Early Stage Assessment (ESA)

Department of Mathematics - Imperial College London
Yanni (John) Papandreou supervised by Dr Andrew Duncan
Project Title: *Bayesian formulations of PDE-based models, with an aim towards physics-informed machine learning*

1 Introduction

Mathematical models of physical systems are often expressed in terms of Partial Differential Equations (PDEs). In such models uncertainty is often introduced, either through a lack of knowledge of the parameters of the system or via inherent randomness in the system itself. Furthermore, these mathematical models and the associated computer simulations are often simplifications of the actual system leading to possible model misspecification [1]. The numerical algorithms used to simulate such models also induce uncertainty [2]. For example, it is often the case that a numerical method involves a finite-dimensional approximation of the unknown function. The computer simulations of these models can also often be very expensive computationally, and as such, these models are rarely used alone in the modelling procedure. Instead, observational data from the actual physical system via measurements is often incorporated as well. Data from measurements is now becoming increasingly available in almost every area of engineering and science, and failure to consider either the data or the model is clearly suboptimal. The issue of combining knowledge from both the model and data is thus of utmost importance and is often referred to as **data assimilation**, especially when the underlying mathematical model is a potentially stochastic dynamical system and the data may be time-ordered [3].

The Bayesian formulation of PDE-based models allows one to naturally incorporate all these sources of uncertainty (while still being able to identify the relevant source) and forces one to deal with modelling issues in a clear and precise manner. It allows measurement data to be considered in order to calibrate and tune mathematical models. Moreover, it allows a full characterization of all possible solutions to be found, together with their relative probabilities [4].

The statistical formulation of PDE-based models is necessary in many applications in order to handle in a precise manner the uncertainty present in the model. It allows this uncertainty to be propagated forward and gives clear answers for how much trust can be placed in the conclusions of the model. The finite element method (FEM) [5] is one of the most widely used methods for numerically approximating the solution of PDEs modelling natural and physical systems. Since FEM is an integral part of the study of many physical systems it is essential that we are able to fully quantify the uncertainty that using FEM introduces to our models and simulations.

In the recent paper "The Statistical Finite Element Method" Girolami et al. introduce a novel unifying approach which provides a fully statistical FEM in which both the finite element model and observational data are combined into a coherent inferential framework. This approach allows observational data to provide us with data adjusted FEM solutions. In particular, this paper considers a large class of linear PDEs and assumes that we have incomplete knowledge of the forcing term. The uncertainty resulting from this lack of knowledge is then formally accounted for by modelling the forcing as being random, having an appropriately defined Gaussian process (GP) distribution. The approximation of the linear PDE using the FE method then yields a multivariate Gaussian distribution on the resulting finite dimensional approximation. This probabilistic representation of the FE method is then used to condition the model on sensor data, providing a systematic methodology by which one can statistically update the Galerkin FEM solution.

Our work aims to provide more detailed error analysis explicitly quantifying the extent by which the distributions obtained using the "true" solution and the FEM solution differ. Once this is investigated we will then explore how this propagates through to any further inference. To be more specific, we will consider placing two different priors for any further inference. The first prior we will consider will be the distribution obtained

using the true solution operator of the PDE. The second prior will be that obtained using the FEM solution. In the case of Gaussian forcing, and under suitable conditions which will be specified, these two priors are both Gaussian measures on appropriate function spaces. We will aim to investigate how these priors differ by utilising the Wasserstein distance between probability measures. In particular, we will obtain an upper-bound for this distance by utilising a connection between the Wasserstein distance and the Procrustes Metric on covariance operators. Having investigated this discrepancy between the priors we will then investigate how this translates to a discrepancy in the subsequent posteriors obtained using observational data. Our treatment aims to follow the guiding principle of "*avoiding discretization until the the last possible moment*" [4]. This principle is a very powerful one used throughout numerical analysis, and we will aim to highlight its importance in our work.

The remainder of the report is structured as follows. Section 2 provides a concise account of the most relevant background material for the project together with a brief survey of the literature behind the topic of this work. In Section 3 we introduce the general framework we will be considering. We then apply the general framework in the context of FEM for an elliptic boundary value problem in Section 4 and then to a parabolic problem in Section 5. Section 6 finally discusses in more general terms the aims of our research before outlining several ideas for future work.

2 Brief Overview of Background Material

Our project is focused on providing detailed analysis of the uncertainty introduced by utilising numerical approximations for solving potentially noisy PDEs. The propagation of this error through to further inference is then investigated, when for instance observational data is incorporated. This project lies at the intersection of the fields of data assimilation, data-centric engineering, probabilistic numerics and Bayesian inference. We now provide a brief overview of the relevant background material for the project.

It is now well established that the language of probabilistic inference can be applied to numerical problems in order to provide a more detailed notion of the uncertainty resulting from numerically approximating an intractable problem [6, 7, 8, 9]. Numerical algorithms can be viewed as estimation rules for a latent, often intractable quantity given the results of tractable computations. Such algorithms can be considered to perform inference and are thus open to being analysed using the formal framework of probability theory. The field of Probabilistic Numerics (PN) [10] involves the study of so called "probabilistic numerical methods"; these are numerical algorithms which take in a probability distribution over its inputs and give out a probability distribution over its output. Several existing numerical methods have even recently been shown to arise from specific probabilistic models (references can be found at [10]). It is worth pointing out that so far we have only been referring to problems of a deterministic nature and probability theory is used as a means of providing a notion of the uncertainty inherent in using a numerical approximation to the solution of an intractable deterministic problem. In our work we will not restrict attention to purely deterministic problems but instead will consider potentially noisy PDEs. We will then seek to analyse the problem from the viewpoint of PN.

Much work has already been undertaken in the field of PN into applications to differential equations, especially for ODEs. Classic numerical algorithms for solving initial value problems (IVPs) provide an approximate solution often defined on a grid of time points. This numerical solution is often computed iteratively by collecting information from evaluations of the vector field associated to the system of differential equations. Probabilistic numerical methods instead provide probability measures, as opposed to point estimates, over the space of possible solutions to the IVP. In the PN literature there are two main approaches to solving ODEs which we now briefly outline.

The first approach introduces probability measures to ODE solvers by representing the distribution of all numerically possible trajectories with a set of sample paths using various different methods of computation (see [11, 2, 12, 13, 14, 15]). [11] draws them from a (Bayesian) Gaussian process regression while [2, 12, 13, 15] perturb classical estimates after an integration step with suitably scaled Gaussian noise and [14] instead perturbs the classical estimate via choosing a stochastic step size.

The second approach [16, 17, 18, 19, 20, 21] recasts IVPs as **stochastic filtering problems**. This method involves assuming *a priori* that the solution of the IVP and a prespecified number of its derivatives follow a Gauss-Markov process that solves a particular stochastic differential equation (SDE). The evaluations of the vector field of the IVP at numerical estimates of the true solution are then regarded as imperfect evaluations of

the time derivative of the solution and are thus used as a Bayesian update for the Gauss-Markov process. This approach gives an algorithm very similar in structure to that of the Kalman filter.

