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Numerical Analysis of some Bayesian Inverse Problems

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Numerical Analysis of some Bayesian Inverse Problems

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A thesis submitted to Nanyang Technological University
in partial fulfillment of the requirement for the degree of
Doctor of Philosophy in Mathematical Sciences

2019

Statement of Originality

I hereby certify that the work embodied in this thesis is the result of original research, is free of plagiarised materials, and has not been submitted for a higher degree to any other University or Institution.

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I have reviewed the content and presentation style of this thesis and declare it is free of plagiarism and of sufficient grammatical clarity to be examined. To the best of my knowledge, the research and writing are those of the candidate except as acknowledged in the Author Attribution Statement. I confirm that the investigations were conducted in accord with the ethics policies and integrity standards of Nanyang Technological University and that the research data are presented honestly and without prejudice.

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Hoang Vut Ha

Authorship Attribution Statement

This thesis contains material from 1 paper accepted for publication in the following peer-reviewed journal where I was the corresponding author. (Author names are alphabetically ordered)

Chapter 2 is published as V. H. Hoang and J. H. Quek, Bayesian inverse problems for recovering coefficients of two scale elliptic equations. *Inverse Problems* (Accepted for publication).

The contributions of the co-authors are as follows:

- I developed the theory under the guidance of Prof Hoang
- I simulated the numerical results using Markov Chain Monte Carlo sampling method to approximate the expectation, with the help from Dr Tan Wee Chin in solving the forward problem using sparse tensor product finite element method.

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Date

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Quek Jia Hao

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Abstract

Bayesian inverse problems for partial differential equations arise from many important real world applications. We find the physical properties of a medium in the form of an unknown coefficient of a partial differential equation, given limited noisy observations on the solution. The noise follows a known probability distribution. The unknown coefficient, or the parameters on which it depends, belong to a prior probability space. We aim to find the posterior probability which is the conditional probability of the unknown given the observations.

The first part of the thesis is devoted to Bayesian inverse problems to find the unknown locally periodic coefficient of a two scale elliptic equation. In the remaining part, we develop the Multilevel Markov Chain Monte Carlo method for approximating posterior expectation of a quantity of interest for Bayesian inverse problems for partial differential equations. The method achieves an approximation within a prescribed accuracy but uses only an optimal number of total degrees of freedom. We develop the method for elliptic forward equations with the Gaussian prior distribution for the log-normal coefficients, and for parabolic equations with both uniform and Gaussian prior distributions for the coefficients.

In Chapter 2, we consider the problem of finding coefficients of locally periodic two scale elliptic problems. We consider both the uniform prior and the Gaussian prior in the space of locally periodic coefficients. In the first case, the coefficient is uniformly coercive and bounded for all the realizations. In the second case, the coefficient is positive but can get arbitrarily large and arbitrarily close to 0. We approximate the posterior by the probability measure obtained from solution of the two scale homogenized equation. We show an explicit error for this approximation with respect to

the Hellinger distance of the two measures, in terms of the microscopic scale. This error estimate holds when the solution of the two scale homogenized equation is sufficiently regular. The two scale homogenized equation provides all the information we need: the solution to the homogenized equation which approximates the solution to the two scale forward equation macroscopically, and the corrector term which encodes the microscopic behavior. Although this equation is posed in a high dimensional tensorized domain, the sparse tensor product finite element method developed in V. H. Hoang and Ch. Schwab, *Multiscale Model. Simul.* Vol 3, pp 168-194 (2005), solves this equation with essentially optimal complexity. We then approximate the posterior measure by the measure obtained from the sparse tensor product finite element solution of the two scale homogenized equation, with an explicit error in terms of the finite element mesh and the microscopic scale. We show numerically that observations on the macroscopic behavior alone are not sufficient to infer the microstructure. We need also observations on the corrector. Solving the two scale homogenized equation, we get both the solution to the homogenized equation and the corrector. Thus our method is particularly suitable for sampling the posterior measure of two scale coefficients.

Chapter 3 reviews the Multilevel Markov Chain Monte Carlo method for approximating posterior expectation of a quantity of interest in Bayesian inverse problems for forward elliptic equations with uniform prior probability. This chapter serves as a basis for the development in the subsequent chapters. We define the uniform prior probability space. We then outline the Multilevel Markov Chain Monte Carlo method developed in V. H. Hoang, Ch. Schwab, A. M. Stuart, *Inverse Problems*, Vol. 29, 085010, 37pp (2013). The method achieves an approximation for the posterior expectation of a

quantity of interest within a prescribed accuracy, using only an optimal level of degrees of freedom (with a possible logarithmic factor). We show that the logarithmic factor in the error can be reduced by slightly increasing the Markov Chain Monte Carlo sample size. The paper by Hoang et al. does not include numerical examples. We perform new numerical examples to illustrate the theory.

The Multilevel Markov Chain Monte Carlo method by Hoang et al. is only valid for the uniform prior probability. Their proof of convergence is not valid for the Gaussian prior probability of the coefficient of a forward elliptic equation as it relies essentially on the uniform boundedness of the solution. In Chapter 4, we develop a new Multilevel Markov Chain Monte Carlo method for elliptic equation with Gaussian prior probability. We show theoretically the convergence of the method together with the explicit optimal convergence rate. We provide numerical examples using both independence sampler and preconditioned Crank-Nicolson (pCN) sampler to verify the rigorously justified theoretical convergence rate.

In Chapter 5, we consider Bayesian inverse problems for finding coefficient of forward parabolic equations with the uniform prior probability. We consider the coefficient of the parabolic equation to be an expansion of random variables each uniformly distributed in a compact interval. We assume that the coefficient is uniformly coercive and bounded for all the realizations. We approximate the posterior measure by the approximated solution of the forward parabolic equation which is solved by backward Euler and finite element method with coefficient taking only a finite number of terms in the expansion. We then develop the Multilevel Markov Chain Monte Carlo method to estimate the posterior expectation of a quantity of interest. As in the paper by Hoang, Schwab and Stuart, the key point to

achieve optimal convergence is to judiciously balance the level of resolution and the sample size of each run of the Markov Chain Monte Carlo algorithm. We establish rigorously the convergence rate. We present numerical examples that support the theory.

We consider Gaussian prior probability where the coefficient of the parabolic equation takes the log-normal form in Chapter 6. We use the backward Euler finite element method to approximate the truncated forward parabolic equation taking only a finite number of terms in the coefficient. This approximation leads to an approximation for the posterior measure where the forward functional is determined from the approximated solution of the forward equation. We then approximate the posterior expectation of a quantity of interest by this approximated posterior measure. We develop the Multilevel Markov Chain Monte Carlo to estimate the posterior expectation in this case of forward parabolic equations with log-normal coefficients. We show theoretically the convergence of the method together with the explicit optimal convergence rate. We present numerical examples for both the independent sampler and the preconditioned Crank-Nicolson sampler. The results for both cases verify the theoretical prediction.

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Chapter 1

Introduction

Inverse problems arise from many important engineering and practical areas such as subsurface flow, oil production, seismology and weather forecast. We need to find the properties of the medium in which a physical process occurs, to construct the governing equations of a physical process, given only limited observations on the solutions to the equations. Solving inverse problems are complicated. The limited observations normally are not sufficient to determine the governing equation precisely. Further, observations are contaminated with errors (noise). The problems can be ill-posed: they can have no solution, or more than one solution. The solutions can also be unstable, i.e. they depend sensitively on small changes of the observation data.

Mathematically, we consider a functional $\mathcal{G} : V \rightarrow \mathbb{R}^N$ where V represents the function space in which we find the unknown quantities, such as coefficients of an equation, from which we construct the governing model or equation; V can also be the space of parameters on which the desired quantities depend on. Normally V is an infinite dimensional space. Here $\mathcal{G}(z)$ represents the forward map which can be found by solving the for-

ward equation if it is known. In the situation of inverse problems, we have available a noisy observation of $\mathcal{G}(z)$ and wish to reconstruct the forward equation. The noisy observation δ of $\mathcal{G}$ is modelled by

$$\delta = \mathcal{G}(z) + \vartheta \quad (1.0.1)$$

where ϑ represents the noise contamination in δ . The inverse problem aims to find z given the noisy observation δ . The forward partial differential equations are well-posed; for every $z \in V$, there is a unique solution and hence a unique $\mathcal{G}(z)$. However, as inverse problems are usually ill-posed as mentioned above, one way to solve an inverse problem is to find a $z \in V$ such that the forward map $\mathcal{G}(z)$ found from solving the forward equation best fits the available observation, i.e we find z such that

$$\|\delta - \mathcal{G}(z)\|_W \quad (1.0.2)$$

is minimum. Here $\|\cdot\|_W$ is a measuring norm. The disadvantage of this approach is that the minimizing problem may not have a solution due to the high oscillation and divergence of the minimizing sequence; that is, the minimizing functional admits an infimum but not an absolute minimum. On the other hand, the minimization problem may have multiple solutions. To overcome this difficulty, classical approach to inverse problems adds a regularizing term that makes the best fit minimization problem well-posed. In particular, instead of considering the functional (1.0.2), the Tikhonov regularizing approach considers the minimization problem of

$$\|\delta - \mathcal{G}(z)\|_W + \|z\|_E, \quad (1.0.3)$$

where $\|z\|_E$ is the regularizing term, with $\|\cdot\|_E$ to be chosen. While regularization makes the best fit problem well-posed, the choice of the regularizing

term is usually ad hoc. Details of the classical method can be found in [21] and [38]. In this thesis, we consider the Bayesian framework for inverse problems which attracts large attention recently (see Stuart [51]). The difference is in the treatment of the noise and the solution of interest. In the classical approach above, the unknown noise is treated as deterministic, and the solution to the inverse problem is a deterministic function. On the other hand, Bayesian approach regards the noise as random variables which follow a predetermined prior probability. The unknown quantity z which we wish to find belongs to the prior probability space. We are interested in finding the conditional probability of z given the noisy observation δ . This conditional probability, also known as the posterior probability, is the solution of the inverse problem. Bayesian approach to inverse problems is discussed thoroughly in the book by Kaipio and Somersalo [43] and Stuart [51]. In particular, the existence of a solution is assured by Bayes theorem in a finite dimensional setting. For problems that involve infinite dimensional space of functions, Kaipio and Somersalo [43] discretize the equation to reduce it to an approximated finite dimensional problem first before applying the Bayesian framework. This could pose difficulties as the approximating discretized space must be of a very high dimension in order to give an accurate representation of the original. In addition, as discussed by Stuart [51], in many problems, discretizing in the last possible moment allows obtaining important information. The pioneering work by Cotter et al. [12] establishes a rigorous mathematical framework for Bayesian inverse problems in Banach spaces V equipped with a prior probability γ . In particular, they show that the Bayes formula holds in the infinite dimensional setting for the posterior probability when the functional $\mathcal{G}$ is γ measurable. Further, if the prior probability is Gaussian, and if $\mathcal{G}$ grows polynomially,

then the posterior probability measure is continuous with respect to δ in the Hellinger distance sense. This shows that the problem is well-posed. While the posterior probability measure is the solution to the Bayesian inverse problem, in many situations, we are more interested in the expectation of some quantity of interest with respect to this posterior. The challenge in finding this posterior expectation is in the high or infinite dimension of the probability space; computing the normalizing constant of the probability density in the Bayes formula of the posterior measure would prove to be difficult or impossible. As such, we look at sampling methods to approximate the expectation. Sampling the posterior probability by Markov Chain Monte Carlo (MCMC) method is a popular choice for approximating the posterior expectation. However, the complexity of the MCMC method can also be very high. This is because, for the MCMC method to provide a reasonable approximation, a large number of samples are needed. Furthermore, the forward partial differential equation needs to be solved with reasonable accuracy as well. Their combined effect, due to the need to solve the forward equation once for each sample generated, results in the high complexity. The issue is far more severe for multiscale forward equations where the forward equations depend also on microscopic scales. The cost of solving a multiscale forward equation using fine mesh to capture the microscopic scale is very large, leading to prohibitively large total computational cost. In this thesis, we devote a chapter to considering Bayesian inverse problems for multiscale problems to infer the microstructure. The rest of the thesis develops the Multilevel MCMC (MLMCMC) method to reduce the sampling cost when approximating the expectation with respect to the posterior measure in Bayesian inverse problems for partial differential equations.

We consider in this thesis an inverse problem to find the two scale coefficient of an elliptic equation given limited noisy observations on the solution of the two scale problem. We assume that the coefficient is locally periodic. We follow the framework of Bayesian inverse problems which assumes that the observation errors follow known probability distributions. Imposing a prior probability measure on the space of locally periodic coefficients, we find the posterior measure which is the conditional probability given the noisy observations. We contribute a method that reduces significantly the complexity of Markov Chain Monte Carlo (MCMC) sampling for the posterior measure in the space of two scale coefficients. We consider two types of prior probability measures. In the first type, the two scale coefficients are uniformly coercive and bounded for all the realizations. We assume that they can be written as an expansion of random variables which are uniformly distributed in a compact interval. The prior probability space is the probability space of countably infinite sequences of these random variables. We note that the uniform prior probability is considered for Bayesian inversion of single scale elliptic equations in Hoang et al. [37]. In the second type, the logarithm of the coefficient is a linear expansion of standard normal random variables. This is the well-known log-gaussian coefficients where the expansion arise from the Kahùnen-Loève expansion of the logarithm of the random coefficient given its covariace (see, e.g., [1], [51], [14]).

As the coefficient of the forward two scale equation is locally periodic, we use two scale convergence ([45], [2]) to study homogenization of the problem. The method produces the two scale homogenized equation for both the solution of the homogenized equation which describes the solution to the two scale equation macroscopically, and the corrector which encodes the microscopic behaviour of the solution to the multiscale equation. These

are the first two terms in the two scale asymptotic expansion of the solution to the two scale equation (see [5], [4], [42]). Solving the two scale homogenized equation, we obtain all the necessary information. The observations obtained from the oscillating solution of the two scale equation can be approximated by the solution of this macroscopic two scale homogenized equation, which leads to an approximation of the posterior measure when the microscopic scale approaches zero. Sampling the posterior by the MCMC method, we can solve this two scale homogenized equation instead of the original two scale equation. Although posed in a high dimensional tensorized domain, the two scale homogenized equation can be solved with an essentially optimal complexity for a prescribed accuracy by the sparse tensor product finite element (FE) method developed by Hoang and Schwab [35]. The cost of the MCMC method is far lower than solving the original two scale equation for a large number of samples, using a fine mesh to capture the microscopic scale. Further, we will demonstrate that for recovering the microstructure, it is not sufficient to have only information on the solution of the homogenized problem. We need information on the corrector term. Our method of using the two scale homogenized equation finds all the necessary information with much less complexity. Although we do not consider multilevel MCMC in the context of two scale problem, the problem is well amenable to this method as developed in [37] and the subsequent chapters of this thesis which reduces the computation to the optimal level.

We only consider two scale problems in this thesis. However, Bayesian inverse problems for finding coefficients that depend on multiple separable scales can be solved in the same way, using multiscale convergence [3] and the essentially optimal method for solving multiscale homogenized equation developed in Hoang and Schwab [35].

Inverse problems for locally periodic two scale problems have been considered before. Nolen et al. [46] study the effective model and thus the multiscale features of the problem are not recovered. Frederick and Engquist [22] assume that the microstructure is known, and find a macroscopic quantity such as the volume fraction or the orientation of the inclusions. We contribute in this thesis a rigorous theory for recovering the microstructure, and an MCMC sampling method for the posterior measure with significantly reduced complexity.

Inverse problems for finding physical properties of multiscale media arise in important application such as oil exploration, subsurface flow... We mention the work by Efendiev et al. [20] (see also the references there) which considers Bayesian inverse problem in the context of subsurface flow, where a procedure for speeding up the MCMC sampling process is developed. General multiscale inverse problems using generalized multiscale finite elements method (GMsFEM) is proposed in Chung et al. [9]. Model reduction in the framework of GMsFEM is studied in [40]. Bayesian inference for multiscale fractional diffusion equations is considered in [41]. These reference employ general method for general multiscale problems. The complexity of general methods for solving multiscale problem such as Multiscale Finite Elements and the Heterogeneous Multiscale Method has complexity comparable to that for directly solve multiscale problem using fine mesh. When running MCMC, many samples of the forward equation have to be solved; the complexity of these methods will be high. For locally periodic multiscale problem, the sparse tensor product FEM that we employ solve the multiscale problem within a prescribed accuracy and requires only an optimal number of degrees of freedom. For performing the MCMC, we need to solve a forward equation of each realisation of sample. The number of

multiscale equations we need to solve is very high, thus the sparse tensor product FEM reduce the complexity significantly.

In the remaining part of the thesis, we consider the MLMCMC method for Bayesian inverse problems to infer unknown coefficients of forward partial differential equation. As described above, simple employment of the MCMC method for Bayesian inverse problems can be highly complex as for each sample of the MCMC, we need to solve the forward partial differential equations. The number of samples required is normally very high leading to very high complexity. Thus a sampling method that can reduce the computation cost for MCMC sampling of the posterior measure to the optimal level will have a far reaching consequence. In Hoang, Schwab and Stuart [37], a MLMCMC method for Bayesian inverse problems to find the coefficient of elliptic equations is developed. The paper considers the case of uniform prior probability in which the coefficient is expressed as a linear expansion of random variables which are uniformly distributed in a compact interval. They proved theoretically that approximation of the expectation of the quantity of interest with respect to the posterior measure can be executed with an essentially optimal number of total degrees of freedom. The computational cost is essentially equal to that for performing only one step of the simple MCMC method to obtain an equal level of accuracy. For a problem in $\mathbb{R}^d$, to obtain an approximation of the posterior expectation of a quantity of interest with error ε , the method requires a total $O(\varepsilon^{-d})$ number of degrees of freedom (ignoring a possible logarithmic factor). This is essentially equal to that for solving a single deterministic elliptic equation. The method is essentially optimal. The main idea of the method is to use a telescopic sum for the posterior expectation with respect to different levels of FE discretization of the posterior measure. In each of the

terms in the telescopic sum, the quantity of interest is discretized with a level of resolution that depends on the discretization level of the posterior in the corresponding term of the telescopic sum. We then use a second telescopic sum for the quantity of interest in terms of the FE resolution of this quantity. Each term in this double telescopic sum is then approximated by MCMC. The key point is that the number of samples for approximating each term is chosen judiciously according to the FE discretization levels of the posterior measure and the quantity of interest in this term. As a consequence, the total number of degrees of freedom we need to achieve a prescribed level of accuracy is optimal. We note that there is another version of MLMCMC algorithm developed in [19] in literature. Comparing to the method developed in Hoang et al. [37], the complexity of this algorithm is not optimal; it requires a computational cost of $O(\varepsilon^{-d-1})$ to achieve a level of accuracy with error $O(\varepsilon)$. There have been papers in the past five years that work on mathematical and computational investigations of a number of methodologies for the Bayesian inversion of PDEs with uncertain inputs. We mention [16, 15] and the references there for a presentation of MCMC methods for PDEs which account explicitly for the dependence on PDE discretization parameters.

Multi-level versions of Sequential Monte Carlo, Particle Filters, EnKF etc. for data assimilation and inference under PDE constraints have been recently proposed and analyzed. They can be found in the papers [39, 6] and the references there, showing the contributions on this. Recent work on multi-level algorithms in uncertainty quantification for PDEs includes in particular the numerical analysis of multilevel methods for the filtering problem, see, e.g. [17, 39, 49]. While also admitting noisy data, in these works, uncertain input of the PDE is limited to the forcing term.

In the paper [47], MLMCFEM and (single-level)QMC FEM for Bayesian PDE inversion under log-gaussian diffusion coefficient and under gaussian prior measure have been considered. Similarly as proposed in [48], ratio estimators were investigated there with MLMC integration to directly estimate the expectation of the quantity of interest under the posterior expectation and the normalization constant of the posterior measure. It was assumed in [[47] Appendix] that the log-gaussian diffusion coefficient is bounded away from zero by a positive constant.

To the best of our knowledge, none of these references addresses the problem of sign-indefiniteness in the exponent of posterior densities in the telescoping sums of the multi-level Bayesian estimators under gaussian priors, and with log-gaussian diffusion coefficients which may become, with positive probability, arbitrary close to zero. This, however, entails mathematical issues (posterior densities of increments between discretization levels may not be integrable with respect to the gaussian prior measure), and can, as we show in the thesis with numerical examples, foil practical realizations of the MLMCMC FEM methods.

In many applications such as subsurface flow, the coefficient of the forward governing equation is modelled in the log-normal form where the logarithm of the coefficient is assumed to follow a Gaussian random field. This is to model the situation when the coefficient is positive but can get arbitrarily large and arbitrarily close to zero. The method by Hoang, Schwab and Stuart in [37] theoretically does not cover this case as it relies on the uniform boundedness of the solution of the forward equation for all realizations. The proof of [37] does not work for the case of log-normal coefficient. Furthermore, we show numerically that the method may not work for the case of log-normal coefficient. In this thesis, we develop the optimal MLMCMC

method for Bayesian inverse problems for forward elliptic partial differential equations with log-normal coefficients. The method of Hoang et al. needs to be modified substantially. The optimal convergence rate of the method we develop for log-normal coefficient with the Gaussian prior probability can be justified mathematically rigorously. We perform numerical examples to verify the theory. We then consider parabolic problems. In the literature, MLMCMC for Bayesian inverse problems to find coefficients of parabolic equations have not been developed. We study Bayesian inverse problems for parabolic equations in the thesis for both uniform and Gaussian prior probability. We develop the MLMCMC method for these problems. We show the theory rigorously and provide numerical examples to illustrate the theory.

The organization of the thesis is as follows.

In Chapter 2, we study Bayesian inverse problems for finding coefficients of locally periodic two scale elliptic equations. We perform rigorous analysis for the existence and well-posedness of the posterior measure. We then study approximation of the posterior measure in terms of the finite element solution of the macroscopic two scale homogenized equation. We perform numerical experiments to illustrate the theory.

In the Section 2.1, we set up the Bayesian inverse problems for two scale equations. We define the prior probability space and introduce the Bayes formula for the posterior measure and the well-posedness results of Bayesian inverse problems that we will prove later for our two scale setting. We recall the definition of two scale convergence and the results of two scale homogenization for elliptic equations in Section 2.2. We prove that the observations on the oscillating solution of the two scale equation can be approximated by the solution of the two scale homogenized equation, leading to an ap-

proximation of the forward functional and the miss-match function. We study the Bayesian inverse problem with the uniform prior probability in Section 2.3. We first establish the existence and well-posedness with respect to the data of the posterior measure. We show that the posterior measure can be approximated by the corresponding measure determined from the solution of the two scale homogenized equation. In particular, we show that the Hellinger distance of these two measures converges to zero in the zero limit of the microscale. When the solution of the two scale homogenized equation is sufficiently regular, we establish a rate for this convergence of the Hellinger distance in terms of the microscale. This uses the well-known homogenization rate of convergence. The Bayesian inverse problem with the Gaussian prior probability is studied in Section 2.4. As in Section 2.3, we first prove the existence and well-posedness of the posterior measure. We then prove that the posterior measure can be approximated by the measure determined from the solution of the two scale homogenized equation with respect to the Hellinger distance, with an explicit bound for the Hellinger distance in terms of the microscopic scale when the solution is sufficiently regular. We review the sparse tensor product FE method for solving the two scale homogenized equation in Section 2.5. This method solves the two scale homogenized equation with essentially equal accuracy as the full tensor product FEs but requires a far less number of degrees of freedom, which is essentially optimal. We define the approximating posterior measure in terms of the FE solutions and prove the convergence of the Hellinger distance of the posterior measure and this FE approximating measure when the meshsize and the microscale converge to zero, with an explicit error bound when the solutions are sufficiently smooth. Numerical examples are presented in Section 2.6. By considering a one dimensional problem, we

show that when we only have observations for the macroscopic behaviour, i.e. when the functions ℓ_i in (2.1.4) do not depend on y , it is not sufficient to recover the microstructure. Indeed, the posterior measure obtained from the MCMC process does not give a clear description of the reference coefficient. Likewise, when the observation is the flux of the two scale equation, which is approximately the flux of the homogenized equation, we only have an observation for the macroscopic behaviour; the recovery of the reference coefficient by MCMC is poor. However, when the functions ℓ_i in (2.1.4) depend also on y , i.e. we have information on the corrector u_1 , the MCMC method provides reasonably good recovery of the reference coefficient. We demonstrate this for both the cases of uniform and Gaussian prior probability measures. We conclude the chapter with some appendices that contain the long proofs of some results in the previous sections.

In Chapter 3, we review the MLMCMC method for Bayesian inverse problems for forward elliptic partial differential equations that is developed in [37]. This paper considers the uniform prior probability where the coefficient of the equation is expressed as a summation of random variables that are uniformly distributed in a compact interval. The coefficient is uniformly coercive and bounded for all the realizations. This paper does not include numerical examples to illustrate the theory. In the thesis, we modify this method slightly by increasing the number of sample size for each Markov Chain to reduce the logarithmic factor in the overall error, with the complexity increased only by a logarithmic factor. In Section 3.1, we define the Bayesian inverse problem. We introduce the prior probability space of infinite sequences of random variables where each random variable is uniformly distributed in a compact interval. The random coefficient of the forward equation is expressed as the sum of these variables. We impose condition on

the supremum norm of the functions which are coefficients of this expansion to ensure that the coefficient is uniformly coercive and bounded. In Section 3.2, we review the existence and well-posedness of the posterior measure that are established in [37]. The forward equation is approximated by FE in Section 3.3 where we truncate the coefficient to take only a finite number of random variables in the expansion. We recall the approximation results for the posterior in terms of the number of chosen random variables in the coefficient and the FE mesh. The MLMCMC algorithm developed in [37] is recalled in Section 3.4. We introduce a slight modification in the number of MCMC sample size to reduce the logarithmic factor in the overall error. We contribute numerical examples to verify the theory in Section 3.5 where we illustrate the MLMCMC errors for the modified method.

Chapter 4 develops the new MLMCMC method for Bayesian inverse problems for finding the log-normal coefficient of the forward elliptic equation.

The MLMCMC method developed in Chapter 3 is only valid in the case of uniform prior probability. We show by an example in Section 4.5 that for equations with log-normal coefficients, the method may fail to work. This is due to the fact that in Chapter 3, we rely on the uniform boundedness of the potential $\Phi(z, \delta)$ for all z in the prior probability space. This is no longer the case for equations with log-normal coefficients. We develop in this chapter a MLMCMC method for equations with log-normal coefficients. We show theoretically the convergence of the method together with the explicit optimal convergence rate. We show numerically that for the example where the MLMCMC method developed in Chapter 3 fails to work, the new method developed in this chapter converges as theoretical prediction. In Section 4.1, we introduce the log-normal coefficient and define the prior

probability space. We then show the existence and well-posedness of the posterior measure in Section 4.2. In Section 4.3, we approximate the forward equation by finitely truncating the coefficient and solving the resulting equation by FE. We then define the approximated posterior measure from the FE solution of the truncated equation and establish an explicit error estimate for the approximation in terms of the Hellinger distance. We then develop the MLMCMC for the Gaussian prior probability and present the convergence rate of the MLMCMC estimator in Section 4.4. In Section 4.5, we show numerical results supporting the convergence of the MLMCMC method developed in this chapter for both the independent sampler and the preconditioned Crank-Nicolson (pCN) sampler. The numerical results show that the MLMCMC method for log-normal coefficients achieves the optimal level of accuracy with respect to the finest level of FE discretization, as theoretically predicted. We then show the example where the MLMCMC method developed in Chapter 3 for uniform prior probability fails to work while the MLMCMC method developed in this chapter does. The appendices give the detailed proofs of some theorems.

Chapter 5 devotes to Bayesian inverse problems for finding coefficient of parabolic equations. We consider uniform prior probability in the chapter. We set up the problem in Section 5.1. We first recall the definition of the uniform prior probability space defined in Chapter 3. We define the posterior measure using Bayes' rule for which we will prove the existence and well-posedness in Section 5.2. Section 5.3 considers the approximation of the posterior measure by solving the forward parabolic equation by Backward Euler and Finite Elements method. We deduce explicit error for the approximation with respect to the Hellinger distance in terms of the finite number of terms chosen in the truncated coefficient, the FE mesh size and

the time step size. We develop the Multilevel Markov Chain Monte Carlo (MLMCMC) in Section 5.4. We establish rigorously the convergence rate of the MLMCMC estimator. In Section 5.5, we present some numerical examples that illustrate the theoretical results. The appendices in the end of the chapter contain the long proofs of some results in the previous sections.

Chapter 6 devotes to Bayesian inverse problems for finding coefficient of parabolic equations with log-normal coefficients. We first recall the definition of the Gaussian prior probability space defined in Chapter 4. We set up the problem by introducing the coefficients of the log-normal form and defining the Gaussian prior probability space in Section 6.1. We show in Section 6.2 the existence and well-posedness of the posterior measure in terms of the Hellinger distance. In Section 6.3, we approximate the forward parabolic equation by taking only a finite number of terms in the coefficient and using Backward Euler and Finite Element method. From the approximated solution of the forward parabolic equation, we establish an approximation for the posterior measure with an explicit error with respect to the Hellinger distance. We develop the MLMCMC method in Section 6.4 and establish rigorously the convergence rate of the MLMCMC estimator. In Section 6.5, we provide numerical results that support the theoretical findings. The chapter concludes with some appendices.

