Early Stage Assessment (ESA)

Department of Mathematics - Imperial College London
Yanni (John) Papandreou supervised by Dr Andrew Duncan
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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 naturally incorporates 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. Section 5 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 several parts. We first outline the general type of problem we will be considering in this report. Having done this we will then aim to describe how two priors for the solution to this problem 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 will consider PDEs which do not have any time dependence in this report. Future work will deal with the case of time dependent PDEs. 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 separable 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 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:

[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.

3.2 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):

3.3 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 a 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 $j = 1, \dots, J$. 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. $\mathcal{I} = (I_1, \dots, I_J)^T$. 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 $\psi(u^N) := \psi(u(x_1), \dots, u(x_N))$ 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 $Ph := (h(x_1), \dots, h(x_N))^T$ 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,

$$h^N := \Sigma_{\mathcal{I}}\Sigma_N^{-1}PQB^{-1}K_{\mathcal{I}}^{-1}\bar{F} = PQ\bar{F} \tag{13}$$
$$\Sigma_{\mathcal{I}} := P(\Sigma + QK_{\mathcal{I}}Q^*)P^* \tag{14}$$
$$B := \left(Q^*P^*\Sigma_N^{-1}PQ + K_{\mathcal{I}}^{-1}\right) \tag{15}$$

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:

$$u|\{\mathcal{I}\mathcal{L}u = F\} \sim \mathcal{N}\left(Q\bar{F}, \Sigma + QK_{\mathcal{I}}Q^*\right) \tag{16}$$

■

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 Section 4 we will obtain, for a specific example, 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.

3.4 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:

$$m_1 = \mathcal{L}^{-1}\bar{f} \tag{17}$$
$$\Sigma_1 = \mathcal{L}^{-1}K(\mathcal{L}^{-1})^* \tag{18}$$

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

$$m_2 = Q\bar{F} \tag{19}$$
$$\Sigma_2 = \Sigma + QK_{\mathcal{I}}Q^* \tag{20}$$

with Q 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 $y_1, \ldots, y_s$ 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 $(h(y_1), \ldots, h(y_s))^T$ 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:

$$\mathbf{v}|u \sim \mathcal{N}(Su, \epsilon^2 I) \tag{21}$$

The goal is to now find the posterior $u|\mathbf{v}$ when our prior is $u \sim \nu_i \equiv \mathcal{N}(m_i, \Sigma_i), \;\; i = 1, 2$. 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 (21) 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:

$$\begin{pmatrix} u \\ \mathbf{v} \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} m_i \\ Sm_i \end{pmatrix}, \begin{pmatrix} \Sigma_i & \Sigma_i S^* \\ S\Sigma_i & \epsilon^2 I + S\Sigma_i S^* \end{pmatrix} \right) \tag{22}$$

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

$$u|\mathbf{v} \sim \mathcal{N}(m^{(i)}_{u|\mathbf{v}}, \Sigma^{(i)}_{u|\mathbf{v}}) \tag{23}$$

where,

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

$$\Sigma^{(i)}_{u|\mathbf{v}} := \Sigma_i - \Sigma_i S^*(\epsilon^2 I + S\Sigma_i S^*)^{-1} S\Sigma_i \tag{25}$$

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

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

$$\begin{aligned} \mathcal{L}u(x) &:= -\nabla \cdot (a(x)\nabla u(x)) = f(x), \quad x \in \Omega \\ u(x) &= 0, \quad x \in \partial\Omega \end{aligned} \tag{26}$$

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 taken from [22]:

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

$$0 < a_{\min} \leq a(x) \leq a_{\max} < \infty \text{ for almost all } x \in \Omega \tag{27}$$

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 (26) 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 (26) 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:

$$Vu(x) := \sum_{i=1}^{J} \lambda_i \phi_i(x) \int_\Omega \phi_i(y) u(y) \mathrm{d}y \tag{28}$$

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:

$$Vu := \sum_{i=1}^{J} \lambda_i \langle u, \phi_i \rangle \phi_i \quad \forall u \in H^{-1}(\Omega) \tag{29}$$

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:

$$k(x, y) := \sum_{i=1}^{J} \lambda_i \phi_i(x) \phi_i(y) \tag{30}$$

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

$$Vu(x) = \langle u(\cdot), k(x, \cdot) \rangle \tag{31}$$

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:

$$I_j \mathcal{L} u = \int_{\Omega} a(x) \nabla u(x) \cdot \nabla \phi_j(x) \mathrm{d}x \tag{32}$$

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:

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

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:

$$Vu(x) = \Phi(x)^* \Lambda \langle u, \Phi \rangle \tag{34}$$

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 $\mathbb{R}^J$:

$$(\langle u, \phi_1 \rangle, \ldots, \langle u, \phi_J \rangle)^T = \mathcal{I} u \tag{35}$$

thus we see that we can write:

$$Vu = \Phi^* \Lambda \mathcal{I} u \quad \forall u \in H^{-1}(\Omega) \tag{36}$$

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 defined by:

$$\Phi^* \mathbf{v} := \sum_{i=1}^{J} v_i \phi_i \tag{37}$$

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

$$\langle u, \Phi^* \mathbf{v} \rangle = (\Phi u, \mathbf{v}) \quad \forall u \in H^{-1}(\Omega)\ \forall \mathbf{v} \in \mathbb{R}^J \tag{38}$$

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:

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

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

$$A_{ij} := I_i \mathcal{L}\phi_j \tag{39}$$

$$= \int_\Omega a(x) \nabla\phi_i(x) \cdot \nabla\phi_j(x) \mathrm{d}x \tag{40}$$

where we have utilised equation (32). 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:

$$\mathcal{N}(\Phi^* A^{-1}\bar{F}, \Phi^* A^{-1} K_{\mathcal{I}} A^{-1}\Phi) \tag{41}$$

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 (41). 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 (26) 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 3.2 provided that the solution operator to the BVP is bounded we can work out that the "true" distribution of u should be:

$$u \sim \mathcal{N}(\mathcal{L}^{-1}\bar{f}, \mathcal{L}^{-1}K(\mathcal{L}^{-1})^*) \tag{42}$$

For the BVP under consideration (26) 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 be taken to be the Gaussian (42). We now move on to quantifying how different the approximate prior (41) and the true prior (42) are.

4.3 Upperbound on the Wasserstein Distance between the two priors

We now have two Gaussian priors for the BVP (26) given by $\nu_i = \mathcal{N}(m_i, \Sigma_i)$ for $i = 1, 2$ where:

$$m_1 := \mathcal{L}^{-1}\bar{f} \tag{43}$$
$$m_2 := \Phi^* A^{-1}\bar{F} \tag{44}$$
$$\Sigma_1 := \mathcal{L}^{-1}K(\mathcal{L}^{-1})^* \tag{45}$$
$$\Sigma_2 := \Phi^* A^{-1} K_{\mathcal{I}} A^{-1}\Phi \tag{46}$$

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 $\mathcal{H}$, $W(\mu, \nu)$:

$$W^2(\mu, \nu) = \inf_{\pi\in\Gamma(\mu,\nu)} \int_{\mathcal{H}\times\mathcal{H}} \|x - y\|^2_{\mathcal{H}} \mathrm{d}\pi(x, y) \tag{47}$$

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

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

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

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],

$$W^2(\mu, \nu) = \|m_1 - m_2\|_{\mathcal{H}}^2 + \mathrm{tr}(\Sigma_1) + \mathrm{tr}(\Sigma_2) - 2\,\mathrm{tr}\sqrt{\Sigma_1^{1/2}\Sigma_2\Sigma_1^{1/2}} \tag{48}$$

This formula is true in both the finite and infinite dimensional cases. The term $\mathrm{tr}\sqrt{\Sigma_1^{1/2}\Sigma_2\Sigma_1^{1/2}}$ 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 $\|A\|_2 = \sqrt{\mathrm{tr}(A^*A)}$. ♦

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

$$W(\mathcal{N}(0, \Sigma_1), \mathcal{N}(0, \Sigma_2)) = \inf_{R:R^*R=I} \|\Sigma_1^{1/2} - R\Sigma_2^{1/2}\|_2 \leq \|\Sigma_1^{1/2} - \Sigma_2^{1/2}\|_2 \tag{49}$$

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]:

$$W^2(\nu_1, \nu_2) = \|m_1 - m_2\|_{\mathcal{H}}^2 + W^2(\nu_1^*, \nu_2^*) \tag{50}$$

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 (26) lies in a subspace $H_0^1(\Omega) \subset L^2(\Omega)$. We have,

$$W^2(\nu_1, \nu_2) = \|m_1 - m_2\|_{L^2(\Omega)}^2 + W^2(\mathcal{N}(0, \Sigma_1), \mathcal{N}(0, \Sigma_2)) \tag{51}$$

where now the $m_i, \Sigma_i, i = 1, 2$ are given by equations (43-46). 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.