Probabilistic numerical methods for PDEs are much more uncommon. However, some methods do exist, and are briefly outlined below. In chapter 9 of "An Introduction to Computational Stochastic PDEs" Lord et al. analyse several different methods for dealing with elliptic PDEs with random data. In particular the following (random) elliptic boundary-value problem (BVP) on a domain $D \subset \mathbb{R}^d$ is considered:

$$\begin{aligned} -\nabla \cdot (a(x)\nabla u(x)) &= f(x), \quad \forall x \in D \\ u(x) &= g(x), \quad \forall x \in \partial D \end{aligned}$$

where $\{a(x)|x \in D\}$ and $\{f(x)|x \in D\}$ are second-order random fields. Lord et al. consider several methods for dealing with such a BVP. To start they first consider a variational formulation on D and show that under suitable assumptions on the diffusion coefficients there is a unique solution to the variational formulation almost surely. A Galerkin FE approximation is then established for this formulation. The FEM is then combined with the Monte Carlo method to yield what the authors call the "Monte Carlo Finite Element Method" (MCFEM) which can be used to estimate the expectation and variance of $u(x)$. This method essentially involves drawing *iid* samples from the random fields in the BVP and then applying the FEM element to the resulting elliptic BVPs. Following this a variational formulation on $D \times \Omega$ is instead considered, where Ω is the underlying sample space for the probability space where the random fields live. The associated weak form is not a convenient starting point for Galerkin approximation as it involves taking expectations with respect to the abstract set Ω and the associated probability measure. This leads the authors to instead consider that the noise arises from a finite number of random-variables (i.e. the random fields are so called *finite-dimensional noise*). Doing so yields an equivalent weak form on $D \times \Gamma$ where Γ is the range of the finite-dimensional noise. Having done this a Stochastic Galerkin FEM is developed to approximate the solution to this new weak form. Both a semi-discrete and fully-discrete version are considered (discretization can now occur in two spaces). After analysing this method the authors finally consider a stochastic collocation FEM which combines collocation on the range of the finite-dimensional noise and FEM approximations on D. It should be pointed out that these methods are quite computationally expensive and become infeasible when the dimension (of both the deterministic and random spaces) increases past 4. Some work has been done on sparse deterministic-stochastic tensor Galerkin finite element methods (sparse sGFEMS) [23] **CHANGE REFERENCE!!!!!**. This method aims to reduce computational complexity by using hierarchic sequences of finite-dimensional approximation spaces to yield sparse tensor product spaces. In Section 4 we will consider a particular example of such a random elliptic BVP and introduce an alternative probabilistic numerical method to tackle this.

Add more on PDE methods!!! In [24] a probabilistic numerical method to solve the strong formulation of a PDE (as opposed to the weak form considered in [2]) is proposed. This method begins with a prior distribution over the solution space of the PDE which is then restricted to a subset of the solution space by utilising information about the true solution of the PDE. This can be viewed as imposing the governing equations of the PDE at a finite number of locations in the domain of interest. The choice of where to impose the equations is what constitutes the discretization of the PDE and this restriction yields the posterior distribution on the solution.

We now give a brief account of additional background material necessary for this project. In particular, it was necessary to learn about methods to approximate solutions of partial differential equations, specifically parabolic and elliptic PDEs. We focused on Finite Element based approaches and sought to find a Bayesian formulation of the conditions which give rise to FEM approximations. As such a proper understanding of Finite Element Methods was necessary; the two main references we consulted for this were [22] and [25].

A thorough understanding of Gaussian processes/measures was also required. It is well known that we cannot have a Lebesgue measure on an infinite dimensional space; Gaussian measures provide a natural substitute [26]. Since solutions to PDEs lie in infinite dimensional function spaces Gaussian measures will prove very useful for our purposes in this project. GPs can be viewed as an infinite-dimensional extension of classical normal random variables. GPs have several advantages [27]:

- they provide a flexible way to model prior belief over function spaces
- computations involving them are often analytically tractable
- they provide a fully probabilistic work-flow which returns robust posterior variance estimates; allowing

uncertainty to be quantified in a natural way

There are two main views on how to work with Gaussian processes, one focuses on the covariance function of the GP [28] whereas the other focuses on the associated covariance operator [26, 29, 30]. Both viewpoints will prove useful in the sequel, though in general it is slightly cumbersome to switch between the two. The main references we followed for GPs include [26, 28, 29, 30].

Ideas from the data assimilation and filtering literature were also very useful. Data assimilation involves the combination of two sources of information:

- a mathematical model of the physical system or a numerical implementation of this model
- observations of the system, typically corrupted by noise

The objective of data assimilation [31] is to combine these two sources of information in order to obtain a more accurate and complete estimate of the system's true state. Doing so will often allow more accurate predictions of the system's future trajectory and can also lead to more accurate uncertainty quantification. Data assimilation methods are usually Bayesian, since the current knowledge of the state of the system can be thought of as a prior and the incorporation of the model dynamics and observations can be considered to be the "data" with which we condition on to obtain a posterior. Often it is desirable for *real time* data assimilation as well as for reasonable computational costs and as such there are two main ideas behind filtering/data assimilation:

- knowledge about the posterior should be built up sequentially
- the unknown state should be split into parts and knowledge should be built up for each of these parts sequentially

The first point seeks to improve overall efficiency and the second helps to reduce the dimensionality of each computational problem. The main references consulted for data assimilation/filtering were [3, 31, 32]. Another reference which proved invaluable was [4] which provided much insight into how to properly perform Bayesian Inference in the function space setting.

3 General Framework

We now introduce the general framework we will be considering. This will be split into two parts. In the first we shall be considering spatial problems without any time dependence, while in the second part we will consider problems with time dependence. We aim to describe how the two priors will be formed and then discuss how further inference will be carried out when observational data from the physical system is available.

3.1 Spatial Boundary Value Problems

We first consider PDEs which do not have any time dependence. Let Ω be a domain with boundary $\partial\Omega$ and let $\mathcal{L}$ be a suitable linear differential operator. We will focus on the following Dirichlet problem:

$$\begin{cases} \mathcal{L}u = f & \text{on } \Omega \\ u = g & \text{on } \partial\Omega \end{cases} \tag{1}$$

where the functions f, g may be noisy, typically Gaussian. The operator $\mathcal{L}$ may also be random. For simplicity we will take $g = 0$ and will assume that $\mathcal{L}$ is deterministic. We will also now assume that f is Gaussian, i.e. $f \sim \mathcal{N}(\bar{f}, K)$. We seek the solution in some appropriate Hilbert space of functions $\mathcal{H}$. We now discuss how the two priors over the solution space are formed. The first prior will essentially come from the true solution of the PDE while the second will be the "output" of a probabilistic numerical method[1] for solving the problem (1). As such we will initially place an appropriate prior on the solution u which encapsulates our prior belief on the solution (such as its smoothness) before utilising detailed knowledge of the specific PDE. We will then

[1]Note that in our discussion of probabilistic numerical methods we referred to the output as being a posterior distribution over the solution of the problem; here we are viewing the output as what we will set our prior to be for further inference.

consider using an approximation to obtain a posterior distribution which will then become our prior for further inference. We start with utilising the true solution:

3.1.1 Prior from the true solution

Formally we have $u = \mathcal{L}^{-1} f$, where $\mathcal{L}^{-1}$ is the solution operator (Green's function) for the problem (1). Since f is random we see that the solution is also random; in particular it is the push-forward of f by the **linear** operator $\mathcal{L}^{-1}$. Provided that the linear operator $\mathcal{L}^{-1}$ is bounded it follows from the theory of Gaussian measures (see Proposition 1.18 of [26]) that u is also Gaussian and in particular has the following distribution:

$$u \sim \mathcal{N}(\mathcal{L}^{-1}\bar{f}, \mathcal{L}^{-1}K(\mathcal{L}^{-1})^*) \tag{2}$$

This will be one of the two priors we will consider. One should note that this prior indeed utilises the true solution to the PDE. However, for most PDEs it will be intractable to actually compute this prior due to the fact that $\mathcal{L}^{-1}$ is inaccessible. This leads us instead to consider a prior based on a probabilistic numerical method for solving (1):

3.1.2 Prior from an approximation

We will now consider placing an initial Gaussian prior on the solution u, $u \sim \mathcal{N}(0, V)$. The covariance operator V will be chosen so as to satisfy the following assumption:

Assumption 1 V is controlled so that u lies almost surely in some appropriate subspace $\mathcal{U} \subset \mathcal{H}$ where the linear operator $\mathcal{L}$ restricted to this subspace is bounded[2], i.e. $\mathcal{L} : \mathcal{U} \to \mathcal{U}'$ is bounded where $\mathcal{U} \subset \mathcal{H} \subset \mathcal{U}'$.
Remark. We shall assume here that the subspace $\mathcal{U}$ is reflexive so that $\mathcal{U}''$ can be identified with $\mathcal{U}$. ♦