Throughout the thesis, by ∇ without indicating the variable, we mean the gradient with respect to x of a function of x , and by ∇_x we mean the partial gradient of a function that depends on x and y . Repeated indices indicate summation. By c we denote a generic constant whose value can change from one appearance to the next. When the constant c depends on the parameter z , we write it as $c(z)$. The symbol $\#$ denotes spaces of periodic functions. For functions that depend on the parameter sequence

z and other space and/or time variables, when we wish to indicate only the dependence on z , we write the variable z only. By $\mathbb{E}^\mu[g]$ we mean expectation of a function g with respect to the probability measure μ .

Chapter 2

Bayesian inverse problems for recovering coefficients of two scale elliptic equations

We consider Bayesian inverse problems for finding the locally periodic coefficient of a two scale elliptic equation. In Section 2.1, we set up the Bayesian inverse problem, we introduce the uniform and Gaussian prior probabilities, and we introduce the basic results. In Section 2.2, we recall the definition of two scale convergence. We use the solution of the two scale homogenized equation to approximate the posterior measure. We study the problem with uniform prior probability in Section 2.3. We show the existence and well-posedness of the posterior measure. We establish the approximation of the posterior measure by that determined by the solution of the two scale homogenized problem with respect to the Hellinger distance. When the solution is sufficiently regular, we derive an explicit error for this approximation in terms of the microscopic scale. Similar results for the Gaussian prior probability are proved in Section 2.4. In Section 2.5, we recall the

sparse tensor product finite element method for solving the two scale homogenized equation. We use the finite element solution to approximate the posterior measure with respect to the Hellinger distance. When the solution is regular, we derive an error of this approximation in terms of the finite element mesh size. Section 2.6 contains numerical results that support the theory. The chapter concludes with some appendices.

2.1 Problem setting

Let $D \subset \mathbb{R}^d$ be a bounded domain. Let Y be the unit cube $(0, 1)^d \subset \mathbb{R}^d$. Let $\varepsilon > 0$ be a small quantity that represents the microscopic scale of the problem. We consider the prior probability space (U, Θ, γ) . Let $A : U \rightarrow C(\bar{D}, C_\#(\bar{Y}))$. We assume that for each $z \in U$, there are constants $c_*(z) > 0$ and $c^*(z) > 0$ such that

$$c_*(z) \leq A(z; x, y) \leq c^*(z) \quad (2.1.1)$$

for all $x \in D$ and $y \in Y$ ¹. We define the two scale coefficient as

$$A^\varepsilon(z; x) = A(z; x, \frac{x}{\varepsilon}).$$

We denote by V the space $H_0^1(D)$. Let $f \in V'$. We consider the forward two scale elliptic problem

$$-\nabla \cdot (A^\varepsilon(z; x) \nabla u^\varepsilon(z; x)) = f(x), \quad u^\varepsilon = 0 \text{ for } x \in \partial D. \quad (2.1.2)$$

Due to condition (2.1.1), problem (2.1.2) has a unique solution which satisfies

$$\|u^\varepsilon(z)\|_V \leq \frac{c^*(z)}{c_*(z)} \|f\|_{V'}. \quad (2.1.3)$$

¹Indeed we can consider the case where the coefficient $A(z; x, y)$ is a uniformly positive definite symmetric matrix but for simplicity we restrict our consideration to the case where it is a scalar function.

For $N \in \mathbb{N}$, we consider N functions $\ell_i(x, y) \in C(\bar{D}, C_\#(\bar{Y}))^d$ for $i = 1, \dots, N$. We define by

$$\mathcal{O}_i^\varepsilon(z) = \int_D \ell_i(x, \frac{x}{\varepsilon}) \cdot \nabla u^\varepsilon(z; x) dx \quad (2.1.4)$$

which represents a bounded linear map in $H^{-1}(D)$. Let the forward function be

$$\mathcal{G}^\varepsilon(z) = (\mathcal{O}_1^\varepsilon(z), \dots, \mathcal{O}_N^\varepsilon(z)) \in \mathbb{R}^N. \quad (2.1.5)$$

We consider a noisy observation δ of $\mathcal{G}^\varepsilon(z)$ which is

$$\delta = \mathcal{G}^\varepsilon(z) + \nu$$

where ν follows a Gaussian distribution $\mathcal{N}(0, \Sigma)$ in $\mathbb{R}^N$ where the $N \times N$ covariance matrix Σ is positive definite. We consider the Bayesian inverse problem of determining the posterior probability $\gamma^{\varepsilon, \delta} = \mathbb{P}(z|\delta)$.

2.1.1 Prior probability space

We consider two types of prior probability measures in this chapter.

2.1.1.1 Uniform prior

We assume that the coefficient $A(z; x, y)$ is represented in the form

$$A(z; x, y) = \bar{A}(x, y) + \sum_{j=1}^{\infty} z_j \psi_j(x, y), \quad (2.1.6)$$

where $\bar{A}$ and ψ_j belong to $C(\bar{D}, C_\#(\bar{Y}))$ with $\inf_{x \in \bar{D}, y \in \bar{Y}} \bar{A}(x, y) > 0$. The random variables z_j are uniformly distributed in $[-1, 1]$ and are pairwise independent. The prior probability space $U = [-1, 1]^{\mathbb{N}}$ is equipped with the σ algebra

$$\Theta = \bigotimes_{j=1}^{\infty} \mathcal{B}([-1, 1])$$

where $\mathcal{B}([-1, 1])$ is the Borel σ algebra in $[-1, 1]$. Here $z = (z_1, z_2, \dots) \in U$.

The prior probability is

$$\gamma = \bigotimes_{j=1}^{\infty} \frac{dz_j}{2}.$$

We assume further that the constants $c_*(z)$ and $c^*(z)$ are uniform with respect to z . For this to hold, we make the following assumption.

Assumption 2.1.1. There is a constant $\kappa > 0$ such that

$$\sum_{j=1}^{\infty} \sup_{x \in D, y \in Y} |\psi_j(x, y)| \leq \frac{\kappa}{1 + \kappa} \inf_{x \in D, y \in Y} \bar{A}(x, y).$$

With this assumption, let

$$c_*(z) = \frac{1}{1 + \kappa} \inf_{x \in D, y \in Y} \bar{A}(x, y) \quad (2.1.7)$$

and

$$c^*(z) = \sup_{x \in D, y \in Y} \bar{A}(x, y) + \frac{\kappa}{1 + \kappa} \inf_{x \in D, y \in Y} \bar{A}(x, y); \quad (2.1.8)$$

here $c^*(z)$ and $c_*(z)$ do not depend on z .

Approximation of the solutions of the forward two scale equations with random/parametric coefficients of the form (2.1.6) by the generalized polynomial chaos method is studied thoroughly in [36].

2.1.1.2 Gaussian prior

We consider the case where the coefficient A is of the form

$$A(z; x, y) = A^*(x, y) + \exp(\bar{A}(x, y) + \sum_{j=1}^{\infty} z_j \psi_j(x, y)). \quad (2.1.9)$$

We assume that z_j follow the standard normal distribution $\mathcal{N}(0, 1)$ in $\mathbb{R}$ and are pairwise independent; here $z = (z_1, z_2, \dots) \in \mathbb{R}^{\mathbb{N}}$. The function

$A^*(x, y) \in C(\bar{D}, C_\#(\bar{Y}))$ is non-negative for all $x \in D$ and $y \in Y$; and $\bar{A}$ and ψ_j belong to $C(\bar{D}, C_\#(\bar{Y}))$ for all $j \in \mathbb{N}$. The functions ψ_j satisfy

$$\sum_{j=1}^{\infty} \sup_{x \in D, y \in Y} |\psi_j(x, y)| < \infty. \quad (2.1.10)$$

We equip $\mathbb{R}^{\mathbb{N}}$ with the σ algebra

$$\Theta = \bigotimes_{j=1}^{\infty} \mathcal{B}(\mathbb{R})$$

where $\mathcal{B}(\mathbb{R})$ is the Borel σ algebra in $\mathbb{R}$; and the probability measure

$$\gamma = \bigotimes_{j=1}^{\infty} \mathcal{N}(0, 1).$$

We define the space

$$U = \{z = (z_1, z_2, \dots) \in \mathbb{R}^{\mathbb{N}} : \sum_{j=1}^{\infty} |z_j| \sup_{x \in D, y \in Y} |\psi_j(x, y)| < \infty\}.$$

For conciseness of notation, we denote by $b_j = \sup_{x \in D, y \in Y} |\psi_j(x, y)|$. With condition (2.1.10), we deduce that the set U has γ measure 1 ([55], [50]). We thus define the prior probability space as U with the σ algebra Θ induced in U , and the probability γ restricted to U , still denoted as γ . For each $z \in U$, coefficient A is well defined. We also have

$$A(z; x, y) \geq \inf_{x \in D, y \in Y} A^*(x, y) + \exp\left(\inf_{x \in D, y \in Y} A(x, y) - \sum_{j=1}^{\infty} |z_j| b_j\right) := c_*(z) > 0, \quad (2.1.11)$$

and

$$A(z; x, y) \leq \sup_{x \in D, y \in Y} A^*(x, y) + \exp\left(\sup_{x \in D, y \in Y} A(x, y) + \sum_{j=1}^{\infty} |z_j| b_j\right) := c^*(z). \quad (2.1.12)$$

Problem (2.1.2) is thus well posed for $z \in U$. We note that if

$\inf_{x \in D, y \in Y} A^*(x, y) = 0$, $c_*(z)$ is positive for all $z \in U$ but can get arbitrarily close to 0.

2.1.2 Posterior probability measure

We define the function $\Phi^\varepsilon(z, \delta)$ as

$$\Phi^\varepsilon(z, \delta) = \frac{1}{2} |\delta - \mathcal{G}^\varepsilon(z)|_\Sigma^2.$$

In Sections 2.3 and 2.4, we will show that the posterior probability $\gamma^{\varepsilon, \delta} = \mathbb{P}(z|\delta)$ is determined by the Bayes formula

$$\frac{d\gamma^{\varepsilon, \delta}}{d\gamma} \propto \exp(-\Phi^\varepsilon(z, \delta)). \quad (2.1.13)$$

We will show further that $\gamma^{\varepsilon, \delta}$ is well posed with respect to δ . In particular, we will show that for $\delta, \delta' \in \mathbb{R}$ such that $|\delta| \leq r$ and $|\delta'| \leq r$,

$$d_{Hell}(\gamma^{\varepsilon, \delta}, \gamma^{\delta', \varepsilon}) \leq c(r) |\delta - \delta'|. \quad (2.1.14)$$

Here the Hellinger distance d_{Hell} of two measures μ and μ' is defined as (see [51])

$$d_{Hell}(\mu, \mu') = \left(\frac{1}{2} \int_U \left(\sqrt{\frac{d\mu}{d\gamma}} - \sqrt{\frac{d\mu'}{d\gamma}} \right)^2 d\gamma \right)^{1/2}.$$

2.2 Two scale convergence

We review in this section the two scale convergence theory to study homogenization of problem (2.1.2). We first recall the definition of two scale convergence which is initiated by Nguetseng [45] and developed further by Allaire [2] and Allaire and Briane [3].

Definition 2.2.1. A sequence $\{w^\varepsilon\}_\varepsilon$ in $L^2(D)$ two scale converges to a function $w_0 \in L^2(D \times Y)$ if for any functions $\phi \in C(D, C_\#(Y))$

$$\lim_{\varepsilon \rightarrow 0} \int_D w^\varepsilon(x) \phi(x, \frac{x}{\varepsilon}) dx = \int_D \int_Y w_0(x, y) \phi(x, y) dy dx.$$

This definition makes sense because of the following result.

Proposition 2.2.2. From a bounded sequence in $L^2(D)$, we can extract a subsequence which two scale converges.

Let $V_1 = L^2(D, H_{\#}^1(Y)/\mathbb{R})$. We define by $\mathbf{V} = V \times V_1$ with the natural norm

$$\|\mathbf{v}\|_{\mathbf{V}} = \|v_0\|_V + \|v_1\|_{V_1},$$

for $\mathbf{v} = (v_0, v_1) \in \mathbf{V}$. Using two scale convergence for the two scale elliptic problem (2.1.2), we have

Proposition 2.2.3. The solution $u^\varepsilon(z; \cdot)$ of (2.1.2) converges weakly to a function $u_0(z; \cdot)$ in V . Further there is a function $u_1(z; \cdot, \cdot) \in V_1$ such that ∇u^ε two scale converges to $\nabla u_0 + \nabla_y u_1$. Denoting $B(z; \mathbf{u}, \phi)$ as

$$\int_D \int_Y A(z; x, y) (\nabla u_0(z; x) + \nabla_y u_1(z; x, y)) \cdot (\nabla \phi_0(x) + \nabla_y \phi_1(x, y)) dy dx,$$

the function $\mathbf{u} = (u_0, u_1) \in \mathbf{V}$ is the unique solution of the problem

$$B(z; \mathbf{u}, \phi) = \int_D f(x) \phi_0(x) dx \quad (2.2.1)$$

$$\forall \phi = (\phi_0, \phi_1) \in V \times V_1.$$

These results are standard. We refer to [2] for the proof. We then have

$$\lim_{\varepsilon \rightarrow 0} \mathcal{O}_i^\varepsilon(z) = \int_D \int_Y \ell_i(x, y) \cdot (\nabla u_0(z; x) + \nabla_y u_1(z; x, y)) dy dx := \mathcal{O}_i^0(z). \quad (2.2.2)$$

Denoting by

$$\mathcal{G}^0(z) = (\mathcal{O}_1^0(z), \dots, \mathcal{O}_N^0(z)),$$

we have

$$\lim_{\varepsilon \rightarrow 0} \mathcal{G}^\varepsilon(z) = \mathcal{G}^0(z). \quad (2.2.3)$$

Letting

$$\Phi^0(z, \delta) = \frac{1}{2} |\delta - \mathcal{G}^0(z)|_{\Sigma}^2,$$

we define the probability measure $\gamma^{0,\delta}$ on U as

$$\frac{d\gamma^{0,\delta}}{d\gamma} \propto \exp(-\Phi^0(z, \delta)). \quad (2.2.4)$$

We will show that the posterior measure $\gamma^{\varepsilon,\delta}$ can be approximated by $\gamma^{0,\delta}$ in Sections 2.3 and 2.4 for the uniform prior and the Gaussian prior respectively. We also find a rate of convergence for $d_{Hell}(\gamma^{\varepsilon,\delta}, \gamma^{0,\delta})$ when the solution of (2.2.1) is sufficiently regular.

It is well known that the homogenized equation for u_0 can be derived from (2.2.1). From (2.2.1), we can write u_1 in terms of u_0 . For $l = 1, \dots, d$, we denote by $w^l(z; x, y)$, as a function of $y \in Y$, the solution of the cell problem

$$\nabla_y \cdot (A(z; x, y) \nabla_y w^l(z; x, y)) = -\nabla_y \cdot (A(z; x, y) e^l), \quad (2.2.5)$$

where $w^l(z; x, \cdot) \in H_{\#}^1(Y)$; e^l is the l th unit vector in $\mathbb{R}^d$ with all the components being zero except the l th component which is 1. The symmetric homogenized coefficient $A^0(z; x)$ is determined by

$$A_{kl}^0(z; x) = \int_Y A(z; x, y) \left(\delta_{kp} + \frac{\partial w^k}{\partial y_p} \right) \left(\delta_{lp} + \frac{\partial w^l}{\partial y_p} \right) dy. \quad (2.2.6)$$

The function u_0 is the solution of the homogenized equation

$$-\nabla \cdot (A^0(z; x) \nabla u_0(z; x)) = f(x). \quad (2.2.7)$$

The function u_1 is determined by

$$u_1(z; x, y) = \frac{\partial u_0}{\partial x_l}(z; x) w^l(z; x, y). \quad (2.2.8)$$

2.3 Uniform prior

We consider the case of the uniform prior probability in this section. We first show the existence and well posedness of the posterior probability $\gamma^{\varepsilon, \delta}$. We then show the approximation of this measure by the measure $\gamma^{0, \delta}$ defined in (2.2.4).

2.3.1 Existence and well-posedness

We have the following result.

Proposition 2.3.1. Under Assumption 2.1.1, the posterior probability measure $\gamma^{\varepsilon, \delta} = \mathbb{P}(z|\delta)$ is determined by (2.1.13). Further the posterior measure is well posed, i.e. the local Lipschitz condition (2.1.14) holds.

Proof The proof of this proposition is essentially the same as that of Proposition 3 in [37]. Although Hoang et al. [37] only consider single scale equations but the proof remains valid in our multiscale setting. $\square$

2.3.2 Approximation by solution of two scale homogenized equation

We establish the approximation of the posterior measure $\gamma^{\varepsilon, \delta}$ by the measure $\gamma^{0, \delta}$ defined in (2.2.4).

Theorem 2.3.2. We have

$$\lim_{\varepsilon \rightarrow 0} d_{Hell}(\gamma^{\varepsilon, \delta}, \gamma^{0, \delta}) = 0.$$

Proof Let $Z^\varepsilon(\delta)$ and $Z^0(\delta)$ be the normalizing constants in (2.1.13) and (2.2.4) respectively, i.e.

$$Z^\varepsilon(\delta) = \int_U \exp(-\Phi^\varepsilon(z, \delta)) d\gamma(z), \quad (2.3.1)$$

and

$$Z^0(\delta) = \int_U \exp(-\Phi^0(z, \delta)) d\gamma(z). \quad (2.3.2)$$

We show that $Z^\varepsilon(\delta)$ is uniformly bounded below from 0 for all ε . From (2.1.3), with $c_*(z)$ and $c^*(z)$ being independent of $z \in U$, we have that u^ε is uniformly bounded in V . This implies that $\Phi^\varepsilon(z, \delta) \leq c(\delta)$ for all $\varepsilon > 0$. Thus $Z^\varepsilon(\delta) \geq \exp(-c(\delta))$. We follow standard procedures of estimating the Hellinger distance of two measures as in [51]. We have that

$$\begin{aligned} & 2d_{Hell}(\gamma^{\varepsilon, \delta}, \gamma^{0, \delta})^2 \\ &= \int_U \left(Z^\varepsilon(\delta)^{-1/2} \exp(-\frac{1}{2}\Phi^\varepsilon(z, \delta)) - Z^0(\delta)^{-1/2} \exp(-\frac{1}{2}\Phi^0(z, \delta)) \right)^2 d\gamma(z) \\ &\leq I_1 + I_2, \end{aligned}$$

where

$$I_1 = \frac{2}{Z(\delta)} \int_U \left(\exp(-\frac{1}{2}\Phi^\varepsilon(z, \delta)) - \exp(-\frac{1}{2}\Phi^0(z, \delta)) \right)^2 d\gamma(z), \quad (2.3.3)$$

and

$$I_2 = 2|Z^\varepsilon(\delta)^{-1/2} - Z^0(\delta)^{-1/2}|^2 \int_U \exp(-\Phi^0(z, \delta)) d\gamma(z). \quad (2.3.4)$$

From (2.2.3) we have $\lim_{\varepsilon \rightarrow 0} \mathcal{G}^\varepsilon(z, \delta) = \mathcal{G}^0(z, \delta)$. Using Lebesgue dominated convergence theorem, we have that

$$\lim_{\varepsilon \rightarrow 0} I_1 = 0.$$

We note further that

$$|Z^\varepsilon(\delta)^{-1/2} - Z^0(\delta)^{-1/2}| = \frac{|Z^0(\delta) - Z^\varepsilon(\delta)|}{Z^\varepsilon(\delta)^{1/2} Z^0(\delta)^{1/2} (Z^0(\delta)^{1/2} + Z^\varepsilon(\delta)^{1/2})}.$$

We have

$$\lim_{\varepsilon \rightarrow 0} |Z^0(\delta) - Z^\varepsilon(\delta)| \leq \lim_{\varepsilon \rightarrow 0} \int_U |\exp(-\Phi^\varepsilon(z, \delta)) - \exp(-\Phi^0(z, \delta))| d\gamma(z) = 0.$$

As $Z^\varepsilon(\delta) > c(\delta)$ uniformly with respect to ε , we deduce that $\lim_{\varepsilon \rightarrow 0} I_2 = 0$.

We then get the conclusion. $\square$

With further regularity assumptions on the functions ψ_j in (2.1.6), we get the following convergence rate. We assume:

Assumption 2.3.3. We assume that the function ψ_j in (2.1.6) belong to $C^1(\bar{D}, C_\#^{1,1}(\bar{Y}))$ such that

$$\sum_{j=1}^{\infty} \|\psi_j\|_{C^1(\bar{D}, C_\#^{1,1}(\bar{Y}))} < \infty.$$

Theorem 2.3.4. Assume that the domain D is convex, and $f \in L^2(D)$. Under Assumptions 2.1.1 and 2.3.3, if $\ell_i \in C^{0,1}(\bar{D}, C_\#(\bar{Y}))^d$ then there is a constant c independent of ε such that

$$d_{Hell}(\gamma^{\varepsilon, \delta}, \gamma^{0, \delta}) \leq c\varepsilon^{1/2}.$$

We show this in Section 2.7

2.4 Gaussian prior

We consider the case of the Gaussian prior probability measure in this section.

2.4.1 Existence and well-posedness

We show the existence and local Lipschitzness with respect to the data of the posterior probability in this section. We have the following result.

Proposition 2.4.1. With the prior probability space (U, Θ, γ) defined in Section 2.1.1.2, the posterior probability measure $\gamma^{\varepsilon, \delta} = \mathbb{P}(z|\delta)$ is determined by (2.1.13). Further, the local Lipschitz condition 2.1.14 holds.

Proof To show that the posterior probability is determined by (2.1.13), we need to show that the forward map $\mathcal{G}^\varepsilon$ defined in (2.1.5) is measurable with respect to the prior γ (see Cotter et al. [12]). The solution u^ε of (2.1.2) is measurable as a map from (U, Θ) to $(V, \mathcal{B}(V))$ (see [24], [23], [8]). This leads to the measurability of $\mathcal{G}^\varepsilon$.

The proof of the local Lipschitz condition (2.1.14) follows the same lines of the proof of Proposition 3.3 in [34]. $\square$

2.4.2 Approximation by solution of the two scale homogenized equation

As for the case of the uniform prior probability measure, we show that the posterior measure $\gamma^{\varepsilon, \delta}$ can be approximated by the measure $\gamma^{0, \delta}$ defined in (2.2.4). We first have the following result.

Theorem 2.4.2. For the Gaussian prior measure defined in Section 2.1.1.2, we have

$$\lim_{\varepsilon \rightarrow 0} d_{Hell}(\gamma^{\varepsilon, \delta}, \gamma^{0, \delta}) = 0.$$

Proof The proof of this theorem is similar to that for Theorem 2.3.2. First we show that the normalizing constant defined in (2.3.1) is uniformly bounded from below with respect to all ε , i.e. $Z^\varepsilon(\delta) > c(\delta) > 0$ for all ε . The proof is identical to that for the single macroscopic scale problem in [34].

Indeed, from (2.1.3), (2.1.11) and (2.1.12), we have

$$\|u^\varepsilon(z)\|_V \leq c \exp(2 \sum_{j=1}^{\infty} |z_j| b_j). \quad (2.4.1)$$

Thus $|\Phi^\varepsilon(z, \delta)| \leq c(1 + \exp(4 \sum_{j=1}^{\infty} |z_j| b_j))$. This implies that $\mathbb{E}^\gamma(\Phi^\varepsilon(z, \delta)) < \Lambda$ for a positive constant Λ (see Lemma 2.8.5 in Section 2.8). Fixing a

constant C , the measure of the set $\{z \in U : \Phi^\varepsilon(z, \delta) > C\}$ is not more than Λ/C . Choosing C sufficiently large so that $1 - \Lambda/C > 0$, we have

$$Z^\varepsilon(\delta) \geq \exp(-C)(1 - \Lambda/C).$$

We show that $\lim_{\varepsilon \rightarrow 0} I_1 = 0$ and $\lim_{\varepsilon \rightarrow 0} I_2 = 0$ where I_1 and I_2 are defined in (2.3.3) and (2.3.4) respectively. From (2.2.3), we have that

$$\lim_{\varepsilon \rightarrow 0} \left| \exp\left(-\frac{1}{2}\Phi^\varepsilon(z, \delta)\right) - \exp\left(-\frac{1}{2}\Phi^0(z, \delta)\right) \right| = 0.$$

From Lebesgue dominated convergence theorem, we deduce that $\lim_{\varepsilon \rightarrow 0} I_1 = 0$. Similarly, $\lim_{\varepsilon \rightarrow 0} I_2 = 0$. $\square$

With regularity conditions, we show a rate for the convergence in the previous theorem. We make the following assumption.

Assumption 2.4.3. We assume that the functions A^* , $\bar{A}$ and ψ_j in (2.1.9) belong to $C^1(\bar{D}, C_{\#}^{1,1}(\bar{Y}))$ such that

$$\sum_{j=1}^{\infty} \|\psi_j\|_{C^1(\bar{D}, C_{\#}^{1,1}(\bar{Y}))} < \infty.$$

Let $\bar{b}_j = \|\psi_j\|_{C^1(\bar{D}, C_{\#}^{1,1}(\bar{Y}))}$. Let $\bar{U} \subset U$ be the set of $z = (z_1, z_2, \dots) \in U$ such that $\sum_{j=1}^{\infty} |z_j| \bar{b}_j$ is finite. We have that $\gamma(\bar{U}) = 1$. For $z \in \bar{U}$, the coefficient A defined in (2.1.9) belongs to $C^1(\bar{D}, C_{\#}^1(\bar{Y}))$ with

$$\|A(z)\|_{C^1(\bar{D}, C_{\#}^1(\bar{Y}))} \leq c(1 + \exp(c \sum_{j=1}^{\infty} |z_j| \bar{b}_j))$$

for $z \in \bar{U}$. We have the following result.

Theorem 2.4.4. Assume that D is convex, and $f \in L^2(D)$. Under Assumption 2.4.3, if $\ell_i \in C^{0,1}(\bar{D}, C_{\#}(\bar{Y}))^d$ then

$$d_{Hell}(\gamma^{\varepsilon, \delta}, \gamma^{0, \delta}) \leq c\varepsilon^{1/2}.$$

We prove this theorem in Section 2.8.

2.5 Finite Element approximation of the posterior measure

Sampling the probability $\gamma^{0,\delta}$, we get an approximation for the posterior probability $\gamma^{\varepsilon,\delta}$. The advantage of sampling $\gamma^{0,\delta}$ is that we only need to solve equation (2.2.1) which only involves the macroscopic scale. Although this problem is posed in the high dimensional tensor product domain $D \times Y$, the sparse tensor product FE method is capable of solving this problem with an essentially optimal complexity to obtain an essentially equal accuracy as that of the full tensor product FE spaces. We review in this section the sparse tensor product FE method originally developed in [35].

2.5.1 Hierarchical finite element spaces

Let D be a polyhedron. We consider in D a hierarchy $\{\mathcal{T}^l\}$ of simplices which are obtained recursively. The set of simplices $\mathcal{T}^l$ of mesh size $h_l = O(2^{-l})$ is obtained by dividing each simplex in $\mathcal{T}^{l-1}$ into 4 congruent triangles for $d = 2$ or 8 tetrahedra for $d = 3$. The cube Y is divided into sets of simplices $\mathcal{T}_\#^l$ which are periodically distributed in a similar manner. We define the following finite element spaces

$$\begin{aligned} V^l &= \{w \in H^1(D) : w|_K \in \mathcal{P}_1(K) \ \forall K \in \mathcal{T}^l\}, \\ V_0^l &= \{w \in H_0^1(D) : w|_K \in \mathcal{P}_1(K) \ \forall K \in \mathcal{T}^l\}, \\ V_\#^l &= \{w \in H_\#^1(Y) : w|_K \in \mathcal{P}_1(K) \ \forall K \in \mathcal{T}_\#^l\}, \end{aligned}$$

where $\mathcal{P}_1(K)$ denotes the set of linear polynomials in K . The following approximation properties hold (see, e.g. Ciarlet [10]).

$$\begin{aligned} \inf_{v \in V^l} \|w - v\|_{H^1(D)} &\leq ch_l^{\min\{1,s\}} \|w\|_{H^{1+s}(D)}, \\ \inf_{v \in V^l} \|w - v\|_{L^2(D)} &\leq ch_l^{1+\min\{1,s\}} \|w\|_{H^{1+s}(D)}, \end{aligned} \quad (2.5.1)$$

for all $w \in H^{1+s}(D)$, and

$$\inf_{v \in V_0^l} \|w - v\|_{H^1(D)} \leq ch_l^{\min\{1,s\}} \|w\|_{H^{1+s}(D)} \quad (2.5.2)$$

for $w \in H^{1+s}(D) \cap V$. For periodic functions in Y we have

$$\begin{aligned} \inf_{v \in V_\#^l} \|w - v\|_{H^1(Y)} &\leq ch_l^{\min\{1,s\}} \|w\|_{H^{1+s}(Y)}, \\ \inf_{v \in V_\#^l} \|w - v\|_{L^2(Y)} &\leq ch_l^{1+\min\{1,s\}} \|w\|_{H^{1+s}(Y)}, \end{aligned} \quad (2.5.3)$$

for all periodic functions $w \in H_\#^{1+s}(Y)$.