Under all of these assumptions we have the following Theorem:

Theorem 4.1. Let u satisfy (26). Assuming that Assumptions 2-4 hold we have that the Wasserstein distance between the two priors ν_1, ν_2 is bounded above by $\mathcal{O}(h)$ as $h \to 0$. In particular, there exists a constant $\gamma > 0$, independent of h, such that the following holds:

$$W(\nu_1, \nu_2) \leq \gamma h + \mathcal{O}(h^2) \tag{52}$$

Furthermore, we observe that as $h \to 0$ the approximate FEM prior ν_2 converges in distribution to the true prior ν_1.

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

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

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:

$$\|m_1 - m_2\|_{L^2(\Omega)} \leq Ch^2\|m_1\|_{H^2(\Omega)} \leq \tilde{C}h^2\|\bar{f}\|_{L^2(\Omega)} \tag{53}$$

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:

$$W^2(\mathcal{N}(0,\Sigma_1),\mathcal{N}(0,\Sigma_2)) \leq \|\Sigma_1^{1/2} - \Sigma_2^{1/2}\|_2^2 \tag{54}$$

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

$$W^2(\mathcal{N}(0,\Sigma_1),\mathcal{N}(0,\Sigma_2)) \leq \|\Sigma_1^{1/2} - \Sigma_2^{1/2}\|_2^2 \leq \|\Sigma_1 - \Sigma_2\|_1 \tag{55}$$

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

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 (53) 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.,

$$\|\mathcal{L}^{-1} - \Phi^*A^{-1}\mathcal{I}\|_\infty \leq \tilde{C}h^2 \tag{56}$$

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:

$$W^2(\mathcal{N}(0,\Sigma_1),\mathcal{N}(0,\Sigma_2)) \leq \|\Sigma_1 - \Sigma_2\|_1 \leq \tilde{C}h^2\|K\|_1\left(2\|\mathcal{L}^{-1}\|_\infty + \tilde{C}h^2\right) \tag{57}$$

Combining (53) and (57) we now have:

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

[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 $H_0^1(\Omega)$. We will consider here the case that $\bar{f}$ is in $L^2(\Omega)$ but this assumption can be relaxed.

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

$$W(\nu_1, \nu_2) \leq h\sqrt{2\tilde{C}\|K\|_1\|\mathcal{L}^{-1}\|_\infty + \mathcal{O}(h^2)} \leq \gamma h + \mathcal{O}(h^2) \tag{58}$$

where $\gamma := \sqrt{2\tilde{C}\|K\|_1\|\mathcal{L}^{-1}\|_\infty} > 0$ is a constant. Note that we have also used that both[5] $\|K\|_1$ and $\|\mathcal{L}^{-1}\|_\infty$ are bounded and independent of h. 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]). ■

Having obtained this upperbound on the distance between the true priors we are now in a position to investigate how this "propagates" forwards to further inference. In particular, we will now look at incorporating sensor data and seeing how different the two resulting posteriors are from using the two different priors ν_1, ν_2 above.

4.4 Upperbound on the Wasserstein Distance between the two posteriors

As discussed in Section 3.4 we will now assume that we have noisy observations of the value of u at some points $y_1, \ldots, y_s \in \Omega$ coming from a sensor. We wish to update our belief in the distribution of u using this sensor data, and as discussed either of the ν_i can be used as prior distributions. We thus obtain two different posteriors and these are given by $u|\mathbf{v} \sim \mathcal{N}(m^{(i)}_{u|\mathbf{v}}, \Sigma^{(i)}_{u|\mathbf{v}})$ where $m^{(i)}_{u|\mathbf{v}} := m_i + \Sigma_i S^* B_i^{-1}(\mathbf{v} - Sm_i)$ and $\Sigma^{(i)}_{u|\mathbf{v}} := \Sigma_i - \Sigma_i S^* B_i^{-1} S\Sigma_i$ as shown in Section 3.4. We have denoted $B_i := \epsilon^2 I + S\Sigma_i S^*$ for convenience. We can no go about obtaining an upperbound for the Wasserstein distance between these two posteriors. The result is given in the following Theorem and we outline a proof of this.

Theorem 4.2. Let u satisfy (26). Assuming that Assumptions 2-4 hold we have that the Wasserstein distance between the two posteriors is bounded above by $\mathcal{O}(h)$ as $h \to 0$. In particular, there exists a constant $\kappa > 0$, independent of h, such that the following holds:

$$W\left(\mathcal{N}(m^{(1)}_{u|\mathbf{v}}, \Sigma^{(1)}_{u|\mathbf{v}}), \mathcal{N}(m^{(2)}_{u|\mathbf{v}}, \Sigma^{(2)}_{u|\mathbf{v}})\right) \leq \sqrt{\kappa} h + \mathcal{O}(h^2) \tag{59}$$

Furthermore, we observe that as $h \to 0$ the second posterior obtained using the prior ν_2 converges in distribution to the first posterior obtained using the prior ν_1.

Proof: We have,

$$\begin{aligned} W^2\left(\mathcal{N}(m^{(1)}_{u|\mathbf{v}}, \Sigma^{(1)}_{u|\mathbf{v}}), \mathcal{N}(m^{(2)}_{u|\mathbf{v}}, \Sigma^{(2)}_{u|\mathbf{v}})\right) &= \|m^{(1)}_{u|\mathbf{v}} - m^{(2)}_{u|\mathbf{v}}\|^2_{L^2(\Omega)} + W^2\left(\mathcal{N}(0, \Sigma^{(1)}_{u|\mathbf{v}}), \mathcal{N}(0, \Sigma^{(2)}_{u|\mathbf{v}})\right) \\ &\leq \|m^{(1)}_{u|\mathbf{v}} - m^{(2)}_{u|\mathbf{v}}\|^2_{L^2(\Omega)} + \|\Sigma^{(1)}_{u|\mathbf{v}} - \Sigma^{(2)}_{u|\mathbf{v}}\|_1 \end{aligned}$$

In order to obtain on upperbound on each of these terms it will help to first figure out an upperbound on $\|B_1^{-1} - B_2^{-1}\|_\infty$. To this end we first compute:

$$\begin{aligned} \|B_1 - B_2\|_\infty &= \|S(\Sigma_1 - \Sigma_2)S^*\|_\infty \\ &\leq \|S\|^2_\infty \|\Sigma_1 - \Sigma_2\|_\infty \\ &\leq \|\Sigma_1 - \Sigma_2\|_1 \\ &\leq \gamma^2 h^2 + \mathcal{O}(h^4) \end{aligned}$$

where we have used the fact that $\|S\|_\infty \leq 1$ since it is a projection. Since B_1 (and B_2) are invertible and for sufficiently small[6] h we have that $\|B_1 - B_2\|_\infty < 1/\|B_1^{-1}\|_\infty$ we can utilise Corollary 8.2 of [37] to deduce that:

$$\|B_1^{-1} - B_2^{-1}\|_\infty \leq \frac{\|B_1^{-1}\|^2_\infty \|B_1 - B_2\|_\infty}{1 - \|B_1^{-1}\|_\infty \|B_1 - B_2\|_\infty} \leq \|B_1^{-1}\|^2_\infty \gamma^2 h^2 + \mathcal{O}(h^4) \tag{60}$$

Note that $\|B_1^{-1}\|_\infty$ is a bounded constant independent of h (but dependent on ϵ).