Having placed this prior on u we will now consider conditioning on the "observation" of a suitable information operator in order to form a posterior distribution which will be taken to be our new prior. This information operator will involve the following discretization $\mathcal{F}_h$ of the function space $\mathcal{H}$, where h is the mesh size. In particular, we will consider the following information operators $I_j : \mathcal{U}' \to \mathbb{R}$ defined by:

$$I_j \cdot = \langle \cdot, \phi_j \rangle$$

where $\langle \cdot, \cdot \rangle$ is the duality pairing between $\mathcal{U}$ and $\mathcal{U}'$ and where the $\phi_j \in \mathcal{F}_h$ for $j = 1, \ldots, J$. Note that J is inversely proportional to the mesh size h, in particular if $\Omega \subset \mathbb{R}^2$ then $J \propto 1/h^2$. It is also important to emphasise that $I_j \in \mathcal{U}''$ and so they are bounded linear operators.
Remark. Think of the $\{\phi_j\}$ as a basis for finite element spaces. ♦

Let $\mathcal{I}$ be the concatenation of these information operators, i.e. $\mathcal{I} = (I_1, \ldots, I_J)^T$. We will refer to $\mathcal{I}$ as the information operator. The probabilistic numerical method will involve conditioning on the "observation" of this information operator. To be more specific consider $\mathcal{I}$ acting on the PDE $\mathcal{L}u = f$. We have,

$$\mathcal{I}\mathcal{L}u = \mathcal{I}f =: F$$

where both $\mathcal{I}\mathcal{L}u$ and F are vectors in $\mathbb{R}^J$. Since, in theory, we know the properties of the forcing term f we have access to F. Our second prior will thus be the distribution of u conditional on "observing" $\mathcal{I}\mathcal{L}u = F$. In order to work out what this distribution is we will first consider the joint distribution of $(u, \mathcal{I}\mathcal{L}u)^T$. It is here that Assumption 1 is necessary, since we will utilise the fact that, under our prior, u lies almost surely in a subspace where the restriction of $\mathcal{L}$ is bounded. This implies that the joint distribution is as follows:

$$\begin{pmatrix} u \\ \mathcal{I}\mathcal{L}u \end{pmatrix} = \begin{pmatrix} I \\ \mathcal{I}\mathcal{L} \end{pmatrix} u \sim \mathcal{N}\left(\begin{pmatrix} 0 \\ \mathbf{0} \end{pmatrix}, \begin{pmatrix} V & V\mathcal{L}^*\mathcal{I}^* \\ \mathcal{I}\mathcal{L}V & \mathcal{I}\mathcal{L}V\mathcal{L}^*\mathcal{I}^* \end{pmatrix} \right) \tag{3}$$

In order to progress we will now consider that we fix a realisation of f (and so the corresponding F is also fixed). Doing so allows us to perform the conditioning step (see the Appendix for a full justification of this conditioning step) yielding the Bayesian update:

$$u | \{\mathcal{I}\mathcal{L}u = F, f\} \sim \mathcal{N}(a, \Sigma) =: \mu_{a,\Sigma} \tag{4}$$

[2] $\mathcal{L}$, being a differential operator, is in general an unbounded operator when viewed on the whole function space $\mathcal{H}$.

where,

$$a = V\mathcal{L}^*\mathcal{I}^*(\mathcal{I}\mathcal{L}V\mathcal{L}^*\mathcal{I}^*)^{-1}F \tag{5}$$

$$\Sigma = V - V\mathcal{L}^*\mathcal{I}^*(\mathcal{I}\mathcal{L}V\mathcal{L}^*\mathcal{I}^*)^{-1}\mathcal{I}\mathcal{L}V \tag{6}$$

Remark. We use the notation $\mu_{m,A}$ to denote a Gaussian measure (in arbitrary dimensions) with mean m and covariance A. The space (and hence the dimension) should be clear from the domain of the covariance operator. ♦

We will now seek to marginalize over f in (4) so as to obtain the "average" conditional distribution over all possible values of the forcing. This will give us our second prior. We state in the proposition below the result of performing this marginalization:

Proposition 3.1. Let u satisfy problem (1) and suppose that we place a prior $u \sim \mathcal{N}(0, V)$ where V satisfies Assumption 1. Also suppose that $g = 0$ and that the forcing f is distributed as $f \sim \mathcal{N}(\bar{f}, K)$. Then the conditional distribution $u|\{\mathcal{I}\mathcal{L}u = F\}$ is given by:

$$u|\{\mathcal{I}\mathcal{L}u = F\} \sim \mathcal{N}(Q\bar{F}, \Sigma + QK_{\mathcal{I}}Q^*) \tag{7}$$

where we have $\bar{F} := \mathcal{I}\bar{f}$, $K_{\mathcal{I}} := \mathcal{I}K\mathcal{I}^*$ and $Q := V\mathcal{L}^*\mathcal{I}^*(\mathcal{I}\mathcal{L}V\mathcal{L}^*\mathcal{I}^*)^{-1}$.

Proof: In order to perform this marginalization over f we first note:

$$f \sim \mathcal{N}(\bar{f}, K) =: \mu_{\bar{f},K} \implies \mathcal{I}f = F \sim \mathcal{N}(\mathcal{I}\bar{f}, \mathcal{I}K\mathcal{I}^*) =: \mu_{\bar{F},K_{\mathcal{I}}} \tag{8}$$

where $\bar{F} := \mathcal{I}\bar{f}$ and $K_{\mathcal{I}} := \mathcal{I}K\mathcal{I}^*$. In order to specify the "average" conditional distribution it suffices to compute the expectation of arbitrary bounded cylindrical test functions $\psi(u^N) := \psi(u(x_1), \ldots, u(x_N))$ since the $\sigma-$algebra generated by cylinder sets coincides with the Borel $\sigma-$algebra (see for instance Theorem 2.1.1 in [30]). We must thus compute:

$$\int\int \psi(u^N)\mu_{a,\Sigma}(\mathrm{d}u)\mu_{\bar{f},K}(\mathrm{d}f) \tag{9}$$

Note that $u^N = Pu$ where the bounded linear operator $P : \mathcal{H} \to \mathbb{R}^N$ is defined by $Ph := (h(x_1), \ldots, h(x_N))^T$ for any function h. Thus, u^N is multivariate normal, i.e., $u^N \sim \mathcal{N}(Pa, P\Sigma P^*) =: \mu_{Pa,\Sigma_N}$ where $\Sigma_N := P\Sigma P^*$ is the $N \times N$ covariance matrix of u^N. We thus have:

$$\int\int \psi(u^N)\mu_{a,\Sigma}(\mathrm{d}u)\mu_{\bar{f},K}(\mathrm{d}f) = \int\int \psi(u^N)\mu_{Pa,\Sigma_N}(\mathrm{d}u^N)\mu_{\bar{f},K}(\mathrm{d}f) \tag{10}$$

We note that $Pa = PQF$ where $Q := V\mathcal{L}^*\mathcal{I}^*(\mathcal{I}\mathcal{L}V\mathcal{L}^*\mathcal{I}^*)^{-1}$. Since the conditional distribution of u, (4), and hence of u^N only depends on f through $F \in \mathbb{R}^J$ we can thus write:

$$\int\int \psi(u^N)\mu_{Pa,\Sigma_N}(\mathrm{d}u^N)\mu_{\bar{f},K}(\mathrm{d}f) = \int\int \psi(u^N)\mu_{PQF,\Sigma_N}(\mathrm{d}u^N)\mu_{\bar{F},K_{\mathcal{I}}}(\mathrm{d}F) \tag{11}$$

Both measures in the above integral are now multivariate normal and so we can utilise the well-known formula for multidimensional Gaussian integrals to conclude that our integral becomes:

$$\int \psi(u^N)\mu_{h^N,\Sigma_{\mathcal{I}}}(\mathrm{d}u^N) \tag{12}$$

where,

$$h^N := \Sigma_{\mathcal{I}}\Sigma_N^{-1}PQB^{-1}K_{\mathcal{I}}^{-1}\bar{F} = PQ\bar{F} \tag{13}$$

$$\Sigma_{\mathcal{I}} := P(\Sigma + QK_{\mathcal{I}}Q^*)P^* \tag{14}$$

The details of this computation are left to the Appendix. From this we can see that we have obtained the expectation of ψ w.r.t. a multivariate Gaussian with mean and covariance given by h^N and $\Sigma_{\mathcal{I}}$. Thus, we can conclude that "averaging" over f gives the following Gaussian posterior:

$$u|\{\mathcal{I}\mathcal{L}u = F\} \sim \mathcal{N}\left(Q\bar{F}, \Sigma + QK_{\mathcal{I}}Q^*\right) \tag{15}$$

■

This posterior will be taken to be our second prior for further inference. One should note that this prior does indeed arise from an approximation to the solution of the PDE as it involves the information operator $\mathcal{I}$ which contains information on only a finite number of FE basis functions (J of them to be precise). The hope is that as the mesh size h decreases to 0 (and so $J \to \infty$) this distribution will become more and more like the true prior (2). In Sections 4 and 5 we will obtain, for specific examples, an upperbound on the distance between these two priors in terms of h and we will see that the two priors do indeed agree in the limit $h \to 0$.