Similarly, if D is a union of squares ($d = 2$) or cubes ($d = 3$), we first divide D into subsquares. The simplices in $\mathcal{T}^l$ are obtained by dividing each simplex in $\mathcal{T}^{l-1}$ into 4 squares for $d = 2$ or 8 cubes for $d = 3$. The simplices in Y are defined similarly. The finite element spaces consist of functions that are linear with respect to each component of x or y in each simplex, i.e. they belong to the space $\mathcal{Q}_1(K)$ for $K \in \mathcal{T}^l$ and $K \in \mathcal{T}_\#^l$.

2.5.2 Full tensor product finite elements for problem

(2.2.1)

As $u_1 \in L^2(D, H_\#^1(Y)) \cong L^2(D) \otimes H_\#^1(Y)$, we choose the finite element subspace $V_1^L \subset V_1$ for approximating u_1 as

$$V_1^L = V^L \otimes V_\#^L. \quad (2.5.4)$$

Let

$$\mathbf{V}^L = V_0^L \times V_1^L. \quad (2.5.5)$$

We consider the full tensor product approximating problem: Find $\mathbf{u}^L(z) = (u_0^L(z), u_1^L(z)) \in \mathbf{V}^L$ such that

$$B(z; \mathbf{u}^L(z), \mathbf{v}^L) = \int_D f v_0^L dx \quad \forall \mathbf{v}^L = (v_0^L, v_1^L) \in \mathbf{V}^L. \quad (2.5.6)$$

To get an explicit error estimate for the finite element approximation, we define the regularity space $\mathcal{H}$ as follows.

Let $\mathcal{H}$ be the space of functions $w(x, y) \in L^2(D, H_{\#}^2(Y))$ such that $w \in L^2(Y, H^1(D))$. The space $\mathcal{H}$ is equipped with the norm

$$\|w\|_{\mathcal{H}} = \|w\|_{L^2(D, H_{\#}^2(Y))} + \|w\|_{L^2(Y, H^1(D))}.$$

We then have the following approximating property whose proof can be found in [7], [35]

Lemma 2.5.1. For $w \in \mathcal{H}$,

$$\inf_{v \in V_1^L} \|w - v\|_{L^2(D, H^1(Y))} \leq ch_L \|w\|_{\mathcal{H}}.$$

We define the space $\mathcal{H}$ by

$$\mathcal{H} = H^2(D) \times \mathcal{H}, \quad (2.5.7)$$

which is equipped with the norm

$$\|\mathbf{w}\|_{\mathcal{H}} = \|w_0\|_{H^2(D)} + \|w_1\|_{\mathcal{H}},$$

where $\mathbf{w} = (w_0, w_1) \in \mathcal{H}$.

From this we deduce the following rate of convergence for the full tensor approximating problem (2.5.6).

Proposition 2.5.2. Assume that the solution $\mathbf{u}(z) = (u_0(z), u_1(z))$ of problem (2.2.1) belongs to $\mathcal{H}$, then for the FE approximating problem (2.5.6), we have

$$\|\mathbf{u}(z) - \mathbf{u}^L(z)\|_{\mathbf{V}} \leq c \frac{c^*(z)}{c_*(z)} h_L \|\mathbf{u}(z)\|_{\mathcal{H}}.$$

The proof uses Cea's lemma and Lemma 2.5.1.

2.5.3 Sparse tensor product finite elements for problem (2.2.1)

The dimension of the full tensor product space $\mathbf{V}^L$ is $O(2^{dL})$ which is prohibitively large when L is large. We develop the sparse tensor product finite element spaces with an essentially optimal dimension but produce essentially equal accuracy as for the full tensor product FE spaces. We assume that for each $l \geq 1$ there is a linear space $W^l \subset V^l$ that is linearly independent of V^{l-1} so that V^l is the linear span of W^l and V^{l-1} . We denote this as $V^l = V^{l-1} \oplus W^l$ with $\dim V^l = \dim W^l + \dim V^{l-1}$. Here $W^0 = V^0$. Let $\{\psi_j^l\}$ where $j \in I_l \subset \mathbb{N}$ be a linear basis of W^l . Then $\{\psi_j^{l'}\}$ for $0 \leq l' \leq l$ and $j \in I_{l'}$ form a basis for V^l . We assume further that this is a Riesz wavelet basis in $L^2(D)$, i.e. there are constants $c_1 > 0$ and $c_2 > 0$ such that for all $w = \sum_{l=0}^{\infty} \sum_{j \in I_l} w_j^l \psi_j^l$, we have the norm equivalence

$$c_1 \sum_{l=0}^{\infty} \sum_{j \in I_l} (w_j^l)^2 \leq \|w\|_{L^2(D)}^2 \leq c_2 \sum_{l=0}^{\infty} \sum_{j \in I_l} (w_j^l)^2. \quad (2.5.8)$$

For $H_{\#}^1(Y)/\mathbb{R}$, we suppose that there are spaces $W_{\#}^{l1} = \text{span}\{\psi_{1j}^l : j \in I_{1l} \subset \mathbb{N}\}$ with $W_{\#}^{01} = V_{\#}^0$ such that $V_{\#}^l = \text{span}\{\psi_{1j}^{l'} : l' = 0, \dots, l \text{ and } j \in I_{1l'}\}$. We further have the norm equivalence

$$c_5 \sum_{l=0}^{\infty} \sum_{j \in I_{1l}} (w_j^l)^2 \leq \|w\|_{H^1(Y)/\mathbb{R}}^2 \leq c_6 \sum_{l=0}^{\infty} \sum_{j \in I_{1l}} (w_j^l)^2 \quad (2.5.9)$$

for $w \in H_{\#}^1(Y)/\mathbb{R}$ where c_5 and c_6 are independent of w . From

$$V^l = \bigoplus_{0 \leq l' \leq l} W^{l'}, \quad V_{\#}^l = \bigoplus_{0 \leq l' \leq l} W_{\#}^{l'1},$$

the full tensor product space V_1^L in (2.5.4) can be written as

$$V_1^L = \bigoplus_{0 \leq l_0, l_1 \leq L} W^{l_0} \otimes W_{\#}^{l_11}.$$

We define the sparse tensor product space $\hat{V}_1^L \subset V_1^L$ as

$$\hat{V}_1^L = \bigoplus_{0 \leq l_0 + l_1 \leq L} W^{l_0} \otimes W_{\#}^{l_11},$$

and the finite element space

$$\hat{\mathbf{V}}^L = V_0^L \times \hat{V}_1^L.$$

We consider the sparse tensor product FE approximating problem: Find $\hat{\mathbf{u}}^L(z) \in \hat{\mathbf{V}}^L$ such that

$$B(z; \hat{\mathbf{u}}^L(z), \hat{\mathbf{v}}^L) = \int_D f(x) \hat{v}_0^L(x) dx \quad (2.5.10)$$

for all $\hat{\mathbf{v}}^L = (\hat{v}_0^L, \hat{v}_1^L) \in \hat{\mathbf{V}}^L$. To get a FE rate of convergence for problem (2.5.10), we define the regularity spaces $\hat{\mathcal{H}}$ of functions $w(x, y)$ that are Y -periodic with respect to y such that for all $\alpha_0, \alpha_1 \in \mathbb{N}_0^d$ with $|\alpha_0| \leq 1$ and $|\alpha_1| \leq 2$,

$$\frac{\partial^{|\alpha_0|+|\alpha_1|} w}{\partial^{\alpha_0} x \partial^{\alpha_1} y} \in L^2(D \times Y),$$

i.e. $w \in H^1(D, H_{\#}^2(Y))$. We then equip the space $\hat{\mathcal{H}}$ with the norm

$$\|w\|_{\hat{\mathcal{H}}} = \sum_{|\alpha_1| \leq 2, |\alpha_0| \leq 1} \left\| \frac{\partial^{|\alpha_0|+|\alpha_1|} w}{\partial^{\alpha_0} x \partial^{\alpha_1} y} \right\|_{L^2(D \times Y)}.$$

We define the regularity space

$$\hat{\mathcal{H}} = H^2(D) \times \hat{\mathcal{H}}$$

with the norm

$$\|\mathbf{w}\|_{\hat{\mathcal{H}}} = \|w_0\|_{H^2(D)} + \|w_1\|_{\hat{\mathcal{H}}}$$

for $w = (w_0, w_1) \in V \times V_1$. For functions in $\hat{\mathcal{H}}$, we have the following estimate (see e.g., [7], [53], for a proof).

Lemma 2.5.3. For $w \in \hat{\mathcal{H}}$:

$$\inf_{v \in \hat{V}_1^L} \|w - v\|_{V_1} \leq cL^{1/2}h_L\|w\|_{\hat{\mathcal{H}}}.$$

We now present some examples of the wavelet basis functions that satisfy the norm equivalence above. For constructions of wavelet basis functions we refer to references such as [11] and [13].

Example (i) A hierarchical basis for $L^2(0, 1)$ can be constructed as follows. We first take three following piecewise linear functions as the basis for level $l = 0$: ψ_1^0 obtains values $(1, 0)$ at $(0, 1/2)$ and is 0 in $(1/2, 1)$, ψ_2^0 is continuous piecewise linear and obtains values $(0, 1, 0)$ at $(0, 1/2, 1)$, and ψ_3^0 obtains values $(0, 1)$ at $(1/2, 1)$ and is 0 in $(0, 1/2)$. The basis functions for other levels are constructed from the wavelet function ψ that takes values $(0, -1, 2, -1, 0)$ at $(0, 1/2, 1, 3/2, 2)$, the left boundary function ψ^{left} taking values $(-2, 2, -1, 0)$ at $(0, 1/2, 1, 3/2)$, and the right boundary function ψ^{right} taking values $(0, -1, 2, -2)$ at $(1/2, 1, 3/2, 2)$. For levels $l \geq 1$, $I_l = \{1, 2, \dots, 2^l\}$. The wavelet basis functions are defined as $\psi_1^l(x) = 2^{-l/2}\psi^{left}(2^l x)$, $\psi_k^l(x) = 2^{-l/2}\psi(2^l x - k + 3/2)$ for $k = 2, \dots, 2^l - 1$ and $\psi_{2^l}^l = \psi^{right}(2^l x - 2^l + 2)$.

(ii) For $Y = (0, 1)$, a hierarchical basis for $H_{\#}^1(Y)/\mathbb{R}$ can be constructed from those in (i). For level 0, we exclude ψ_1^0, ψ_3^0 . At other levels, the functions ψ^{left} and ψ^{right} are replaced by the piecewise linear functions that take values $(0, 2, -1, 0)$ at $(0, 1/2, 1, 3/2)$ and values $(0, -1, 2, 0)$ at $(1/2, 1, 3/2, 2)$ respectively.

For the d dimensional cube $(0, 1)^d$, the basis functions can be constructed by taking the tensor products of the basis functions in $(0, 1)$. They satisfy the norm equivalence after appropriate scaling, see [27].

We then have the following error estimate for sparse tensor product FE approximation.

Proposition 2.5.4. Assume that the solution $\mathbf{u}$ of (2.2.1) belongs to $\hat{\mathcal{H}}$. Then the solution $\hat{\mathbf{u}}^L$ of the finite element approximating problem (2.5.10) satisfies

$$\|\mathbf{u}(z) - \hat{\mathbf{u}}^L(z)\|_{\mathbf{V}} \leq c \frac{c^*(z)}{c_*(z)} L^{1/2} h_L \|\mathbf{u}(z)\|_{\hat{\mathcal{H}}}. \quad (2.5.11)$$

The proof of this proposition uses Cea's lemma and Lemma 2.5.3.

2.5.4 FE approximation of the posterior measure

We define an approximation to the posterior measure using the FE solution $\hat{\mathbf{u}}^L(z) = (\hat{u}_0^L(z), \hat{u}_1^L(z))$ in (2.5.10). We define for $i = 1, \dots, N$

$$\mathcal{O}_i^{0,L}(z) = \int_D \int_Y \ell_i(x, y) \cdot (\nabla \hat{u}_0^L + \nabla_y \hat{u}_1^L) dy dx;$$

and

$$\mathcal{G}^{0,L}(z) = (\mathcal{O}_1^{0,L}(z), \dots, \mathcal{O}_N^{0,L}(z)).$$

The function $\Phi^{0,L}$ which approximates Φ^0 is defined as

$$\Phi^{0,L}(z, \delta) = \frac{1}{2} |\delta - \mathcal{G}^{0,L}(z)|_{\Sigma}^2.$$

We define the measure $\gamma^{0,L,\delta}$ as

$$\frac{d\gamma^{0,L,\delta}}{d\gamma} \propto \exp(-\Phi^{0,L}(z, \delta)).$$

We then have the following result.

Theorem 2.5.5. For both the cases of uniform prior measure (2.1.6) and Gaussian prior measure (2.1.9), we have the following approximation

$$\lim_{\varepsilon \rightarrow 0, L \rightarrow \infty} d_{Hell}(\gamma^{\varepsilon, \delta}, \gamma^{0, L, \delta}) = 0.$$

Proof As $\lim_{L \rightarrow \infty} \Phi^{0, L}(\delta, z) = \Phi^0(\delta, z)$, by arguing as in the proofs of Theorems 2.3.2 and 2.4.2 we have

$$\lim_{L \rightarrow \infty} d_{Hell}(\gamma^{0, \delta}, \gamma^{0, L, \delta}) = 0.$$

We then get the conclusion from Theorems 2.3.2 and 2.4.2. $\square$

With regularity assumptions, we get an explicit rate of convergence for the convergence in Theorem 2.5.5.

Theorem 2.5.6. Assume that D is a convex polygon and $f \in L^2(D)$. We assume Assumption 2.3.3 for the case of uniform prior (2.1.6) and Assumption 2.4.3 for the case of Gaussian prior (2.1.9). Then

$$d_{Hell}(\gamma^{\varepsilon, \delta}, \gamma^{0, L, \delta}) \leq c(\varepsilon^{1/2} + L^{1/2}2^{-L}).$$

Proof For the case of uniform prior probability (2.1.6), under Assumption 2.3.3 we have that $\hat{\mathbf{u}}(z) = (\hat{u}_0(z), \hat{u}_1(z))$ is uniformly bounded in $\hat{\mathcal{H}}$ (see [36] Proposition 4.2). Thus

$$|\mathcal{G}^0(z) - \mathcal{G}^L(z)| \leq c \|\mathbf{u}(z) - \hat{\mathbf{u}}^L(z)\|_{\mathbf{V}} \leq cL^{1/2}2^{-L} \quad \forall z \in \bar{U},$$

where $|\cdot|$ denotes the Euclidean norm in $\mathbb{R}^N$. By a similar procedure as in the proof of Theorem 2.3.4, using $\gamma(\bar{U}) = 1$, we show that

$$d_{Hell}(\gamma^{0, \delta}, \gamma^{0, L, \delta}) \leq cL^{1/2}2^{-L}.$$

From this and Theorem 2.3.4 we get the conclusion.

For the Gaussian prior in (2.1.9), we have that

$$|\mathcal{G}^0(z) - \mathcal{G}^L(z)| \leq c \|\mathbf{u}(z) - \hat{\mathbf{u}}^L(z)\|_{\mathbf{V}} \leq c \|\mathbf{u}(z)\|_{\hat{\mathcal{H}}} L^{1/2} 2^{-L}.$$

From Lemmas 2.8.2 and 2.8.3, and from (2.2.8), we have that

$$\|\mathbf{u}(z)\|_{\hat{\mathcal{H}}} \leq c(1 + \exp(c \sum_{j=1}^{\infty} |z_j| \bar{b}_j))$$

for $z \in \bar{U}$. By an identical proof as that of Theorem 2.4.4 using the fact that $\gamma(\bar{U}) = 1$ and Lemma 2.8.5, we have

$$d_{Hell}(\gamma^{0,\delta}, \gamma^{0,L,\delta}) \leq c L^{1/2} 2^{-L}.$$

From this and Theorem 2.4.4 we get the conclusion. $\square$

Remark 2.5.7. We do not analyze approximation of the forward problem by choosing only a finite number of J terms in the expansion of A . However, if the functions ψ_j in (2.1.6) and (2.1.9) have a decay rate $O(1/j^s)$ for $s > 1$ with respect to the $L^\infty(D \times Y)$ norm, we can establish a rate of convergence in terms of J for the approximated posterior measure which is similar to that considered in [37].

2.6 Numerical examples

We perform the MCMC method in this section for some particular examples of recovering two scale coefficients. We use independent sampler for MCMC in all the numerical simulations in this section. We first consider the case of the uniform prior probability measure. We consider a reference solution by taking a random realization of z in (2.1.6) or (2.1.9). The data are obtained by adding a random realization of the noise into $\mathcal{O}_i^0$ in (2.2.2). We note

that when ε is sufficiently small, this is a good approximation of the data generated in (2.1.4). First for the one dimensional domain $D = (0, 1)$, we consider the coefficient of the form

$$A(z; x, y) = 9 + z_1(1 + x) \sin(2\pi y) + z_2(1 + x) \cos(2\pi y) \quad (2.6.1)$$

where z_1 and z_2 are uniformly distributed in $[-1, 1]$. We consider first the case where the functions ℓ_i in (2.1.4) do not depend on y . As $u^\varepsilon \rightharpoonup u_0$ in V , we have that

$$\lim_{\varepsilon \rightarrow 0} \int_D \ell_i(x) \cdot \nabla u^\varepsilon(x) dx = \int_D \ell_i(x) \cdot \nabla u_0(x) dx$$

so that when ℓ_i do not depend on y , we essentially get information on u_0 only. Let $\ell_1(x, y) = x$ and $\ell_2(x, y) = x^2$. The observations become

$$\begin{aligned} \mathcal{O}_1^\varepsilon(z) &= \int_D x \nabla u^\varepsilon(z; x) dx \approx \int_D x \nabla u_0(z; x) dx = \mathcal{O}_1^0(z), \\ \mathcal{O}_2^\varepsilon(z) &= \int_D x^2 \nabla u^\varepsilon(z; x) dx \approx \int_D x^2 \nabla u_0(z; x) dx = \mathcal{O}_2^0(z). \end{aligned}$$

The covariance of the noise is $10^{-3}I$ where I is the 2×2 identity matrix. We choose a reference pair (z_1, z_2) at random. In Figure 2.1, we plot the first 60000 MCMC samples. We see that the samples are evenly scattered over a curve; the figure does not indicate clearly the value of the reference (z_1, x_2) . In Figure 2.2, we show the reference coefficient A and the arithmetic average of 60000 MCMC samples. The figure shows that the average of the MCMC samples does not describe the reference coefficient accurately.

Now we consider the case where the observation is the flux of the two scale equation. This case can be analysed in the same way as in the previous sections. The coefficient is (2.6.1). We consider one observation

$$\mathcal{O}_1^\varepsilon(z) = \int_D A(z; x, \frac{x}{\varepsilon}) \nabla u^\varepsilon(z; x) dx$$

Figure 2.1: MCMC samples for 1D two scale problem with uniform prior
where observations are independent of y

Figure 2.2: The reference coefficient and the average of the MCMC
samples for 1D two scale problem with uniform prior where observations
are independent of y

$$\approx \int_D \int_Y A(z; x, y) (\nabla u_0(z; x) + \nabla_y u_1(z; x, y)) dy dx = \mathcal{O}_1^0(z)$$

Figure 2.3 shows the 60000 MCMC samples for $z = (z_1, z_2)$. The posterior does not provide good information on the reference $z = (z_1, z_2)$. Figure 2.4 shows the reference coefficient and the arithmetic average of the coefficients

obtained from the 60000 MCMC samples. We see that we cannot recover any details of the reference coefficient from the average of the MCMC samples. We note that the flux of the two scale equation converges to the flux of the homogenized equation, i.e.

$$\lim_{\varepsilon \rightarrow 0} \int_D A^\varepsilon(z; x, \frac{x}{\varepsilon}) \nabla u^\varepsilon(z; x) dx = \int_D A^0(z; x) \nabla u_0(z; x) dx.$$

Thus an observation on the flux essentially provides only the information on the homogenized equation, i.e. only the macroscopic information. This explains why we cannot recover accurately the reference coefficient. These examples show that it is necessary to have observations on u_1 to recover the microscopic structures.

Figure 2.3: MCMC samples for 1D two scale problem with uniform prior where observation is the flux

Next we consider the case where ℓ_i in (2.1.4) depend also on y . The coefficient A is of the form (2.6.1). The functions

$$\ell_1(x, y) = x(1 + \sin(2\pi y)), \quad \ell_2(x, y) = x(1 + \cos(2\pi y)).$$

The observations are:

Figure 2.4: The reference coefficient and the average of the MCMC samples for 1D two scale problem with uniform prior where observation is the flux

$$\begin{aligned}\mathcal{O}_1^\varepsilon(z) &= \int_D x(1 + \sin(2\pi \frac{x}{\varepsilon})) \nabla u^\varepsilon(x) dx \\ &\approx \int_D \int_Y [x(1 + \sin(2\pi y))] (\nabla u_0 + \nabla_y u_1) dy dx = \mathcal{O}_1^0(z),\end{aligned}$$

and

$$\begin{aligned}\mathcal{O}_2^\varepsilon(z) &= \int_D x(1 + \cos(2\pi \frac{x}{\varepsilon})) \nabla u^\varepsilon(x) dx \\ &\approx \int_D \int_Y [x(1 + \cos(2\pi y))] (\nabla u_0 + \nabla_y u_1) dy dx = \mathcal{O}_2^0(z).\end{aligned}$$

In Figure 2.5 we plot the 60000 MCMC samples for the pair (z_1, z_2) . The figure shows that the posterior measure provides very good prediction on the reference $z = (z_1, z_2)$. In Figure 2.6, we show the reference coefficient and the average of the coefficient obtained from the MCMC samples. The figure shows that we have a good recovery of the reference coefficient.

Now we consider a two dimensional problem in the domain $D = (0, 1)^2$. Here $x = (x_1, x_2) \in D$ and $y = (y_1, y_2) \in Y = (0, 1)^2$ – the unit cube in $\mathbb{R}^2$.

Figure 2.5: MCMC samples for 1D two scale problem with uniform prior where observations are dependent of y

Figure 2.6: The reference coefficient and the average of the MCMC samples for 1D two scale problem with uniform prior where observations are dependent of y

We consider the coefficient of the form

$$a(x, y, z) = 10 + \frac{1}{4}(1 + x_1)(1 + x_2) \sum z_{F_1, F_2} F_1(y_1) F_2(y_2)$$

where the summation is over all

$F_i(y_i) \in \{\sin(2\pi y_i), \cos(2\pi y_i), \frac{1}{4} \sin(4\pi y_i), \frac{1}{4} \cos(4\pi y_i)\}$, $i = 1, 2$. The ran-

dom variables z_{F_1, F_2} are uniformly distributed in $[-1, 1]$. We consider the observations of the form

$$\begin{aligned} & \int_D (1+x_1)(1+x_2) G_1\left(\frac{x_1}{\varepsilon}\right) G_2\left(\frac{x_2}{\varepsilon}\right) \frac{\partial u^\varepsilon}{\partial x_p} dx \\ & \approx \int_D \int_Y (1+x_1)(1+x_2) G_1(y_1) G_2(y_2) \left(\frac{\partial u_0}{\partial x_p}(z; x) + \frac{\partial u_1}{\partial y_p}(z; x, y) \right) dy dx \end{aligned}$$

for all $G_i(y_i) \in \{\sin(2\pi y_i), \cos(2\pi y_i), \sin(4\pi y_i), \cos(4\pi y_i), \sin(6\pi y_i), \cos(6\pi y_i)\}$, $i = 1, 2$, $p = 1, 2$. Figure 2.7 presents the reference coefficient and the average of 120000 MCMC samples fixing $x = (0.2, 0.2)$. It shows that we have a reasonably good recovery of the two scale coefficient.

Figure 2.7: The reference coefficient and the average of the MCMC samples for $x = (0.2, 0.2)$ for 2D two scale problem with uniform prior

We now consider the case of an equation in the two dimensional domain $D = (0, 1)^2$ with the Gaussian prior probability. Let $\psi_i(x)$, $i = 1, \dots, 9$ be the 9 eigenfunctions of $-\Delta_x^{-1}$ with periodic boundary condition on $D = (0, 1)^2$ that are of the form $\sin(\cos)(2k\pi x_1) \sin(\cos)(2l\pi x_2)$ with $k, l = 0, 1$ (excluding the zero function), with eigenvalues λ_i . Let $\phi_j(y)$, $j = 1, \dots, 9$,

be the 9 eigenfunctions of $-\Delta_y^{-1}$ with periodic boundary condition on $Y = (0, 1)^2$ that are of the form $\phi_j(x) = \sin(\cos)(2k\pi y_1) \sin(\cos)(2l\pi y_2)$ with $k, l = 0, 1$ (excluding the zero function) with eigenvalues μ_j . We let $\psi_1(x) = 1$, $\lambda_1 = 0$ and $\phi_1(y) = 1$ with $\mu_1 = 0$. We consider the coefficient

$$a(z; x, y) = \exp \left(\sum_{\substack{i,j=1,\dots,9 \\ (i,j) \neq (1,1)}} z_{i,j} \frac{1}{(\lambda_i + \mu_j)^2} \psi_i(x) \psi_j(y) \right)$$

where $z_{ij} \sim \mathcal{N}(0, 1)$. All together we have 80 terms in the summation. We consider all the observations of the form

$$\begin{aligned} \int_D 1000 F_1(x_1) F_2(x_2) G_1\left(\frac{x_1}{\varepsilon}\right) G_2\left(\frac{x_2}{\varepsilon}\right) \frac{\partial u^\varepsilon}{\partial x_p}(z; x) dx \approx \\ \int_D \int_Y 1000 F_1(x_1) F_2(x_2) G_1(y_1) G_2(y_2) \left(\frac{\partial u_0}{\partial x_p}(z; x) + \frac{\partial u_1}{\partial y_p}(z; x, y) \right) dy dx \end{aligned}$$

for all $F_i(x_i) \in \{1, 1 + \sin(2\pi k x_i), 1 + \cos(2\pi k x_i), k = 1, 2\}$ and $G_i(y_i) \in \{1, 1 + \sin(2\pi k y_i), 1 + \cos(2\pi k y_i), k = 1, 2\}$; $p = 1, 2$. In Figure 2.8 we show the reference coefficient for $x = (0.25, 0.25)$ and the average of 120000 MCMC samples. The figure shows that the MCMC method provides a reasonably good recovery of the coefficient. Similarly, for $x = (0.25, 0.75)$ we show the reference coefficient and the average of the MCMC samples in Figure 2.9.

2.7 Appendix A

We show Theorem 2.3.4 in this appendix. We show that I_1 and I_2 in (2.3.3) and (2.3.4) have upper bound $c\varepsilon$. We first recall the following result.

Figure 2.8: The reference coefficient and the average of the MCMC samples for $x = (0.25, 0.25)$ for 2D two scale problem with Gaussian prior

Figure 2.9: The reference coefficient and the average of the MCMC samples for $x = (0.25, 0.75)$ for 2D two scale problem with Gaussian prior

Lemma 2.7.1. For the coefficient of the form (2.1.6), under Assumption 2.3.3, there is a constant c independent of $z \in U$ such that

$$\|\nabla u^\varepsilon(z) - [\nabla u_0(z) + \nabla_y u_1(z; \cdot, \frac{\cdot}{\varepsilon})]\|_{L^2(D)} \leq c\varepsilon^{1/2}.$$

Proof This result is indeed Theorem 5.2 of Hoang and Schwab [36]. From Assumption 2.3.3, we have that $A(z; x, y)$ is uniformly bounded in $C^1(\bar{D}, C^{1,1}(\bar{Y}))$. The result follows from Theorem 5.2 of [36]. $\square$

From Lemma 2.7.1, we have that

$$\left| \int_D \ell_i(x, \frac{x}{\varepsilon}) \cdot \nabla u^\varepsilon(z; x) dx - \int_D \ell_i(x, \frac{x}{\varepsilon}) \cdot (\nabla u_0(z; x) + \nabla_y u_1(z; x, \frac{x}{\varepsilon})) dx \right| \leq c\varepsilon^{1/2}. \quad (2.7.1)$$

Next we show the following result.

