular preserves steady states of (1) better than the usual techniques like splitting (see [Tor09]) or direct incorporation (see [Ul01]). The exact derivation is based on the nature of broad solutions to semilinear systems of balance laws and can be found in [HS17b] where also a comparison of different strategies to incorporate source terms is provided. The initial conditions are imposed weakly through

$$p_j^0 = \frac{1}{h_j} \int_{x_{j-1/2}}^{x_{j+1/2}} p_0(x) dx, \quad q_j^0 = \frac{1}{h_j} \int_{x_{j-1/2}}^{x_{j+1/2}} q_0(x) dx \quad \forall j = 1, \dots, N_h,$$

and the boundary conditions are realized through ghost cells yielding

$$q_0^n = g_L(t_n), \quad q_{N_h+1}^n = g_R(t_n) \quad \text{for all } t_n.$$

Since the boundary conditions merely prescribe q , the boundary values of p have to be computed. Here the flow into the ghost cells based on characteristic lines is utilized again, providing

$$p_{0/N_h+1}^{n+1} = p_{1/N_h}^n \mp \frac{1}{c} q_{1/N_h}^n \pm \frac{1}{c} q_{0/N_h+1}^{n+1} \mp \frac{\Delta t}{c} \lambda_{1/N_h} a(q_{1/N_h}^n, p_{1/N_h}^n).$$

We again refer to [HS17b] for details. The discrete pressure drop at time t_n is defined by

$$\delta p_h^n := \left| \|p_h^n\|_{L^2(0,\epsilon)} - \|p_h^n\|_{L^2(1-\epsilon,1)} \right|,$$

where $p_h^n \in L^2(\Omega)$ and $q_h^n \in L^2(\Omega)$ are piecewise approximate solutions of the form

$$p_h^n(x) = \sum_{j=1}^{N_h} p_j^n \mathbf{1}_{I_j}(x), \quad q_h^n(x) = \sum_{j=1}^{N_h} q_j^n \mathbf{1}_{I_j}(x) \quad \forall x \in \Omega.$$

Here $\mathbf{1}_{I_j}(x)$ is the characteristic function of the interval $I_j = (x_{j-1/2}, x_{j+1/2}]$. When discretizing the infinite-dimensional setting, the discrete uncertainty-to-observation operator $\mathcal{G}_h : \mathbb{R}^{2N+1} \rightarrow \mathbb{R}^K$ is defined by

$$\mathcal{G}_h(\lambda^N) := (\delta p_h^{n_1}, \delta p_h^{n_2}, \dots, \delta p_h^{n_K}).$$

4.1 Markov Chain Monte Carlo

Following the discretization of the forward problem and representing the friction function by a truncated series we can use the Bayesian framework (3) and obtain the posterior density function by

$$\pi(\lambda^N | y) = \frac{1}{Z} \exp\left(-\frac{1}{2}|y - \mathcal{G}_h(\lambda^N)|_\Gamma^2\right) \pi_0(\lambda^N), \quad (24)$$

where $Z > 0$ is the normalization constant and $\pi_0(\cdot)$ is the prior density function. MCMC is a method to sample from a given distribution whose normalization constant is unknown or intractable to compute. In our context, we use the MCMC algorithm as stated in Algorithm 4.1.

Algorithm 4.1 (Metropolis-Hastings). 1: Given $\lambda_{(0)} \in \mathbb{R}^{2N+1}$, a proposal distribution $q(\lambda'|\lambda)$, $y \in \mathbb{R}^K$ and $M \in \mathbb{N}$.
2: Define $\pi_y(\lambda) := \exp\left(-\frac{1}{2}|y - \mathcal{G}_h(\lambda)|_\Gamma^2\right)\pi_0(\lambda)$.
3: Define an empty list $\text{output} = []$.
4: **for** $0 \leq i \leq M$ **do**
5: Draw a proposal λ' from the proposal distribution function, i.e., $q(\lambda'|\lambda_{(i)})$.
6: Compute
$$\alpha = \min \left\{ 1, \frac{\pi_y(\lambda') q(\lambda_{(i)}|\lambda')}{\pi_y(\lambda_{(i)}) q(\lambda'|\lambda_{(i)})} \right\}.$$
7: Set $\lambda_{(i+1)} := \lambda'$ with probability α and $\lambda_{(i+1)} := \lambda_{(i)}$ with probability $1 - \alpha$.
8: Append λ' into output .
9: $i \leftarrow i + 1$.
10: **end for**
11: **return** output