It is also worth pointing out that the approximate prior (7) contains details of $V, \mathcal{I}, \bar{f}, K$ i.e. it contains information from all of: the original prior on u, the information operator and the statistical properties of the forcing term.

3.1.3 Incorporating Observational Data

We now have two prior distributions for the solution u to our boundary value problem (1), $\nu_i = \mathcal{N}(m_i, \Sigma_i)$ for $i = 1, 2$. The first is the prior from the true solution to (1) which has mean and covariance given by:

$$m_1 = \mathcal{L}^{-1}\bar{f} \tag{16}$$
$$\Sigma_1 = \mathcal{L}^{-1}K(\mathcal{L}^{-1})^* \tag{17}$$

The second is the prior from using an approximation to the solution of (1) and this has mean and covariance given by:

$$m_2 = Q\bar{F} \tag{18}$$
$$\Sigma_2 = \Sigma + QK_{\mathcal{I}}Q^* \tag{19}$$

with A as in Proposition 3.1.

We will now also assume that we have observational data, coming from sensors say, which give us noisy observations of the value of u at some points $y_1, \dots, y_s$ in Ω. We wish to update our belief in the distribution of u using this sensor data. In theory we can use either of the ν_i as prior distributions. However, as mentioned previously the true prior will often be intractable and as such we will be forced to use the second approximate prior. Our goal will thus be to investigate how different the two resulting posteriors are. This analysis will be carried out in the next section where we will consider a particular PDE and a particular choice of V which will correspond to a statistical version of FEM. For now we will outline the computation of the posterior distributions for the general framework under consideration.

Let $S : \mathcal{H} \to \mathbb{R}^s$ be the operator which maps a function $h \in \mathcal{H}$ to $(h(y_1), \dots, h(y_s))^T$ in $\mathbb{R}^s$. Assuming that the sensors make observations at each y_j with a normally distributed error we have that the likelihood for our sensor readings, $\mathbf{v}$, is:

$$\mathbf{v}|u \sim \mathcal{N}(Su, \epsilon^2 I) \tag{20}$$

The goal is to now find the posterior $u|\mathbf{v}$ when our prior is $u \sim \nu_i \equiv \mathcal{N}(m_i, \Sigma_i), \quad i = 1, 2$. In order to do so we will first find the joint distribution of $(u, \mathbf{v})^T$. To do this we note that our assumption that $\mathbf{v}|u$ is distributed according to (20) is equivalent to the assertion that:

$$\mathbf{v} = Su + \boldsymbol{\delta}$$

where $\boldsymbol{\delta} \sim \mathcal{N}(\mathbf{0}, \epsilon^2 I)$ is independent of u. From this we can see that the joint distribution of $(u, \boldsymbol{\delta})^T$ is:

$$\begin{pmatrix} u \\ \boldsymbol{\delta} \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} m_i \\ \mathbf{0} \end{pmatrix}, \begin{pmatrix} \Sigma_i & 0 \\ 0 & \epsilon^2 I \end{pmatrix} \right)$$

We now note that $(u, \mathbf{v})$ can be expressed as:

$$\begin{pmatrix} u \\ \mathbf{v} \end{pmatrix} = \begin{pmatrix} I & 0 \\ S & I \end{pmatrix} \begin{pmatrix} u \\ \boldsymbol{\delta} \end{pmatrix} + \begin{pmatrix} 0 \\ \mathbf{0} \end{pmatrix}$$

Since this is just a linear transformation of $(u, \boldsymbol{\delta})^T$ we have that the joint distribution of $(u, \mathbf{v})^T$ is given by:

$$\begin{pmatrix} u \\ \mathbf{v} \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} m_i \\ Sm_i \end{pmatrix}, \begin{pmatrix} \Sigma_i & \Sigma_i S^* \\ S\Sigma_i & \epsilon^2 I + S\Sigma_i S^* \end{pmatrix} \right) \tag{21}$$

From this it is simply a matter of conditioning to obtain the posterior distribution of $u|\mathbf{v}$. We thus obtain:

$$u|\mathbf{v} \sim \mathcal{N}(m^{(i)}_{u|\mathbf{v}}, \Sigma^{(i)}_{u|\mathbf{v}}) \tag{22}$$

where,

$$m^{(i)}_{u|\mathbf{v}} := m_i + \Sigma_i S^*(\epsilon^2 I + S\Sigma_i S^*)^{-1}(\mathbf{v} - Sm_i) \tag{23}$$

$$\Sigma^{(i)}_{u|\mathbf{v}} := \Sigma_i - \Sigma_i S^*(\epsilon^2 I + S\Sigma_i S^*)^{-1} S\Sigma_i \tag{24}$$

The next step in the analysis will be to quantify how different these two posteriors are by utilizing the Wasserstein Distance. In order to do this we must first investigate the distance between the priors ν_i. This will be done in the next section where we look at a particular PDE and a particular choice of V. We note that the presentation here has been quite general and that with a little bit of work it will even be possible to generalise this procedure to PDEs which have time dependence.

4 Statistical FEM for Elliptic Boundary Value Problem

AAIn this section we will focus on the following standard elliptic stationary conductivity problem:

$$\begin{aligned} \mathcal{L}u(x) &:= -\nabla \cdot (a(x)\nabla u(x)) = f(x), \quad x \in \Omega \\ u(x) &= 0, \quad x \in \partial\Omega \end{aligned} \tag{25}$$

where f is random and has distribution $f \sim \mathcal{N}(\bar{f}, K)$ as in Section 3. We assume that the diffusion coefficient satisfies the following assumption:

Assumption 2 (regularity of coefficients) The diffusion coefficient $a(x)$ satisfies:

$$0 < a_{\min} \leq a(x) \leq a_{\max} < \infty \text{ for almost all } x \in \Omega \tag{26}$$

for some real constants $a_{\min}, a_{\max}$. In particular, $a \in L^\infty(\Omega)$.

We will first work out the approximate prior for a specific choice of initial prior covariance V. This choice will correspond to solving the weak formulation of (25) via a finite element method. Once we work out this approximate prior we will give some conditions on the domain Ω so that the true prior is well-defined and so that we will be able to proceed with obtaining an upper-bound on the Wasserstein distance between these two priors. For now we will assume that Ω is a bounded domain and we will proceed to work out the approximate prior which corresponds to the FEM:

4.1 FEM prior

Throughout this section we will take the Hilbert space of functions to be $\mathcal{H} = L^2(\Omega)$. As noted in Section 3 we require that the initial prior covariance operator satisfies Assumption 1. In order to check if a candidate V satisfies this assumption we must first identify a subspace of $L^2(\Omega)$ on which the restriction of the operator $\mathcal{L}$ in (25) is bounded. This can easily be done in this case, as standard energy estimates give that $\mathcal{L}$ is a bounded operator from $H^1_0(\Omega)$ to $H^{-1}(\Omega)$. Thus, it suffices to check that the choice of V ensures that u lies almost surely in $H^1_0(\Omega) \subset L^2(\Omega)$. We are now in a position to define the initial prior.