Lemma 2.7.2. Under Assumption 2.3.3, when $\ell_i \in C^{0,1}(\bar{D}, C(\bar{Y}))^d$, we have

$$\left| \int_D \ell_i(x, \frac{x}{\varepsilon}) \cdot (\nabla u_0(z; x) + \nabla_y u_1(z; x, \frac{x}{\varepsilon})) dx - \int_D \int_Y \ell_i(x, y) \cdot (\nabla u_0(z; x) + \nabla_y u_1(z; x, y)) dy dx \right| \leq c\varepsilon^{1/2}. \quad (2.7.2)$$

Proof From Proposition 4.2 of [36], we have that $u_0(z; \cdot)$ is uniformly bounded in $H^2(D)$ with respect to z . Let D_m , $m = 1, \dots, M$ be the cubes of the form $\varepsilon \mathbf{n} + \varepsilon Y$ where $\mathbf{n} \in \mathbb{N}^d$, that are entirely contained in D . We denote by $D^\varepsilon = \bigcup_{m=1}^M D_m$. We have that

$$\begin{aligned} & \left| \int_{D \setminus D^\varepsilon} \ell_i(x, \frac{x}{\varepsilon}) \cdot \nabla u_0(z; x) dx \right| \\ & \leq c \int_{D \setminus D^\varepsilon} |\nabla u_0(z; x)| dx \leq c |D \setminus D^\varepsilon|^{1/2} \left(\int_{D \setminus D^\varepsilon} |\nabla u_0(z; x)|^2 dx \right)^{1/2} \leq c\varepsilon^{1/2}. \end{aligned} \quad (2.7.3)$$

From the proof of Lemma 5.5 in [36], we have

$$\int_D \int_Y \left| \frac{\partial u_0}{\partial x_k}(z; x) - \frac{\partial u_0}{\partial x_k} \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right) \right| dt dx \leq c\varepsilon, \quad (2.7.4)$$

where c is independent of z ; $\frac{\partial u_0}{\partial x_k}$ is continuously extended outside D . We therefore have

$$\left| \int_{D^\varepsilon} \ell_i(x, \frac{x}{\varepsilon}) \cdot \nabla u_0(z; x) - \int_{D^\varepsilon} \ell_i(x, \frac{x}{\varepsilon}) \cdot \left(\int_Y \nabla u_0 \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right) dt \right) dx \right| \leq c\varepsilon. \quad (2.7.5)$$

We have

$$\begin{aligned} & \int_{D^\varepsilon} \ell_i(x, \frac{x}{\varepsilon}) \cdot \left(\int_Y \nabla u_0 \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right) dt \right) dx \\ &= \sum_{m=1}^M \int_{D_m} \ell_i(x, \frac{x}{\varepsilon}) \cdot \left(\int_Y \nabla u_0 \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right) dt \right) dx. \end{aligned}$$

Let x_m be the centre of D_m . We have

$$\begin{aligned} & \left| \sum_{m=1}^M \int_{D_m} \ell_i(x, \frac{x}{\varepsilon}) \cdot \left(\int_Y \nabla u_0 \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right) dt \right) dx - \sum_{m=1}^M \int_{D_m} \ell_i(x_m, \frac{x}{\varepsilon}) \cdot \left(\int_Y \nabla u_0 \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right) dt \right) dx \right| \\ & \leq \sum_{m=1}^M c\varepsilon \int_{D_m} \left| \int_Y \nabla u_0 \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right) dt \right| \\ & = c\varepsilon \int_{D^\varepsilon} \left| \int_Y \nabla u_0 \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right) dt \right| dx \leq c\varepsilon. \end{aligned} \quad (2.7.6)$$

As $\int_Y \nabla u_0 \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right) dt$ is constant for $x \in D_m$, with a simple change of variable, for $x \in D_m$

$$\begin{aligned} & \int_{D_m} \ell_i(x_m, \frac{x}{\varepsilon}) \cdot \left(\int_Y \nabla u_0 \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right) dt \right) dx \\ &= \varepsilon^d \int_Y \nabla u_0 \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right) dt \cdot \int_Y \ell_i(x_m, y) dy \\ &= \int_{D_m} \int_Y \ell_i(x_m, y) \cdot \left(\int_Y \nabla u_0 \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right) dt \right) dy dx. \end{aligned}$$

As for $x \in D_m$, $|\ell_i(x, y) - \ell_i(x_m, y)| \leq c\varepsilon$, from this equality, we have

$$\left| \int_{D_m} \ell_i(x_m, \frac{x}{\varepsilon}) \cdot \left(\int_Y \nabla u_0 \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right) dt \right) dx \right|$$

$$\begin{aligned}
& \left| - \int_{D_m} \int_Y \ell_i(x, y) \cdot \left(\int_Y \nabla u_0 \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right) dt \right) dy dx \right| \\
& \leq c\varepsilon \varepsilon^d \int_Y |\nabla u_0 \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right)| dt \\
& = c\varepsilon \int_{D_m} |\nabla u_0(z; x)| dx
\end{aligned}$$

as $\varepsilon[x/\varepsilon] + \varepsilon t \in D_m$ for $x \in D_m$ and $t \in Y$, the last equality is obtained from a simple change of variable. Thus

$$\begin{aligned}
& \left| \sum_{m=1}^M \int_{D_m} \ell_i(x_m, \frac{x}{\varepsilon}) \cdot \left(\int_Y \nabla u_0 \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right) dt \right) dx \right. \\
& \quad \left. - \int_{D^\varepsilon} \int_Y \ell_i(x, y) \cdot \left(\int_Y \nabla u_0 \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right) dt \right) dy dx \right| \\
& \leq c\varepsilon \int_{D^\varepsilon} |\nabla u_0(z; x)| dx \leq c\varepsilon.
\end{aligned} \tag{2.7.7}$$

From (2.7.4), we have

$$\begin{aligned}
& \left| \int_{D^\varepsilon} \int_Y \ell_i(x, y) \cdot \left(\int_Y \nabla u_0 \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right) dt \right) dy dx \right. \\
& \quad \left. - \int_{D^\varepsilon} \int_Y \ell_i(x, y) \cdot \nabla u_0(z; x) dy dx \right| \\
& = \left| \int_{D^\varepsilon} \left(\int_Y \ell_i(x, y) dy \right) \cdot \int_Y \left(\nabla u_0 \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right) - \nabla u_0(z; x) \right) dt dx \right| \\
& \leq c \int_{D^\varepsilon} \int_Y \left| \nabla u_0 \left(z; \varepsilon \left[\frac{x}{\varepsilon} \right] + \varepsilon t \right) - \nabla u_0(z; x) \right| dt dx \leq c\varepsilon.
\end{aligned} \tag{2.7.8}$$

Further,

$$\left| \int_{D \setminus D^\varepsilon} \int_Y \ell_i(x, y) \cdot \nabla u_0(z; x) dy dx \right| \leq \int_{D \setminus D^\varepsilon} |\nabla u_0(z; x)| dx \leq c\varepsilon^{1/2}. \tag{2.7.9}$$

We then deduce that

$$\left| \int_D \ell_i(x, \frac{x}{\varepsilon}) \cdot \nabla u_0(z; x) dx - \int_D \int_Y \ell_i(x, y) \cdot \nabla u_0(z; x) dx \right| \leq c\varepsilon^{1/2}. \tag{2.7.10}$$

From Proposition 4.2 of [36], as $A(z; \cdot, \cdot)$ is uniformly bounded in $C^1(\bar{D}, C_\#^1(\bar{Y}))$, we have that w^l is uniformly bounded in $C^1(\bar{D}, C_\#(\bar{Y}))$ with respect to $z \in U$. Using

$$u_1(z; x, y) = \frac{\partial u_0}{\partial x_l}(z; x) w^l(z; x, y)$$

we deduce that

$$\left| \int_D \ell_i(x, \frac{x}{\varepsilon}) \cdot \nabla_y u_1(z; x, \frac{x}{\varepsilon}) dx - \int_D \int_Y \ell_i(x, y) \cdot \nabla_y u_1(z; x, y) dy dx \right| \leq c\varepsilon^{1/2}.$$

This can be shown in the same way as for (2.7.10). We then get the conclusion. $\square$

From Lemmas 2.7.1 and 2.7.2, we have

$$|\mathcal{O}_i^\varepsilon(z) - \mathcal{O}_i^0(z)| \leq c\varepsilon^{1/2}, \quad \forall z \in U.$$

Thus

$$|\mathcal{G}^\varepsilon(z) - \mathcal{G}^0(z)| \leq c\varepsilon^{1/2} \quad \forall z \in U.$$

Using inequality $|\exp(-x) - \exp(-y)| \leq |x - y|$ for $x, y \geq 0$, we have

$$\begin{aligned} & \left| \exp\left(-\frac{1}{2}\Phi^\varepsilon(z, \delta)\right) - \exp\left(-\frac{1}{2}\Phi^0(z, \delta)\right) \right| \\ & \leq c |\Phi^\varepsilon(z, \delta) - \Phi^0(z, \delta)| \\ & \leq c \left| \langle \Sigma^{-1/2} (\mathcal{G}^\varepsilon(z) - \mathcal{G}^0(z)), \Sigma^{-1/2} (2\delta - \mathcal{G}^\varepsilon(z) - \mathcal{G}^0(z)) \rangle \right|. \end{aligned} \tag{2.7.11}$$

From (2.7.11), and the uniform boundedness of $\mathcal{G}^\varepsilon(z)$ and $\mathcal{G}^0(z)$ with respect to z , we have $I_1 \leq c\varepsilon$. Similarly, we have $I_2 \leq c\varepsilon$. Thus

$$d_{Hell}(\gamma^{\varepsilon, \delta}, \gamma^{0, \delta}) \leq c\varepsilon^{1/2}.$$

2.8 Appendix B

We show Theorem 2.4.4 in this appendix. For each $z \in \bar{U}$, the $O(\varepsilon^{1/2})$ homogenization rate of convergence in Lemma 2.7.1 holds. However, the

constant c now depends on z . We specify the dependence of this constant on z .

We have the following result.

Lemma 2.8.1. There are constants $c_1 > 0$, $c_2 > 0$, and $c_3 > 0$ such that the homogenized coefficient $A^0(z; x)$ satisfies

$$\exp(-c_1 \sum_{j=1}^{\infty} |z_j| b_j) |\xi|^2 \leq A_{kl}^0(z; x) \xi_k \xi_l \leq c_2 (1 + \exp(c_3 \sum_{j=1}^{\infty} |z_j| b_j)) |\xi|^2$$

for all $\xi \in \mathbb{R}^d$.

Proof From (2.2.6), we have that

$$A_{kl}^0(z; x) \xi_k \xi_l = \int_Y A(z; x, y) \left(\xi_p + \frac{\partial(w^k \xi_k)}{\partial y_p} \right) \left(\xi_p + \frac{\partial(w^l \xi_l)}{\partial y_p} \right) dy.$$

We therefore have

$$A_{kl}^0(z; x) \xi_k \xi_l \geq c_*(z) \int_Y \left(\xi_p + \frac{\partial(w^k \xi_k)}{\partial y_p} \right) \left(\xi_p + \frac{\partial(w^l \xi_l)}{\partial y_p} \right) dy \geq c_*(z) |\xi|^2.$$

On the other hand,

$$\begin{aligned} A_{kl}^0(z; x) \xi_k \xi_l &\leq c^*(z) \left(\sum_{p=1}^d \xi_p^2 + \sum_{p=1}^d \int_Y \frac{\partial(w^l \xi_l)}{\partial y_p} \frac{\partial(w^k \xi_k)}{\partial y_p} dy \right) \\ &\leq c^*(z) \left(\sum_{p=1}^d \xi_p^2 + \sum_{p=1}^d \left(\sum_{k=1}^d \xi_k^2 \right) \left(\sum_{k=1}^d \int_Y \left(\frac{\partial w^k}{\partial y_q} \right)^2 dy \right) \right). \end{aligned}$$

From (2.2.5), we deduce that

$$\|w^l(z; x, \cdot)\|_{H_{\#}^1(Y)/\mathbb{R}} \leq \frac{c^*(z)}{c_*(z)} \|A(z; x, \cdot) e^l\|_{L^2(Y)} \leq c (1 + \exp(c \sum_{j=1}^{\infty} |z_j| b_j)).$$

From these we deduce

$$A_{kl}^0(z; x) \xi_k \xi_l \leq c \left(1 + \exp(c \sum_{j=1}^{\infty} |z_j| b_j) \right) |\xi|^2.$$

□

Lemma 2.8.2. There are constants $c_4 > 0$ and $c_5 > 0$ such that for $z \in \bar{U}$

$$\|w^l(z)\|_{C^1(\bar{D}, H^2(Y)) \cap L^\infty(\bar{D}, C^1(\bar{Y}))} \leq c_4(1 + \exp(c_5 \sum_{j=1}^{\infty} |z_j| \bar{b}_j)).$$

Proof From equation (2.2.5), we have that

$$\int_Y A(z; x, y) \nabla_y (w^l(z; x, y) + e^l \cdot y) \cdot \nabla_y \phi dy = 0, \quad \forall \phi \in H_{\#}^1(Y).$$

As any functions in $\mathcal{D}(\mathbb{R})$ can be decomposed by partition of unity to functions of small supports which can be extended to a periodic function, this equation holds also for all $\phi \in \mathcal{D}(\mathbb{R})$. Thus from theorem 4.16 of McLean [44], we have that

$$\|w^l(z; x, \cdot) + e^l \cdot y\|_{H^3(Y)} \leq c \|w^l(z; x, \cdot)\|_{H^1(Y)}$$

where c only depends on the $C^{1,1}$ norm of A (with respect to y) in a polynomial manner. It is clear that

$$\|w^l(z; x, \cdot)\|_{H^1(Y)/\mathbb{R}} \leq \frac{c^*(z)}{c_*(z)} \|A(z; x, \cdot) e^l\|_{L^2(Y)} \leq c(1 + \exp(c \sum_{j=1}^{\infty} |z_j| b_j)).$$

We thus deduce that

$$\|w^l(z; x, \cdot)\|_{H^3(Y)/\mathbb{R}} \leq c(1 + \exp(c \sum_{j=1}^{\infty} |z_j| \bar{b}_j)).$$

For $d = 2, 3$, $H^3(Y) \subset C^1(\bar{Y})$ so $\|w^l(z; x, \cdot)\|_{C^1(\bar{Y})} \leq c(1 + \exp(c \sum_{j=1}^{\infty} |z_j| \bar{b}_j))$.

For $l, k = 1, \dots, d$

$$-\nabla_y \cdot \left(A \nabla_y \frac{\partial w^l}{\partial x_k} \right) = \nabla_y \cdot \left(\frac{\partial A}{\partial x_k} (e^l + \nabla_y w^l) \right).$$

Therefore,

$$\left\| \frac{\partial w^l}{\partial x_k} \right\|_{H^1(Y)/\mathbb{R}} \leq \frac{c^*(z)}{c_*(z)} \left\| \frac{\partial A}{\partial x_k} (e^l + \nabla w^l) \right\|_{L^2(Y)} \leq c(1 + \exp(c \sum_{j=1}^{\infty} |z_j| \bar{b}_j)).$$

Thus from Theorem 4.16 of [44], we have

$$\left\| \frac{\partial w^l}{\partial x_k}(z; x, \cdot) \right\|_{H^2(Y)/\mathbb{R}} \leq c \left(\left\| \frac{\partial w^l}{\partial x_k}(z; x, \cdot) \right\|_{H^1(Y)/\mathbb{R}} + \left\| \frac{\partial A}{\partial x_k}(e^l + \nabla w^l(z; x, \cdot)) \right\|_{H^1(Y)} \right)$$

where the constant c depends only on $c^*(z)$, $c_*(z)$ and the $C^{0,1}$ norm of $A(z; x, \cdot)$ polynomially. We thus deduce

$$\left\| \frac{\partial w^l}{\partial x_k}(z; x, \cdot) \right\|_{H^2(Y)/\mathbb{R}} \leq c \left(1 + \exp\left(c \sum_{j=1}^{\infty} |z_j| \bar{b}_j\right) \right).$$

□

Lemma 2.8.3. Assume that D is a convex domain, and $f \in L^2(D)$. Under Assumption 2.4.3, there are constants $c_6 > 0$ and $c_7 > 0$ such that for all $z \in \bar{U}$

$$\|u_0(z; \cdot)\|_{H^2(D)} \leq c_6 \left(1 + \exp\left(c_7 \sum_{i=1}^{\infty} |z_i| \bar{b}_i\right) \right).$$

Proof The solution $u_0(z; \cdot)$ of (2.2.7) belongs to $H^2(D)$ when the domain D is convex. Examining the proof of Theorem 3.1.3.1 of Grisvard [28], we find that

$$\|u_0(z; \cdot)\|_{H^2(D)} \leq c \|f\|_{L^2(D)}$$

where the constant c depends polynomially on the Lipschitz norm of $A_{kl}^0(z; \cdot)$, the upper bound of the entries of $R = A^0(z; x)^{-1/2}$, and the constant of the Friedrichs inequality in the domain RD . From (2.2.6) and Lemma 2.8.2, the Lipschitz norm of A_{kl}^0 is bounded by $c(1 + \exp(c \sum_{j=1}^{\infty} |z_j| \bar{b}_j))$. From Lemma 2.8.1, the eigenvalues of A^0 are bounded below by $c \exp(-c \sum_{j=1}^{\infty} |z_j| b_j)$ and bounded above by $c(1 + \exp(c \sum_{j=1}^{\infty} |z_j| b_j))$. Thus the eigenvalues of $A^0(z; x)^{-1/2}$ is bounded above by $c \exp(c \sum_{j=1}^{\infty} |z_j| b_j)$. Let ξ be the vector in $\mathbb{R}^d$ whose components are all zero except the k th and the l th components which are 1. As $A^0(z; x)^{-1/2}$ is symmetric,

$$(A^0)_{kl}^{-1/2}(z; x) = \frac{1}{2} (A^0)^{-1/2}(z; x) \xi \cdot \xi$$

so the entries of $(A^0)^{-1/2}(z; x)$ are bounded above by $c(1 + \exp(c \sum_{j=1}^{\infty} |z_j| b_j))$. We note that the constant in the Friedrichs inequality in RD is bounded polynomially by the diameter of RD (see, e.g., Wloka [54] page 116) so is also bounded by $c(1 + \exp(c \sum_{j=1}^{\infty} |z_j| b_j))$. We get the conclusion. $\square$

Proposition 2.8.4. Assume that the domain D is convex, and $f \in L^2(D)$. Under Assumption 2.4.3, there are constants $c_8 > 0$ and $c_9 > 0$ such that for $z \in \bar{U}$

$$\|\nabla u^\varepsilon(z) - [\nabla u_0(z) + \nabla_y u_1(z; \cdot, \frac{\cdot}{\varepsilon})]\|_{L^2(D)} \leq C(z) \varepsilon^{1/2},$$

where

$$C(z) = c_8(1 + \exp(c_9 \sum_{i=1}^{\infty} |z_i| \bar{b}_i)).$$

Proof We check the dependence on the parameters of the constants in the proof of the homogenization convergence rate for parametric two scale elliptic problem. We follow closely the proof of Proposition 5.1 in [36]. The proof is an extension of the homogenization proof in [42] for the case of smooth u_0 to the case where u_0 is only in $H^2(D)$.

Let

$$u_1^\varepsilon(z; x) = u_0(z; x) + \varepsilon w^l(z; x, \frac{x}{\varepsilon}) \frac{\partial u_0(z; x)}{\partial x_l}.$$

We first show that

$$\|\operatorname{div} A^\varepsilon \nabla u_1^\varepsilon - \operatorname{div} A^0 \nabla u_0\|_{H^{-1}(D)} \leq c(z) \varepsilon,$$

where $c(z)$ is of the form

$$c(1 + \exp(c \sum_{j=1}^{\infty} |z_j| \bar{b}_j)). \quad (2.8.1)$$

We note that

$$(A^\varepsilon(z; x) \nabla u_1^\varepsilon(z; x))_i$$

$$\begin{aligned}
&= \left(A_{ij}^\varepsilon(z; x) + A_{ik}^\varepsilon(z; x) \frac{\partial w^j}{\partial y_k} \left(z; x, \frac{x}{\varepsilon} \right) \right) \frac{\partial u_0}{\partial x_j} (z; x) \\
&\quad + \varepsilon A_{ij}^\varepsilon(z; x) w^k \left(z; x, \frac{x}{\varepsilon} \right) \frac{\partial^2 u_0}{\partial x_j \partial x_k} (z; x) \\
&= A_{ij}^0(z; x) \frac{\partial u_0}{\partial x_j} (z; x) \\
&\quad + \left(A_{ij}^\varepsilon(z; x) + A_{ik}^\varepsilon(z; x) \frac{\partial w^j}{\partial y_k} \left(z; x, \frac{x}{\varepsilon} \right) - A_{ij}^0(z; x) \right) \frac{\partial u_0}{\partial x_j} (z; x) \\
&\quad + \varepsilon A_{ij}^\varepsilon(z; x) w^k \left(z; x, \frac{x}{\varepsilon} \right) \frac{\partial^2 u_0}{\partial x_j \partial x_k} (z; x) \\
&= A_{ij}^0(z; x) \frac{\partial u_0}{\partial x_j} (z; x) + g_i^j(z; x, \frac{x}{\varepsilon}) \frac{\partial u_0}{\partial x_j} (z; x) \\
&\quad + \varepsilon A_{ij}^\varepsilon(z; x) w^k \left(z; x, \frac{x}{\varepsilon} \right) \frac{\partial^2 u_0}{\partial x_j \partial x_k} (z; x),
\end{aligned}$$

where the functions $g_i^j(z; x, y)$ which are periodic in y are defined as

$$g_i^j(z; x, y) = A_{ij}(z; x, y) + A_{ik}(z; x, y) \frac{\partial w^j}{\partial y_k} (z; x, y) - A_{ij}^0(z; x).$$

We have

$$\int_Y g_i^j(z; x, y) dy = 0, \text{ and } \frac{\partial}{\partial y_i} g_i^j(z; x, y) = 0.$$

Following Jikov et al. [42], we write $g_i^k(z; x, y) = \frac{\partial}{\partial y_j} \alpha_{ij}^k(z; x, y)$ where $\alpha_{ij}^k(z; x, y)$ are periodic in y and $\alpha_{ij}^k = -\alpha_{ji}^k$. As $w^l(z; \cdot, \cdot) \in C^1(\bar{D}, H_{\#}^2(Y))$ and $A(z; \cdot, \cdot) \in C^1(\bar{D}, C_{\#}^1(\bar{Y}))$, $g_i^j(z; \cdot, \cdot) \in C^1(\bar{D}, H_{\#}^1(Y))$. From Lemma 2.8.2, the $C^1(\bar{D}, H^1(\bar{Y}))$ norm of $g_i^j(z; \cdot, \cdot)$ is bounded above a constant of the form (2.8.1). Consider the Fourier series of $\mathbf{g}^k$

$$\mathbf{g}^k(z; x, y) = \sum_{l \in \mathbb{R}^d, l \neq 0} \mathbf{g}_l^k(z; x) \exp(\sqrt{-1}l \cdot y).$$

As $\mathbf{g}^k(z; \cdot, \cdot) \in C^1(\bar{D}, H_{\#}^1(Y))^d$, $\mathbf{g}_l^k(z; \cdot) \in C^1(\bar{D})^d$ and, for all $r = 1, \dots, d$, there is a constant $c_r(z)$ such that

$$\sum_{l \in \mathbb{R}^d, l \neq 0} |\mathbf{g}_l^k(z; x)|^2 l_r^2 < c_r(z) \quad (2.8.2)$$

where $c_r(z)$ is of the form (2.8.1) due to the bound of $\|\mathbf{g}^k(z; \cdot, \cdot)\|_{C^1(\bar{D}, H_{\#}^1(Y))^d}$.

From [42], the functions α_{ij}^k are defined as

$$\alpha_{ij}^k(z; x, y) = -\sqrt{-1} \sum_{l \in \mathbb{R}^d, l \neq 0} \frac{(\mathbf{g}_l^k(z; x))_j l_i - (\mathbf{g}_l^k(z; x))_i l_j}{|l|^2} \exp(\sqrt{-1} l \cdot y).$$

For $r, s = 1, \dots, d$

$$\sum_{l \in \mathbb{R}^d, l \neq 0} \frac{|(\mathbf{g}_l^k(z; x))_j l_i - (\mathbf{g}_l^k(z; x))_i l_j|^2}{|l|^4} l_r^2 l_s^2 < c_{rs}(z).$$

From (2.8.2), the constant $c_{rs}(z)$ can be taken to be of the form (2.8.1).

Therefore for dimension $d \leq 3$, $\alpha_{ij}^k(z; \cdot, \cdot) \in C^1(\bar{D}, H_{\#}^2(Y) \subset C^1(\bar{D}, C(\bar{Y}))$; and the $C^1(\bar{D}, C(\bar{Y}))$ norm of $\alpha_{ij}^k(z; \cdot, \cdot)$ is bounded above by a constant of the form (2.8.1).

We note that

$$(A^\varepsilon \nabla u_1^\varepsilon(z; x) - A_0 \nabla u_0(z; x))_i = \varepsilon \frac{\partial}{\partial x_j} \left(\alpha_{ij}^k(z; x, \frac{x}{\varepsilon}) \frac{\partial u_0(z; x)}{\partial x_k} \right) + (r_\varepsilon)_i(z; x),$$

where

$$\begin{aligned} (r_\varepsilon)_i(z; x) = & -\varepsilon \frac{\partial \alpha_{ij}^k(z; x, y)}{\partial x_j} \Big|_{y=x/\varepsilon} \frac{\partial u_0(z; x)}{\partial x_k} - \varepsilon \alpha_{ij}^k(z; x, \frac{x}{\varepsilon}) \frac{\partial^2 u_0(z; x)}{\partial x_k \partial x_j} \\ & + \varepsilon w^k(z; x, \frac{x}{\varepsilon}) A_{ij}^\varepsilon(z; x, \frac{x}{\varepsilon}) \frac{\partial^2 u_0(z; x)}{\partial x_k \partial x_j}. \end{aligned}$$

As $\alpha_{ij}^k(z; \cdot, \cdot) \in C^1(\bar{D}, C(\bar{Y}))$, $\|(r_\varepsilon)_i(z; \cdot)\|_{L^2(D)} \leq c(z)\varepsilon$ where the constant $c(z)$ is of the form (2.8.1). As $\alpha_{ij}^k = \alpha_{ji}^k$,

$$\|\operatorname{div} A^\varepsilon \nabla u_1^\varepsilon(z; x) - \operatorname{div} A^0 \nabla u_0(z; x)\|_{H^{-1}(D)} \leq c(z)\varepsilon,$$

where the constant $c(z)$ is of the form (2.8.1).

As $\operatorname{div} A^0 \nabla u_0 = \operatorname{div} A^\varepsilon \nabla u^\varepsilon$, we find that

$$\|\operatorname{div} A^\varepsilon \nabla u_1^\varepsilon(z; x) - \operatorname{div} A^\varepsilon \nabla u^\varepsilon(z; x)\|_{H^{-1}(D)} \leq c(z)\varepsilon,$$

where the constant $c(z)$ is of the form (2.8.1).

Let $\tau^\varepsilon \in \mathcal{D}(D)$ be such that $\tau^\varepsilon = 1$ outside an ε neighbourhood of ∂D and $\varepsilon|\nabla\tau^\varepsilon(x)| \leq c$ for all ε . We consider the function

$$\begin{aligned} w_1^\varepsilon(z; x) &= u_0(z; x) + \varepsilon\tau^\varepsilon(x)w^k(z; x, \frac{x}{\varepsilon})\frac{\partial u_0(z; x)}{\partial x_k} \\ &= u_1^\varepsilon(z; x) - \varepsilon(1 - \tau^\varepsilon(x))w^k(z; x, \frac{x}{\varepsilon})\frac{\partial u_0(z; x)}{\partial x_k}. \end{aligned}$$

We then get

$$\begin{aligned} \frac{\partial}{\partial x_j}(u_1^\varepsilon - w_1^\varepsilon)(z; x) &= -\varepsilon\frac{\partial\tau^\varepsilon}{\partial x_j}(x)w^k(z; x, \frac{x}{\varepsilon})\frac{\partial u_0(z; x)}{\partial x_k} \\ &\quad + (1 - \tau^\varepsilon(x))\frac{\partial w^k}{\partial y_j}(z; x, \frac{x}{\varepsilon})\frac{\partial u_0}{\partial x_k}(z; x) \\ &\quad + \varepsilon(1 - \tau^\varepsilon(x))w^k(z; x, \frac{x}{\varepsilon})\frac{\partial^2 u_0(z; x)}{\partial x_k \partial x_j}. \end{aligned}$$

Let D^ε be the ε neighbourhood of ∂D . As ∂D is Lipschitz; for all smooth functions $\phi(x)$

$$\|\phi\|_{L^2(D^\varepsilon)}^2 \leq c\varepsilon^2\|\phi\|_{H^1(D)}^2 + c\varepsilon\|\phi\|_{L^2(\partial D)}^2,$$

where c only depends on the domain D ; so for all $\phi \in H^1(D)$

$$\|\phi\|_{L^2(D^\varepsilon)} \leq c\varepsilon^{1/2}\|\phi\|_{H^1(D)}.$$

Therefore from Lemmas 2.8.3 and 2.8.2 we get

$$\|u_1^\varepsilon(z; \cdot) - w_1^\varepsilon(z; \cdot)\|_{H^1(D)} \leq c(z)\varepsilon^{1/2},$$

where the constant $c(z)$ is of the form (2.8.1). Thus,

$$\|\operatorname{div}(A^\varepsilon(\nabla u_1^\varepsilon(z; \cdot) - \nabla w_1^\varepsilon(z; \cdot)))\|_{H^{-1}(D)} \leq c(z)\varepsilon^{1/2},$$

so

$$\|\operatorname{div}(A^\varepsilon(\nabla u^\varepsilon(z; \cdot) - \nabla w_1^\varepsilon(z; \cdot)))\|_{H^{-1}(D)} \leq c(z)\varepsilon^{1/2}$$

where the constant $c(z)$ is of the form (2.8.1). From (2.1.1), we get

$$\|u^\varepsilon(z; \cdot) - w_1^\varepsilon(z; \cdot)\|_{H_0^1(D)} \leq c(z)\varepsilon^{1/2},$$

where $c(z)$ is of the form (2.8.1). Hence

$$\|u^\varepsilon(z; \cdot) - u_1^\varepsilon(z; \cdot)\|_{H^1(D)} \leq c(z)\varepsilon^{1/2}$$

where $c(z)$ is of the form (2.8.1). □

Proof of Theorem 2.4.4

The proof of Theorem 2.4.4 is largely similar to that in Section 2.7 except that the constants depend on z .