Algorithm 4.1 generates a Markov chain with stationary distribution $\pi(\lambda|y)$ (under additional assumptions on the proposal kernel). The first few samples are usually discarded for inference and are called *burn-in* samples. The Metropolis Hastings algorithm will be used in the following with two different proposal kernels, the Gaussian random walk proposal and the preconditioned Crank Nicolson variant. For the Gaussian random walk proposal function and throughout this paper (when referring to MCMC) we use

$$q(\lambda|\lambda') = \exp(-|\lambda - \lambda'|^2/2\sigma^2)/\sqrt{2\pi\sigma^2}. \quad (25)$$

4.2 Preconditioned Crank-Nicolson

Since the Gaussian random walk is known not to be robust with respect to the dimension of the underlying friction coefficient, we use a robust variant of the Metropolis-Hastings algorithm called *preconditioned Crank-Nicolson*. Already in its basic form pCN is suitable for centered Gaussian priors, i.e., $\pi_0 \sim \mathcal{N}(0, C)$ where C is the covariance matrix. Algorithm 4.2 describes this method; see [CDPS18].

Algorithm 4.2 (pCN with Gaussian prior). 1: Given $\lambda_{(0)} \in \mathbb{R}^{2N+1}$, $\beta \in (0, 1]$, $y \in \mathbb{R}^K$ and $M \in \mathbb{N}$.
2: Define $\Phi(\lambda; y) := \frac{1}{2}|y - \mathcal{G}_h(\lambda)|_\Gamma^2$.
3: Define an empty list $\text{output} = []$.
4: **for** $0 \leq i \leq M$ **do**
5: Propose $\lambda' = (1 - \beta^2)^{\frac{1}{2}}\lambda_{(i)} + \beta\zeta_{(i)}$ with $\zeta_{(i)} \sim \mathcal{N}(0, I)$.
6: Compute
$$\alpha = \min \left\{ 1, \exp\left(\Phi(\lambda_{(i)}; y) - \Phi(\lambda'; y)\right) \right\}$$
7: Set $\lambda_{(i+1)} := \lambda'$ with probability α and $\lambda_{(i+1)} := \lambda_{(i)}$ with probability $1 - \alpha$.
8: Append λ' into output .
9: $i \leftarrow i + 1$.
10: **end for**
11: **return** output

In order to use pCN in our setting, i.e., with a uniform prior instead of a Gaussian prior, we need to rewrite the random representation of $\lambda(x)$ in a way suitable for Algorithm 4.2. Recall that the truncated random friction function is defined by

$$\lambda^N(x) = m_0 + \sum_{j=1}^N \lambda_j \phi_j(x),$$

where $\lambda_j = \gamma_j \xi_j$. Here $\{\gamma_j\}_{j=1}^N$ is a deterministic sequence and $\{\xi_j\}_{j=1}^N$ is an i.i.d. random sequence where $\xi_j \sim U([-1, 1])$. We now represent ξ_j by $\xi_j = G(\zeta_j)$ with

$$G(\zeta_j) := 2F(\zeta_j) - 1, \quad \zeta_j \sim \mathcal{N}(0, I),$$

and $F(z)$ is the cumulative distribution function of a standard normal distribution. Therefore λ^N can be represented using random numbers with normal distribution, i.e.,

$$\lambda^N = m_0 + \sum_{j=1}^N \gamma_j G(\zeta_j) \phi_j.$$

This enables us to define Algorithm 4.2 using uniform priors which we describe in Algorithm 4.3.

Algorithm 4.3 (pCN with uniform prior). 1: Given $\lambda_{(0)} \in \mathbb{R}^{2N+1}$, $\beta \in (0, 1]$, $y \in \mathbb{R}^K$ and $M \in \mathbb{N}$.

2: Define $\Phi(\lambda; y) := \frac{1}{2} \|y - \mathcal{G}_h(\lambda)\|_{\Gamma}^2$.

3: Define an empty list `output = []`.

4: **for** $0 \leq i \leq M$ **do**

5: Define $\hat{\zeta}_{(i)} := (G^{-1}(\lambda_{(i),0}), \dots, G^{-1}(\lambda_{(i),2N+1}))^\top$.

6: Propose $\zeta' = (1 - \beta^2)^{\frac{1}{2}} \hat{\zeta}_{(i)} + \beta \zeta_{(i)}$ with $\zeta_{(i)} \sim \mathcal{N}(0, I)$.

7: Define $\lambda' := (G(\zeta'_0), \dots, G(\zeta'_{2N+1}))^\top$

8: Compute

$$\alpha = \min \left\{ 1, \exp \left(\Phi(\lambda_{(i)}; y) - \Phi(\lambda'; y) \right) \right\}$$

9: Set $\lambda_{(i+1)} := \lambda'$ with probability α and $\lambda_{(i+1)} := \lambda_{(i)}$ with probability $1 - \alpha$.