Let $V : L^2(\Omega) \to L^2(\Omega)$ be defined as follows:

$$Vu(x) := \sum_{i=1}^{J} \lambda_i \phi_i(x) \int_\Omega \phi_i(y)u(y)\mathrm{d}y \tag{27}$$

where the λ_i are non-zero real numbers. Now the support of a Gaussian measure $\mathcal{N}(m, \Sigma)$ on a Hilbert space $\mathcal{H}$ is the space $m + \overline{\mathrm{Im}(\Sigma)}$ (see [33] for the general case of a Gaussian measure on a Banach space) where the bar denotes closure with respect to $\mathcal{H}$ and $\mathrm{Im}(\Sigma)$ is the image of Σ. The image of V can easily be seen to be

contained in the span of the $\{\phi_i\}_{i=1}^J$ which itself is strictly contained in $H_0^1(\Omega)$. Thus, the support of $\mathcal{N}(0,V)$ is clearly contained in $H_0^1(\Omega)$ and so if u is distributed according to this measure then u lies almost surely in $H_0^1(\Omega)$. This choice of V therefore satisfies Assumption 1.

Remarks. *Remark 1.* Since u lies almost surely in $H_0^1(\Omega)$ we can view $\mathcal{N}(0,V)$ as a Gaussian measure on $H_0^1(\Omega) \subset L^2(\Omega)$ and as such the covariance operator V can be instead viewed as a function from $H^{-1}(\Omega) \to H_0^1(\Omega)$ defined by:

$$Vu := \sum_{i=1}^{J} \lambda_i \langle u, \phi_i \rangle \phi_i \quad \forall u \in H^{-1}(\Omega) \tag{28}$$

where now $\langle \cdot, \cdot \rangle$ is now the $H^{-1}(\Omega), H_0^1(\Omega)$ duality pairing.

Remark 2. Note that taking $u \sim \mathcal{N}(0,V)$ is equivalent to saying that u has a Gaussian process distribution $u \sim \mathcal{GP}(0,k)$ where the k is the covariance function $k : \Omega \times \Omega \to \mathbb{R}$ given by:

$$k(x,y) := \sum_{i=1}^{J} \lambda_i \phi_i(x) \phi_i(y) \tag{29}$$

To link this with the covariance operator V note that we have:

$$Vu(x) = \langle u(\cdot), k(x, \cdot) \rangle \tag{30}$$

This connection between the two frameworks will be useful when we move to time-dependent PDEs. ♦

Now we recall the information operators. Let $\{\phi_j\}_{j=1}^J$ be a truncated set of FE basis functions. Since we have taken $\mathcal{U} = H_0^1(\Omega)$ we have that $\mathcal{U}' = H^{-1}(\Omega)$ and thus our info operators are maps $I_j : H^{-1}(\Omega) \to \mathbb{R}$ given by $I_j \cdot = \langle \cdot, \phi_j \rangle$.

Remark. Note that when $v \in L^2(\Omega) \subset H^{-1}(\Omega)$ we have, since $\phi_j \in H_0^1(\Omega)$, that

$$I_j v = \langle v, \phi_j \rangle = (v, \phi_j)_{L^2}$$

where $(\cdot, \cdot)_{L^2}$ is the standard $L^2(\Omega)$ inner product. This is essentially because of the identification of L^2 functions with linear functionals on $H_0^1(\Omega)$. ♦

It can be shown that for these information operators we have:

$$I_j \mathcal{L} u = \int_\Omega a(x) \nabla u(x) \cdot \nabla \phi_j(x) \mathrm{d}x \tag{31}$$

In order to continue with the derivation of the approximate prior as in Section 3 it will prove useful to express V in a different form as follows. We note that we can write:

$$Vu = \Phi^* \Lambda \langle u, \Phi \rangle \tag{32}$$

where $\Phi := (\phi_1, \ldots, \phi_J)^T$ and $\Lambda := \mathrm{diag}\{\lambda_i\}_{i=1}^J$ is a $J \times J$ matrix. To be precise we note that the above equation means:

$$Vu(x) = \Phi(x)^* \Lambda \langle u, \Phi \rangle \tag{33}$$

where $\Phi(x)^* = (\phi_1(x), \ldots, \phi_J(x))^T$ is a vector in R^J. It should also be pointed out that $\langle u, \Phi \rangle$ should be interpreted as the following column vector in $\mathbb{R}^J$:

$$(\langle u, \phi_1 \rangle, \ldots, \langle u, \phi_J \rangle)^T = \mathcal{I} u \tag{34}$$

thus we see that we can write:

$$Vu = \Phi^* \Lambda \mathcal{I} u \quad \forall u \in H^{-1}(\Omega) \tag{35}$$

i.e. $V = \Phi^* \Lambda \mathcal{I}$.

Remark. It will also prove useful later to notice that Φ^* is actually the same operator as $\mathcal{I}^*$. To see this we note that $\Phi^* : \mathbb{R}^J \to H_0^1(\Omega)$ is given by:

$$\Phi^* \mathbf{v} := \sum_{i=1}^{J} v_i \phi_i \tag{36}$$

where the vector $\mathbf{v}$ has components $v_i, \quad i = 1, \ldots, J$. Thus, Φ, the adjoint of Φ^* is a mapping from $H^{-1}(\Omega) \to \mathbb{R}^J$ which is determined by the relation:

$$\langle u, \Phi^* \mathbf{v} \rangle = (\Phi u, \mathbf{v}) \quad \forall u \in \ H^{-1}(\Omega) \ \forall \mathbf{v} \in \mathbb{R}^J \tag{37}$$

where $(\cdot, \cdot)$ is the standard inner product in $\mathbb{R}^J$. Using this equation it is a simple matter to show that $\Phi = \mathcal{I}$ and so $\Phi^* = \mathcal{I}^*$ as claimed. We can thus also express V as $V = \mathcal{I}^* \Lambda \mathcal{I} = \Phi^* \Lambda \Phi$. ♦

We are now in a position to work out the distribution of u conditional on "observing" $\mathcal{I}\mathcal{L}u = F$ for a fixed realistion of f. This distribution is given by $\mathcal{N}(a, \Sigma)$ where the definitions of a and Σ are given by equations (5) and (6) respectively. We work out each of these separately. First we compute the mean:

$$\begin{aligned} a &= V\mathcal{L}^*\mathcal{I}^*(\mathcal{I}\mathcal{L}V\mathcal{L}^*\mathcal{I}^*)^{-1}F \\ &= \Phi^*\Lambda\mathcal{I}\mathcal{L}^*\mathcal{I}^*(\mathcal{I}\mathcal{L}\Phi^*\Lambda\mathcal{I}\mathcal{L}^*\mathcal{I}^*)^{-1}F \\ &= \Phi^*\Lambda(\mathcal{I}\mathcal{L}\mathcal{I}^*)^*(\mathcal{I}\mathcal{L}\Phi^*\Lambda(\mathcal{I}\mathcal{L}\mathcal{I}^*)^*)^{-1}F \\ &= \Phi^*\Lambda(\mathcal{I}\mathcal{L}\Phi^*)^*(\mathcal{I}\mathcal{L}\Phi^*\Lambda(\mathcal{I}\mathcal{L}\Phi^*)^*)^{-1}F \end{aligned}$$

where we have used that $\mathcal{I}^* = \Phi^*$.

In order to simplify the mean we will work out what $\mathcal{I}\mathcal{L}\Phi^*$ is. We compute:

$$\begin{aligned} \mathcal{I}\mathcal{L}\Phi^* &= \begin{pmatrix} I_1 \\ \vdots \\ I_J \end{pmatrix} \begin{pmatrix} \mathcal{L}\phi_1 & \ldots & \mathcal{L}\phi_J \end{pmatrix} \\ &=: A \end{aligned}$$

where the $J \times J$ matrix A has $ij-th$ entry given by:

$$A_{ij} := I_i \mathcal{L}\phi_j \tag{38}$$

$$= \int_\Omega a(x) \nabla\phi_i(x) \cdot \nabla\phi_j(x) \mathrm{d}x \tag{39}$$

where we have utilised equation (31). This matrix A is the standard Galerkin stiffness matrix which appears in the finite element method. This matrix is a real symmetric matrix and so $A^* = A$. Further, this matrix can be shown to be invertible since the diffusion coefficient $a(x)$ satisfies Assumption 2 (for details of this see the Appendix). We can thus simplify the mean as follows:

$$\begin{aligned} a &= \Phi^*\Lambda(\mathcal{I}\mathcal{L}\Phi^*)^*(\mathcal{I}\mathcal{L}\Phi^*\Lambda(\mathcal{I}\mathcal{L}\Phi^*)^*)^{-1}F \\ &= \Phi^*\Lambda A^*(A\Lambda A^*)^{-1}F \\ &= \Phi^*\Lambda A A^{-1}\Lambda^{-1}A^{-1}F \\ &= \Phi^* A^{-1} F \end{aligned}$$