Consider $z \in \bar{U}$. From Proposition 2.8.4, the constant in (2.7.1) is of the form (2.8.1). From Lemma 2.8.3, the constant c in (2.7.3) is also of the form (2.8.1). The proof of Lemma 5.5 of [36] shows that the constant c in (2.7.4) is of the form $c\|u_0\|_{H^2(D)}$ so is of the form (2.8.1). The constant c in (2.7.6) depends on $\int_D \int_Y \nabla u_0(z; \varepsilon[\frac{x}{\varepsilon}] + \varepsilon t) dt dx$. From (2.7.4), this is bounded by $\|\nabla u_0\|_{L^2(D)}$ so the constant c in (2.7.6) is of the form (2.8.1). Similarly, the constant c in equations (2.7.7), (2.7.8), (2.7.9), and (2.7.10) are all of the form (2.8.1). Arguing in the same way, from Lemma 2.8.2, we have that

$$\left| \int_D \ell_i(x, \frac{x}{\varepsilon}) \cdot \nabla_y u_1(z; x, \frac{x}{\varepsilon}) dx - \int_D \int_Y \ell_i(x, y) \cdot \nabla_y u_1(z; x, y) dy dx \right| \leq c(z)\varepsilon^{1/2}$$

where $c(z)$ is of the form (2.8.1). Thus for $z \in \bar{U}$, Lemma 2.7.2 holds for the case of Gaussian prior with the constant c depending on z and is of the form (2.8.1).

We therefore deduce that

$$|\mathcal{G}^\varepsilon(z) - \mathcal{G}^0(z)| \leq c(z)\varepsilon^{1/2} \tag{2.8.3}$$

where $c(z)$ is of the form (2.8.1). From (2.4.1), we have that

$$|\mathcal{G}^\varepsilon(z)| \leq c(z) \quad (2.8.4)$$

where $c(z)$ is of the form (2.8.1). From Lemmas 2.8.2 and 2.8.3, and equation (2.2.8), we deduce that

$$|\mathcal{G}^0(z)| \leq c(z) \quad (2.8.5)$$

where $c(z)$ is of the form (2.8.1). From (2.8.3), (2.8.4) and (2.8.5), the right hand side of (2.7.11) is bounded by $c(z)\varepsilon^{1/2} \forall z \in \bar{U}$ where $c(z)$ is of the form (2.8.1). Thus from (2.3.3), as the set $\bar{U}$ has γ measure 1 the integral in (2.3.3) over $U \setminus \bar{U}$ is 0, we deduce that $I_1 \leq c\varepsilon$ (see Lemma 2.8.5 below). Similarly, $I_2 \leq c\varepsilon$. The conclusion then follows.

Lemma 2.8.5. For any constants α and β ,

$$\int_{\bar{U}} \alpha(1 + \exp(\beta \sum_{j=1}^{\infty} |z_j| \bar{b}_j)) d\gamma(z)$$

is finite.

Proof We use the inequality for $s > 0$

$$\int_{-\infty}^{\infty} \exp(-t^2/2 + |t|s) \frac{dt}{\sqrt{2\pi}} \leq \exp(s^2/2) \exp(s\sqrt{2/\pi})$$

which is proved in Lemma 4.6.1. We have

$$\begin{aligned} \int_{\bar{U}} \alpha(1 + \exp(\beta \sum_{j=1}^{\infty} |z_j| \bar{b}_j)) d\gamma(z) \\ \leq \alpha + \alpha \exp\left(\frac{1}{2}\beta^2 \sum_{j=1}^{\infty} \bar{b}_j^2\right) \exp\left(\sqrt{\frac{2}{\pi}}\beta \sum_{j=1}^{\infty} \bar{b}_j\right) \end{aligned}$$

which is finite. □

Chapter 3

Bayesian Inverse Problems for Elliptic problems with Uniform Prior

In this chapter, we review the MLMCMC method for Bayesian inverse problems for forward elliptic partial differential equations that is developed in [37]. This paper considers the uniform prior probability where the coefficient of the equation is expressed as a summation of random variables that are uniformly distributed in a compact interval. The coefficient is uniformly coercive and bounded for all the realizations. This paper does not include numerical examples to illustrate the theory. In the thesis, we modify this method slightly by increasing the sample size for each Markov chain to reduce the logarithmic factor in the overall error, with the complexity increased only by a logarithmic factor. In Section 3.1, we define the Bayesian inverse problem. We introduce the prior probability space of infinite sequences of random variables, each is uniformly distributed in a compact interval. The random coefficient of the forward equation is expressed as the sum of these variables. We impose condition on the supremum norm of the functions which are coefficients of this expansion to ensure that the

coefficient is uniformly coercive and bounded. In Section 3.2, we review the existence and well-posedness of the posterior measure that are established in [37]. The forward equation is approximated by FE in Section 3.3 where we truncate the coefficient to take only a finite number of random variables in the expansion. We recall the approximation results in terms of the number of chosen random variables in the coefficient and the FE mesh. The MLMCMC algorithm developed in [37] is recalled in Section 3.4. We introduce a slight modification in the number of MCMC sample size to reduce the logarithmic factor in the overall error. We contribute numerical examples to verify the theory in Section 3.5 where we illustrate the MLMCMC errors for the modified method.

3.1 Problem Setting

Let D be a bounded polygonal domain in $\mathbb{R}^d$ ($d = 1, 2, 3$). The uniform prior probability measures are considered in detail in Hoang et al. [37]. We consider uncertain diffusion coefficients K of the form

$$K(x, z) = \bar{K}(x) + \sum_{j=1}^{\infty} z_j \psi_j(x), \quad x \in D, \quad z = (z_j)_{j \geq 1} \in U, \quad (3.1.1)$$

where $\bar{K}, \psi_j \in L^\infty(D)$ for $j \in \mathbb{N}$, and where the parameters $z = (z_j)_{j \geq 1}$ are assumed to be independent and uniformly identically distributed in $[-1, 1]$.

Therefore, we consider the product probability space (U, Θ, γ) given by

$$U = [-1, 1]^{\mathbb{N}}, \quad \Theta = \bigotimes_{i=1}^{\infty} \mathcal{B}([-1, 1]) \quad \text{and} \quad \gamma = \bigotimes_{i=1}^{\infty} \frac{dz_i}{2} \quad (3.1.2)$$

where $\mathcal{B}([-1, 1])$ is the Borel σ -algebra in $[-1, 1]$, and where dz_i denotes the Lebesgue measure in $\mathbb{R}$. For the coefficient K to be uniformly coercive and bounded for all $z \in U$, we impose the following assumption on the decay of the sequence $(\psi_j)_{j \geq 1}$.

Assumption 3.1.1. The functions $\bar{K}, \psi_j \in L^\infty(D)$. Further, there exists a constant $\kappa > 0$ such that

$$\sum_{j=1}^{\infty} \|\psi_j\|_{L^\infty(D)} \leq \frac{\kappa}{1+\kappa} \bar{K}_{\min}$$

where $\bar{K}_{\min} = \operatorname{ess\,inf} \bar{K}(x) > 0$.

With Assumption 3.1.1,

$$\forall z \in U : \quad \frac{1}{1+\kappa} \bar{K}_{\min} \leq K(x, z) \leq \bar{K}_{\max} + \frac{\kappa}{1+\kappa} \bar{K}_{\min}$$

where $\bar{K}_{\max} = \operatorname{ess\,sup}_{x \in D} \bar{K}(x)$. The forward problem is

$$-\nabla \cdot (K(\cdot, z) \nabla P(\cdot, z)) = f, \quad P(x, z) = 0, \quad \text{when } x \in \partial D, \quad (3.1.3)$$

where $f \in V'$ with $V := H_0^1(D)$. Under Assumption 3.1.1, for each $z \in U$ the parametric forward problem (3.1.3) admits a unique solution. We assume further:

Assumption 3.1.2. The functions $\bar{K}$ and ψ_j ($j = 1, 2, \dots$) in (3.1.1) belong to $W^{1,\infty}(D)$ and $\sum_{j=1}^{\infty} \|\psi_j\|_{W^{1,\infty}(D)}$ is finite. Moreover, there exist constants $C > 0$ and $s > 1$ so that $\|\psi_j\|_{L^\infty(D)} < Cj^{-s}$ for all $j \in \mathbb{N}$.

Let $\ell_1, \dots, \ell_N \in V'$. Then, the forward data to observation map $\mathcal{G}(z) : U \rightarrow \mathbb{R}^N$ is defined as

$$\mathcal{G}(z) = (\ell_1(P(\cdot, z)), \dots, \ell_N(P(\cdot, z))). \quad (3.1.4)$$

We assume the noisy observation

$$\delta = \mathcal{G}(z) + \vartheta$$

where ϑ is a random variable in $\mathbb{R}^N$ which follows the normal distribution $\mathcal{N}(0, \Sigma)$, where Σ is a known $N \times N$ symmetric and positive definite covariance matrix. The aim is to compute expectations of a quantity of interest

under the posterior probability measure γ^δ , which is the conditional probability $\gamma(z|\delta)$. We assume that the quantity of interest is a continuous, linear functional of the solution of the forward equation. We define the misfit, or potential, functional

$$\Phi(z, \delta) = \frac{1}{2}|\delta - \mathcal{G}(z)|_\Sigma^2 = \frac{1}{2}(\delta - \mathcal{G}(z))^\top \Sigma^{-1}(\delta - \mathcal{G}(z)). \quad (3.1.5)$$

We will show in the following section that, by Bayes' rule, we will have

$$\frac{d\gamma^\delta}{d\gamma} \propto \exp(-\Phi(z, \delta)) \quad (3.1.6)$$

where we denote by

$$Z(\delta) = \int_U \exp(-\Phi(z, \delta)) d\gamma(z)$$

the normalising constant of (3.1.6).

3.2 Existence and Well-posedness of Posterior measure

The existence and well-posedness of the posterior γ^δ follow the standard results ([51]).

Cotter et al. [12] proved the following general result on the existence of the posterior γ^δ (see also [51]).

Proposition 3.2.1. If, in (3.1.5), the parametric forward map $\mathcal{G} : U \rightarrow \mathbb{R}^N$ is measurable on (U, Θ) , then the posterior γ^δ is absolutely continuous with respect to the prior γ . The Radon-Nikodym derivative is given by

$$\frac{d\gamma^\delta}{d\gamma} \propto \exp(-\Phi(z, \delta)). \quad (3.2.1)$$

For the well-posedness of the posterior measure, we recall the following results in [32] and [37] which slightly generalize [12]. We work under the following assumption.

Assumption 3.2.2. The potential function Φ in (3.1.5) satisfies:

- (i) For each $r > 0$ there is a constant $\Lambda(r) > 0$ such that if $|\delta| < r$ where $|\cdot|$ denotes the Euclidean norm in $\mathbb{R}^N$

$$\int_U \Phi(z, \delta) d\gamma(z) < \Lambda.$$

- (ii) There is a function $G : \mathbb{R} \times U \rightarrow \mathbb{R}$ so that for each $r > 0$, $G(r, \cdot) \in L^2(U, \gamma)$ and for all $\delta, \delta' \in \mathbb{R}^N$ with $|\delta|, |\delta'| < r$ we have

$$|\Phi(z, \delta) - \Phi(z, \delta')| \leq G(r, z) |\delta - \delta'|.$$

Under this assumption, we have the following well-posedness result.

Proposition 3.2.3. Under Assumption 3.2.2 the posterior γ^δ is locally Lipschitz with respect to the Hellinger distance, i.e. for each $r > 0$, there is a positive constant $C = C(r)$ so that

$$d_{\text{Hell}}(\gamma^\delta, \gamma^{\delta'}) \leq C |\delta - \delta'| \quad \forall |\delta|, |\delta'| < r. \quad (3.2.2)$$

The estimate 3.2.3 implies that if $g \in L^2(U, \gamma)$ then

$$\left| \mathbb{E}^{\gamma^\delta}[g] - \mathbb{E}^{\gamma^{\delta'}}[g] \right| \leq C |\delta - \delta'|$$

This means that a small change in δ will only result in a small change in the posterior expectation (see [51]). Hoang et al. [37] show that under Assumption 3.1.1(i), the forward functional $\mathcal{G}$ in (3.1.4) is measurable and Assumption 3.2.2 holds. Thus, from Propositions 3.2.1 and 3.2.3 we have:

Proposition 3.2.4. For the coefficient K in (3.1.1), under Assumption 3.1.1, with the prior probability space (U, Θ, γ) defined in (3.1.2), the posterior probability γ^δ is absolutely continuous with respect to the prior probability γ , and is locally Lipschitz with respect to data $\delta \in \mathbb{R}^N$. In particular, the Radon-Nikodym derivative admits a density as in (3.1.6) and the Lipschitz estimate (3.2.2) hold.

3.3 Approximation by FE method

We recall in this section the MLMCMC FE method developed in Hoang et al. in [37]. We first summarize the approximation of the forward problem (3.1.3) with the coefficient (3.1.1) obtained by a finite truncation of the infinite series representation of K and by subsequent numerical solution of the resulting truncated equation by finite element discretization.

For each $J \in \mathbb{N}$, we consider the J -term truncated coefficient

$$K^J(\cdot, z) = \bar{K}(\cdot) + \sum_{j=1}^J z_j \psi_j(\cdot). \quad (3.3.1)$$

The forward problem (3.1.3) is approximated by the problem

$$-\nabla \cdot (K^J(\cdot, z) \nabla P^J(\cdot, z)) = f, \quad P^J \in V. \quad (3.3.2)$$

We approximate the solution of (3.3.2) numerically by a standard FE discretization. We assume that D is a bounded polygonal domain. We consider in D a nested sequence $\{\mathcal{T}^l\}_{l=0}^\infty$ of regular, simplicial triangulations of D ; each triangle $\mathcal{T}^l$ is obtained by dividing each simplex in $\mathcal{T}^{l-1}$ into 4 congruent triangles when $d = 2$ or into 8 tetrahedra when $d = 3$. We define a nested sequence $\{V^l\}_{l \geq 1}$ of spaces of continuous, piecewise linear functions on $\mathcal{T}^l$ as

$$V^l = \{w \in V : w|_T \in \mathbb{P}^1(T) \ \forall T \in \mathcal{T}^l\}, \quad (3.3.3)$$

where $\mathbb{P}^1(T)$ is the set of linear polynomials in T . The finite element approximation is to find $P^{J,l}(z) \in V^l$ such that

$$\int_D K^J(x, z) \nabla P^{J,l}(x, z) \cdot \nabla \phi(x) dx = \int_D f(x) \phi(x) dx, \quad \forall \phi \in V^l. \quad (3.3.4)$$

Under Assumption 3.1.2, for $f \in L^2(D)$ and D a convex polygon, Hoang et al. [37] show that $P^J(\cdot, z) \in H^2(D) \cap V$, with $\|P^J(\cdot, z)\|_{H^2(D)}$ uniformly bounded with respect to J and z . This allow us to establish the following error estimate for the approximate solution $P^{J,l}$ in (3.3.4).

Proposition 3.3.1. Assume that the domain D is convex, and that $f \in L^2(D)$. Under Assumption 3.1.2, there exists a constant $C > 0$ such that for every $J, l \in \mathbb{N}$

$$\|P - P^{J,l}\|_V \leq C(J^{-q} + 2^{-l})\|f\|_{L^2(D)} \quad (3.3.5)$$

where $q = s - 1$.

With the approximate solution $P^{J,l}(\cdot, z)$ of problem (3.3.4) we consider the approximate forward map

$$\mathcal{G}^{J,l}(z) = (\ell_1(P^{J,l}(\cdot, z)), \dots, \ell_N(P^{J,l}(\cdot, z))). \quad (3.3.6)$$

The approximate Bayesian potential is defined as

$$\Phi^{J,l}(\delta, z) = \frac{1}{2}|\delta - \mathcal{G}^{J,l}(z)|_\Sigma^2, \quad (3.3.7)$$

and the approximate posterior on (U, Θ) is given by

$$\frac{d\gamma^{J,l,\delta}}{d\gamma} \propto \exp(-\Phi^{J,l}(\delta, z)). \quad (3.3.8)$$

Hoang et al. [37] Proposition 10 prove the following result on the approximation property of the measure $\gamma^{J,l}$.

Proposition 3.3.2. Under Assumptions 3.1.1, 3.1.2, if the domain D is a convex polygon and $f \in L^2(D)$, then there is a constant C which only depends on δ so that

$$d_{\text{Hell}}(\gamma^\delta, \gamma^{J,l,\delta}) \leq C(J^{-q} + 2^{-l})\|f\|_{L^2(D)}.$$

To balance the two errors from truncating the coefficient K and from finite element approximation, respectively, for each level l of finite element discretization we choose $J = J_l = \lceil 2^{l/q} \rceil$.

3.4 Multilevel MCMC

We do a recap on the MCMC. Let $g : U \rightarrow \mathbb{R}$ be γ^δ -measurable. The expectation $\mathbb{E}^{\gamma^\delta}[g]$ can be approximated numerically by Metropolis-Hastings MCMC sampling. A Markov chain $\{z^{(k)}\}_{k=1}^\infty \subset U$ is constructed as follows: given the current state $z^{(k)}$, we draw a proposal $s^{(k)}$ from a probability distribution $q(z^{(k)}, ds^{(k)})$. Let $\{w^{(k)}\}_{k \geq 1}$ denote an i.i.d sequence with $w^{(k)} \sim \mathcal{U}[0, 1]$ and with $w^{(k)}$ independent of both $z^{(k)}$ and $s^{(k)}$. The next state $z^{(k+1)}$ is determined by

$$z^{(k+1)} = \mathbf{1}(\alpha(z^{(k)}, s^{(k)}) \geq w^{(k)})s^{(k)} + \left(1 - \mathbf{1}(\alpha(z^{(k)}, s^{(k)}) \geq w^{(k)})\right)z^{(k)} \quad (3.4.1)$$

where the acceptance probability is

$$\alpha(z, s) = \min\left(1, \frac{d\nu^T(z, s)}{d\nu(z, s)}\right)$$

with $\nu(dz, ds) = q(z, ds)\gamma^\delta(dz)$. We suppose that the transition kernel q is chosen so that $\nu^T \ll \nu$, and in particular,

$$\frac{d\nu^T(z, s)}{d\nu(z, s)} = \exp(\Phi(z, \delta) - \Phi(s, \delta)) \quad (3.4.2)$$

so that

$$\alpha(z, s) = \min(1, \exp(\Phi(z, \delta) - \Phi(s, \delta))) . \quad (3.4.3)$$

This means that, for each sample to be generated, we need to compute the acceptance probability once, which requires the solving of the forward equation in order to compute the potential function Φ with the new proposal as the input. Together with the slow convergence rate of $O(M^{-1/2})$ of the MCMC method, we are forced to solve a large number of equations to get a reasonable error, hence explains the well-known high computational complexity. We summarise the algorithm in the table below:

Step	Details
1	Generate initial sample $z^{(0)}$ from some probability distribution of choice. Initialise $k = 0$.
2	Generate a proposal $s^{(k)}$ from a probability distribution $q(z^{(k)}, ds^{(k)})$
3	Compute the acceptance probability $\alpha(z^{(k)}, s^{(k)}) = \min(1, \exp(\Phi(z^{(k)}, \delta) - \Phi(s^{(k)}, \delta)))$
4	Generate $\omega^{(k)} \sim \mathcal{U}[0, 1]$
5	If $\omega^{(k)} \leq \alpha(z^{(k)}, s^{(k)})$, then $z^{(k+1)} = s^{(k)}$ If $\omega^{(k)} > \alpha(z^{(k)}, s^{(k)})$, then $z^{(k+1)} = z^{(k)}$
6	$k = k + 1$, repeat step 2 – 6

Table 3.1: Metropolis-Hastings algorithm

We note that (3.4.2) is not strictly necessary, although the independence

and the pCN samplers satisfy (3.4.2), for example. Thus we choose to move from $z^{(k)}$ to $s^{(k)}$ with probability $\alpha(z^{(k)}, s^{(k)})$, and to remain at $z^{(k)}$ with probability $1 - \alpha(z^{(k)}, s^{(k)})$.

We summarise the derivation of the Multilevel MCMC FE method for the uniform prior from Hoang et al. [37]. For conciseness, with the choice $J_l = \lceil 2^{l/q} \rceil$, we denote $\gamma^{J_l, l, \delta}$ simply as γ^l , $P^{J_l, l}$ as P^l and $\Phi^{J_l, l}$ as Φ^l . For every $L \in \mathbb{N}$, we have the telescoping sum

$$\begin{aligned} \mathbb{E}^{\gamma^L}[\ell(P(\cdot, z))] &= \sum_{l=1}^L \left(\mathbb{E}^{\gamma^l}[\ell(P(\cdot, z))] - \mathbb{E}^{\gamma^{l-1}}[\ell(P(\cdot, z))] + \mathbb{E}^{\gamma^0}[\ell(P(\cdot, z))] \right) \\ &= \sum_{l=1}^L \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [\ell(P(\cdot, z))] + \mathbb{E}^{\gamma^0}[\ell(P(\cdot, z))] . \end{aligned} \quad (3.4.4)$$

For each l , with a discretization level $L'(l) \leq L$ to be determined, we approximate $\mathbb{E}^{\gamma^L}[\ell(P(\cdot, z))]$ by (omitting the arguments of P and its approximations for conciseness)

$$\sum_{l=1}^L \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [\ell(P^{L'(l)})] + \mathbb{E}^{\gamma^0}[\ell(P^{L'(0)})]. \quad (3.4.5)$$

For each l , this results in

$$\begin{aligned} &\left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [\ell(P^{L'(l)})] \\ &= \sum_{l'=1}^{L'(l)} \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [\ell(P^{l'}) - \ell(P^{l'-1})] + \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [\ell(P^0)] . \end{aligned} \quad (3.4.6)$$

Similarly,

$$\mathbb{E}^{\gamma^0}[\ell(P^{L'(0)})] = \sum_{l'=1}^{L'(0)} \mathbb{E}^{\gamma^0}[\ell(P^{l'}) - \ell(P^{l'-1})] + \mathbb{E}^{\gamma^0}[\ell(P^0)].$$

Thus, for each level L of approximation,

$$\begin{aligned}
& \sum_{l=1}^L \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [\ell(P^{L'(l)})] + \mathbb{E}^{\gamma^0} [\ell(P^{L'(0)})] \\
&= \sum_{l=1}^L \sum_{\substack{l'=1 \\ L'(0)}}^{L'(l)} \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [\ell(P^{l'}) - \ell(P^{l'-1})] + \sum_{l=1}^L \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [\ell(P^0)] \\
& \quad + \sum_{l'=1}^{L'(0)} \mathbb{E}^{\gamma^0} [\ell(P^{l'}) - \ell(P^{l'-1})] + \mathbb{E}^{\gamma^0} [\ell(P^0)].
\end{aligned} \tag{3.4.7}$$

We approximate each expectation $\mathbb{E}^{\gamma^l}$ in (3.4.7) by sample averages of $M_{ll'}$ many realizations, upon choosing $L'(l)$ judiciously. In order to do so, we rearrange the integration into a sum of expectations with respect to posterior measures approximated at different mesh-levels l of some quantity of interest. This then allows the use of MCMC to approximate each of these expectations. We observe that, for any measurable function $Q : U \rightarrow \mathbb{R}$ which is integrable with respect to the approximate posterior measures γ^l ,

$$\begin{aligned}
& \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [Q] \\
&= \frac{1}{Z^l} \int_U \exp(-\Phi^l(z, \delta)) Q(z) d\gamma(z) - \frac{1}{Z^{l-1}} \int_U \exp(-\Phi^{l-1}(z, \delta)) Q(z) d\gamma(z) \\
&= \frac{1}{Z^l} \int_U \exp(-\Phi^l(z, \delta)) (1 - \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta))) Q(z) d\gamma(z) \\
& \quad + \left(\frac{Z^{l-1}}{Z^l} - 1 \right) \frac{1}{Z^{l-1}} \int_U \exp(-\Phi^{l-1}(z, \delta)) Q(z) d\gamma(z)
\end{aligned} \tag{3.4.8}$$

where Φ^l denotes the approximate potential defined in (3.3.7) and Z^l denotes the approximate normalizing constant in (3.3.8) with $J = J_l$. We remark that under Assumption 3.1.1, the normalization constants Z_l are uniformly (with respect to l) bounded from below away from zero. We note further that

$$\frac{Z^{l-1}}{Z^l} - 1 = \frac{1}{Z^l} \int_U (\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) - 1) \exp(-\Phi^l(z, \delta)) d\gamma(z).$$

Thus an approximation for $Z^{l-1}/Z^l - 1$ can be computed by running MCMC with respect to the approximate posterior γ^l to sample $\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) -$

1. To estimate the expectation with respect to the approximated posteriors γ^l and γ^{l-1} , we apply the MCMC algorithm introduced in Section 3.1. The acceptance probability $\alpha(z, s)$ in (3.4.3) is, however, replaced by that derived from the FE solution of the truncated forward problem. In particular, we define by $E_{M_{ll'}}^{\gamma^l}$ the MCMC FE estimator obtained with the acceptance probability in (3.4.3) replaced by

$$\alpha^l(z, s) = \min(1, \exp(\Phi^l(z, \delta) - \Phi^l(s, \delta))), \quad (3.4.9)$$

with $M_{ll'}$ samples.

This leads to the *Multilevel Markov Chain Monte Carlo* (MLMCMC) estimator $E_L^{MLMCMC}[\ell(P)]$ of $\mathbb{E}^{\gamma^\delta}[\ell(P)]$ defined by

$$\begin{aligned} E_L^{MLMCMC}[\ell(P)] = & \sum_{l=1}^L \sum_{l'=1}^{L'(l)} E_{M_{ll'}}^{\gamma^l} \left[\left(1 - \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) \right) (\ell(P^{l'}) - \ell(P^{l'-1})) \right] \\ & + \sum_{l=1}^L \sum_{l'=1}^{L'(l)} E_{M_{ll'}}^{\gamma^l} \left[\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) - 1 \right] \cdot E_{M_{ll'}}^{\gamma^{l-1}} \left[\ell(P^{l'}) - \ell(P^{l'-1}) \right] \\ & + \sum_{l=1}^L E_{M_{l0}}^{\gamma^l} \left[\left(1 - \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) \right) (\ell(P^0)) \right] \\ & + \sum_{l=1}^L E_{M_{l0}}^{\gamma^l} \left[\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) - 1 \right] \cdot E_{M_{l0}}^{\gamma^{l-1}} \left[\ell(P^0) \right] \\ & + \sum_{l'=1}^{L'(0)} E_{M_{0l'}}^{\gamma^0} \left[\ell(P^{l'}) - \ell(P^{l'-1}) \right] + E_{M_{00}}^{\gamma^0}[\ell(P^0)]. \end{aligned} \quad (3.4.10)$$

As in Hoang et al. [37], we choose the parameters

$$L'(l) = L - l, \quad M_{ll'} = 2^{2(L-(l+l'))}. \quad (3.4.11)$$

When evaluating the MLMCMC estimator for each approximation level l ,

we generate a Markov chain $C_l \subset \mathbb{R}^{J_l}$. We thus generate L pairwise uncorrelated chains. For each L , we denote the probability space of these chains as $\mathbf{C}_L = \{\mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_L\}$. Let $\mathcal{P}^{\gamma, J_l, l}$ denote the probability measure in the space of all chains run from the initial sample $z^{(0)}$, distributed according to the prior γ . Then, we define the probability on $\mathbf{C}_L$ as

$$\mathbf{P}_L = \mathcal{P}^{\gamma, J_1, 1} \otimes \mathcal{P}^{\gamma, J_2, 2} \otimes \dots \otimes \mathcal{P}^{\gamma, J_L, L}.$$

Let $\mathbf{E}_L$ be the expectation in $\mathbf{C}_L$ with respect to $\mathbf{P}_L$. Using any basis of the FE spaces V^l , the multilevel MCMC method achieves an approximation with a prescribed error using an essentially optimal number of degrees of freedom. In terms of the computing time, if a Riesz basis is used, Hoang et al. [37] show that the method uses also an essentially optimal number of floating point operations. We make the following assumption on the availability of a Riesz finite element basis. This assumption is valid for polygonal domains in space dimensions $d = 1, 2, 3$.