10: Append λ' into `output`.

11: $i \leftarrow i + 1$.

12: **end for**

13: **return** `output`

5 Numerical experiments

In this section we report on numerical experiments using the forward scheme and the MCMC algorithm as described in Section 4. The forward solver is implemented in C++ in order to perform fast numerical computation while the MCMC algorithm is implemented in Python scripting language with calls to the C++ code. The software package can be downloaded from <http://github.com/fg8/UQ> for academic purposes.

In the first numerical experiment we choose the truncation parameter in the friction coefficient to be $N = 0$ and choose $m_0 = 0$. This yields a scalar friction coefficient, i.e., $\lambda^0(x) = \beta_0$. As the prior we choose a uniform one, i.e.,

$$\pi_0(\lambda) := \frac{1}{Z} \mathbf{1}_{[\bar{\lambda}, \lambda]}(\lambda),$$

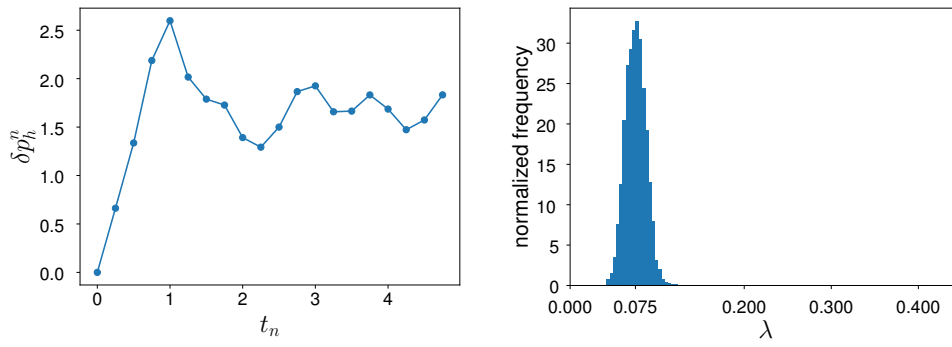


Figure 1: Pressure drop for a scalar friction coefficient with $\lambda_{\text{true}} = 0.075$ (left) and its corresponding histogram of the samples obtained from MCMC algorithm (right).

where $\underline{\lambda} < \bar{\lambda}$ are two fixed constants and $Z = \bar{\lambda} - \underline{\lambda}$ is the normalization constant. We choose the boundary conditions for $q(x, t)$ on $\partial\Omega$ as

$$q(0, t) = q(1, t) = 10 - \sin(2\pi t),$$

and the initial conditions as

$$p(x, 0) = q(x, 0) = 10 + \sin(2\pi x).$$

The model problem is completed by choosing the friction function $a(\cdot, \cdot)$ as

$$a(p, q) = -q|q|.$$

In order to validate the forward and the MCMC solvers, we set $\Gamma = I$ and $y_{\text{true}} = \mathcal{G}(\lambda_{\text{true}})$, with $\lambda_{\text{true}} = 0.075$. Then we choose $\underline{\lambda} = 0$ and $\bar{\lambda} = 0.5$ to fix the prior distribution. We fix the number of cells for the forward solver to be $N_h = 200$ and measure the pressure drop at t_{n_ℓ} for $\ell = 1, \dots, 20$, which are distributed uniformly in the interval $t \in [0, 5]$ (see Figure 1). We then run the MCMC of Algorithm 4.1 with 10,000 iterations to generate the Markov chain and we let 1,000 burn-in iterations. For the proposal function $q(\lambda|\lambda')$, see (25), we choose $\sigma = 0.25$ throughout this section. The histogram of the Markov Chain is plotted in Figure 1 (right). Observe that the samples cluster around the true value, i.e., $\lambda_{\text{true}} = 0.075$ while the starting point of the Markov Chain was set to be $\lambda_{(0)} = 0.45$, i.e., far from the true value.

We then add a mean zero Gaussian noise $\eta \in \mathbb{R}^K$ to y with covariance $\Gamma = 0.25 \times I_K$, where I_K is the identity matrix of size $K = 20$; see Figure 2 (left) for the comparison between true and noisy pressure drop. More precisely we set $y = \mathcal{G}_h(\lambda_{\text{true}}) + \eta$, and use MCMC to sample from the posterior distribution. The settings are the same as in the previous example. In Figure 2 (right) we see that the posterior distribution clusters around the true friction constant, i.e., $\lambda_{\text{true}} = 0.075$, despite the initial sample of MCMC to be $\lambda = 0.45$.