We thus see that when expressed in terms of the finite element basis the mean function has coefficients given by the vector $\hat{a} := A^{-1}F$ just like FEM gives. We now turn to the covariance and compute:

$$\begin{aligned} \Sigma &= V - V\mathcal{L}^*\mathcal{I}^*(\mathcal{I}\mathcal{L}V\mathcal{L}^*\mathcal{I}^*)^{-1}\mathcal{I}\mathcal{L}V \\ &= V - \Phi^*\Lambda\mathcal{I}\mathcal{L}^*\mathcal{I}^*(A\Lambda A)^{-1}\mathcal{I}\mathcal{L}\Phi^*\Lambda\mathcal{I} \\ &= V - \Phi^*\Lambda(\mathcal{I}\mathcal{L}\mathcal{I}^*)^* A^{-1}\Lambda^{-1}A^{-1}A\Lambda\mathcal{I} \\ &= V - \Phi^*\Lambda A A^{-1}\mathcal{I} \\ &= V - \Phi^*\Lambda\mathcal{I} = V - V = 0 \end{aligned}$$

We can thus see that when we choose our covariance operator V as above that the posterior (for a fixed realisation of F) collapses to a point measure located at the FEM solution to the PDE.

We now move on to work out the marginalization over f. Proposition 3.1 tells us that we should expect to obtain a Gaussian distribution with mean and covariance given by $Q\bar{F}$ and $\Sigma + QK_{\mathcal{I}}Q^*$ respectively. We have

shown by the above that for the FEM case we have $Q = \Phi^* A^{-1}$ and $\Sigma = 0$. We thus should expect to obtain the following:

$$\mathcal{N}(\Phi^* A^{-1} \bar{F}, \Phi^* A^{-1} K_{\mathcal{I}} A^{-1} \Phi) \tag{40}$$

as our averaged distribution. However, in the proof of Proposition 3.1 the calculations required the existence of the inverse of $\Sigma_N = P \Sigma P^*$ which in the FEM case is the 0 matrix since $\Sigma = 0$. However, it is still possible to redo the calculation of the expectation of an arbitrary bounded cylindrical test function which we performed in Section 3. The details of this are left to the Appendix, but the result is the same as expected from Proposition 3.1. Thus, the approximate prior arising from this choice of V is given by (40). It should be noted that this Gaussian measure directly links to what is found at the end of section 2 in the Statistical FEM paper [1]. It is also worth pointing out that this probabilistic numerical method for solving the BVP (25) gives a distribution whose mean coincides with the weak solution obtained by solving the problem with forcing given by $\bar{f}$ using FEM. Thus, this PNM recovers a classical method. We now move onto discussing the true prior.

4.2 Prior from the true solution

As discussed in Section 3.1.1 provided that the solution operator to the BVP is bounded we can work out that the "true" distribution of u should be:

$$u \sim \mathcal{N}(\mathcal{L}^{-1} \bar{f}, \mathcal{L}^{-1} K (\mathcal{L}^{-1})^*) \tag{41}$$

For the BVP under consideration (25) the following assumptions on Ω and its boundary $\partial\Omega$ will prove to be sufficient for our purposes here:

Assumption 3 Ω is a bounded, convex polygonal [3] domain whose boundary $\partial\Omega$ is thus a piecewise smooth curve.

Under this assumption on the domain and its boundary we have that the solution operator $\mathcal{L}^{-1}$ to the BVP is indeed bounded and so the "true" prior can indeed be taken to be the Gaussian (41). We now move on to quantifying how different the approximate prior (40) and the true prior (41) are.

4.3 Upperbound on the Wasserstein Distance between the two priors

We now have two Gaussian priors for the BVP (25) given by $\nu_i = \mathcal{N}(m_i, \Sigma_i)$ for $i = 1, 2$ where:

$$m_1 := \mathcal{L}^{-1} \bar{f} \tag{42}$$

$$m_2 := \Phi^* A^{-1} \bar{F} \tag{43}$$

$$\Sigma_1 := \mathcal{L}^{-1} K (\mathcal{L}^{-1})^* \tag{44}$$

$$\Sigma_2 := \Phi^* A^{-1} K_{\mathcal{I}} A^{-1} \Phi \tag{45}$$

We will now consider quantifying how close these two distributions ν_1, ν_2 are as a function of the FEM mesh size h. This will be achieved by obtaining an upperbound for the Wasserstein distance between ν_1, ν_2. In order to establish this upperbound a connection between the Wasserstein distance between Gaussian measures and the Procrustes Metric on covariance operators [34] will be exploited. We start by first giving the definition of the Wasserstein distance between two probability measures μ, ν on a normed space $\mathcal{H}$, $W(\mu, \nu)$:

$$W^2(\mu, \nu) = \inf_{\pi \in \Gamma(\mu, \nu)} \int_{\mathcal{H} \times \mathcal{H}} \|x - y\|_{\mathcal{H}}^2 \mathrm{d}\pi(x, y) \tag{46}$$

where $\Gamma(\mu, \nu)$ is the set of couplings of μ and ν, i.e.

$$\Gamma(\mu, \nu) := \{\text{Borel probability measures } \pi \text{ on } \mathcal{H} \times \mathcal{H} \mid \pi(E \times \mathcal{H}) = \mu(E) \text{ and } \pi(\mathcal{H} \times F) = \nu(F) \text{ for all Borel } E, F \subset \mathcal{H}\}$$

When μ, ν are both Gaussian measures an explicit expression can be obtained for the Wasserstein distance. Suppose $\mu = \mathcal{N}(m_1, \Sigma_1)$ and $\nu = \mathcal{N}(m_2, \Sigma_2)$. One has [34],

$$W^2(\mu, \nu) = \|m_1 - m_2\|_{\mathcal{H}}^2 + \mathrm{tr}(\Sigma_1) + \mathrm{tr}(\Sigma_2) - 2\,\mathrm{tr}\sqrt{\Sigma_1^{1/2} \Sigma_2 \Sigma_1^{1/2}} \tag{47}$$

[3] The polygonal assumption can easily be relaxed but we assume it here for simplicity.

This formula is true in both the finite and infinite dimensional cases. The term $\operatorname{tr}\sqrt{\Sigma_1^{1/2}\Sigma_2\Sigma_1^{1/2}}$ is difficult to analyse in our situation and as such we will make use of Proposition 3 from [34] which states:

Proposition 4.1. The Procrustes distance between two trace-class operators Σ_1 and Σ_2 on $\mathcal{H}$ coincides with the Wasserstein distance between two second-order Gaussian processes $\mathcal{N}(0,\Sigma_1)$ and $\mathcal{N}(0,\Sigma_2)$ on $\mathcal{H}$,

$$\Pi(\Sigma_1,\Sigma_2) := \inf_{R:R^*R=I} \|\Sigma_1^{1/2} - R\Sigma_2^{1/2}\|_2 = W(\mathcal{N}(0,\Sigma_1),\mathcal{N}(0,\Sigma_2))$$

where $\|\cdot\|_2$ is the Hilbert-Schmidt norm defined by $\|A\|_2 = \sqrt{\operatorname{tr}(A^*A)}$. ♦

Using this result one can obtain a simple upperbound on the Wasserstein distance by choosing $R = I$ in the infimum:

$$W(\mathcal{N}(0,\Sigma_1),\mathcal{N}(0,\Sigma_2)) = \inf_{R:R^*R=I} \|\Sigma_1^{1/2} - R\Sigma_2^{1/2}\|_2 \leq \|\Sigma_1^{1/2} - \Sigma_2^{1/2}\|_2 \tag{48}$$

Now since in our case we have un-centered Gaussian measures ν_1, ν_2 we must first link the Wasserstein distance between ν_1, ν_2 to the Wasserstein distance of the centred measures ν_1^*, ν_2^* using a general result mentioned in [35]:

$$W^2(\nu_1,\nu_2) = \|m_1 - m_2\|_{\mathcal{H}}^2 + W^2(\nu_1^*,\nu_2^*) \tag{49}$$