Assumption 3.4.1. For $l \in \mathbb{N}$, there is a set of indices $I^l \subset \mathbb{N}^d$ of cardinality $N_l = O(2^{-dl})$ and a family of basis functions $w_k^l \in V$ with $k \in \mathcal{I}^l$ such that V^l is the linear span of w_k^l for $k \in \mathcal{I}^l$. Further there are positive constants c_1 and c_2 which are independent of l such that if $w = \sum_{k \in \mathcal{I}^l} c_k^l w_k^l \in V^l$, then

$$c_1 \sum_{k \in \mathcal{I}^l} (c_k^l)^2 \leq \|w\|_V^2 \leq c_2 \sum_{k \in \mathcal{I}^l} (c_k^l)^2.$$

For all $l \in \mathbb{N}_0$ and all $k \in \mathcal{I}^l$, for each $l' \in \mathbb{N}_0$, $\text{supp}(w_k^l) \cap \text{supp}(w_{k'}^{l'})$ has positive measure for at most $O(\max(1, 2^{l'-l}))$ functions $w_{k'}^{l'}$ for $k' \in \mathcal{I}^{l'}$.

Hoang et al. [37] establish the following result on the error and complexity of the MLMCMC procedure for sampling the posterior measure γ^δ

corresponding to uniform prior probability measure γ , using the independence sampler.

Theorem 3.4.2. For $d = 2, 3$, under Assumption 3.1.2, and with the parameter choices (3.4.11), there exists a constant $c(\delta) > 0$ such that for all $L \geq 1$,

$$\mathbf{E}_L[|\mathbb{E}^{\gamma(\delta)}[\ell(P)] - E_L^{MLMCMC}[\ell(P)]|] \leq C(\delta)L^2 2^{-L}. \quad (3.4.12)$$

The total number of degrees of freedom used in running the MLMCMC sampler is bounded by $O(L2^{2L})$ for $d = 2$ and $O(2^{3L})$ for $d = 3$. Under Assumption 3.4.1 on the availability of a Riesz finite element basis, the total number of floating point operations required for computing the MLMCMC estimator is bounded by $O(L^{d-1}2^{(d+1/q)L})$. Denoting the total number of degrees of freedom in running the chain on all discretization level by N_{dof} , the error in (3.4.12) is bounded by $O((\log N_{dof})^{3/2}N_{dof}^{-1/2})$ for $d = 2$ and by $O((\log N_{dof})^2 N_{dof}^{-1/3})$ for $d = 3$. The total number of floating point operations is bounded by $O((\log N_{dof})^{-1/(2q)}N_{dof}^{1+1/(2q)})$ for $d = 2$ and by $O((\log N_{dof})^2 N_{dof}^{1+1/(3q)})$ for $d = 3$.

This shows that with a small sacrifice in the error by a L^2 factor, we will be able to save a great amount of computational cost, as we have seen in terms of the total degrees of freedom. We have worked out that the logarithmic factor L^2 in the error bounds, may be reduced by slightly increasing the sample numbers $M_{ll'}$. The following error bounds are a refinement of those in [37]: choosing in (3.4.10) the sample numbers $M_{ll'} = (l + l')^a 2^{2(L-(l+l'))}$ when $l \geq 1$ and $l' \geq 1$, the error due to the first two terms of (3.4.10) is bounded by an absolute multiple of $2^{-L} \sum_{l,l'=1}^L (l + l')^{-a/2}$. The following table shows the resulting asymptotic bounds, for various values of a .

a	$M_{ll'}, l, l' > 1$	$M_{l0} = M_{0l}$	M_{00}	Total error
0	$2^{2(L-(l+l'))}$	$2^{2(L-l)}/L^2$	$2^{2L}/L^4$	$O(L^2 2^{-L})$
2	$(l+l')^2 2^{2(L-(l+l'))}$	$2^{2(L-l)}$	$2^{2L}/L^2$	$O(L \log L 2^{-L})$
3	$(l+l')^3 2^{2(L-(l+l'))}$	$l 2^{2(L-l)}$	$2^{2L}/L$	$O(L^{1/2} 2^{-L})$
4	$(l+l')^4 2^{2(L-(l+l'))}$	$l^2 2^{2(L-l)}$	$2^{2L}/(\log L^2)$	$O(\log L 2^{-L})$

Table 3.2: Relation of total error with different a

3.5 Numerical experiments

In this section, we present numerical experimental results that supports the theory for the rate of convergence in the previous sections when FE method is used to solve the forward problem and MLMCMC to approximate the conditional expectation. We point out that experimental results for testing the modified version of MLMCMC, which has the sample size $M_{ll'}$ as described in Table 3.2, are new and support the theory discussed previously. We only consider equations with one random variable z , and thus the numerical results illustrate the effect of balancing the number of MCMC samples $M_{ll'}$ and the mesh size. This is because we need a highly accurate reference posterior expectation to compare the numerical results of the MLMCMC to. The reference expectation is computed by taking a large number of Gauss-Legendre quadrature points; this is not possible if we consider many variables z_j . We note that the main idea of the method is to choose the number of MCMC samples judiciously according to the mesh size. Our numerical examples illustrate this idea. However, the numerical simulation can compute the MLMCMC approximation for the case where the coefficients depends on many parameters z_j .

We first consider the forward equations in one dimensional domain $D = (0, 1)$. In particular, we consider the forward problem

$$-\frac{d}{dx} \left(K(x, z) \frac{dP}{dx} \right) = f, \quad \text{for } 0 < x < 1 \quad (3.5.1)$$

$$P(0, z) = 0, \quad P(1, z) = 0$$

where $K(x, z) = 2 + z \sin(2\pi x)$ and $f = 10$.

The observation functional:

$$\mathcal{G}(z) = \int_0^1 x \frac{dP}{dx}(x, z) dx \quad (3.5.2)$$

The quantity of interest:

$$\ell(P(z)) = \int_0^1 x^{1.5} \frac{dP}{dx}(x, z) dx \quad (3.5.3)$$

The reference expectation of the quantity of interest with respect to the posterior probability,

$$\mathbb{E}^{\gamma^\delta}[\ell(P(z))] = \int_{-1}^1 \ell(P(z)) d\gamma^\delta(z) = \int_{-1}^1 \ell(P(z)) \exp\left(-\frac{1}{2} |\delta - \mathcal{G}(z)|^2\right) d\gamma(z) \quad (3.5.4)$$

is computed by solving the forward equation exactly with the use of Gauss-Legendre quadrature rule to compute any needed integration. The result is plotted in Figure 3.1 with MLMCMC error plotted against the finest mesh level h_L for $a = 0$, where the MLMCMC error were computed from taking arithmetic average of absolute errors from 64 independent runs. The gradient of the best fit straight line is 1.096.

We now consider a forward equation in the two dimensional domain $D = (0, 1) \times (0, 1)$. We consider the periodic boundary condition. The theory above holds also for periodic boundary conditions. We choose to performs numerical examples with periodic boundary condition as we can

Figure 3.1: MLMCMC error for 1D elliptic equation with uniform prior probability

solve the forward equation for each sample $z \in U$ very accurately with Fourier collocation method. Thus we can compute a reference posterior expectation very accurately to compare the MLMCMC results to. The forward problem is

$$\begin{aligned}
 -\nabla \cdot ((2 + z \sin(2\pi x_1) \sin(2\pi x_2)) \nabla P(x, z)) &= 200 (\sin(2\pi x_1) + \sin(2\pi x_2)) \\
 \text{for } x = (x_1, x_2) \in D = (0, 1) \times (0, 1)
 \end{aligned}
 \tag{3.5.5}$$

with periodic boundary condition. The observational functional is

$$\mathcal{G}(z) = \int_D x_1 \frac{\partial P}{\partial x_1}(x, z) + x_2 \frac{\partial P}{\partial x_2}(x, z) dx.
 \tag{3.5.6}$$

The quantity of interest is

$$\ell(P(z)) = \int_D x_1^{1.5} \frac{\partial P}{\partial x_1}(x, z) + x_2^{1.5} \frac{\partial P}{\partial x_2}(x, z) dx.
 \tag{3.5.7}$$

The reference expectation is computed by first using Gauss-Legendre quadrature rule to approximate the integration with respect to $z \in [-1, 1]$ to compute the expectation. Then at each quadrature point z , we solve the forward problem using Fourier Collocation method (see [30]) to obtain a highly accurate approximation of the solution $P(z)$. This results in a highly accurate approximation for the observation $\mathcal{G}(z)$ and the posterior expectation. The MLMCMC error is computed in the same way as before, by taking the arithmetic average of absolute errors from 64 independent runs.

With the new choice of sample size M_{ll} , we experiment with different a , in particular $a = 0, 2, 3$. Results are presented in Figures 3.2, 3.3 and 3.4, with gradients of the best fit straight line 1.049, 1.123 and 1.386, in the same respective order $a = 0, 2, 3$. The results support the theory.

Figure 3.2: MLMCMC error for 2D elliptic equation with uniform prior probability, $a = 0$

Figure 3.3: MLMCMC error for 2D elliptic equation with uniform prior probability, $a = 2$

Figure 3.4: MLMCMC error for 2D elliptic equation with uniform prior probability, $a = 3$

Chapter 4

Bayesian Inverse Problems for Elliptic problems with Gaussian Prior

The Multilevel Markov Chain Monte Carlo (MLMCMC) method developed in Chapter 3 is only valid in the case of uniform prior probability. We show by an example in Section 4.5 that for equations with log-normal coefficients, the method may fail to work. This is due to the fact that in Chapter 3, we rely on the uniform boundedness of the potential $\Phi(z, \delta)$ for all z in the prior probability space. This is no longer the case for the equations with log-normal coefficients. We develop in this chapter a MLMCMC method for equations with log-normal coefficients. We show theoretically the convergence of the method together with the explicit optimal convergence rate. We show numerically that for the example where the MLMCMC method developed in Chapter 3 fails to work, the new method developed in this chapter converges as theoretical prediction. The chapter is organised as follows: In Section 4.1, we introduce the log-normal coefficient and define the prior probability space. We then show the existence and well-posedness of the posterior measure in Section 4.2. In Section 4.3, we approximate the for-

ward equation by finitely truncating the coefficient and solving the resulting equation by Finite Element (FE) method. We then define the approximated posterior measure from the FE solution of the truncated equation and establish an explicit error estimate for this approximated posterior in terms of the Hellinger distance. We then develop the MLMCMC for the Gaussian prior probability and present the convergence rate of the MLMCMC estimator in Section 4.4. In Section 4.5, we show numerical results supporting the convergence of the MLMCMC developed in this chapter for both the independent sampler and the preconditioned Crank-Nicolson (pCN) sampler. The appendices that come after give the detailed proofs of the theorems.

4.1 Problem Setting

Let D be a bounded polygonal domain in $\mathbb{R}^d$ ($d = 1, 2, 3$). We consider the forward elliptic equation in D . Denote by $\mathbb{R}^{\mathbb{N}}$ the set of all infinite sequences $(z_1, z_2, \dots)$ of real numbers. Let $\{\psi_j\}_{j \geq 1} \subset L^\infty(D)$ be a sequence of bounded functions in D . We denote $b_j = \|\psi_j\|_{L^\infty(D)}$ and assume that $\sum_{j=1}^{\infty} b_j$ is finite. Ignoring for now the questions of convergence, we formally introduce the parametric, deterministic coefficient $K : D \times \mathbb{R}^{\mathbb{N}} \rightarrow \mathbb{R}$ as

$$K(\cdot, z) = K_*(\cdot) + \exp \left(\bar{K}(\cdot) + \sum_{j=1}^{\infty} z_j \psi_j(\cdot) \right) \quad (4.1.1)$$

for $z = (z_1, z_2, \dots) \in \mathbb{R}^{\mathbb{N}}$. We assume that the functions K_* and $\bar{K}$ belong to $L^\infty(D)$ and that K_* is non-negative. We note that if $\inf K_*(x) = 0$, then $K(x, z)$ can be arbitrarily close to 0. To specify a prior probability measure on the coefficient space, we assume that the random variables z_j are independently, identically distributed according to the standard Gaussian measure, i.e. $z_j \sim \mathcal{N}(0, 1)$. We denote by γ_1 the standard Gaussian

measure in $\mathbb{R}$. We equip $\mathbb{R}^{\mathbb{N}}$ with the product σ -algebra $\otimes_{j=1}^{\infty} \mathcal{B}(\mathbb{R})$ where $\mathcal{B}$ denotes the Borel σ -algebra on $\mathbb{R}$. The Gaussian probability measure γ on $(\mathbb{R}^{\mathbb{N}}, \mathcal{B}(\mathbb{R}^{\mathbb{N}}))$ is the product measure

$$\gamma = \bigotimes_{j=1}^{\infty} \gamma_1. \quad (4.1.2)$$

We deduce that the set

$$U := \{z \in \mathbb{R}^{\mathbb{N}}, \sum_{j=1}^{\infty} b_j |z_j| < \infty\} \in \mathcal{B}(\mathbb{R}^{\mathbb{N}}), \quad (4.1.3)$$

has full Gaussian measure, i.e. $\gamma(U) = 1$ (see [50, Lemma 2.28]), and that for every $z \in U$, the coefficient (4.1.1) is well-defined as an element of $L^{\infty}(D)$.

We consider the restriction of the σ -algebra $\otimes_{j=1}^{\infty} \mathcal{B}(\mathbb{R})$ to U and denote this σ -algebra by Θ . We consider the restriction of the Gaussian measure γ to U as the prior probability measure. For $z \in U$, we define

$$K_{\max}(z) = \text{esssup}_{x \in D} K_*(x) + \exp \left(\|\bar{K}\|_{L^{\infty}(D)} + \sum_{j=1}^{\infty} \|\psi_j\|_{L^{\infty}(D)} |z_j| \right), \quad (4.1.4)$$

and

$$K_{\min}(z) = \text{essinf}_{x \in D} K_*(x) + \exp \left(\text{essinf}_{x \in D} \bar{K}(x) - \sum_{j=1}^{\infty} \|\psi_j\|_{L^{\infty}(D)} |z_j| \right), \quad (4.1.5)$$

which are (U, Θ) measurable. For $z \in U$ and for almost all $x \in D$, $0 < K_{\min}(z) \leq K(x, z) \leq K_{\max}(z) < \infty$. Consider the forward elliptic problem

$$-\nabla \cdot (K(\cdot, z) \nabla P(\cdot, z)) = f(\cdot), \quad P(x, z) = 0, \quad \text{when } x \in \partial D, \quad (4.1.6)$$

where $f \in V'$ with $V := H_0^1(D)$. The equation has a unique solution $P(\cdot, z) \in V$ for every $z \in U$. We consider observations

$$\mathcal{G}(z) = (\ell_1(P(\cdot, z)), \dots, \ell_N(P(\cdot, z)))$$

where $\ell_i \in V'$ for $i = 1, \dots, N$. We consider the noisy observation of $\mathcal{G}$

$$\delta = \mathcal{G}(z) + \vartheta$$

where ϑ follows the Gaussian distribution $\mathcal{N}(0, \Sigma)$ in $\mathbb{R}^N$; Σ is the $N \times N$ covariance matrix that is symmetric and positive definite. We aim to find the posterior probability measure $\gamma^\delta = \mathbb{P}(z|\delta)$, which we will show by Bayes' rule that

$$\frac{d\gamma^\delta}{d\gamma} \propto \exp(-\Phi(z, \delta)) \quad (4.1.7)$$

where

$$\Phi(z, \delta) = \frac{1}{2} |\delta - \mathcal{G}(z)|_\Sigma^2$$

is the misfit or potential function, with $|\cdot|_\Sigma^2 = \left\langle \Sigma^{-\frac{1}{2}} \cdot, \Sigma^{-\frac{1}{2}} \cdot \right\rangle$, $\langle \cdot, \cdot \rangle$ denoting the inner product in $\mathbb{R}^N$. We denote by

$$Z(\delta) = \int_U \exp(-\Phi(z, \delta)) d\gamma(z)$$

the normalising constant of (4.1.7).

4.2 Existence and Well-posedness of Posterior measure

The solution P of (4.1.6), when interpreted as a map from (U, Θ) to $(V, \mathcal{B}(V))$, is measurable (see, for example, in [25] and [23, 8]) so that the forward functional $\mathcal{G}$ is measurable in the measurable space (U, Θ) . Further, Hoang and Schwab [31] show that Assumption 3.2.2 holds. From Propositions 3.2.1 and 3.2.3, we have

Proposition 4.2.1. For the log-normal coefficient K defined in (4.1.1) with the prior probability space (U, Θ, γ) , the posterior probability measure γ^δ

is absolutely continuous with respect to the prior measure γ , and is locally Lipschitz. The Radon-Nikodym derivative is given as

$$\frac{d\gamma^\delta}{d\gamma} \propto \exp(-\Phi(z, \delta)), \quad (4.2.1)$$

and the local Lipschitz condition

$$d_{\text{Hell}}(\gamma^\delta, \gamma^{\delta'}) \leq C|\delta - \delta'| \quad \forall |\delta|, |\delta'| < r. \quad (4.2.2)$$

holds.

4.3 Approximation by FE method

The numerical analysis of the forward problem for Gaussian prior was studied in detail in Hoang and Schwab [31], Gittelsohn [25], [8] and in the references there. We review some of the results in these references, as needed in the convergence analysis of the MLMCMC method.

We approximate the forward equation (4.1.6) by truncating the coefficient and by discretizing the resulting equation by the FE method.

For $z = (z_1, z_2, \dots) \in \mathbb{R}^\mathbb{N}$, for $J \in \mathbb{N}$, we define

$$K^J(\cdot, z) = K_*(\cdot) + \exp\left(\bar{K}(\cdot) + \sum_{j=1}^J z_j \psi_j(\cdot)\right). \quad (4.3.1)$$

For each $z \in U$, the parametric equation with J -term truncated coefficient is

$$P^J \in V : \quad -\nabla \cdot (K^J(\cdot, z) \nabla P^J(\cdot, z)) = f \text{ in } H^{-1}(D). \quad (4.3.2)$$

We define

$$\mathcal{G}^J(z) = (\ell_1(P^J(\cdot, z)), \dots, \ell_N(P^J(\cdot, z)))$$

where $\ell_i \in V'$ for $i = 1, \dots, N$. We further define

$$\Phi^J(z, \delta) = \frac{1}{2} \left| \delta - \mathcal{G}^J(z) \right|_{\Sigma}^2 \quad (4.3.3)$$

and

$$\frac{d\gamma^{J,\delta}}{d\gamma} \propto \exp(-\Phi^J(z, \delta)), \quad (4.3.4)$$

the approximation of the posterior measure. We make the following assumption.

Assumption 4.3.1. There are $c > 0$ and $s > 1$ such that $\|\psi_j\|_{L^\infty(D)} \leq cj^{-s}$.

We have the following result:

Proposition 4.3.2. Let D be a convex domain. Let f belong to $L^2(D)$. Under Assumptions 4.3.1 and 4.3.3, for $q = s - 1 > 0$, there is a positive constant c depending on δ such that for every $J \in \mathbb{N}$,

$$d_{Hell}(\gamma^\delta, \gamma^{J,\delta}) \leq cJ^{-q}$$

We prove this in Section 4.6. This indicates the error bound for approximating the posterior probability measure γ^δ by the approximated one $\gamma^{J,\delta}$ from solving the forward equation by truncating the coefficient. The effect is observed when we are approximating the expectation with respect to the posterior probability measure by the approximated posterior probability measure.

We approximate (4.3.2) by FE: Find $P^{J,l} \in V^l$ so that

$$\int_D K^J(x, z) \nabla P^{J,l}(x, z) \cdot \nabla \phi(x) dx = \int_D f(x) \phi(x) dx \quad \forall \phi \in V^l \quad (4.3.5)$$

where V^l is the finite element space defined in (3.3.3) and K^J is the J -term truncated coefficient in (4.3.1). This problem has a unique solution that satisfies

$$\|P^{J,l}(\cdot, z)\|_V \leq \frac{\|f\|_{V'}}{K_{\min}^J(z)} \leq c \exp\left(\sum_{j=1}^{\infty} b_j |z_j|\right). \quad (4.3.6)$$

To obtain an order of convergence for the FE approximation of the forward equation, we impose the following regularity assumption on the parametric coefficient.

Assumption 4.3.3. The functions K_* , $\bar{K}$ and ψ_j in expansion (4.1.1) belong to $W^{1,\infty}(D)$. Further, let $\bar{b}_j = \|\psi_j\|_{W^{1,\infty}(D)}$ and that

$$\sum_{j=1}^{\infty} \bar{b}_j < \infty.$$

To estimate the complexity of solving the linear system in (4.3.5), we assume a Riesz basis as in Assumption 3.4.1, we have the following result.

Lemma 4.3.4. Fix $\epsilon > 0$ arbitrary. Then, under Assumption 3.4.1, for any $z \in U$ and for every $l \in \mathbb{N}$, the number $j^*(z, l)$ of iterations of the conjugate gradient method to solve the linear system in the finite element method, to solve the forward truncated equation, for the $H^1(D)$ norm of the FE error to be smaller than ϵ is bounded from below by

$$j^*(z, l) \geq C(|\log \epsilon| + |\log K_{\min}(z)|) \sqrt{\frac{K_{\max}(z)}{K_{\min}(z)}}. \quad (4.3.7)$$

Here, the constant $C > 0$ is independent of $J, l \in \mathbb{N}$ and of $z \in U$.

This is proved in [34].

For the FE solution $P^{J,l}$ in (4.3.5), the approximate forward operator $\mathcal{G}^{J,l}$ is defined as

$$\mathcal{G}^{J,l}(z) = (\ell_1(P^{J,l}(z)), \dots, \ell_N(P^{J,l}(z))) : U \rightarrow \mathbb{R}^N. \quad (4.3.8)$$

With this approximate forward mapping, the approximate potential $\Phi^{J,l}$ is

$$\Phi^{J,l}(z, \delta) := \frac{1}{2} |\delta - \mathcal{G}^{J,l}(z)|_{\Sigma}^2 \quad (4.3.9)$$

and the corresponding approximate posterior is

$$\frac{d\gamma^{J,l,\delta}}{d\gamma}(z) \propto \exp(-\Phi^{J,l}(z, \delta)). \quad (4.3.10)$$

We then have

Proposition 4.3.5. Under Assumption 4.3.1, for $q = s - 1 > 0$ there is a positive constant c depending on δ , such that for every $J, l \in \mathbb{N}$

$$d_{\text{Hell}}(\gamma^\delta, \gamma^{J,l,\delta}) \leq c(J^{-q} + 2^{-l}).$$

We prove this in Section 4.7. This shows the corresponding error for approximating the posterior probability measure by solving the forward equation by truncating the coefficient and solving the truncated equation using FEM. In our numerical experiments when we are approximating the expectation with respect to the posterior probability measure by the expectation with respect to the approximated one, we observed the effect as described by this error bound.

Choosing $J = J_l = \lceil 2^{l/q} \rceil$, we obtain $d_{\text{Hell}}(\gamma^\delta, \gamma^{J,l,\delta}) \leq c2^{-l}$. For the Multilevel MCMC method that we will develop in the next section, we estimate $|\Phi^{J_l,l}(z, \delta) - \Phi^{J_{l-1},l-1}(z, \delta)|$.

Lemma 4.3.6. For $|\delta| < r$, there is a constant $C(r)$ that depends only on r and on δ , and $c > 0$, such that, for every $l \in \mathbb{N}$,

$$\begin{aligned} & |\Phi^{J_l,l}(z, \delta) - \Phi^{J_{l-1},l-1}(z, \delta)| \\ & \leq C(r) \exp\left(c \sum_{j=1}^{J_l} b_j |z_j|\right) \left(2^{-l} \left(1 + \sum_{j=1}^{J_l} b_j |z_j|\right) + \sum_{j=J_{l-1}+1}^{J_l} b_j |z_j|\right). \end{aligned}$$

Proof From (4.3.9), we have

$$|\Phi^{J_l,l}(z, \delta) - \Phi^{J_{l-1},l-1}(z, \delta)|$$

$$\leq c(|\delta| + |\mathcal{G}^{J_l, l}(z)| + |\mathcal{G}^{J_{l-1}, l-1}(z)|)|\mathcal{G}^{J_l, l}(z) - \mathcal{G}^{J_{l-1}, l-1}(z)|.$$

We note that

$$|\mathcal{G}^{J_l, l}(z) - \mathcal{G}^{J_{l-1}, l-1}(z)| \leq c \max_{0 \leq i \leq N} \{\|\ell_i\|_{V'}\} \|P^{J_l, l}(\cdot, z) - P^{J_{l-1}, l-1}(\cdot, z)\|_V.$$

We have from (4.3.2) that

$$\begin{aligned} & -\nabla \cdot (K^{J_l}(\cdot, z) \nabla (P^{J_l}(\cdot, z) - P^{J_{l-1}}(\cdot, z))) \\ & = \nabla \cdot ((K^{J_l}(\cdot, z) - K^{J_{l-1}}(\cdot, z)) \nabla P^{J_{l-1}}(\cdot, z)). \end{aligned}$$

Therefore

$$\begin{aligned} \|P^{J_l}(\cdot, z) - P^{J_{l-1}}(\cdot, z)\|_V & \leq \frac{1}{K_{\min}^{J_l}(z)} \|K^{J_l}(\cdot, z) - K^{J_{l-1}}(\cdot, z)\|_{L^\infty(D)} \|P^{J_{l-1}}(\cdot, z)\|_V \\ & \leq \frac{1}{K_{\min}^{J_l}(z) K_{\min}^{J_{l-1}}(z)} \|K^{J_l}(\cdot, z) - K^{J_{l-1}}(\cdot, z)\|_{L^\infty(D)} \|f\|_{V'}. \end{aligned}$$

Using the inequality $|e^x - e^y| \leq |x - y|(e^x + e^y)$ for $x, y \in \mathbb{R}$, we have

$$\|K^{J_l}(\cdot, z) - K^{J_{l-1}}(\cdot, z)\|_{L^\infty(D)} \leq C \exp \left(\sum_{j=1}^{J_l} b_j |z_j| \right) \sum_{j=J_{l-1}+1}^{J_l} b_j |z_j|.$$

Thus there are constants $C, c > 0$ independent of J and l such that

$$\|P^{J_l}(\cdot, z) - P^{J_{l-1}}(\cdot, z)\|_V \leq C \exp \left(c \sum_{j=1}^{J_l} b_j |z_j| \right) \sum_{j=J_{l-1}+1}^{J_l} b_j |z_j|.$$

From this and (4.7.1) we deduce that

$$\begin{aligned} & \|P^{J_l, l}(\cdot, z) - P^{J_{l-1}, l-1}(\cdot, z)\|_V \\ & \leq C \exp \left(c \sum_{j=1}^{J_l} b_j |z_j| \right) \left(2^{-l} (1 + \sum_{j=1}^{J_l} b_j |z_j|) + \sum_{j=J_{l-1}+1}^{J_l} b_j |z_j| \right). \quad (4.3.11) \end{aligned}$$

Together with (4.3.6) this gives the conclusion. $\square$

4.4 Multilevel MCMC

The Multilevel MCMC FE method for uniform prior in [37] uses the uniform boundedness of the potential $\Phi(z, \delta)$ and its approximation $\Phi^{J_l, l}(z, \delta)$ for all $z \in U = [-1, 1]^{\mathbb{N}}$. For the log-normal coefficient K in (4.1.1) this is no longer true. We derive the MLMCMC FE method for the Gaussian prior. We run the MCMC with the acceptance probability α in (3.4.3) i.e., we use the acceptance probability

$$\alpha^{J_l}(z, s) = \min(1, \exp(\Phi^{J_l}(z, \delta) - \Phi^{J_l}(s, \delta))) \quad (4.4.1)$$

where Φ^{J_l} is defined in (4.3.9). We denote the MCMC average of $M_{ll'}$ samples for approximating the posterior expectation of a function g as $E_{M_{ll'}}^{\gamma^{J_l}}[g]$. We choose $J = J_l$ where $J_l = \lceil 2^{l/q} \rceil$. To simplify notation, we denote $\gamma^{J_l, l, \delta}$ by γ^l , $P^{J_l, l}$ by P^l and $\Phi^{J_l, l}$ by Φ^l . Let $\ell \in V^l$. The derivation of the MLMCM FE method to approximate the expectation of $\ell(P(\cdot))$ with respect to the posterior probability measure γ^δ on U is as follows.

From Proposition 4.3.5, there is a constant $c > 0$ such that, for every $L \in \mathbb{N}$,

$$\left| \mathbb{E}^{\gamma^\delta}[\ell(P(z))] - \mathbb{E}^{\gamma^L}[\ell(P(z))] \right| \leq c2^{-L}.$$

This is due to the estimate, as in ([51] in Lemma 6.37) ,

$$\left| \mathbb{E}^{\gamma^\delta}[\ell(P(z))] - \mathbb{E}^{\gamma^L}[\ell(P(z))] \right| \leq C \|\ell(P(z))\|_{L^2(U, \gamma)} d_{Hell}(\gamma^\delta, \gamma^L).$$

We recall the approximation (3.4.7). To obtain convergence rate bounds for the multilevel MCMC sampling strategy in Section 3.4, we found it essential that $|\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)|$ be uniformly bounded.