[5] K is trace-class since it is a covariance operator and thus its trace-norm is bounded.

[6] It suffices to take $h < h_*$ where h_* satisfies $\gamma^2 h_*^2 + \tilde{C}^2 h_*^4 < 1/\|B_1^{-1}\|_\infty$.

We are now in a good position to derive an upper bound on the Wasserstein distance between the two posteriors. We first focus on the difference of the two means:

$$\begin{aligned}
\|m^{(1)}_{u|\mathbf{v}} - m^{(2)}_{u|\mathbf{v}}\|_{L^2(\Omega)} &= \|m_1 + \Sigma_1 S^* B_1^{-1}(\mathbf{v} - Sm_1) - m_2 - \Sigma_2 S^* B_2^{-1}(\mathbf{v} - Sm_2)\|_{L^2(\Omega)} \\
&= \|m_1 - m_2 + \Sigma_1 S^* B_1^{-1}\mathbf{v} - \Sigma_1 S^* B_1^{-1} S m_1 - \Sigma_2 S^* B_2^{-1}\mathbf{v} + \Sigma_2 S^* B_2^{-1} S m_2\|_{L^2(\Omega)} \\
&\leq \|m_1 - m_2\|_{L^2(\Omega)} + \|(\Sigma_1 S^* B_1^{-1} - \Sigma_2 S^* B_2^{-1})\mathbf{v}\|_{L^2(\Omega)} + \|\Sigma_1 S^* B_1^{-1} S m_1 - \Sigma_2 S^* B_2^{-1} S m_2\|_{L^2(\Omega)}
\end{aligned}$$

We now focus on these three terms separately. For the first term we already have from (53) that

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

The other two terms can be bounded above by utilising the bounds on $\|\Sigma_1 - \Sigma_2\|_1$ and $\|B_1^{-1} - B_2^{-1}\|_\infty$. Details of these calculations are left to the Appendix. Upon performing these calculations we obtain:

$$\|m^{(1)}_{u|\mathbf{v}} - m^{(2)}_{u|\mathbf{v}}\|_{L^2(\Omega)} \leq \tilde{\gamma} h^2 + \mathcal{O}(h^4) \tag{61}$$

where $\tilde{\gamma} > 0$ is a constant independent of h. Similarly (see Appendix for details) one can obtain the following upperbound for the difference of the covariance operators:

$$\|\Sigma^{(1)}_{u|\mathbf{v}} - \Sigma^{(2)}_{u|\mathbf{v}}\|_1 \leq \kappa h^2 + \mathcal{O}(h^4) \tag{62}$$

where $\kappa > 0$ is a constant independent of h. Combining these two upper bounds we obtain,

$$W^2\left(\mathcal{N}(m^{(1)}_{u|\mathbf{v}}, \Sigma^{(1)}_{u|\mathbf{v}}), \mathcal{N}(m^{(2)}_{u|\mathbf{v}}, \Sigma^{(2)}_{u|\mathbf{v}})\right) \leq \kappa h^2 + \mathcal{O}(h^4) \tag{63}$$

and so the Wasserstein distance between the posteriors is bounded above by $\mathcal{O}(h)$ and thus goes to 0 as $h \to 0$. Thus, the posterior obtained using the approximate prior converges in distribution to the posterior obtained using the true prior as the mesh size goes to 0. ■

5 Conclusions and Research Plan

The statistical FEM method introduced in [1] allowed both the FE model and observational data to be combined into a coherent inferential framework. The main goal of our work was to provide more detailed error analysis explicitly quantifying the extent by which the distributions obtained using the "true" solution and the FEM solution differ, and then seeing how this carried forward to further inference. In particular, Theorems 4.1 and 4.2 provide a full probabilistic description of the uncertainty due to using a FEM approximation for the noisy BVP (26). In arriving at these results the guiding principle of "*avoiding discretization until the last possible moment*" [4] was very important.

Our work carries out one of the first detailed error analysis of a probabilistic numerical method for solving a noisy PDE. However, future work and research is needed. In particular, we plan on extending this framework to time-dependent PDEs. We hope to obtain Kalman Filter-like update rules for our belief in the distribution of solutions to noisy time-dependent PDEs. We are especially interested in investigating how incorporating observational data will control the error as time progresses.

Further work is also needed for the case of spatial PDEs as investigated in this report. We will aim to perform numerical methods illustrating the methodology and results presented in Sections 3 and 4. On a more theoretical side, it will also be interesting to investigate in greater depth how the upperbound on the Wasserstein distance between the posteriors given by (59) depends on the sensor sensitivity ϵ. This dependence can be potentially useful in answering questions such as "if we have a finite budget for both computation and sensor equipment how should we allocate these resources efficiently?" and other related questions.

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6 Appendix

In this section we provide the omitted details for the proofs and methodology presented in Sections 3 and 4.

6.1 Justification of the conditioning step yielding equation (4) in Section 3

We now provide a full justification for the conditioning step yielding equation (4) in Section 3. The justification essentially follows from Theorem 3.3 in [38]. This theorem is given below (we only give the part of the theorem we require):

Theorem 6.1. Consider a Gaussian measure μ on an orthogonal direct sum $H = H_1 \oplus H_2$ of separable Hilbert spaces with mean m and covariance operator C. Then for all $t \in H_2$, the conditional measure μ_t is a Gaussian measure with covariance operator $\mathcal{H}_1(C)$, the short of C to H_1.

If the covariance operator C is compatible with H_2, then for any oblique projection Q in $\mathcal{P}(C, H_2) \neq \emptyset$, the mean m_t of the conditional measure μ_t is

$$m_t = \begin{pmatrix} m_1 + \hat{Q}^*(t - m_2) \\ t \end{pmatrix}$$

Where

$$Q = \begin{pmatrix} 0 & 0 \\ \hat{Q} & I \end{pmatrix}$$

and $\mathcal{P}(C, H_2)$ is the set of (C-symmetric) oblique projections onto H_2. *Note: the terms shorted operator, compatible and oblique projections are all defined in [38].*

To apply this theorem to our problem we note that our pair $(u, \mathcal{IL}u)^T$ lies in the orthogonal direct sum $\mathcal{H}_1 \oplus \mathcal{H}_2$ of the separable Hilbert spaces $\mathcal{H}_1 := \mathcal{H} \times \{0\}$ and $\mathcal{H}_2 := \{0\} \times \mathbb{R}^J$. The corresponding Gaussian measure we are dealing with on this space is given by (3). Theorem 6.1 states that the conditional distribution is a Gaussian measure with covariance operator being the short of the covariance operator of the distribution (3) to $\mathcal{H}_2$. This operator,

$$\begin{pmatrix} V & V\mathcal{L}^*\mathcal{I}^* \\ \mathcal{IL}V & \mathcal{IL}V\mathcal{L}^*\mathcal{I}^* \end{pmatrix}$$

is already written in its $(\mathcal{H}_1, \mathcal{H}_2)$ partition representation. In the section on shorted operators in [38] it is stated that provided the lower right partition of the covariance operator of (3) corresponding to the covariance in $\mathcal{H}_2$, i.e. $\mathcal{IL}V(\mathcal{IL})^*$, is invertible then the shorted operator is given by:

$$\begin{pmatrix} V - V\mathcal{L}^*\mathcal{I}^*(\mathcal{IL}V\mathcal{L}^*\mathcal{I}^*)^{-1}\mathcal{IL}V & 0 \\ 0 & 0 \end{pmatrix}$$

We assume the invertibility of this partition.