We finish this experiment by numerically checking for posterior consistency, i.e., the noise level in the observation will be reduced. In Figure 3, the histogram of the identified friction constant is plotted for different noise levels, i.e., $\eta = \mathcal{N}(0, \sigma \cdot I_K)$ for $\sigma = 0.05, \dots, 0.15$. Observe that the maximum of the posterior density function approaches the true value $\lambda_{\text{true}} = 0.075$ as the noise tends to zero.

In the next numerical example, we consider $\lambda(x)$ to be a function of the type (21) with $N = 3$. We set the true friction coefficient to be

$$\lambda_{\text{true}}(x) = 0.075 + \sum_{k=1}^N a_k \left(\alpha_k \sin(2\pi kx) + \beta_k \cos(2\pi kx) \right),$$

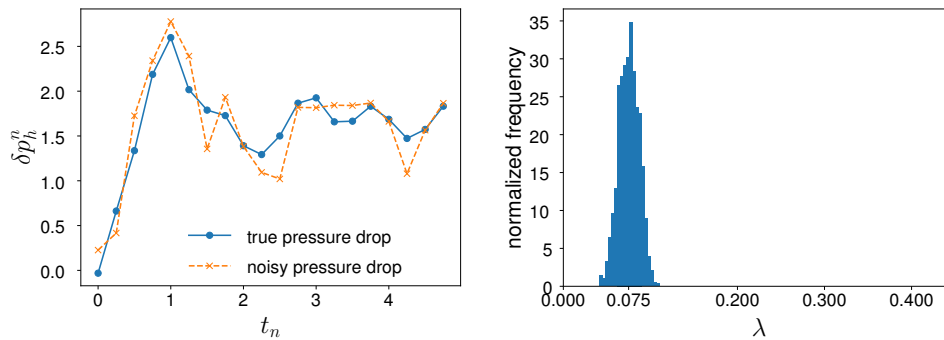


Figure 2: True and noisy pressure drop for a scalar friction coefficient with $\lambda_{\text{true}} = 0.075$ (left) and its corresponding histogram of the samples obtained from MCMC algorithm (right).

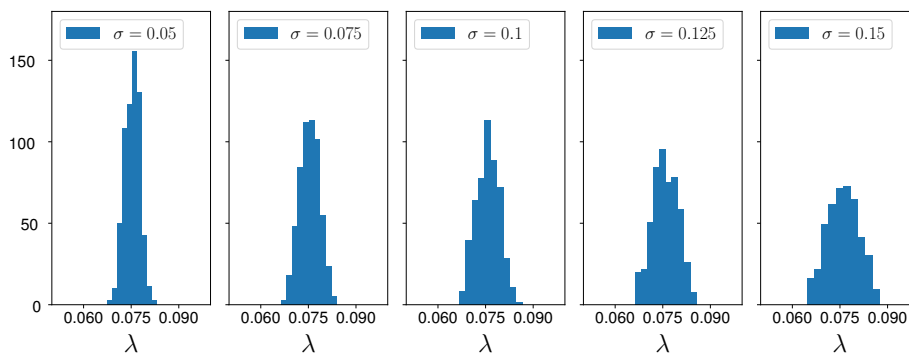


Figure 3: Effect of the noise in the observation on the posterior distribution.

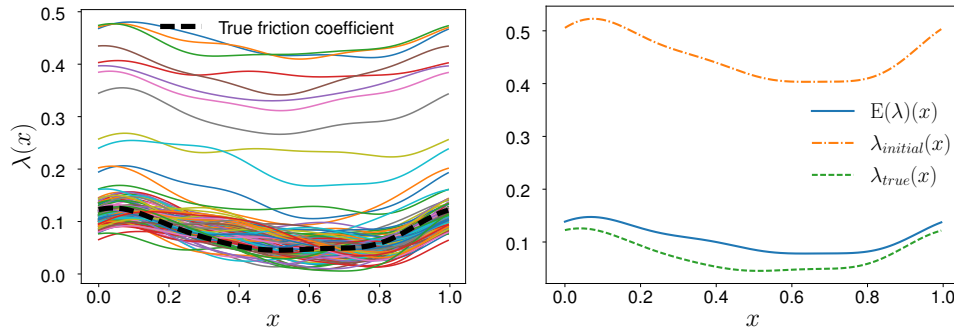


Figure 4: True and MCMC samples of the friction coefficient (left) and the pointwise mean friction function (right).

where

$$\alpha_1 = \frac{15}{1000}, \quad \beta_1 = \frac{35}{1000}, \quad \alpha_2 = \frac{25}{1000}, \quad \beta_2 = \frac{35}{1000}, \quad \alpha_3 = \frac{1}{1000}, \quad \beta_3 = \frac{30}{1000}.$$