For our particular case, as mentioned previously, we will consider the underlying Hilbert space of functions to be $\mathcal{H} = L^2(\Omega)$. As such the norm for the difference in means is the L^2 norm. However, note that the solution to our BVP (25) lies in a subspace $H_0^1(\Omega) \subset L^2(\Omega)$. We have,

$$W^2(\nu_1,\nu_2) = \|m_1 - m_2\|_{L^2(\Omega)}^2 + W^2(\mathcal{N}(0,\Sigma_1),\mathcal{N}(0,\Sigma_2)) \tag{50}$$

where now the $m_i, \Sigma_i, i = 1, 2$ are given by equations (42-45). We now go about obtaining an upperbound on each of these two terms. We want to control each term by the FEM mesh size h. For brevity we will now assume that $\Omega \subset \mathbb{R}^2$ so we have a 2-dimensional problem. The analysis follows in almost exactly the same way for $\mathbb{R}^d$. We will assume that Ω satisfies Assumption 3. The convexity asssumption gives us that the $H^2(\Omega)$ norm of the variational solution of our PDE is controlled by the L^2 norm of the RHS. WE now take our FEM mesh to be a triangulation of Ω with H being the maximum side length of any triangle in the triangulation. We require a further technical assumption:

Assumption 4 The meshes under consideration remain regular in the sense that as we refine the mesh by decreasing h to 0 the angles of all triangles are bounded below independently of h.

Since $m_1 = \mathcal{L}^{-1}\bar{f}$ is the solution to the following elliptic BVP:

$$\begin{aligned} -\nabla\cdot(a(x)\nabla v(x)) &= \bar{f}(x), \quad x \in \Omega \\ v &= 0, \quad x \in \partial\Omega \end{aligned}$$

and since $m_2 = \Phi^* A^{-1}\bar{F} = \Phi^* A^{-1}\mathcal{I}\bar{f}$ is the FEM solution to the variational formulation of the above problem the error analysis of FEM transfers over to allow us to bound the norm of the difference of the means as follows:

$$\|m_1 - m_2\|_{L^2(\Omega)} \leq Ch^2\|m_1\|_{H^2(\Omega)} \leq \tilde{C}h^2\|\bar{f}\|_{L^2(\Omega)} \tag{51}$$

for some constances $C, \tilde{C} > 0$. We have utilised in the last inequality above the assumption that the H^2 norm of the true solution can be controlled by the L^2 norm of $\bar{f}$. The assumptions and error analysis is taken from Chapter 5 of [25] (see in particular Theorem 5.4).

We now move on to getting an upperbound for the second term. Using the link with the Procrustes distance discussed above we have:

$$W^2(\mathcal{N}(0,\Sigma_1),\mathcal{N}(0,\Sigma_2)) \leq \|\Sigma_1^{1/2} - \Sigma_2^{1/2}\|_2^2 \tag{52}$$

The RHS of the above is still difficult to deal with so we make use of Lemma 4.1 from [36] to obtain:

$$W^2(\mathcal{N}(0,\Sigma_1),\mathcal{N}(0,\Sigma_2)) \leq \|\Sigma_1^{1/2} - \Sigma_2^{1/2}\|_2^2 \leq \|\Sigma_1 - \Sigma_2\|_1 \tag{53}$$

where $\|\cdot\|_1$ is the trace norm or nuclear norm defined by $\|A\|_1 = \operatorname{tr}(\sqrt{A^*A})$.

We now investigate this term:

$$\begin{aligned}\|\Sigma_1 - \Sigma_2\|_1 &= \|\mathcal{L}^{-1}K(\mathcal{L}^{-1})^* - \Phi^* A^{-1} K_{\mathcal{I}} A^{-1}\Phi\|_1 \\ &= \|\mathcal{L}^{-1}K(\mathcal{L}^{-1})^* - \Phi^* A^{-1}\mathcal{I}K\mathcal{I}^* A^{-1}\Phi\|_1 \\ &= \|\mathcal{L}^{-1}K(\mathcal{L}^{-1})^* - \Phi^* A^{-1}\mathcal{I}K(\Phi^* A^{-1}\mathcal{I})^*\|_1\end{aligned}$$

where we have used the defintion of $K_{\mathcal{I}}$ and the fact that A and hence A^{-1} is self-adjoint. From this simplification we can see that we can control how "close" the two covariance operators are because we can control how "close" $\Phi^* A^{-1}\mathcal{I}$ is to $\mathcal{L}^{-1}$. To be more precise:

$$\begin{aligned}\|\Sigma_1 - \Sigma_2\|_1 &= \|\mathcal{L}^{-1}K(\mathcal{L}^{-1})^* - \Phi^* A^{-1}\mathcal{I}K(\Phi^* A^{-1}\mathcal{I})^*\|_1 \\ &= \|\mathcal{L}^{-1}K(\mathcal{L}^{-1})^* - \Phi^* A^{-1}\mathcal{I}K(\mathcal{L}^{-1})^* + \Phi^* A^{-1}\mathcal{I}K(\mathcal{L}^{-1})^* - \Phi^* A^{-1}\mathcal{I}K(\Phi^* A^{-1}\mathcal{I})^*\|_1 \\ &\leq \|\mathcal{L}^{-1}K(\mathcal{L}^{-1})^* - \Phi^* A^{-1}\mathcal{I}K(\mathcal{L}^{-1})^*\|_1 + \|\Phi^* A^{-1}\mathcal{I}K(\mathcal{L}^{-1})^* - \Phi^* A^{-1}\mathcal{I}K(\Phi^* A^{-1}\mathcal{I})^*\|_1 \\ &= \|(\mathcal{L}^{-1} - \Phi^* A^{-1}\mathcal{I})K(\mathcal{L}^{-1})^*\|_1 + \|\Phi^* A^{-1}\mathcal{I}K(\mathcal{L}^{-1} - \Phi^* A^{-1}\mathcal{I})^*\|_1 \\ &\leq \|\mathcal{L}^{-1} - \Phi^* A^{-1}\mathcal{I}\|_\infty \|K\mathcal{L}^{-1}\|_1 + \|\Phi^* A^{-1}\mathcal{I}K\|_1 \|(\mathcal{L}^{-1} - \Phi^* A^{-1}\mathcal{I})^*\|_\infty \\ &\leq \|\mathcal{L}^{-1} - \Phi^* A^{-1}\mathcal{I}\|_\infty (\|K\|_1 \|\mathcal{L}^{-1}\|_\infty + \|\Phi^* A^{-1}\mathcal{I}\|_\infty \|K\|_1)\end{aligned}$$

where we have utilized Holder's inequality and the sub-multiplicativity of Schatten-p norms (*note: the* $\|\cdot\|_\infty$ *is the operator norm here and is a special case of the Schatten-p norm for p being infinity*). As mentioned, we can control how "close" $\Phi^* A^{-1}\mathcal{I}$ is to $\mathcal{L}^{-1}$. To do this we note that (51) holds for all $\bar{f}$ in $L^2(\Omega)$, i.e. we have:

$$\|m_1 - m_2\|_{L^2(\Omega)} = \|(\mathcal{L}^{-1} - \Phi^* A^{-1}\mathcal{I})\bar{f}\|_{L^2(\Omega)} \leq \tilde{C}h^2 \|\bar{f}\|_{L^2(\Omega)} \quad \forall \bar{f} \in L^2(\Omega)$$

This implies that we can bound the operator norm[4] of $\mathcal{L}^{-1} - \Phi^* A^{-1}\mathcal{I}$ by $\tilde{C}h^2$, i.e.,

$$\|\mathcal{L}^{-1} - \Phi^* A^{-1}\mathcal{I}\|_\infty \leq \tilde{C}h^2 \tag{54}$$

Utilising this upper bound together with the fact that this implies that $\|\Phi^* A^{-1}\mathcal{I}\|_\infty$ is bounded by $\|\mathcal{L}^{-1}\|_\infty + \tilde{C}h^2$ we have:

$$W^2(\mathcal{N}(0,\Sigma_1),\mathcal{N}(0,\Sigma_2)) \leq \|\Sigma_1 - \Sigma_2\|_1 \leq \tilde{C}h^2 \|K\|_1 \left(2\|\mathcal{L}^{-1}\|_\infty + \tilde{C}h^2\right) \tag{55}$$