Remark. This part of the partition reduces to the $J \times J$ matrix $A\Lambda A^*$ when we choose the FEM prior and FEM information operator as was discussed in Section 4. The invertibility of this matrix is then equivalent to the invertibility of the Galerkin Stiffness Matrix A (since we assume the entries of Λ are non-zero). ♦

We thus see that the conditional distribution (4) has the correct covariance operator. Theorem 6.1 also goes on to give the mean of the conditional distribution in the case that the covariance operator of the joint distribution is compatible with H_2. For our problem this is in fact the case as we now show. We first denote the covariance operator of the joint distribution by:

$$\begin{pmatrix} V & V\mathcal{L}^*\mathcal{I}^* \\ \mathcal{IL}V & \mathcal{IL}V\mathcal{L}^*\mathcal{I}^* \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix}$$

i.e. $C_{11} := V, C_{12} := V\mathcal{L}^*\mathcal{I}^*, C_{21} = \mathcal{IL}V, C_{22} := \mathcal{IL}V\mathcal{L}^*\mathcal{I}^*$. If we now define the following bounded operator $Q : H \to H$ by

$$Q = \begin{pmatrix} 0 & 0 \\ C_{22}^{-1}C_{21} & I \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ \hat{Q} & I \end{pmatrix}$$

where $\hat{Q} := C_{22}^{-1}C_{21} : H_1 \to H_2$ we can easily check that such an operator Q is an (C-symmetric) oblique projection onto H_2. Since Q is not 0 we have by Theorem 6.1 that the mean of the conditional distribution (4) is given by $\hat{Q}^*F$. Now C_{22} and therefore C_{22}^{-1} are self-adjoint and further we have $C_{12}^* = C_{21}$ and so we can easily deduce that $\hat{Q}^* = C_{12}C_{22}^{-1}$ and so the mean is given by:

$$\hat{Q}^*F = C_{12}C_{22}^{-1}F = V\mathcal{L}^*\mathcal{I}^*(\mathcal{IL}V\mathcal{L}^*\mathcal{I}^*)^{-1}F = a \tag{64}$$

where a is what we had in (5). We thus see that the conditioning step is justified and we indeed obtain what was claimed in Section 3. ■

6.2 Detailed computations for the proof of Proposition 3.1

We provide here details of the computation of the following integral needed for the proof of Proposition 3.1:

$$\int\int \psi(u^N)\mu_{PQF,\Sigma_N}(\mathrm{d}u^N)\mu_{\bar{F},K_\mathcal{I}}(\mathrm{d}F)$$

Both measures in the above integral are multivariate normal and so we have:

$$\begin{aligned}\int\int &\psi(u^N)\mu_{Pa,\Sigma_N}(\mathrm{d}u^N)\mu_{\bar{F},K_\mathcal{I}}(\mathrm{d}F) = \\ &= \frac{1}{Z_u}\int\int \psi(u^N)\exp\left(-\frac{1}{2}\left\langle u^N - PQF, \Sigma_N^{-1}(u^N - PQF)\right\rangle\right)\mu_{\bar{F},K_\mathcal{I}}(\mathrm{d}F)\mathrm{d}u^N \\ &= \frac{1}{Z_uZ_f}\int\int \psi(u^N)\exp\left(-\frac{1}{2}\left\langle u^N - PQF, \Sigma_N^{-1}(u^N - PQF)\right\rangle\right)\exp\left(-\frac{1}{2}\left\langle F - \bar{F}, K_\mathcal{I}^{-1}(F - \bar{F})\right\rangle\right)\mathrm{d}F\mathrm{d}u^N\end{aligned} \tag{65}$$

where the normalization constants are $Z_u := (2\pi)^{N/2}\det(\Sigma_N)^{1/2}$ and $Z_f := (2\pi)^{J/2}\det(K_{\mathcal{I}})^{1/2}$. We now need to compute the integral over F. In order to do so we combine the exponents in (11) into a quadratic in F in order to be able to use the well-known formula of a multidimensional Gaussian integral. Going through the algebra we obtain:

$$\begin{aligned}
&\frac{1}{Z_u Z_f}\int\int \psi(u^N)\exp\Bigg(-\frac{1}{2}\Big(\left\langle u^N, \Sigma_N^{-1}u^N\right\rangle - 2\left\langle \Sigma_N^{-1}PQF, u^N\right\rangle + \left\langle F, Q^*P^*\Sigma_N^{-1}PQF\right\rangle \\
&\qquad + \left\langle F, K_{\mathcal{I}}^{-1}F\right\rangle - 2\left\langle K_{\mathcal{I}}^{-1}\bar{F}, F\right\rangle + \left\langle \bar{F}, K_{\mathcal{I}}^{-1}\bar{F}\right\rangle\Big)\Bigg)\mathrm{d}F\mathrm{d}u^N = \\
&\qquad = \frac{1}{Z_u Z_f}\int \psi(u^N)\exp\left(-\frac{1}{2}\left(\left\langle u^N, \Sigma_N^{-1}u^N\right\rangle + \left\langle \bar{F}, K_{\mathcal{I}}^{-1}\bar{F}\right\rangle\right)\right)\cdot \\
&\qquad \left(\int \exp\left(-\frac{1}{2}\left\langle F, BF\right\rangle + \left\langle Q^*P^*\Sigma_N^{-1}u^N + K_{\mathcal{I}}^{-1}\bar{F}, F\right\rangle\right)\mathrm{d}F\right)\mathrm{d}u^N
\end{aligned} \tag{66}$$

where $B := \left(Q^*P^*\Sigma_N^{-1}PQ + K_{\mathcal{I}}^{-1}\right)$. Computing the inner integral over F we thus obtain:

$$\begin{aligned}
\frac{(2\pi)^{J/2}}{Z_u Z_f \det(B)^{1/2}}\int \psi(u^N)\exp\Bigg(&\frac{1}{2}\left\langle Q^*P^*\Sigma_N^{-1}u^N + K_{\mathcal{I}}^{-1}\bar{F}, B^{-1}\left(Q^*P^*\Sigma_N^{-1}u^N + K_{\mathcal{I}}^{-1}\bar{F}\right)\right\rangle \\
&-\frac{1}{2}\left(\left\langle u^N, \Sigma_N^{-1}u^N\right\rangle + \left\langle \bar{F}, K_{\mathcal{I}}^{-1}\bar{F}\right\rangle\right)\Bigg)\mathrm{d}u^N
\end{aligned} \tag{67}$$