The prior distribution function is then defined as

$$\pi_0(\boldsymbol{\lambda}) := \mathbf{1}_{[0.0,0.5] \times [0.0,0.05]^4}(\boldsymbol{\lambda}),$$

and the starting point of MCMC $\boldsymbol{\lambda}_{(0)} = (0.45, 0.04, 0.04, 0.04, 0.04, 0.04, 0.04)^\top$. In Figure 4 (left) we observe the samples drawn from the MCMC. Note that the initial starting point of the MCMC is far from the true friction coefficient and as the Markov Chain grows we converge to the true friction coefficient. In Figure 4 (right) we observe the pointwise mean friction coefficient obtained from the samples.

5.1 A double bump friction function

In this section we perform experiments with a true friction coefficient that can be approximated only in the limit by the truncated prior model (21). Throughout this section we use the following double bump friction function:

$$\lambda_{true}(x) = \frac{1}{10} + \mathbf{1}_{[\frac{1}{8}, \frac{3}{8}]}(x) \left(\frac{1}{8} - \left| x - \frac{1}{4} \right| \right) + 4 \times \mathbf{1}_{[\frac{5}{8}, \frac{7}{8}]}(x) \left(\frac{1}{8} - \left| x - \frac{3}{4} \right| \right). \quad (26)$$

In Figure 5 (left) we have plotted its approximation by the prior model (21) for $N = 0, \dots, 20$.

The discretization settings are defined as in the previous section. We choose at first $N = 4$ and set the prior distribution function to

$$\pi_0(\boldsymbol{\lambda}) := \frac{1}{Z} \mathbf{1}_{[0.0,0.45] \times [-0.025,0.025]^4 \times [-0.01,0.01]^4}(\boldsymbol{\lambda}),$$

where $Z > 0$ is the normalization constant and the starting point of the Markov chain is chosen as

$$\boldsymbol{\lambda}_{(0)} = (0.25, 0, 0, 0, 0, 0, 0, 0, 0)^\top.$$

We fix $\Gamma = I$, $y_{true} := \mathcal{G}(\lambda_{true})$ and run the MCMC to sample from the posterior distribution function.

In Figure 5, we plot the value of the posterior distribution function (upto a constant) evaluated at samples of the Markov chain obtained from Algorithm 4.1. Observe that there are three distinctive regions

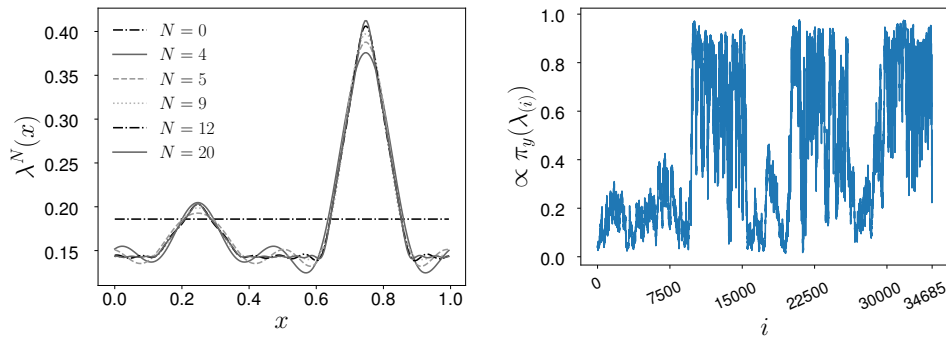


Figure 5: Fourier approximations of (26) (left) and posterior density function (upto a constant) for the Markov chain obtained from MCMC (right).

where the posterior density function is maximized, i.e., for i in $[7500, 15000]$, $[22000, 27000]$ and $[30000, 34685]$. This observation may hint that there are multiple friction functions that maximize the posterior distribution. In other words, for a given pressure drop, there might exist multiple friction functions, i.e., the uncertainty-to-observation operator is not injective. In such situations, the conditional mean might lead to unlikely estimates of the unknown parameters and to a poor fit of the measurement data, which is usually indicated by a wider variance. Thus, we propose a different strategy which is based on identifying regions in which the posterior is maximized.