Combining (51) and (55) we now have:

$$\begin{aligned}W^2(\nu_1,\nu_2) &= \|m_1 - m_2\|^2_{L^2(\Omega)} + W^2(\mathcal{N}(0,\Sigma_1),\mathcal{N}(0,\Sigma_2)) \\ &\leq \tilde{C}^2 h^4 \|\bar{f}\|^2_{L^2(\Omega)} + \tilde{C}h^2 \|K\|_1 \left(2\|\mathcal{L}^{-1}\|_\infty + \tilde{C}h^2\right) \\ &= 2\tilde{C}h^2 \|K\|_1 \|\mathcal{L}^{-1}\|_\infty + \mathcal{O}(h^4)\end{aligned}$$

We thus have an upper bound on the Wasserstein distance between ν_1, ν_2 in terms of the FEM mesh size h:

$$W(\nu_1,\nu_2) \leq h\sqrt{2\tilde{C}\|K\|_1 \|\mathcal{L}^{-1}\|_\infty + \mathcal{O}(h^2)} \leq \gamma h + \mathcal{O}(h) \tag{56}$$

where $\gamma > 0$ is a constant. We also see that as $h \to 0$ the Wasserstein distance between ν_1, ν_2 goes to 0 and so the approximate prior converges (in distribution) to the true prior as $h \to 0$ (see Proposition 4 in [34]).

[4]Note that here we are viewing both $\mathcal{L}^{-1}$ and $\Phi^* A^{-1}\mathcal{I}$ as operators from $L^2(\Omega)$ to itself. They are however more generally operators from $H^{-1}(\Omega)$ to $H^1_0(\Omega)$. We will consider here the case that $\bar{f}$ is in $L^2(\Omega)$ but this assumption can be relaxed.

5 FEM for Parabolic Problem

6 Conclusions and Research Plan

7 Appendix

References

[1] Mark Girolami, Alastair Gregory, Ge Yin, and Fehmi Cirak. The statistical finite element method. *arXiv preprint arXiv:1905.06391*, 2019.

[2] Patrick R Conrad, Mark Girolami, Simo Särkkä, Andrew Stuart, and Konstantinos Zygalakis. Statistical analysis of differential equations: introducing probability measures on numerical solutions. *Statistics and Computing*, 27(4):1065–1082, 2017.

[3] Kody Law, Andrew Stuart, and Kostas Zygalakis. Data assimilation. *Cham, Switzerland: Springer*, 2015.

[4] Andrew M Stuart. Inverse problems: a bayesian perspective. *Acta numerica*, 19:451–559, 2010.

[5] Gilbert Strang and George J Fix. An analysis of the finite element method. *Journal of Applied Mathematics and Mechanics*, 1973.

[6] Persi Diaconis. Bayesian numerical analysis. *Statistical decision theory and related topics IV*, 1:163–175, 1988.

[7] A O'Hagan. Bayesian statistics 4. some bayesian numerical analysis, 1992.

[8] John Skilling. Bayesian solution of ordinary differential equations. In *Maximum entropy and Bayesian methods*, pages 23–37. Springer, 1992.

[9] Philipp Hennig, Michael A Osborne, and Mark Girolami. Probabilistic numerics and uncertainty in computations. *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 471(2179): 20150142, 2015.

[10] URL `http://probabilistic-numerics.org/`.

[11] Oksana A Chkrebtii, David A Campbell, Ben Calderhead, Mark A Girolami, et al. Bayesian solution uncertainty quantification for differential equations. *Bayesian Analysis*, 11(4):1239–1267, 2016.

[12] Onur Teymur, Kostas Zygalakis, and Ben Calderhead. Probabilistic linear multistep methods. In *Advances in Neural Information Processing Systems*, pages 4321–4328, 2016.

[13] Han Cheng Lie, AM Stuart, and TJ Sullivan. Strong convergence rates of probabilistic integrators for ordinary differential equations. *Statistics and Computing*, 29(6):1265–1283, 2019.

[14] Assyr Abdulle and Giacomo Garegnani. Random time step probabilistic methods for uncertainty quantification in chaotic and geometric numerical integration. *Statistics and Computing*, pages 1–26, 2020.

[15] Onur Teymur, Han Cheng Lie, Tim Sullivan, and Ben Calderhead. Implicit probabilistic integrators for odes. In *Advances in Neural Information Processing Systems*, pages 7244–7253, 2018.

[16] Michael Schober, David K Duvenaud, and Philipp Hennig. Probabilistic ode solvers with runge-kutta means. In *Advances in neural information processing systems*, pages 739–747, 2014.

[17] Hans Kersting and Philipp Hennig. Active uncertainty calibration in bayesian ode solvers. *arXiv preprint arXiv:1605.03364*, 2016.

[18] Emilia Magnani, Hans Kersting, Michael Schober, and Philipp Hennig. Bayesian filtering for odes with bounded derivatives. *arXiv preprint arXiv:1709.08471*, 2017.

[19] Michael Schober, Simo Särkkä, and Philipp Hennig. A probabilistic model for the numerical solution of initial value problems. *Statistics and Computing*, 29(1):99–122, 2019.

[20] Filip Tronarp, Hans Kersting, Simo Särkkä, and Philipp Hennig. Probabilistic solutions to ordinary differential equations as nonlinear bayesian filtering: a new perspective. *Statistics and Computing*, 29(6): 1297–1315, 2019.

[21] Hans Kersting, TJ Sullivan, and Philipp Hennig. Convergence rates of gaussian ode filters. *arXiv preprint arXiv:1807.09737*, 2018.

[22] Gabriel J Lord, Catherine E Powell, and Tony Shardlow. *An introduction to computational stochastic PDEs*, volume 50. Cambridge University Press, 2014.

[23] Marcel Bieri, Roman Andreev, and Christoph Schwab. Sparse tensor discretization of elliptic spdes. *SIAM Journal on Scientific Computing*, 31(6):4281–4304, 2010.

[24] Jon Cockayne, Chris Oates, Tim Sullivan, and Mark Girolami. Probabilistic numerical methods for partial differential equations and bayesian inverse problems. *arXiv preprint arXiv:1605.07811*, 2016.

[25] Stig Larsson and Vidar Thomée. *Partial differential equations with numerical methods*, volume 45. Springer Science & Business Media, 2008.

[26] Giuseppe Da Prato. *An introduction to infinite-dimensional analysis*. Springer Science & Business Media, 2006.

[27] Maziar Raissi, Paris Perdikaris, and George Em Karniadakis. Machine learning of linear differential equations using gaussian processes. *Journal of Computational Physics*, 348:683–693, 2017.

[28] Carl Edward Rasmussen. Gaussian processes for machine learning. MIT Press, 2006.

[29] Mikhail Lifshits. Lectures on gaussian processes. In *Lectures on Gaussian Processes*, pages 1–117. Springer, 2012.

[30] Alessandra Lunardi, Michele Miranda, and Diego Pallara. Infinite dimensional analysis. In *19th Internet Seminar*, volume 2016, 2015.

[31] Timothy John Sullivan. *Introduction to uncertainty quantification*, volume 63. Springer, 2015.

[32] Simo Särkkä. *Bayesian filtering and smoothing*, volume 3. Cambridge University Press, 2013.

[33] NN Vakhania. The topological support of gaussian measure in banach space. *Nagoya Mathematical Journal*, 57:59–63, 1975.

[34] Valentina Masarotto, Victor M Panaretos, and Yoav Zemel. Procrustes metrics on covariance operators and optimal transportation of gaussian processes. *Sankhya A*, 81(1):172–213, 2019.

[35] JA Cuesta-Albertos, C Matrán-Bea, and A Tuero-Diaz. On lower bounds for the l2-wasserstein metric in a hilbert space. *Journal of Theoretical Probability*, 9(2):263–283, 1996.

[36] Robert T Powers and Erling Størmer. Free states of the canonical anticommutation relations. *Communications in Mathematical Physics*, 16(1):1–33, 1970.