We now focus on the terms in the exponent and simplify these as follows:

$$\begin{aligned}
&\frac{1}{2}\left\langle Q^*P^*\Sigma_N^{-1}u^N + K_{\mathcal{I}}^{-1}\bar{F}, B^{-1}\left(Q^*P^*\Sigma_N^{-1}u^N + K_{\mathcal{I}}^{-1}\bar{F}\right)\right\rangle - \frac{1}{2}\left(\left\langle u^N, \Sigma_N^{-1}u^N\right\rangle + \left\langle \bar{F}, K_{\mathcal{I}}^{-1}\bar{F}\right\rangle\right) = \\
&= -\frac{1}{2}\Big(\left\langle u^N, \Sigma_N^{-1}u^N\right\rangle + \left\langle \bar{F}, K_{\mathcal{I}}^{-1}\bar{F}\right\rangle - \left\langle Q^*P^*\Sigma_N^{-1}u^N + K_{\mathcal{I}}^{-1}\bar{F}, B^{-1}\left(Q^*P^*\Sigma_N^{-1}u^N + K_{\mathcal{I}}^{-1}\bar{F}\right)\right\rangle\Big) \\
&= -\frac{1}{2}\Big(\left\langle u^N, \Sigma_N^{-1}u^N\right\rangle + \left\langle \bar{F}, K_{\mathcal{I}}^{-1}\bar{F}\right\rangle - \left\langle u^N, \Sigma_N^{-1}PQB^{-1}Q^*P^*\Sigma_N^{-1}u^N\right\rangle \\
&- 2\left\langle u^N, \Sigma_N^{-1}PQB^{-1}K_{\mathcal{I}}^{-1}\bar{F}\right\rangle - \left\langle \bar{F}, K_{\mathcal{I}}^{-1}B^{-1}K_{\mathcal{I}}^{-1}\bar{F}\right\rangle\Big) \\
&= -\frac{1}{2}\Big(\left\langle u^N, (\Sigma_N^{-1} - \Sigma_N^{-1}PQB^{-1}Q^*P^*\Sigma_N^{-1})u^N\right\rangle - 2\left\langle u^N, \Sigma_N^{-1}PQB^{-1}K_{\mathcal{I}}^{-1}\bar{F}\right\rangle + \left\langle \bar{F}, (K_{\mathcal{I}}^{-1} - K_{\mathcal{I}}^{-1}B^{-1}K_{\mathcal{I}}^{-1})\bar{F}\right\rangle\Big) \\
&= -\frac{1}{2}\Big(\left\langle u^N, \Sigma_{\mathcal{I}}^{-1}u^N\right\rangle - 2\left\langle u^N, \Sigma_N^{-1}PQB^{-1}K_{\mathcal{I}}^{-1}\bar{F}\right\rangle + \left\langle \bar{F}, (K_{\mathcal{I}}^{-1} - K_{\mathcal{I}}^{-1}B^{-1}K_{\mathcal{I}}^{-1})\bar{F}\right\rangle\Big)
\end{aligned} \tag{68}$$

where $\Sigma_{\mathcal{I}} := \Sigma_N + PQK_{\mathcal{I}}Q^*P^*$. The inverse of $\Sigma_{\mathcal{I}}$ is indeed the coefficient matrix for the quadratic term in u^N in (68). This can be seen by utilizing the Woodbury matrix identity as follows:

$$\begin{aligned}
\Sigma_{\mathcal{I}}^{-1} &= (\Sigma_N + PQK_{\mathcal{I}}Q^*P^*)^{-1} \\
&= \Sigma_N^{-1} - \Sigma_N^{-1}PQ(K_{\mathcal{I}}^{-1} + Q^*P^*\Sigma_N^{-1}PQ)^{-1}Q^*P^*\Sigma_N^{-1} \\
&= \Sigma_N^{-1} - \Sigma_N^{-1}PQB^{-1}Q^*P^*\Sigma_N^{-1}
\end{aligned}$$

We now complete the square (in terms of u^N) to obtain:

$$\begin{aligned}
&-\frac{1}{2}\Big(\left\langle u^N - h^N, \Sigma_{\mathcal{I}}^{-1}(u^N - h^N)\right\rangle + \left\langle \bar{F}, (K_{\mathcal{I}}^{-1} - K_{\mathcal{I}}^{-1}B^{-1}K_{\mathcal{I}}^{-1})\bar{F}\right\rangle - \left\langle \Sigma_N^{-1}PQB^{-1}K_{\mathcal{I}}^{-1}\bar{F}, \Sigma_{\mathcal{I}}\Sigma_N^{-1}PQB^{-1}K_{\mathcal{I}}^{-1}\bar{F}\right\rangle\Big) = \\
&\quad = -\frac{1}{2}\Big(\left\langle u^N - h^N, \Sigma_{\mathcal{I}}^{-1}(u^N - h^N)\right\rangle + \left\langle \bar{F}, (K_{\mathcal{I}}^{-1} - K_{\mathcal{I}}^{-1}B^{-1}K_{\mathcal{I}}^{-1} - K_{\mathcal{I}}^{-1}B^{-1}Q^*P^*\Sigma_N^{-1}\Sigma_{\mathcal{I}}\Sigma_N^{-1}PQB^{-1}K_{\mathcal{I}}^{-1})\bar{F}\right\rangle\Big)
\end{aligned} \tag{69}$$

where $h^N := \Sigma_{\mathcal{I}}\Sigma_N^{-1}PQB^{-1}K_{\mathcal{I}}^{-1}\bar{F}$. We now show that the term quadratic in $\bar{F}$ vanishes by showing that the coefficient matrix of $\bar{F}$ is equal to the zero matrix. Note that this coefficent matrix can be rewritten as:

$$\begin{aligned}
&K_{\mathcal{I}}^{-1} - K_{\mathcal{I}}^{-1}B^{-1}K_{\mathcal{I}}^{-1} - K_{\mathcal{I}}^{-1}B^{-1}Q^*P^*\Sigma_N^{-1}\Sigma_{\mathcal{I}}\Sigma_N^{-1}PQB^{-1}K_{\mathcal{I}}^{-1} = \\
&= K_{\mathcal{I}}^{-1}K_{\mathcal{I}}K_{\mathcal{I}}^{-1} - K_{\mathcal{I}}^{-1}B^{-1}K_{\mathcal{I}}^{-1} - K_{\mathcal{I}}^{-1}B^{-1}Q^*P^*\Sigma_N^{-1}\Sigma_{\mathcal{I}}\Sigma_N^{-1}PQB^{-1}K_{\mathcal{I}}^{-1} \\
&= K_{\mathcal{I}}^{-1}(K_{\mathcal{I}} - B^{-1} - B^{-1}Q^*P^*\Sigma_N^{-1}\Sigma_{\mathcal{I}}\Sigma_N^{-1}PQB^{-1})K_{\mathcal{I}}^{-1} \\
&= K_{\mathcal{I}}^{-1}B^{-1}(BK_{\mathcal{I}}B - B - Q^*P^*\Sigma_N^{-1}\Sigma_{\mathcal{I}}\Sigma_N^{-1}PQ)B^{-1}K_{\mathcal{I}}^{-1}
\end{aligned}$$

and so showing that it is the zero matrix is equivalent to showing that $(BK_{\mathcal{I}}B - B - Q^*P^*\Sigma_N^{-1}\Sigma_{\mathcal{I}}\Sigma_N^{-1}PQ)$ is the zero matrix. This can be shown as follows:

$$\begin{aligned}
&BK_{\mathcal{I}}B - B - Q^*P^*\Sigma_N^{-1}\Sigma_{\mathcal{I}}\Sigma_N^{-1}PQ = \\
&= (Q^*P^*\Sigma_N^{-1}PQ + K_{\mathcal{I}}^{-1})K_{\mathcal{I}}B - B - Q^*P^*\Sigma_N^{-1}\Sigma_{\mathcal{I}}\Sigma_N^{-1}PQ \\
&= Q^*P^*\Sigma_N^{-1}PQK_{\mathcal{I}}B + B - B - Q^*P^*\Sigma_N^{-1}\Sigma_{\mathcal{I}}\Sigma_N^{-1}PQ \\
&= Q^*P^*\Sigma_N^{-1}PQK_{\mathcal{I}}(Q^*P^*\Sigma_N^{-1}PQ + K_{\mathcal{I}}^{-1}) - Q^*P^*\Sigma_N^{-1}\Sigma_{\mathcal{I}}\Sigma_N^{-1}PQ \\
&= Q^*P^*\Sigma_N^{-1}PQK_{\mathcal{I}}Q^*P^*\Sigma_N^{-1}PQ + Q^*P^*\Sigma_N^{-1}PQ - Q^*P^*\Sigma_N^{-1}\Sigma_{\mathcal{I}}\Sigma_N^{-1}PQ \\
&= Q^*P^*\Sigma_N^{-1}(PQK_{\mathcal{I}}Q^*P^* + \Sigma_N - \Sigma_{\mathcal{I}})\Sigma_N^{-1}PQ = 0
\end{aligned}$$

where the last equality follows by the definition of $\Sigma_{\mathcal{I}}$. Thus, our integral simplifies to:

$$\frac{(2\pi)^{J/2}}{Z_u Z_f \det(B)^{1/2}} \int \psi(u^N) \exp\Big(-\frac{1}{2}\left\langle u^N - h^N, \Sigma_{\mathcal{I}}^{-1}(u^N - h^N)\right\rangle\Big)\mathrm{d}u^N \tag{70}$$