In order to identify these friction functions we use a clustering algorithm to categorize friction functions that maximize the posterior distribution. Recall that given the truncation constant N we have for each sample in the Markov chain that $\lambda_{(i)} \in \mathbb{R}^{2N+1}$. We first select the samples in the Markov chain that maximize the posterior distribution upto a threshold. Let us denote the number of such samples by N_{\max} . Then, we concatenate the maximizing samples to form a feature matrix $F \in \mathbb{R}^{N_{\max} \times (2N+1)}$, i.e.,

$$F := (\lambda_{(i_0)}, \lambda_{(i_1)}, \dots, \lambda_{(i_{N_{\max}})})^\top. \quad (27)$$

Using the feature matrix F and a clustering algorithm, e.g., k -means, we can classify samples that maximize the posterior distribution. We summarize the above post-processing step in the following algorithm:

Algorithm 5.1 (Post-processing). 1: Given the Markov chain $\{\lambda_{(i)}\}_{i=0}^{N_{\text{samples}}}$, number of clusters, i.e., n_{cluster} , and a threshold $\text{threshold} < 1$.
2: Compute maximizing samples: $\{\lambda_{(i_j)}\}_{j=0}^{N_{\max}}$ such that

$$\lambda_{(i_j)} > \text{threshold} \times \left(\max_{i=1, \dots, N_{\text{samples}}} \pi_y(\lambda_{(i)}) \right).$$

- 3: Set the feature matrix F using (27).
4: Compute the clusters using k -means:

$$\{\Lambda_1, \Lambda_2, \dots, \Lambda_{n_{\text{cluster}}}\} = \text{KMeans}(F, n_{\text{cluster}}),$$

where Λ_ℓ contains samples that form the ℓ th cluster.

- 5: **return** $\{\Lambda_\ell\}_{\ell=1}^{n_{\text{cluster}}}$

We apply Algorithm 5.1 to our Markov chain with $\text{threshold} = 0.95$ and $n_{\text{cluster}} = 3$. In Figure 6, we plot the mean function obtained from samples of each of the three clusters. Note that all three mean functions maximize the posterior density function. However the first mean function, i.e., $E(\Lambda_1)(x)$,

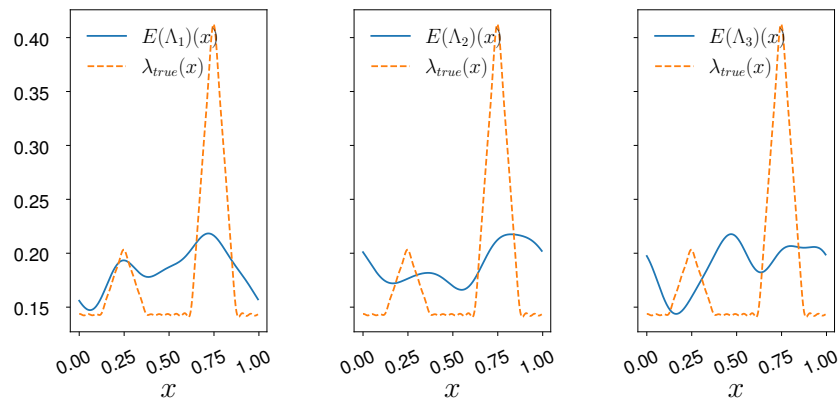


Figure 6: Mean functions of the three clusters obtained from Algorithm 5.1 ($N = 4$).

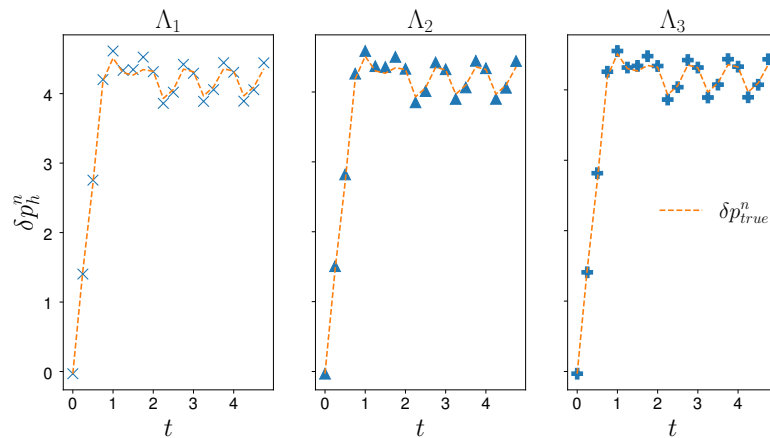


Figure 7: True pressure drop and the pressure drop associated to mean functions of the three clusters obtained from Algorithm 5.1 ($N = 4$).

captures the true friction function in the sense that it captures the right position of the bumps. In Figure 7, the pressure drops from the above mean functions are plotted against the true pressure drop. Note that all pressure drops are a good approximation of the true one which shows that the uncertainty-to-observation is not injective.