For log-Gaussian coefficient and for the Gaussian prior measure, this is no longer the case. To address this, we develop a new method for sampling

the terms in (3.4.7). We recall that in the uniform case, we can rearrange the terms as in (3.4.8) which introduces the difference $\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)$. In the log-normal case, the bound for this difference is dependent on the exponential of the linear summation of z_j . This makes the integration with respect to the prior measure of the upper bound to be unbounded as it involves a term which is the exponential of an exponential of a linear summation of z_j . The idea of the new method is that, when $\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta))$ is bounded for some particular realisation of z , we continue using the method developed for uniform prior, when $\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta))$ is large, we rearrange it differently, which we will see shortly, where we can choose to deal with $\Phi^{l-1}(z, \delta) - \Phi^l(z, \delta)$ instead. This explains the introduction of the control function $I_l(z)$ to be defined next. As a summary, the new method of sampling uses the sampling method developed in Section 3.4 when $\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta) \leq 0$, and the new arrangement of terms when $\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta) > 0$.

We denote by

$$I^l(z) = \begin{cases} 1 & \text{if } \Phi^l(z, \delta) - \Phi^{l-1}(z, \delta) \leq 0, \\ 0 & \text{otherwise.} \end{cases} \quad (4.4.2)$$

Let Q be a measurable function from U to $\mathbb{R}$. For $l \geq 1$, we have

$$\begin{aligned} & \mathbb{E}^{\gamma^l}[Q(z)] - \mathbb{E}^{\gamma^{l-1}}[Q(z)] \\ &= \frac{1}{Z^l} \int_U \exp(-\Phi^l(z, \delta)) Q(z) I^l(z) d\gamma(z) \\ & \quad - \frac{1}{Z^{l-1}} \int_U \exp(-\Phi^{l-1}(z, \delta)) Q(z) I^l(z) d\gamma(z) \\ & \quad + \frac{1}{Z^l} \int_U \exp(-\Phi^l(z, \delta)) Q(z) (1 - I^l(z)) d\gamma(z) \\ & \quad - \frac{1}{Z^{l-1}} \int_U \exp(-\Phi^{l-1}(z, \delta)) Q(z) (1 - I^l(z)) d\gamma(z) \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{Z^l} \int_U (\exp(-\Phi^l(z, \delta)) - \exp(-\Phi^{l-1}(z, \delta))) Q(z) I^l(z) d\gamma(z) \\
&\quad + \left(\frac{1}{Z^l} - \frac{1}{Z^{l-1}} \right) \int_U \exp(-\Phi^{l-1}(z, \delta)) Q(z) I^l(z) d\gamma(z) \\
&\quad - \frac{1}{Z^{l-1}} \int_U (\exp(-\Phi^{l-1}(z, \delta)) - \exp(-\Phi^l(z, \delta))) Q(z) (1 - I^l(z)) d\gamma(z) \\
&\quad + \left(\frac{1}{Z^l} - \frac{1}{Z^{l-1}} \right) \int_U \exp(-\Phi^l(z, \delta)) Q(z) (1 - I^l(z)) d\gamma(z).
\end{aligned}$$

With the notation $A_1^l = (1 - \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta))) Q(z) I^l(z)$, we have

$$\begin{aligned}
&\frac{1}{Z^l} \int_U (\exp(-\Phi^l(z, \delta)) - \exp(-\Phi^{l-1}(z, \delta))) Q(z) I^l(z) d\gamma(z) \\
&= \mathbb{E}^{\gamma^l}[(1 - \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta))) Q(z) I^l(z)] = \mathbb{E}^{\gamma^l}[A_1^l].
\end{aligned}$$

Introducing $A_2^l = (\exp(\Phi^{l-1}(z, \delta) - \Phi^l(z, \delta)) - 1) Q(z) (1 - I^l(z))$, we write

$$\begin{aligned}
&-\frac{1}{Z^{l-1}} \int_U (\exp(-\Phi^{l-1}(z, \delta)) - \exp(-\Phi^l(z, \delta))) Q(z) (1 - I^l(z)) d\gamma(z) \\
&= \mathbb{E}^{\gamma^{l-1}}[(\exp(\Phi^{l-1}(z, \delta) - \Phi^l(z, \delta)) - 1) Q(z) (1 - I^l(z))] = \mathbb{E}^{\gamma^{l-1}}[A_2^l].
\end{aligned}$$

We note that

$$\begin{aligned}
&\frac{1}{Z^l} - \frac{1}{Z^{l-1}} \\
&= \frac{1}{Z^l Z^{l-1}} \int_U (\exp(-\Phi^{l-1}(z, \delta)) - \exp(-\Phi^l(z, \delta))) (I^l(z) + 1 - I^l(z)) d\gamma(z) \\
&= \frac{1}{Z^l Z^{l-1}} \int_U \exp(-\Phi^l(z, \delta)) (\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) - 1) I^l(z) d\gamma(z) \\
&\quad + \frac{1}{Z^l Z^{l-1}} \int_U \exp(-\Phi^{l-1}(z, \delta)) (1 - \exp(\Phi^{l-1}(z, \delta) - \Phi^l(z, \delta))) (1 - I^l(z)) d\gamma(z) \\
&= \frac{1}{Z^{l-1}} \mathbb{E}^{\gamma^l}[(\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) - 1) I^l(z)] + \\
&\quad + \frac{1}{Z^l} \mathbb{E}^{\gamma^{l-1}}[(1 - \exp(\Phi^{l-1}(z, \delta) - \Phi^l(z, \delta))) (1 - I^l(z))].
\end{aligned}$$

Thus

$$\left(\frac{1}{Z^l} - \frac{1}{Z^{l-1}} \right) \int_U \exp(-\Phi^{l-1}(z, \delta)) Q(z) I^l(z) d\gamma(z)$$

$$\begin{aligned}
&= \mathbb{E}^{\gamma^l}[(\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) - 1)I^l(z)] \cdot \\
&\quad \frac{1}{Z^{l-1}} \int_U \exp(-\Phi^{l-1}(z, \delta))Q(z)I^l(z)d\gamma(z) \\
&+ \mathbb{E}^{\gamma^{l-1}}[(1 - \exp(\Phi^{l-1}(z, \delta) - \Phi^l(z, \delta)))(1 - I^l(z))] \cdot \\
&\quad \frac{1}{Z^l} \int_U \exp(-\Phi^l(z, \delta)) \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta))Q(z)I^l(z)d\gamma(z) \\
&= \mathbb{E}^{\gamma^l}[A_3^l] \mathbb{E}^{\gamma^{l-1}}[A_4^l] + \mathbb{E}^{\gamma^{l-1}}[A_5^l] \mathbb{E}^{\gamma^l}[A_6^l]
\end{aligned}$$

where

$$\begin{aligned}
A_3^l &= (\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) - 1)I^l(z), \\
A_4^l &= Q(z)I^l(z), \\
A_5^l &= (1 - \exp(\Phi^{l-1}(z, \delta) - \Phi^l(z, \delta)))(1 - I^l(z)), \\
A_6^l &= \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta))Q(z)I^l(z).
\end{aligned}$$

Similarly, defining for $l \geq 1$

$$A_7^l = Q(z)(1 - I^l(z)) \text{ and } A_8^l = \exp(\Phi^{l-1}(z, \delta) - \Phi^l(z, \delta))Q(z)(1 - I^l(z)) ,$$

we have

$$\begin{aligned}
&\left(\frac{1}{Z^l} - \frac{1}{Z^{l-1}} \right) \int_U \exp(-\Phi^l(z, \delta))Q(z)(1 - I^l(z))d\gamma(z) \\
&= \mathbb{E}^{\gamma^{l-1}}[(1 - \exp(\Phi^{l-1}(z, \delta) - \Phi^l(z, \delta)))(1 - I^l(z))] \cdot \\
&\quad \frac{1}{Z^l} \int_U \exp(-\Phi^l(z, \delta))Q(z)(1 - I^l(z))d\gamma(z) \\
&+ \mathbb{E}^{\gamma^l}[(\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) - 1)I^l(z)] \cdot \\
&\quad \frac{1}{Z^{l-1}} \int_U \exp(-\Phi^{l-1}(z, \delta)) \exp(\Phi^{l-1}(z, \delta) - \Phi^l(z, \delta))Q(z)(1 - I^l(z))d\gamma(z) \\
&= \mathbb{E}^{\gamma^{l-1}}[A_5^l] \mathbb{E}^{\gamma^l}[A_7^l] + \mathbb{E}^{\gamma^l}[A_3^l] \mathbb{E}^{\gamma^{l-1}}[A_8^l] .
\end{aligned}$$

We conclude that, for every $l \geq 1$,

$$\mathbb{E}^{\gamma^l}[Q(z)] - \mathbb{E}^{\gamma^{l-1}}[Q(z)]$$

$$\begin{aligned}
&= \mathbb{E}^{\gamma^l}[A_1^l] + \mathbb{E}^{\gamma^{l-1}}[A_2^l] + \mathbb{E}^{\gamma^l}[A_3^l] \cdot \mathbb{E}^{\gamma^{l-1}}[A_4^l + A_8^l] \\
&\quad + \mathbb{E}^{\gamma^{l-1}}[A_5^l] \cdot \mathbb{E}^{\gamma^l}[A_6^l + A_7^l].
\end{aligned}$$

In (3.4.7), when $Q = \ell(P^{l'} - P^{l'-1})$, we denote A_1^l as $A_1^{l'}$, A_2^l as $A_2^{l'}$, A_4^l as $A_4^{l'}$, A_6^l as $A_6^{l'}$, A_7^l as $A_7^{l'}$ and A_8^l as $A_8^{l'}$. In the case of $Q = \ell(P^0)$, we denote A_1^l as $A_1^{l_0}$, A_2^l as $A_2^{l_0}$, A_4^l as $A_4^{l_0}$, A_6^l as $A_6^{l_0}$, A_7^l as $A_7^{l_0}$ and A_8^l as $A_8^{l_0}$.

We therefore approximate $\mathbb{E}^{\gamma^L}[\ell(P(z))]$ by

$$\begin{aligned}
&\sum_{l=1}^L \sum_{l'=1}^{L'(l)} \left[\mathbb{E}^{\gamma^l}[A_1^{l'}] + \mathbb{E}^{\gamma^{l-1}}[A_2^{l'}] + \mathbb{E}^{\gamma^l}[A_3^l] \cdot \mathbb{E}^{\gamma^{l-1}}[A_4^{l'} + A_8^{l'}] \right. \\
&\quad \left. + \mathbb{E}^{\gamma^{l-1}}[A_5^l] \cdot \mathbb{E}^{\gamma^l}[A_6^{l'} + A_7^{l'}] \right] \\
&+ \sum_{l=1}^L \left[\mathbb{E}^{\gamma^l}[A_1^{l_0}] + \mathbb{E}^{\gamma^{l-1}}[A_2^{l_0}] + \mathbb{E}^{\gamma^l}[A_3^l] \cdot \mathbb{E}^{\gamma^{l-1}}[A_4^{l_0} + A_8^{l_0}] \right. \\
&\quad \left. + \mathbb{E}^{\gamma^{l-1}}[A_5^l] \cdot \mathbb{E}^{\gamma^l}[A_6^{l_0} + A_7^{l_0}] \right] \\
&+ \sum_{l'=1}^{L'(0)} \mathbb{E}^{\gamma^0}[\ell(P^{l'} - P^{l'-1})] + \mathbb{E}^{\gamma^0}[\ell(P^0)].
\end{aligned} \tag{4.4.3}$$

The Multilevel Markov Chain Monte Carlo estimator is now defined by replacing the expectations in the preceding expression by finite sample MCMC averages, i.e.

$$\begin{aligned}
&E_L^{MLMCMC}(\ell(P)) \\
&= \sum_{l=1}^L \sum_{l'=1}^{L'(l)} \left[E_{M_{l'}}^{\gamma^l}[A_1^{l'}] + E_{M_{l'}}^{\gamma^{l-1}}[A_2^{l'}] + E_{M_{l'}}^{\gamma^l}[A_3^l] \cdot E_{M_{l'}}^{\gamma^{l-1}}[A_4^{l'} + A_8^{l'}] \right. \\
&\quad \left. + E_{M_{l'}}^{\gamma^{l-1}}[A_5^l] \cdot E_{M_{l'}}^{\gamma^l}[A_6^{l'} + A_7^{l'}] \right] \\
&+ \sum_{l=1}^L \left[E_{M_{l_0}}^{\gamma^l}[A_1^{l_0}] + E_{M_{l_0}}^{\gamma^{l-1}}[A_2^{l_0}] + E_{M_{l_0}}^{\gamma^l}[A_3^l] \cdot E_{M_{l_0}}^{\gamma^{l-1}}[A_4^{l_0} + A_8^{l_0}] \right. \\
&\quad \left. + E_{M_{l_0}}^{\gamma^{l-1}}[A_5^l] \cdot E_{M_{l_0}}^{\gamma^l}[A_6^{l_0} + A_7^{l_0}] \right] \\
&+ \sum_{l'=1}^{L'(0)} E_{M_{0l'}}^{\gamma^0}[\ell(P^{l'} - P^{l'-1})] + E_{M_{00}}^{\gamma^0}[\ell(P^0)],
\end{aligned}$$

where $E_{M_{l'}}^{\gamma^l}$ denotes the average of the MCMC with $M_{l'}$ samples with the acceptance probability in (4.4.1). For each discretization level $l \in \mathbb{N}_0$, we introduce the Markov chains

$$\mathcal{C}_l = \{z^{(k)}\}_{k \in \mathbb{N}_0} \subset \mathbb{R}^{J_l}$$

which are started with $z^{(0)} \in \mathbb{R}^{J_l}$ and then generated by the MCMC process with the acceptance probability α in (4.4.1) with $J = J_l = \lceil 2^{l/q} \rceil$. From (4.3.6), there are positive constants c_1 and c_2 such that for all $z \in U$

$$\Phi^{J_l}(z) \leq c_1 + c_2 \exp \left(2 \sum_{j=1}^{\infty} b_j |z_j| \right).$$

We define by

$$\kappa = \int_U \exp \left(-c_2 \exp \left(2 \sum_{j=1}^{\infty} b_j |z_j| \right) \right) d\gamma(z).$$

As shown in [31], κ is strictly positive. Following [31], we define the probability measure $\bar{\gamma}$ by

$$d\bar{\gamma}(z) = \frac{1}{\kappa} \exp \left(-c_2 \exp \left(2 \sum_{j=1}^{\infty} b_j |z_j| \right) \right) d\gamma(z), \quad z \in U. \quad (4.4.4)$$

Then, there exists a constant $c > 0$ such that

$$\sup_{z \in U} \sup_{J, l \in \mathbb{N}} \frac{d\bar{\gamma}}{d\gamma^{J, l, \delta}}(z) < c < \infty \quad (4.4.5)$$

We denote by $\mathcal{P}^{\bar{\gamma}, l}$ the probability measure of the probability space that describes the randomness of this Markov chain when the initial state $z^{(0)}$ is distributed according to $\bar{\gamma}$. The purpose of introducing $\bar{\gamma}$ is to make the initial distribution of $z^{(0)}$ independent of the approximating parameters in the probability $\mathbf{P}_L$ below.

Then, for each discretization level $l = 1, 2, \dots$, the chains $\mathcal{C}_l$ are pairwise independent. For every fixed discretization level L , we denote by $\mathbf{C}_L =$

$\{\mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_L\}$ the set of Markov chains obtained from the discretizations at level $l = 0, 1, 2, \dots, L$, and by $\mathbf{P}_L$ the product probability measure on the probability space generated by these L independent Markov chains. For each fixed discretization level L , the measure $\mathbf{P}_L$ describes the law of $\mathbf{C}_L = \{\mathcal{C}_l\}_{l=0}^L$:

$$\mathbf{P}_L := \mathcal{P}^{\bar{\gamma},0} \otimes \mathcal{P}^{\bar{\gamma},1} \otimes \mathcal{P}^{\bar{\gamma},2} \otimes \dots \otimes \mathcal{P}^{\bar{\gamma},L}.$$

Let $\mathbf{E}_L$ denote the expectation over all realizations of the collection $\mathbf{C}_L$ of chains $\{\mathcal{C}_l\}_{l=0}^L$ with respect to the product measure $\mathbf{P}_L$.

With the parameter choice

$$\begin{aligned} L'(l) &= L - l, \quad M_{ll'} = 2^{2(L-(l+l'))} \quad \text{for } l \geq 1, \quad l' \geq 1, \\ M_{0l} &= M_{l0} = 2^{2L}/L^2, \quad M_{00} = 2^{2L}/L^4, \end{aligned} \tag{4.4.6}$$

we have the following result.

Theorem 4.4.1. Assume that the domain D is convex and $f \in L^2(D)$. Under Assumptions 4.3.3, and 4.8.2 for $d = 2, 3$, with the choices (4.4.6) there exists a constant $C(\delta) > 0$ such that for every $L \in \mathbb{N}$,

$$\mathbf{E}_L \left[\left| \mathbb{E}^{\gamma^\delta}[\ell(P)] - E_L^{MLMCMC}[\ell(P)] \right| \right] \leq C(\delta) L^2 2^{-L}. \tag{4.4.7}$$

The expectation of the total number of degrees of freedom required in running the MLMCMC sampler, in the probability space $\mathbf{C}_L$, is bounded by $O(L2^{2L})$ for $d = 2$ and $O(2^{3L})$ for $d = 3$. Further, with the availability of a Riesz finite element basis as in 3.4.1, the expectation of the total number of floating point operations is bounded by $O(L^{d-1}2^{(d+1/q)L})$. Denoting the expectation of the total number of degrees of freedom in running MLMCMC by N , the error in (4.4.7) is bounded by $O((\log N)^{3/2}N^{-1/2})$ for $d = 2$ and by $O((\log N)^2N^{-1/3})$ for $d = 3$. The expectation of the total number of

floating point operations is bounded by $O((\log N)^{-1/(2q)} N^{1+1/(2q)})$ for $d = 2$ and by $O((\log N)^2 N^{1+1/(3q)})$ for $d = 3$.

We prove this theorem in Section 4.8. As in the previous chapter, this shows the huge cut in computational cost, in terms of the total degrees of freedom, with only a small sacrifice in the error by the L^2 factor.

As done for the uniform prior, we can reduce the multiplying logarithmic factor L^2 by increasing $M_{ll'}$ as in the table below:

a	$M_{ll'}, l, l' > 1$	$M_{l0} = M_{0l}$	M_{00}	Total error
0	$2^{2(L-(l+l'))}$	$2^{2(L-l)}/L^2$	$2^{2L}/L^4$	$O(L^2 2^{-L})$
2	$(l+l')^2 2^{2(L-(l+l'))}$	$2^{2(L-l)}$	$2^{2L}/L^2$	$O(L \log L 2^{-L})$
3	$(l+l')^3 2^{2(L-(l+l'))}$	$l 2^{2(L-l)}$	$2^{2L}/L$	$O(L^{1/2} 2^{-L})$
4	$(l+l')^4 2^{2(L-(l+l'))}$	$l^2 2^{2(L-l)}$	$2^{2L}/(\log L^2)$	$O(\log L 2^{-L})$

Table 4.1: Relation of total error with different a

4.5 Numerical experiments

We show in this section numerical examples for two dimensional elliptic equations in the cube $(0, 1) \times (0, 1)$ with the periodic boundary condition, with a coefficient of the log-normal class with the Gaussian prior probability measure. As explained in Chapter 3, we first present examples whose coefficient contains one random variable z here, as we need a highly accurate approximation of the reference posterior expectation as the benchmark to compare the MLMCMC approximations to. Such a highly accurate refer-

ence is difficult to obtain when the number of random variables is large. We thus basically illustrate the approximation due to judiciously choosing the number of MCMC samples $M_{ll'}$ according to the mesh size h_l . Note that our numerical simulations can produce results for any number of random variables z_j . This explains the choice of the periodic boundary too; the periodic boundary condition allows the forward equation to be solved by Fourier collocation method with very high accuracy, leading to a highly accurate approximation of the reference posterior expectation. We also present an example where we consider the whole random coefficient K without truncation (i.e. we consider all the coordinates z_j). The Gaussian random field is sampled by circulant embedding. We can numerically illustrate the theoretical results in this example as the reference posterior expectation can be computed exactly.

We consider the parametric forward equation

$$-\nabla \cdot (K(x, z) \nabla P(x)) = f(x) \quad \text{for } x = (x_1, x_2) \in D,$$

with $D = (0, 1) \times (0, 1)$ and periodic boundary condition where $z \in \mathbb{R}$ is normally distributed and

$$K(x, z) = e^{z(\sin(2\pi x_1) + \sin(2\pi x_2))}, \quad \text{and } f(x) = 200 (\sin(2\pi x_1) + \sin(2\pi x_2)).$$

The forward observation functional is

$$\mathcal{G}(z) = \int_D x_1 \frac{\partial P}{\partial x_1}(x, z) + x_2 \frac{\partial P}{\partial x_2}(x, z) dx;$$

and the quantity of interest is

$$\ell(P(z)) = \int_D x_1^{1.5} \frac{\partial P}{\partial x_1}(x, z) + x_2^{1.5} \frac{\partial P}{\partial x_2}(x, z) dx.$$

The centered Gaussian observation noise ϑ is generated by MATLAB generator for normally distributed random numbers.

To compute a reference posterior expectation, we compute

$$\begin{aligned}\mathbb{E}^{\gamma^\delta} [\ell(P)] &= \int_{-\infty}^{\infty} \ell(P(z)) \, d\gamma^\delta(z) \\ &= \int_{-\infty}^{\infty} \ell(P(z)) \exp\left(-\frac{1}{2} |\delta - G(z)|^2\right) \, d\gamma(z)\end{aligned}$$

using 1200 Gauss-Hermite quadrature points. At each quadrature point, the forward equation is solved by a Fourier collocation method with 1024 collocation points, with very high accuracy.

First we present the numerical experiments with the independence sampler. In the figures below, we plot the error of the MLMCMC approximation versus the finest resolution meshwidth 2^{-L} used in the MLMCMC.

In Figure 4.1, we plot the error versus the meshsize 2^{-L} for the case where a in Table 4.1 equals 0. The gradient of the best fit straight line is 0.9312. In Figure 4.2, we plot the MLMCMC error versus the meshwidth 2^{-L} for $a = 2$. The gradient of the best fit straight line is 0.93257. Similarly, for $a = 3$ and $a = 4$, the MLMCMC error versus 2^{-L} is plotted in Figures 4.3 and 4.4 with the gradient of the best fit straight line is 1.0072 and 1.0804 respectively. These results support the theory. We now present the results for the MLMCMC method with the pCN sampler (see [51]) where the proposal $s^{(k)}$ is chosen from the current sample $z^{(k)}$ as follows,

$$s^{(k)} = \sqrt{1 - \beta^2} z^{(k)} + \beta \xi,$$

where ξ is the standard normal variable, for different values of β . First for $\beta = 1/\sqrt{2}$, we plot the MLMCMC error versus the meshwidth 2^{-L} for $a = 0, 2, 3$ and 4 in Figures 4.5, 4.6, 4.7 and 4.8 respectively. The slope of the best fit straight lines are 0.73977, 1.0392, 1.0111 and 0.99257 respectively. We see that except when $a = 0$ (in which case the method slightly

Figure 4.1: MLMCMC error for 2D elliptic equation with Gaussian prior probability using independence sampler, $a = 0$

underperforms possibly due to the large L^2 multiplying factor in the error bound), the MLMCMCFE method using the pCN sampler performs as expected from our theoretical results. We now compare the acceptance probability when generating the Markov Chain for both the independent sampler and the pCN sampler when $\beta = 1/\sqrt{2}$. We observe that the probability of accepting a proposal for the independent sampler is 0.54 while the probability of accepting a proposal for the pCN with $\beta = 1/\sqrt{2}$ is 0.71. This is as expected from the pCN sampler to have a higher rate of acceptance, but from our numerical results, it is not conclusive that the rate of convergence is better than using the independent sampler.

For $\beta = 1/\sqrt{10}$, we plot the results for $a = 0, 2, 3$ and 4 in Figures 4.9, 4.10, 4.11 and 4.12 respectively. The slopes of the best fit straight lines in the error plots are 0.44129, 0.97061, 0.9058 and 0.92827, respectively. Again

Figure 4.2: MLMCMC error for 2D elliptic equation with Gaussian prior probability using independence sampler, $a = 2$

when $a = 0$ the convergence rate is inferior to the optimal rate $O(2^{-L})$ due to the large multiplying factor L^2 in the error, but for other values of a , the observed convergence rate essentially corresponds to the rates in our theorems.

To test the CPU time performance of the method, we record the average CPU time for 5 different runs of the MLMCMC method, choosing $M_{ll'}$ according to Table 4.1 with $a = 0$ and 2, for different values of L (corresponding to the finest discretization level 2^{-L}) for the independence sampler. The timings are summarised in Table 4.2 and Table 4.3. The CPU time behaves like $O(2^{2L})$ which is essentially optimal. We have similar results for the pCN sampler.

Figure 4.3: MLMCMC error for 2D elliptic equation with Gaussian prior probability using independence sampler, $a = 3$

We now present an example where the whole random field K is sample. In this case, the reference posterior expectation can be computed exactly. We can then compute the numerical errors to illustrate the theory. The homogeneous Gaussian random field is sampled at the finite element nodes by circulant embedding.

We consider the problem

$$-\nabla \cdot (K(x, z) \nabla P(x)) = \cos(2\pi x_1) \sin(2\pi x_2), \quad (4.5.1)$$

for $x = (x_1, x_2) \in D = (0, 1) \times (0, 1)$ with boundary conditions

$$\begin{aligned} P(0, x_2) &= 0, P(1, x_2) = 1, \\ \frac{\partial P}{\partial x_2}(x_1, 0) &= 0, \frac{\partial P}{\partial x_2}(x_1, 1) = 0. \end{aligned}$$

Figure 4.4: MLMCMC error for 2D elliptic equation with Gaussian prior probability using independence sampler, $a = 4$

We assume that

$$K = \exp(R)$$

where R is a Gaussian random field with mean $\mu = 0$ and with covariance function given by

$$C(x, y) = \exp(-|x - y|^2), \quad x, y \in D.$$

Here $|\cdot|$ denotes the Euclidean norm in $\mathbb{R}^2$. The observation is

$$\mathcal{G}(K) = \int_D (0.5 - x_1)^2 \frac{\partial P}{\partial x_1}(x, K) + (0.5 - x_2)^2 \frac{\partial P}{\partial x_2}(x, K) dx$$

and the quantity of interest is

$$\ell(P(K)) = \int_D P(x, K) dx.$$

Following Graham et al. [26], we consider the map $\rho : D \rightarrow D$ given by $\rho(x) = (1 - x_1, 1 - x_2)$. Let $K_\rho(x) = K(\rho(x))$ and $P_\rho(x) = 1 - P(\rho(x))$.

Figure 4.5: MLMCMC error for 2D elliptic equation with Gaussian prior probability using pCN sampler, $\beta = \frac{1}{\sqrt{2}}$, $a = 0$

Then P_ρ is the solution of problem (4.5.1) with coefficient $K = K_\rho$. Further

$$\mathcal{G}(K) = \mathcal{G}(K_\rho).$$

As K and K_ρ define Gaussian random fields with the same mean and with homogeneous covariance, they have the same probability law, which is the prior γ on the space U of continuous functions. Its law is invariant under the map $K \rightarrow K_\rho$. We have the normalising constant

$$Z = \int_U \exp\left(-\frac{1}{2} |\delta - \mathcal{G}(K)|^2\right) d\gamma(K) = \int_U \exp\left(-\frac{1}{2} |\delta - \mathcal{G}(K_\rho)|^2\right) d\gamma(K_\rho).$$

Thus the posterior expectation is

$$\mathbb{E}^{\rho^\delta}[\ell(P(K))] = \frac{1}{Z} \int_U \ell(P(K)) \exp\left(-\frac{1}{2} |\delta - \mathcal{G}(K)|^2\right) d\gamma(K).$$

As

$$\int_D P(x) dx = \int_D P(\rho(x)) dx,$$

Figure 4.6: MLMCMC error for 2D elliptic equation with Gaussian prior probability using pCN sampler, $\beta = \frac{1}{\sqrt{2}}$, $a = 2$

and $\mathcal{G}(K) = \mathcal{G}(K_\rho)$, we have that

$$\mathbb{E}^{\rho^\delta}[\ell(P(K))] = \frac{1}{Z} \int_U (1 - \ell(P(K_\rho)) \exp\left(-\frac{1}{2} |\delta - \mathcal{G}(K_\rho)|^2\right) d\gamma(K).$$

As γ is invariant under the mapping that maps K to K_ρ , we have that

$$\mathbb{E}^{\gamma^\delta}[\ell(P(K))] = 1 - \mathbb{E}^{\gamma^\delta}[\ell(P(K))]$$

so

$$\mathbb{E}^{\gamma^\delta}[\ell(P(K))] = 0.5.$$

In Figure 4.13, we plot the error of $\mathbb{E}^{\gamma^\delta}[\ell(P(K))]$ approximated by the MLMCMC method. The stationary Gaussian random field is numerically sampled by circulant embedding (see, [18], [26]) to generate the samples for the nodes of the finite element mesh in D . Here we choose $a = 3$. We use independent sampler. The slope of the best fit straight line in the error

Figure 4.7: MLMCMC error for 2D elliptic equation with Gaussian prior probability using pCN sampler, $\beta = \frac{1}{\sqrt{2}}$, $a = 3$

convergence plot is 0.910. The MLMCMC error plotted is the arithmetic average of the errors of 64 independent runs of MLMCMC. In Figure 4.14, we plot the MLMCMC error for the pCN sampling method where β is chosen as $1/\sqrt{2}$ and a is also chosen as 3. The slope of the best fit straight line is 0.912. Again, the error plotted is the arithmetic average of the errors of 64 independent runs of the MLMCMC. These numerical results support the theory. We now present a numerical example of an equation with a log-normal coefficient where the MLMCMC method developed for the uniform prior measure in [37] does not converge but the MLMCMC method presented above for the Gaussian prior provides accurate approximation. In the one dimensional domain $D = (0, 1)$ we consider the problem

$$-\frac{d}{dx}\left(K(x, z)\frac{dP}{dx}\right) = f(x),$$

Figure 4.8: MLMCMC error for 2D elliptic equation with Gaussian prior probability using pCN sampler, $\beta = \frac{1}{\sqrt{2}}$, $a = 4$

with

$$K(x, z) = \exp(z \sin(4\pi x)) \text{ and } f(x) = 200.$$

The observation is

$$\mathcal{G}(z) = \int_0^1 x \frac{dP}{dx}(x, z) dx$$

and the quantity of interest is

$$\ell(P(z)) = \int_0^1 x^{1.5} \frac{dP}{dx}(x, z) dx.$$

The data is generated again by solving the equation exactly for one randomly chosen realization of z and by generating the noise by the MATLAB random generator. The reference posterior expectation is computed by solving the equation exactly and by using many Gauss-Legendre quadrature points. The tables below show the arithmetic average of the errors for 64 runs of the MLMCMC using independent sampler. In Table 4.4, we present

Figure 4.9: MLMCMC error for 2D elliptic equation with Gaussian prior probability using pCN sampler, $\beta = \frac{1}{\sqrt{10}}$, $a = 0$

the error for the MLMCMC sampler developed for uniform prior measure in [37]. It shows that the method does not converge, supporting our theory that it is essential for the difference of the potential function solved with different mesh-size, $|\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)|$, to be uniformly bounded with respect to z .