We now focus on simplifying the normalizing constants in front of the integral:

$$\begin{aligned}
\frac{(2\pi)^{J/2}}{Z_u Z_f \det(B)^{1/2}} &= \frac{(2\pi)^{J/2}}{(2\pi)^{N/2}\det(\Sigma_N)^{1/2}(2\pi)^{J/2}\det(K_{\mathcal{I}})^{1/2}\det(B)^{1/2}} = \\
&= \frac{1}{(2\pi)^{N/2}\det(\Sigma_N)^{1/2}\det(K_{\mathcal{I}})^{1/2}\det(B)^{1/2}}
\end{aligned}$$

To proceed we note that $\det B$ can be rewritten as follows:

$$\begin{aligned}
\det(B) &= \det(Q^*P^*\Sigma_N^{-1}PQ + K_{\mathcal{I}}^{-1}) \\
&= \det(K_{\mathcal{I}}^{-1}(I + K_{\mathcal{I}}Q^*P^*\Sigma_N^{-1}PQ)) \\
&= \det(K_{\mathcal{I}}^{-1})\det(I + (K_{\mathcal{I}}Q^*P^*)(\Sigma_N^{-1}PQ))) \\
&= \det(K_{\mathcal{I}})^{-1}\det(I + \Sigma_N^{-1}PQK_{\mathcal{I}}Q^*P^*)
\end{aligned}$$

where we have utilized Sylvester's determinant theorem (*note: the identity matrices in the last two lines are of different sizes*). We can now finish up the simplification of the constants outside the integral:

$$\begin{aligned}
&\frac{1}{(2\pi)^{N/2}\det(\Sigma_N)^{1/2}\det(K_{\mathcal{I}})^{1/2}\det(B)^{1/2}} \\
&= \frac{1}{(2\pi)^{N/2}\det(\Sigma_N)^{1/2}\det(K_{\mathcal{I}})^{1/2}\det(K_{\mathcal{I}})^{-1/2}\det(I + \Sigma_N^{-1}PQK_{\mathcal{I}}Q^*P^*)^{1/2}} \\
&= \frac{1}{(2\pi)^{N/2}\det(\Sigma_N + PQK_{\mathcal{I}}Q^*P^*)^{1/2}} \\
&= \frac{1}{(2\pi)^{N/2}\det(\Sigma_{\mathcal{I}})^{1/2}}
\end{aligned}$$

Thus, our integral becomes:

$$\begin{aligned}
&\int \psi(u^N)\frac{1}{(2\pi)^{N/2}\det(\Sigma_{\mathcal{I}})^{1/2}}\exp\left(-\frac{1}{2}\left\langle u^N - h^N, \Sigma_{\mathcal{I}}^{-1}(u^N - h^N)\right\rangle\right)\mathrm{d}u^N = \\
&= \int \psi(u^N)\mu_{h^N,\Sigma_{\mathcal{I}}}(\mathrm{d}u^N)
\end{aligned} \tag{71}$$

from which we see that we have obtained the expectation of ψ w.r.t. a multivariate Gaussian with mean and covariance given by:

$$h^N := \Sigma_{\mathcal{I}}\Sigma_N^{-1}PQB^{-1}K_{\mathcal{I}}^{-1}\bar{F} = PQ\bar{F} \tag{72}$$

$$\Sigma_{\mathcal{I}} = P(\Sigma + QK_{\mathcal{I}}Q^*)P^* \tag{73}$$

Note that we have simplified the mean h^N of this multivariate Gaussian as follows:

$$\begin{aligned}
h^N &= \Sigma_{\mathcal{I}}\Sigma_N^{-1}PQB^{-1}K_{\mathcal{I}}^{-1}\bar{F} \\
&= (\Sigma_N + PQK_{\mathcal{I}}Q^*P^*)\Sigma_N^{-1}PQ(K_{\mathcal{I}}B)^{-1}\bar{F} \\
&= PQ(K_{\mathcal{I}}B)^{-1}\bar{F} + PQK_{\mathcal{I}}Q^*P^*\Sigma_N^{-1}PQ(K_{\mathcal{I}}B)^{-1}\bar{F} \\
&= PQ(I + K_{\mathcal{I}}Q^*P^*\Sigma_N^{-1}PQ)(K_{\mathcal{I}}B)^{-1}\bar{F} \\
&= PQ(I + K_{\mathcal{I}}Q^*P^*\Sigma_N^{-1}PQ)(K_{\mathcal{I}}(K_{\mathcal{I}}^{-1} + Q^*P^*\Sigma_N^{-1}PQ))^{-1}\bar{F} \\
&= PQ(I + K_{\mathcal{I}}Q^*P^*\Sigma_N^{-1}PQ)(I + K_{\mathcal{I}}Q^*P^*\Sigma_N^{-1}PQ)^{-1}\bar{F} \\
&= PQ\bar{F}
\end{aligned}$$

We thus obtain (12) as claimed in the proof of Proposition 3.1. ■

6.3 Proof of the invertibility of the Galerkin Stiffness matrix A introduced in Section 4

We prove here that that Galerkin Stiffness matrix A with ij-*th* entry given by $A_{ij} := \int_\Omega a(x)\nabla\phi_i(x)\cdot\nabla\phi_j(x)\mathrm{d}x$ is invertible. The proof comes from [22]. As mentioned we assume that the diffusion coefficent $a(x)$ satisfies Assumption 2.

Proof: In order to show that A is invertible we shall show that it is (strictly) positive definite. Under Assumption 2 it is a simple exercise to show that the following bilinear form from $H_0^1(\Omega)\times H_0^1(\Omega)$ to $\mathbb{R}$ defined by:

$$\tilde{a}(u,w) := \int_\Omega a(x)\nabla u(x)\cdot\nabla w(x)\mathrm{d}x \tag{74}$$

defines a norm $|\cdot|_E$ on $H_0^1(\Omega)$ via $|v|_E := \tilde{a}(u,u)^{1/2}$. We can now show that the Galerkin stiffness matrix A is (strictly) positive definite. To this end let $\mathbf{v}\in\mathbb{R}^J\backslash\{0\}$ and define $v = \Phi^*\mathbf{v} = \sum_{i=1}^J v_i\phi_i$ where Φ^* is the operator in Section 4 defined by equation (37). Note that v so defined is a function in $H_0^1(\Omega)$. We can now compute:

$$\begin{aligned}
\mathbf{v}^T A\mathbf{v} &= \sum_{i,j=1}^J v_j A_{ij} v_i \\
&= \sum_{i,j=1}^J v_j\left(\int_\Omega a(x)\nabla\phi_i(x)\cdot\nabla\phi_j(x)\mathrm{d}x\right)v_i \\
&= \sum_{i,j=1}^J v_j\tilde{a}(\phi_i,\phi_j)v_i \\
&= \tilde{a}\left(\sum_{i=1}^J v_i\phi_i, \sum_{j=1}^J v_j\phi_j\right) \\
&= \tilde{a}(v,v) \\
&= |v|_E^2 > 0
\end{aligned}$$

where the strict inequality follows since $\tilde{a}(v,v) = 0$ iff $|v|_E = 0$ iff $v = 0$ (since $|\cdot|_E$ is a norm of $H_0^1(\Omega)$) iff $\mathbf{v} = 0$ since the $\{\phi_i\}$ are linearly independent. ■