Adding noise

In this section we add noise to the observation, i.e., we consider $y = \mathcal{G}(\lambda) + \eta$ where η is a Gaussian noise centered at zero with standard deviation 10^{-4} . Therefore $\Gamma = 10^{-4} \times I$. The setting is the same as in the noise-free experiment and Algorithm 4.1 is used for sampling along with the post-processing step of Algorithm 5.1 with $n_{\text{cluster}} = 3$. The result is depicted in Figure 8.

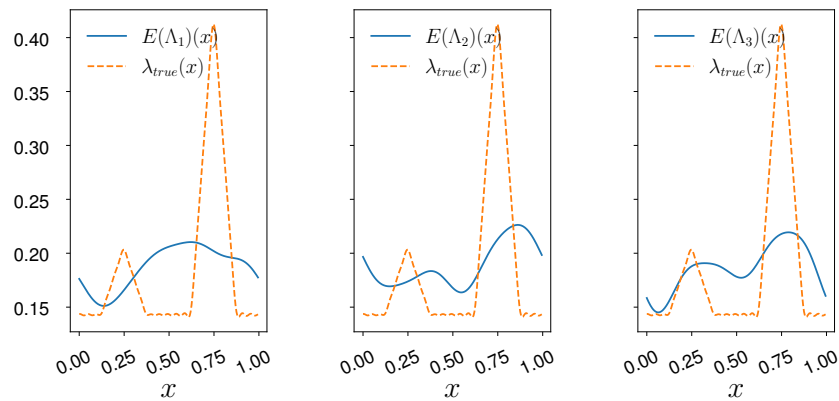


Figure 8: Mean functions of the three clusters obtained from Algorithm 5.1 when noise is present ($N = 4$).

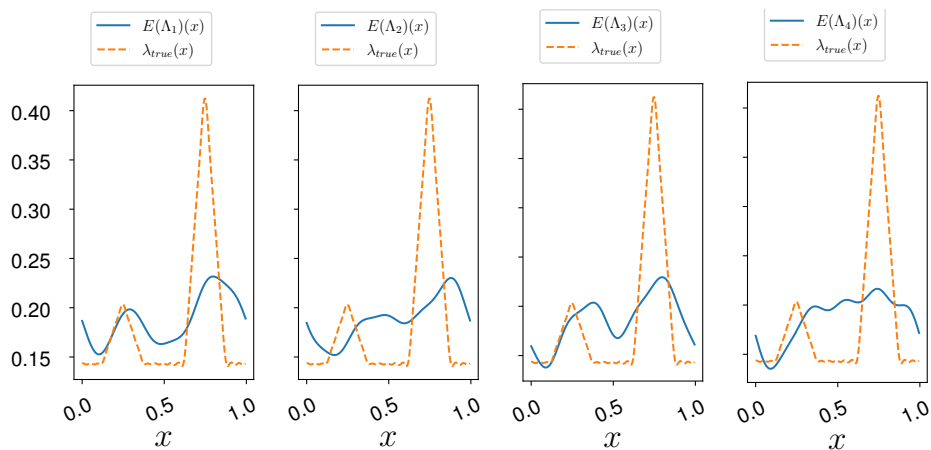


Figure 9: Mean functions of the four clusters obtained from Algorithm 5.1 ($N = 5$).

Increasing the truncation parameter

We now increase the truncation parameter N in the prior model (21). Observe that in Figure 9, the approximation has improved in the sense that we can capture the second bump located at $x = 0.75$ more accurately, and the gap between the first and second gap in the interval $[0.25, 0.75]$ is better approximated compare to Figure 6 (where $N = 4$). Similar results can be obtained for $N = 6$, which we plot in Figure 10. For the last experiment, we have chosen the number of clusters to be $n_{\text{cluster}} = 6$ and plotted the first four clusters.

Finally, we investigate the dimension robust behavior of the pCN (in comparison to the Gaussian random walk). The same setting as in the previous section with $N = 5$, $\Gamma = 5 \times 10^{-2}$ and 2500 is used. In Figure 11 we show the result obtained from pCN as a solver and the post-processing step of Algorithm 5.1. Note that pCN captures the right peak locations but with fewer iterations.