6.4 Detailed computations for proving equation (41) in Section 4

We provide here the detailed computation for showing that the averaged distribution is indeed given by (41). As explained in Section 4 we must redo the calculation of the expectation of an arbitrary bounded cylindrical test function. We are thus again interested in computing the following integral:

$$\int\int \psi(u^N)\mu_{a,\Sigma}(\mathrm{d}u)\mu_{\bar{f},K}(\mathrm{d}f) \tag{75}$$

where now $a = \Phi^* A^{-1} F$ and $\Sigma = 0$. Thus, $\mu_{a,\Sigma} = \delta_a$, that is to say that the measure is in fact a Dirac point mass at $a = \Phi^* A^{-1} F$. We thus have:

$$\int\int \psi(u^N)\mu_{a,\Sigma}(\mathrm{d}u)\mu_{\bar{f},K}(\mathrm{d}f) = \int\int \psi(u^N)\delta_{\Phi^* A^{-1}F}(\mathrm{d}u)\mu_{\bar{f},K}(\mathrm{d}f)$$

Now since the posterior for u for a fixed realisation of f is a point mass we have that the posterior for $u^N = Pu$ is $\delta_{P\Phi^* A^{-1}F}$. Thus, we can write:

$$\int\int \psi(u^N)\delta_{\Phi^* A^{-1}F}(\mathrm{d}u)\mu_{\bar{f},K}(\mathrm{d}f) = \int\int \phi(u^N)\delta_{P\Phi^* A^{-1}F}(\mathrm{d}u^N)\mu_{\bar{f},K}(\mathrm{d}f)$$

It is now important to point out that $P\Phi^*$ is to be interpreted[7] as the following $N \times J$ matrix:

$$\begin{aligned} P\Phi^* &= P(\phi_1, \dots, \phi_J) \\ &= (P\phi_1, \dots, P\phi_J) \\ &= \begin{pmatrix} \phi_1(x_1) & \dots & \phi_J(x_1) \\ \vdots & & \vdots \\ \phi_1(x_N) & \dots & \phi_J(x_N) \end{pmatrix} =: \Theta \end{aligned}$$

i.e. the matrix with $ijth$ entry $\Theta_{i,j} := \phi_j(x_i)$ for $i \in \{1, \dots, N\}, j \in \{1, \dots, J\}$. We thus have that $Y := P\Phi^* A^{-1} F = \Theta A^{-1} F \sim \mathcal{N}(\Theta A^{-1} \bar{F}, \Theta A^{-1} K_{\mathcal{I}} A^{-1} \Theta^*)$. Together with this and with the fact that the posterior of u^N only depends on f through F we can write:

$$\begin{aligned} \int\int \psi(u^N)\delta_{P\Phi^* A^{-1}F}(\mathrm{d}u^N)\mu_{\bar{f},K}(\mathrm{d}f) &= \int\int \phi(u^N)\delta_{\Theta A^{-1}F}(\mathrm{d}u^N)\mu_{\bar{F},K_{\mathcal{I}}}(\mathrm{d}F) \\ &= \int\int \psi(u^N)\delta_Y(\mathrm{d}u^N)\mu_{\Theta A^{-1}\bar{F},\Theta A^{-1}K_{\mathcal{I}}A^{-1}\Theta^*}(\mathrm{d}Y) \\ &= \int \psi(u^N)\left(\int \delta_Y(\mathrm{d}u^N)\mu_{\Theta A^{-1}\bar{F},\Theta A^{-1}K_{\mathcal{I}}A^{-1}\Theta^*}(\mathrm{d}Y)\right) \\ &= \int \psi(u^N)\mu_{\Theta A^{-1}\bar{F},\Theta A^{-1}K_{\mathcal{I}}A^{-1}\Theta^*}(\mathrm{d}u^N) \end{aligned}$$

which we recognize as a finite dimensional projection of a Gaussian measure. Thus, we conclude that "averaging" over f gives the expected Gaussian posterior under these choices:

$$\mathcal{N}(\Phi^* A^{-1} \bar{F}, \Phi^* A^{-1} K_{\mathcal{I}} A^{-1} \Phi) \tag{76}$$

■

6.5 Detailed computations for the proof of Theorem 4.2

Detailed computations to obtain the upper-bounds in Theorem 4.2 are now presented. For convenience we will denote $\beta := \|B_1^{-1}\|_\infty$ which, as mentioned in Section 4 is a bounded constant independent of h. We will now give a detailed derivation of the upper-bound on the two remaining terms in the bound on $\|m^{(1)}_{u|\mathbf{v}} - m^{(2)}_{u|\mathbf{v}}\|_{L^2(\Omega)}$. We start with the second term:

$$\|(\Sigma_1 S^* B_1^{-1} - \Sigma_2 S^* B_2^{-1})\mathbf{v}\|_{L^2(\Omega)} \leq \|\Sigma_1 S^* B_1^{-1} - \Sigma_2 S^* B_2^{-1}\|_\infty \|\mathbf{v}\|$$

where $\|\mathbf{v}\|$ denotes the standard Euclidean norm of $\mathbf{v}$. We proceed by bounding the operator norm in the inequality above:

$$\begin{aligned} \|\Sigma_1 S^* B_1^{-1} - \Sigma_2 S^* B_2^{-1}\|_\infty &= \|\Sigma_1 S^* B_1^{-1} - \Sigma_2 S^* B_1^{-1} + \Sigma_2 S^* B_1^{-1} - \Sigma_2 S^* B_2^{-1}\|_\infty \\ &\leq \|(\Sigma_1 - \Sigma_2) S^* B_1^{-1}\|_\infty + \|\Sigma_2 S^*(B_1^{-1} - B_2^{-1})\|_\infty \\ &\leq \|\Sigma_1 - \Sigma_2\|_\infty \|B_1^{-1}\|_\infty + \|\Sigma_2\|_\infty \|B_1^{-1} - B_2^{-1}\|_\infty \\ &\leq \|\Sigma_1 - \Sigma_2\|_1 \beta + (\|\Sigma_2 - \Sigma_1\|_1 + \|\Sigma_1\|_\infty)(\beta^2\gamma^2 h^2 + \mathcal{O}(h^4)) \\ &\leq \beta(\gamma^2 h^2 + \mathcal{O}(h^4)) + (\|\Sigma_1\|_\infty + \gamma^2 h^2 + \mathcal{O}(h^4))(\beta^2\gamma^2 h^2 + \mathcal{O}(h^4)) \\ &= (\beta\gamma^2 + \|\Sigma_1\|_\infty \beta^2\gamma^2) h^2 + \mathcal{O}(h^4) \\ &= \gamma_1 h^2 + \mathcal{O}(h^4) \end{aligned}$$

[7] By this we mean that $P\Phi^*$ is actually interpreted as $P \otimes \Phi^*$

where $\gamma_1 := \beta\gamma^2 + \|\Sigma_1\|_\infty \beta^2\gamma^2 > 0$ is a constant independent of h. Note that we have utilised the fact that the operator norm is bounded above by the trace norm together with the bounds on $\|\Sigma_1 - \Sigma_2\|_1$ and $\|B_1^{-1} - B_2^{-1}\|_\infty$. Thus, the second term in the bound on the norm of the difference in posterior means is bounded above as follows:

$$\|(\Sigma_1 S^* B_1^{-1} - \Sigma_2 S^* B_2^{-1})\mathbf{v}\|_{L^2(\Omega)} \leq \gamma_1 \|\mathbf{v}\| h^2 + \mathcal{O}(h^4)$$

We now proceed to obtain an upper-bound on the third and final term in the bound on the norm of the difference in means:

$$\begin{aligned}
\|\Sigma_1 S^* B_1^{-1} S m_1 - \Sigma_2 S^* B_2^{-1} S m_2\|_{L^2(\Omega)} &= \|\Sigma_1 S^* B_1^{-1} S m_1 - \Sigma_1 S^* B_1^{-1} S m_2 + \Sigma_1 S^* B_1^{-1} S m_2 - \Sigma_2 S^* B_2^{-1} S m_2\|_{L^2(\Omega)} \\
&\leq \|\Sigma_1 S^* B_1^{-1}(m_1 - m_2)\|_{L^2(\Omega)} + \|(\Sigma_1 S^* B_1^{-1} - \Sigma_2 S^* B_2^{-1}) S m_2\|_{L^2(\Omega)} \\
&\leq \|\Sigma_1\|_\infty \beta \|m_1 - m_2\|_{L^2(\Omega)} + \|\Sigma_1 S^* B_1^{-1} - \Sigma_2 S^* B_2^{-1}\|_\infty \|m_2\|_{L^2(\Omega)} \\
&\leq \beta \tilde{C} \|\bar{f}\|_{L^2(\Omega)} \|\Sigma_1\|_\infty h^2 + (\gamma_1 h^2 + \mathcal{O}(h^4))(\|m_1\|_{L^2(\Omega)} + \tilde{C} h^2 \|\bar{f}\|_{L^2(\Omega)}) \\
&= (\beta \tilde{C} \|\bar{f}\|_{L^2(\Omega)} \|\Sigma_1\|_\infty + \|m_1\|_{L^2(\Omega)} \gamma_1) h^2 + \mathcal{O}(h^4) \\
&= \gamma_2 h^2 + \mathcal{O}(h^4)
\end{aligned}$$

where $\gamma_2 := \beta \tilde{C} \|\bar{f}\|_{L^2(\Omega)} \|\Sigma_1\|_\infty + \|m_1\|_{L^2(\Omega)} \gamma_1 > 0$ is a constant independent of h. Now, using these two bounds, together with the bound on $\|m_1 - m_2\|_{L^2(\Omega)}$ we have:

$$\begin{aligned}
\|m^{(1)}_{u|\mathbf{v}} - m^{(2)}_{u|\mathbf{v}}\|_{L^2(\Omega)} &\leq \tilde{C} h^2 \|\bar{f}\|_{L^2(\Omega)} + \gamma_1 \|\mathbf{v}\| h^2 + \gamma_2 h^2 + \mathcal{O}(h^4) \\
&= (\tilde{C} \|\bar{f}\|_{L^2(\Omega)} + \gamma_1 \|\mathbf{v}\| + \gamma_2) h^2 + \mathcal{O}(h^4) \\
&= \tilde{\gamma} h^2 + \mathcal{O}(h^4)
\end{aligned}$$

where $\tilde{\gamma} := \tilde{C} \|\bar{f}\|_{L^2(\Omega)} + \gamma_1 \|\mathbf{v}\| + \gamma_2 > 0$ is a constant independent of h. Having dealt with the difference of the posterior means we now move onto the term involving the difference of the posterior covariances. We compute:

$$\begin{aligned}
\|\Sigma^{(1)}_{u|\mathbf{v}} - \Sigma^{(2)}_{u|\mathbf{v}}\|_1 &= \|\Sigma_1 - \Sigma_1 S^* B_1^{-1} S \Sigma_1 - \Sigma_2 + \Sigma_2 S^* B_2^{-1} S \Sigma_2\|_1 \\
&\leq \|\Sigma_1 - \Sigma_2\|_1 + \|\Sigma_1 S^* B_1^{-1} S \Sigma_1 - \Sigma_2 S^* B_2^{-1} S \Sigma_2\|_1
\end{aligned}$$

We now bound the second term above as follows:

$$\begin{aligned}
\|\Sigma_1 S^* B_1^{-1} S \Sigma_1 - \Sigma_2 S^* B_2^{-1} S \Sigma_2\|_1 &= \|\Sigma_1 S^* B_1^{-1} S \Sigma_1 - \Sigma_2 S^* B_2^{-1} S \Sigma_1 + \Sigma_2 S^* B_2^{-1} S \Sigma_1 - \Sigma_2 S^* B_2^{-1} S \Sigma_2\|_1 \\
&\leq \|(\Sigma_1 S^* B_1^{-1} - \Sigma_2 S^* B_2^{-1}) S \Sigma_1\|_1 + \|\Sigma_2 S^* B_2^{-1} S (\Sigma_1 - \Sigma_2)\|_1 \\
&\leq \|\Sigma_1 S^* B_1^{-1} - \Sigma_2 S^* B_2^{-1}\|_\infty \|\Sigma_1\|_1 + \|\Sigma_2\|_\infty \|B_2^{-1}\|_\infty \|\Sigma_1 - \Sigma_2\|_1 \\
&\leq \gamma_1 h^2 \|\Sigma_1\|_1 + (\|\Sigma_1\|_\infty + \|\Sigma_1 - \Sigma_2\|_1)(\|B_1^{-1}\|_\infty + \|B_1^{-1} - B_2^{-1}\|_\infty) \|\Sigma_1 - \Sigma_2\|_1 + \mathcal{O}(h^4) \\
&\leq \gamma_1 \|\Sigma_1\|_1 h^2 + \|\Sigma_1\|_\infty \beta \gamma^2 h^2 + \mathcal{O}(h^4) \\
&= (\gamma_1 \|Sigma_1\|_1 + \beta \|\Sigma_1\|_\infty \gamma^2) h^2 + \mathcal{O}(h^4) \\
&= \gamma_3 h^2 + \mathcal{O}(h^4)
\end{aligned}$$

where $\gamma_3 := \gamma_1 \|Sigma_1\|_1 + \beta \|\Sigma_1\|_\infty \gamma^2 > 0$ is a constant independent of h. Using this we can conclude:

$$\begin{aligned}
\|\Sigma^{(1)}_{u|\mathbf{v}} - \Sigma^{(2)}_{u|\mathbf{v}}\|_1 &\leq \gamma^2 h^2 + \gamma_3 h^2 + \mathcal{O}(h^4) \\
&= (\gamma^2 + \gamma_3) h^2 + \mathcal{O}(h^4) \\
&= \kappa h^2 + \mathcal{O}(h^4)
\end{aligned}$$

where $\kappa := \gamma^2 + \gamma_3 > 0$ is a constant independent of h. We can now combine the bounds on terms involving the posterior means and covariances to obtain:

$$\begin{aligned}
W^2 \left(\mathcal{N}(m^{(1)}_{u|\mathbf{v}}, \Sigma^{(1)}_{u|\mathbf{v}}), \mathcal{N}(m^{(2)}_{u|\mathbf{v}}, \Sigma^{(2)}_{u|\mathbf{v}}) \right) &\leq \kappa h^2 + \tilde{\gamma}^2 h^4 + \mathcal{O}(h^2) \\
&\leq \kappa h^2 + \mathcal{O}(h^4)
\end{aligned}$$

We can thus conclude that $W \left(\mathcal{N}(m^{(1)}_{u|\mathbf{v}}, \Sigma^{(1)}_{u|\mathbf{v}}), \mathcal{N}(m^{(2)}_{u|\mathbf{v}}, \Sigma^{(2)}_{u|\mathbf{v}}) \right) \leq \sqrt{\kappa} h + \mathcal{O}(h^2)$ as required. ■