In Table 5.1, the number of accepted proposals (out of 10 000 proposals) for both Gaussian random walk and pCN algorithms is presented. For these numerical experiments, we let $N = 0, \dots, 7$ and we

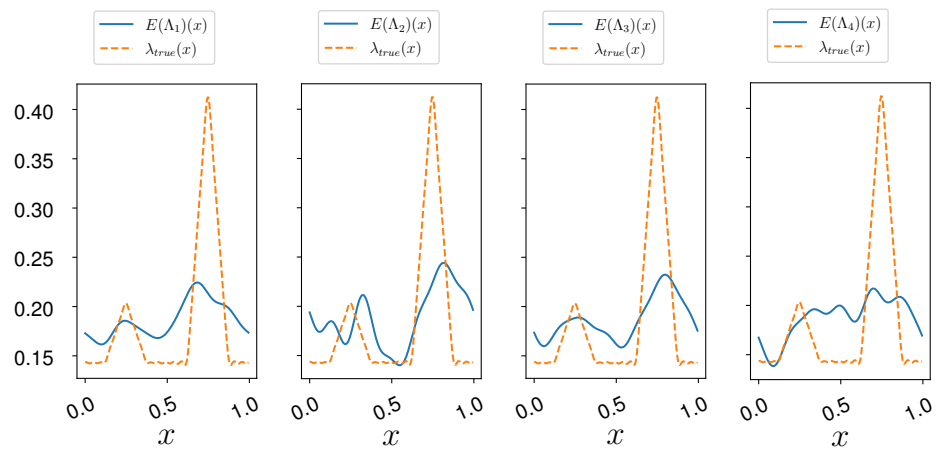


Figure 10: Mean functions of the four clusters obtained from Algorithm 5.1 ($N = 6$).

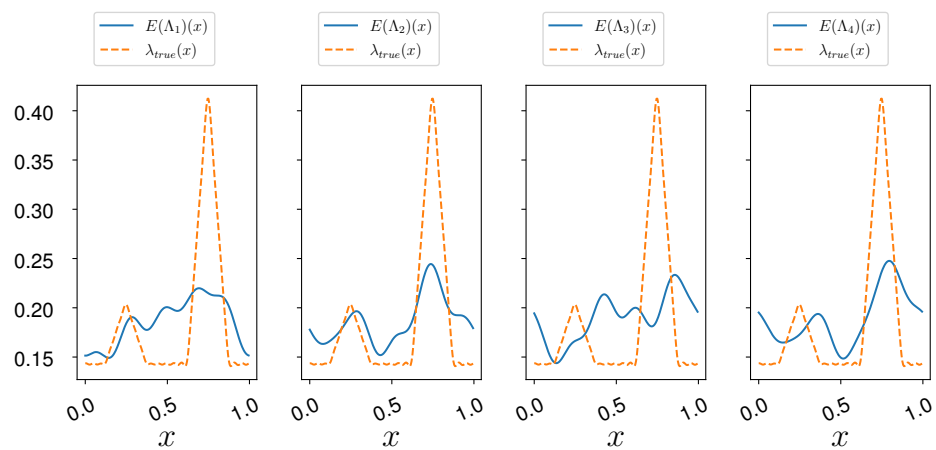


Figure 11: Mean functions of the four clusters obtained from pCN with $N = 5$.

Table 1: Number of accepted proposals for different N (total number of samples are 10 000).

N	0	1	2	3	4	5	6	7
MCMC	582	175	65	27	13	5	0	1
pCN	1802	2148	2022	1902	2127	2046	1907	2150

choose $\beta = 0.1$ for pCN. Observe that the acceptance rate for the Gaussian random walk decreases as N grows while pCN is robust with respect to N .

6 Conclusion and outlook

In this paper we considered a semi-linear isothermal Euler equation for the modelling of the gas flow in pipes and showed well-posedness of the underlying PDE as well as continuous dependence of the unknowns with respect to the friction function. More precisely, provided that the friction function is of Lipschitz class, the underlying PDE has a strong solution (Definition 2.2) and is Lipschitz continuous with respect to the friction function. We then focused on the Bayesian inverse problem of the identification of the friction coefficient using finite (noisy) observations of the pressure drop along the pipe. We showed that the underlying Bayesian inverse problem is well-posed. This enabled us to have a well-posed formulation of the MCMC algorithm both at the continuous and the discrete level. We then discretized the underlying friction coefficient and the PDE in order to identify numerically the friction function using MCMC. The numerical results revealed that the uncertainty-to-observation operator lacks injectivity which leads to multiple friction functions that maximize the likelihood function. Finally, in order to characterize these friction coefficients, we have used a clustering algorithm.

The results of this paper builds a foundation for problems arising from gas networks. As a natural extension of this work, we are working towards Bayesian inverse problems related to leakage detection in gas pipes. Moreover, our results will be used to provide a robust friction function as an input parameter for gas pipe models within the collaborative research center SFB-TRR 154 on *Modelling, Simulation and Optimization at the Example of Gas Networks* (see <https://trr154.fau.de/index.php/en/>) for projects which relate to real applications. We would like to finish this conclusion by mentioning that the convergence of the overall numerical method, i.e., discretization of the forward problem, friction coefficient, MCMC and the post-processing step, is an interesting question on its own.

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