In Table 4.5, we present the average error of 64 runs of the MLMCMC sampler developed in Section 4.4. The results clearly shows that the MLMCMC method for Gaussian prior converges as proved theoretically. Indeed, the slope of the best fit straightline is 0.95.

Figure 4.10: MLMCMC error for 2D elliptic equation with Gaussian prior probability using pCN sampler, $\beta = \frac{1}{\sqrt{10}}$, $a = 2$

4.6 Appendix A

We prove Proposition 4.3.2 in this appendix. We first prove a useful lemma:

Lemma 4.6.1. For $s > 0$,

$$\int_{-\infty}^{\infty} \exp(-t^2/2 + |t|s) \frac{dt}{\sqrt{2\pi}} \leq c \exp(s^2/2) \exp(s\sqrt{2/\pi}),$$

$$\int_{-\infty}^{\infty} t^2 \exp(-t^2/2 + |t|s) \frac{dt}{\sqrt{2\pi}} \leq c \exp(s^2/2) (1 + s^2),$$

and

$$\int_{-\infty}^{\infty} |t| \exp(-t^2/2 + |t|s) \frac{dt}{\sqrt{2\pi}} \leq c \exp(s^2/2) (1 + s).$$

Proof These estimates are proved in [34]. We include them here for completeness. For any $t > 0$, we have

$$\int_{-\infty}^{\infty} \exp(-t^2/2 + |t|s) \frac{dt}{\sqrt{2\pi}}$$

Figure 4.11: MLMCMC error for 2D elliptic equation with Gaussian prior probability using pCN sampler, $\beta = \frac{1}{\sqrt{10}}$, $a = 3$

$$\begin{aligned}
&= \exp(s^2/2) \int_{-\infty}^{\infty} \exp(-(|t| - s)^2/2) \frac{dt}{\sqrt{2\pi}} \\
&= \exp(s^2/2) \left(\int_{-\infty}^0 \exp(-(t + s)^2/2) \frac{dt}{\sqrt{2\pi}} + \int_0^{\infty} \exp(-(t - s)^2/2) \frac{dt}{\sqrt{2\pi}} \right) \\
&= \exp(s^2/2) \left(\int_{-\infty}^s \exp(-t^2/2) \frac{dt}{\sqrt{2\pi}} + \int_{-s}^{\infty} \exp(-t^2/2) \frac{dt}{\sqrt{2\pi}} \right) \\
&= \exp(s^2/2) \left(1 + \int_{-s}^s \exp(-t^2/2) \frac{dt}{\sqrt{2\pi}} \right) \\
&\leq \exp(s^2/2) (1 + s\sqrt{2/\pi}) \leq \exp(s^2/2) \exp(s\sqrt{2/\pi}) .
\end{aligned}$$

For the second inequality we have,

$$\begin{aligned}
&\int_{-\infty}^{\infty} t^2 \exp(-t^2/2 + |t|s) \frac{dt}{\sqrt{2\pi}} \\
&= \exp(s^2/2) \left(\int_{-\infty}^0 t^2 \exp(-(t + s)^2/2) \frac{dt}{\sqrt{2\pi}} + \int_0^{\infty} t^2 \exp(-(t - s)^2/2) \frac{dt}{\sqrt{2\pi}} \right) \\
&= \exp(s^2/2) \left(\int_{-\infty}^s (t - s)^2 \exp(-t^2/2) \frac{dt}{\sqrt{2\pi}} + \int_{-s}^{\infty} (t + s)^2 \exp(-t^2/2) \frac{dt}{\sqrt{2\pi}} \right)
\end{aligned}$$

Figure 4.12: MLMCMC error for 2D elliptic equation with Gaussian prior probability using pCN sampler, $\beta = \frac{1}{\sqrt{10}}$, $a = 4$

$$\begin{aligned}
&\leq 2 \exp(s^2/2) \left(\int_{-\infty}^s (t^2 + s^2) \exp(-t^2/2) \frac{dt}{\sqrt{2\pi}} + \int_{-s}^{\infty} (t^2 + s^2) \exp(-t^2/2) \frac{dt}{\sqrt{2\pi}} \right) \\
&\leq 4 \exp(s^2/2) \int_{-\infty}^{\infty} (t^2 + s^2) \exp(-t^2/2) \frac{dt}{\sqrt{2\pi}} \\
&\leq c \exp(s^2/2) (1 + s^2) .
\end{aligned}$$

For the last inequality, we have

$$\begin{aligned}
&\int_{-\infty}^{\infty} |t| \exp(-t^2/2 + |t|s) \frac{dt}{\sqrt{2\pi}} \\
&= \exp(s^2/2) \left(\int_{-\infty}^0 |t| \exp(-(t+s)^2/2) \frac{dt}{\sqrt{2\pi}} + \int_0^{\infty} |t| \exp(-(t-s)^2/2) \frac{dt}{\sqrt{2\pi}} \right) \\
&= \exp(s^2/2) \left(\int_{-\infty}^s |t-s| \exp(-t^2/2) \frac{dt}{\sqrt{2\pi}} + \int_{-s}^{\infty} |t+s| \exp(-t^2/2) \frac{dt}{\sqrt{2\pi}} \right) \\
&\leq 2 \exp(s^2/2) \int_{-\infty}^{\infty} (|t| + s) \exp(-t^2/2) \frac{dt}{\sqrt{2\pi}} \leq c \exp(s^2/2) (1 + s) .
\end{aligned}$$

□

We prove the following proposition:

Mesh-Level (L)	Mean CPU time
2	0.052
3	0.067
4	0.105
5	0.256
6	0.767
7	2.387
8	8.863
9	35.467
10	146.463

Table 4.2: CPU time for $a = 0$

Proposition 4.6.2. Under Assumption 4.3.1, there exist constants $C, c > 0$ dependent on f such that for all $J \in \mathbb{N}$ and $z \in U$,

$$\|P(z) - P^J(z)\|_V \leq C \exp\left(c \sum_{j=1}^{\infty} b_j |z_j|\right) \left(\sum_{j>J} b_j |z_j|\right)$$

Proof Subtracting (4.3.2) from (4.1.6), we have

$$-\nabla \cdot (K(z) \nabla (P(z) - P^J(z))) = \nabla \cdot ((K(z) - K^J(z)) \nabla P^J(z)).$$

Multiplying by $P(z) - P^J(z)$ and integrating over D , we get

$$\begin{aligned} \int_D (K(z) \nabla (P(z) - P^J(z))) \cdot \nabla (P(z) - P^J(z)) dx \\ = - \int_D (K(z) - K^J(z)) \nabla P^J(z) \cdot \nabla (P(z) - P^J(z)) dx. \end{aligned}$$

Using the coerciveness of K , we have

$$K_{\min}^J(z) \|\nabla (P(z) - P^J(z))\|_{L^2(D)}^2$$

Mesh-Level (L)	Mean CPU time
2	0.046
3	0.088
4	0.342
5	1.512
6	6.321
7	27.256
8	115.612
9	490.272
10	2097.376

Table 4.3: CPU time for $a = 2$

$$\leq \|K(z) - K^J(z)\|_{L^\infty(D)} \|\nabla P^J(z)\|_{L^2(D)} \|\nabla(P(z) - P^J(z))\|_{L^2(D)}. \quad (4.6.1)$$

This implies that

$$\|\nabla(P(z) - P^J(z))\|_{L^2(D)} \leq \frac{1}{K_{\min}^J(z)} \|K(z) - K^J(z)\|_{L^\infty(D)} \|\nabla P^J(z)\|_{L^2(D)}. \quad (4.6.2)$$

To bound $\|\nabla P^J(z)\|_{L^2(D)}$, we follow the standard procedure; multiplying (4.3.2) by P^J and integrating in D to get

$$\|\nabla P^J(z)\|_{L^2(D)} \leq \frac{\|f\|_{V'}}{K_{\min}^J(z)} \leq C \exp\left(\sum_{j=1}^J b_j |z_j|\right). \quad (4.6.3)$$

Figure 4.13: MLMCMC error for example (4.5.1): Independence sampler,
 $a = 3$

To bound $\|K(z) - K^J(z)\|_{L^\infty(D)}$, we note that

$$\begin{aligned}
 & \|K(z) - K^J(z)\|_{L^\infty(D)} \\
 &= \left\| \exp \left(\bar{K}(\cdot) + \sum_{j=1}^{\infty} z_j \psi_j(\cdot) \right) - \exp \left(\bar{K}(\cdot) + \sum_{j=1}^J z_j \psi_j(\cdot) \right) \right\|_{L^\infty(D)} \\
 &\leq \left(\sum_{j>J} b_j |z_j| \right) \left\| \exp \left(\bar{K}(\cdot) + \sum_{j=1}^{\infty} z_j \psi_j(\cdot) \right) + \exp \left(\bar{K}(\cdot) + \sum_{j=1}^J z_j \psi_j(\cdot) \right) \right\|_{L^\infty(D)} \\
 &\leq \left(\sum_{j>J} b_j |z_j| \right) C \exp \left(\|\bar{K}(x)\|_{L^\infty(D)} + \sum_{j=1}^{\infty} b_j |z_j| \right) \\
 &\leq C \left(\sum_{j>J} b_j |z_j| \right) \exp \left(\sum_{j=1}^{\infty} b_j |z_j| \right)
 \end{aligned} \tag{4.6.4}$$

Figure 4.14: MLMCMC error for example (4.5.1): pCN sampler, $\beta = \frac{1}{\sqrt{2}}$,
 $a = 3$

This concludes from (4.6.2) that

$$\|P(z) - P^J(z)\|_V \leq C \exp\left(c \sum_{j=1}^{\infty} b_j |z_j|\right) \left(\sum_{j>J} b_j |z_j|\right).$$

□

We are now ready to prove Proposition 4.3.2.

Proof of Proposition 4.3.2: From equation (4.6.3), we have that

$$|\mathcal{G}(z)| \leq C \exp\left(\sum_{j=1}^{\infty} |z_j| b_j\right), \quad |\mathcal{G}^J(z)| \leq C \exp\left(\sum_{j=1}^{\infty} |z_j| b_j\right)$$

for a constant $C > 0$. From Proposition 4.6.2, we have

$$|\mathcal{G}(z) - \mathcal{G}^J(z)| \leq C \left(\sum_{j>J} |z_j| b_j\right) \exp\left(c \sum_{j=1}^{\infty} |z_j| b_j\right).$$

Let $Z(\delta)$ and $Z^J(\delta)$ be the normalizing constants in (4.1.7) and (4.3.4) respectively. We first show that Z^J is uniformly bounded below from 0

Mesh-Level (L)	Average MLMCMC error
8	2.77959E+23
9	1.96933E+46
10	1683671.3
11	2.8192E+19
12	3.29498E+32
13	2.89131E+41

Table 4.4: MLMCMC error from using MLMCMC sampler developed for uniform prior

with respect to J . From (4.3.3) and equation (4.6.3), we have that

$$|\Phi^J(z, \delta)| \leq c(\delta) \exp\left(c \sum_{j=1}^J |z_j| b_j\right).$$

From Lemma 4.6.1, we have that

$$\int_U \Phi^J(z, \delta) d\gamma(z) < \Lambda$$

uniformly for all J . Fixing a constant $C > 0$, the γ measure of the set z such that $\Phi^J(z, \delta) > C$ is less than Λ/C so the γ measure of the set of z such that $\Phi^J(z, \delta) \leq C$ is more than $1 - \Lambda/C$ which is positive when C is sufficiently large. Thus

$$Z^J(\delta) = \int_U \exp(-\Phi^J(z, \delta)) d\gamma(z) > (1 - \Lambda/C) \exp(-C) > 0.$$

Mesh-Level (L)	Average MLMCMC error
8	1.72670013
9	1.05627325
10	0.5178982
11	0.4255921
12	0.11905266
13	0.06412478

Table 4.5: MLMCMC error from using MLMCMC sampler developed in Section 4.4

Following the procedure in [51], we have

$$\begin{aligned}
& 2d_{Hell}(\gamma^\delta, \gamma^{J,\delta})^2 \\
&= \int_U \left(\sqrt{\frac{d\gamma^\delta}{d\gamma}} - \sqrt{\frac{d\gamma^{J,\delta}}{d\gamma}} \right)^2 d\gamma(z) \\
&= \int_U \left[Z(\delta)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}\Phi(z, \delta)\right) - Z^J(\delta)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}\Phi^J(z, \delta)\right) \right]^2 d\gamma(z) \\
&\leq 2 \int_U \left(Z(\delta)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}\Phi(z, \delta)\right) - Z(\delta)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}\Phi^J(z, \delta)\right) \right)^2 d\gamma(z) \\
&\quad + 2 \int_U \left(Z(\delta)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}\Phi^J(z, \delta)\right) - Z^J(\delta)^{-\frac{1}{2}} \exp\left(-\frac{1}{2}\Phi^J(z, \delta)\right) \right)^2 d\gamma(z) \\
&= I_1 + I_2
\end{aligned} \tag{4.6.5}$$

where

$$I_1 = \frac{2}{Z(\delta)} \int_U \left(\exp\left(-\frac{1}{2}\Phi(z, \delta)\right) - \exp\left(-\frac{1}{2}\Phi^J(z, \delta)\right) \right)^2 d\gamma(z), \tag{4.6.6}$$

and

$$I_2 = 2|Z(\delta)^{-1/2} - Z^J(\delta)^{-1/2}|^2 \int_U \exp(-\Phi^J(z, \delta)) d\gamma(z). \tag{4.6.7}$$

We then have

$$\begin{aligned} \left| \exp\left(-\frac{1}{2}\Phi(z, \delta)\right) - \exp\left(-\frac{1}{2}\Phi^J(z, \delta)\right) \right| &\leq c(|\delta| + |\mathcal{G}(z)| + |\mathcal{G}^J(z)|)|\mathcal{G}(z) - \mathcal{G}^J(z)| \\ &\leq c(\delta) \exp\left(c \sum_{j=1}^{\infty} |z_j| b_j\right) \left(\sum_{j>J} |z_j| b_j\right). \end{aligned} \quad (4.6.8)$$

Thus

$$I_1 \leq c(\delta) \int_U \exp\left(c \sum_{j=1}^{\infty} |z_j| b_j\right) \left(\sum_{j>J} |z_j| b_j\right)^2 d\gamma(z).$$

Now we show that the right hand side of this inequality is not more than $c(\delta)J^{-2q}$. Denoting by γ_1 the standard normal probability measure in $\mathbb{R}$, we have

$$\begin{aligned} &\int_U \exp\left(c \sum_{j=1}^{\infty} b_j |z_j|\right) \left(\sum_{j=J+1}^{\infty} b_j |z_j|\right)^2 d\gamma(z) \\ &= \int_U \exp\left(c \sum_{j=1}^{\infty} b_j |z_j|\right) \left(\sum_{i,j=J+1}^{\infty} b_i b_j |z_i| |z_j|\right) d\gamma(z) \\ &\leq \sum_{i=J+1}^{\infty} b_i^2 \int_{-\infty}^{\infty} \exp(cb_i |z_i|) z_i^2 d\gamma_1(z_i) \prod_{\substack{k=1 \\ k \neq i}}^{\infty} \int_{-\infty}^{\infty} \exp(cb_k |z_k|) d\gamma_1(z_k) \\ &\quad + \sum_{\substack{i,j=J+1 \\ i \neq j}}^{\infty} b_i b_j \int_{-\infty}^{\infty} \exp(cb_i |z_i|) |z_i| d\gamma_1(z_i) \cdot \int_{-\infty}^{\infty} \exp(cb_j |z_j|) |z_j| d\gamma_1(z_j) \\ &\quad \cdot \prod_{\substack{k=1 \\ k \neq i,j}}^{\infty} \int_{-\infty}^{\infty} \exp(cb_k |z_k|) d\gamma_1(z_k). \end{aligned}$$

From Lemma 4.6.1, there exists $c > 0$ (independent of b_j) such that

$$\int_{-\infty}^{\infty} t^2 \exp(-t^2/2 + |t|s) \frac{dt}{\sqrt{2\pi}} \leq c \exp(s^2/2)(1 + s^2),$$

and

$$\int_{-\infty}^{\infty} |t| \exp(-t^2/2 + |t|s) \frac{dt}{\sqrt{2\pi}} \leq c \exp(s^2/2)(1 + s).$$

We deduce that there exists $C > 0$ such that for all $J \geq 1$

$$\begin{aligned}
& \int_U \exp \left(c \sum_{j=1}^{\infty} b_j |z_j| \right) \left(\sum_{j=J+1}^{\infty} b_j |z_j| \right)^2 d\gamma(z) \\
& \leq C \sum_{i=J+1}^{\infty} b_i^2 (1 + b_i^2) \exp \left(\sum_{k=1}^{\infty} c^2 b_k^2 / 2 + c b_k \sqrt{2/\pi} \right) \\
& \quad + C \sum_{\substack{i,j=J+1 \\ i \neq j}}^{\infty} b_i b_j (1 + b_i)(1 + b_j) \exp \left(\sum_{k=1}^{\infty} c^2 b_k^2 / 2 + c b_k \sqrt{2/\pi} \right) \\
& \leq C \left(\sum_{j=J+1}^{\infty} b_j \right)^2 \leq C J^{-2q}.
\end{aligned}$$

Thus $I_1 \leq C J^{-2q}$. To bound I_2 , we observe that

$$\begin{aligned}
\left| Z(\delta)^{-\frac{1}{2}} - Z^J(\delta)^{-\frac{1}{2}} \right| & \leq C \max\{Z(\delta)^{-3}, Z^J(\delta)^{-3}\} |Z(\delta) - Z^J(\delta)|^2 \\
& \leq C |Z(\delta) - Z^J(\delta)|^2.
\end{aligned} \tag{4.6.9}$$

From (4.6.8),

$$\begin{aligned}
|Z(\delta) - Z^J(\delta)| & \leq \int_U |\exp(-\Phi(z, \delta)) - \exp(-\Phi^J(z, \delta))| d\gamma(z) \\
& \leq C J^{-2q}.
\end{aligned} \tag{4.6.10}$$

Therefore,

$$I_2 \leq C J^{-2q}.$$

□

4.7 Appendix B

We prove Proposition 4.3.5 in this appendix. We first prove the proposition:

Proposition 4.7.1. Let D be convex. Let f belong to $L^2(D)$. Under Assumption 4.3.3, there exist constants $C, c > 0$ dependent on f , but independent of z , J and l such that for all $J \in \mathbb{N}$ and $z \in U$,

$$\|P^J(\cdot, z) - P^{J,l}(\cdot, z)\|_V \leq C \exp\left(c \sum_{j=1}^J b_j |z_j|\right) \left(1 + \sum_{j=1}^J b_j |z_j|\right) 2^{-l} \quad (4.7.1)$$

Proof From Cea's lemma, we have

$$\begin{aligned} \|P^J(\cdot, z) - P^{J,l}(\cdot, z)\|_V &\leq \frac{K_{\max}^J(z)}{K_{\min}^J(z)} \inf_{Q \in V^l} \|P^J(\cdot, z) - Q\|_V \\ &\leq \frac{K_{\max}^J(z)}{K_{\min}^J(z)} 2^{-l} \|P^J(\cdot, z)\|_{H^2(D)}. \end{aligned}$$

We prove that when the domain D is convex and for $f \in L^2(D)$, there exist constants $C, c > 0$ such that, for every $z \in U$ and for every finite $J \in \mathbb{N}$ such that

$$\begin{aligned} \|P^J(\cdot, z)\|_{H^2(D)} &\leq C \frac{1}{K_{\min}^J(z)} (\|\nabla K^J(\cdot, z)\|_{L^\infty(D)} \frac{\|f\|_{V'}}{K_{\min}^J(z)} + \|f\|_{L^2(D)}) \\ &\leq C \exp\left(c \sum_{j=1}^J b_j |z_j|\right) \left(1 + \sum_{j=1}^J b_j |z_j|\right). \end{aligned}$$

We write equation (4.3.2) as

$$-\Delta P^J(\cdot, z) = \frac{1}{K^J(x, z)} (f + \nabla K^J(x, z) \cdot \nabla P^J(\cdot, z)).$$

From [28], we have

$$\|P^J(\cdot, z)\|_{H^2(D)} \leq \frac{1}{K_{\min}^J(z)} \left(\|f\|_{L^2(D)} + \|\nabla K^J(x, z)\|_{L^\infty(D)} \|\nabla P^J(\cdot, z)\|_{L^2(D)} \right).$$

To bound $\|\nabla P^J(\cdot, z)\|_{L^2(D)}$, we follow the standard procedure; multiplying (4.3.2) by P^J and integrating in D to get

$$K_{\min}^J(z) \|\nabla P^J(\cdot, z)\|_{L^2(D)}^2 \leq \|f\|_{V'} \|\nabla P^J(\cdot, z)\|_{L^2(D)}$$

$$\|\nabla P^J(\cdot, z)\|_{L^2(D)} \leq \frac{\|f\|_{V'}}{K_{\min}^J(z)}.$$

To bound $\|\nabla K^J(x, z)\|_{L^\infty(D)}$, we note that

$$\begin{aligned} \nabla K^J(\cdot, z) \\ = \nabla K_*(\cdot) + \exp\left(\bar{K}(\cdot) + \sum_{j=1}^J z_j \psi_j(\cdot)\right) \left(\nabla \bar{K}(\cdot) + \sum_{j=1}^J z_j \nabla \psi_j(\cdot)\right), \end{aligned}$$

implying that

$$\begin{aligned} & \|\nabla K^J(\cdot, z)\|_{L^\infty(D)} \\ & \leq \|\nabla K_*(\cdot)\|_{L^\infty(D)} + \left\| \exp\left(\bar{K}(\cdot) + \sum_{j=1}^J z_j \psi_j(\cdot)\right) \right\|_{L^\infty(D)} \left\| \nabla \bar{K}(\cdot) + \sum_{j=1}^J z_j \nabla \psi_j(\cdot) \right\|_{L^2(D)} \\ & \leq c + \exp\left(c + \sum_{j=1}^J |z_j| b_j\right) \left(c + \sum_{j=1}^J |z_j| \bar{b}_j\right). \end{aligned}$$

Therefore we have

$$\|P^J(\cdot, z) - P^{Jl}(\cdot, z)\|_V \leq C \exp\left(c \sum_{j=1}^J b_j |z_j|\right) \left(1 + \sum_{j=1}^J b_j |z_j|\right) 2^{-l}.$$

□

We then have the next proposition.

Proposition 4.7.2. Under Assumption 4.3.3, if D is convex and $f \in L^2(D)$, there exist constants $C, c > 0$ such that, for every $J, l \in \mathbb{N}$ and for every $z \in U$,

$$\begin{aligned} & \|P(\cdot, z) - P^{Jl}(\cdot, z)\|_V \\ & \leq C \exp\left(c \sum_{j=1}^J b_j |z_j|\right) \left(2^{-l} \left(1 + \sum_{j=1}^J b_j |z_j|\right) + \sum_{j=J+1}^{\infty} b_j |z_j|\right). \quad (4.7.2) \end{aligned}$$

Proof Using triangle inequality and Propositions 4.6.2 and 4.7.1, we get the result. □

We are now ready to prove Proposition 4.3.5.

Proof of Proposition 4.3.5: Following Proposition 4.3.2, we have that

$$|\mathcal{G}^{J,l}(z)| \leq c \exp\left(c \sum_{j=1}^{\infty} |z_j| b_j\right)$$

for a constant $c > 0$, and that

$$\begin{aligned} |\mathcal{G}^J(z) - \mathcal{G}^{J,l}(z)| &\leq \max_{0 \leq i \leq N} \{\|\ell_i\|_{V'}\} \|P^J(\cdot, z) - P^{J,l}(\cdot, z)\|_V \\ &\leq C \exp\left(c \sum_{j=1}^J b_j |z_j|\right) \left(1 + \sum_{j=1}^J b_j |z_j|\right) 2^{-l}. \end{aligned}$$

Let $Z^J(\delta)$ and $Z^{J,l}(\delta)$ be the normalizing constants in (4.3.4) and (4.3.10) respectively. We have

$$|\Phi^{J,l}(z, \delta)| \leq \frac{1}{2} \left| |\delta|^2 + |\mathcal{G}^{J,l}(z)|^2 \right| \leq C \exp\left(c \sum_{j=1}^{\infty} |z_j| b_j\right).$$

From Lemma 4.6.1, we have that

$$\int_U \Phi^{J,l}(z, \delta) d\gamma(z) < \Lambda$$

uniformly for all J, l . Fixing a constant $C > 0$, the γ measure of the set z such that $\Phi^{J,l}(z, \delta) > C$ is less than Λ/C so the γ measure of the set of z such that $\Phi^{J,l}(z, \delta) \leq C$ is more than $1 - \Lambda/C$ which is positive when C is sufficiently large. Thus

$$Z^{J,l}(\delta) = \int_U \exp(-\Phi^{J,l}(z, \delta)) d\gamma(z) > (1 - \Lambda/C) \exp(-C) > 0.$$

We note that it is sufficient to prove that $d_{Hell}(\gamma^{J,\delta}, \gamma^{J,l,\delta}) \leq c2^{-l}$. Following the procedure in Proposition 4.3.2, we have

$$2d_{Hell}(\gamma^{J,\delta}, \gamma^{J,l,\delta})^2 \leq I_1 + I_2,$$

where

$$I_1 = \frac{2}{Z^J(\delta)} \int_U \left(\exp(-\frac{1}{2}\Phi^J(z, \delta)) - \exp(-\frac{1}{2}\Phi^{J,l}(z, \delta)) \right)^2 d\gamma(z), \quad (4.7.3)$$

and

$$I_2 = 2|Z^J(\delta)^{-1/2} - Z^{J,l}(\delta)^{-1/2}|^2 \int_U \exp(-\Phi^{J,l}(z, \delta)) d\gamma(z). \quad (4.7.4)$$

We then have

$$\begin{aligned} \left| \exp(-\frac{1}{2}\Phi^J(z, \delta)) - \exp(-\frac{1}{2}\Phi^{J,l}(z, \delta)) \right| & \leq c(|\delta| + |\mathcal{G}^J(z)| + |\mathcal{G}^{J,l}(z)|) |\mathcal{G}^J(z) - \mathcal{G}^{J,l}(z)| \\ & \leq C \exp\left(c \sum_{j=1}^J b_j |z_j|\right) \left(1 + \sum_{j=1}^J b_j |z_j|\right) 2^{-l}. \end{aligned} \quad (4.7.5)$$

Thus

$$I_1 \leq c(\delta) \int_U \exp\left(c \sum_{j=1}^J b_j |z_j|\right) \left(1 + \sum_{j=1}^J b_j |z_j|\right)^2 2^{-2l} d\gamma(z).$$

From Lemma 4.6.1, we can show that

$$\int_U \exp\left(c \sum_{j=1}^J b_j |z_j|\right) \left(1 + \sum_{j=1}^J b_j |z_j|\right)^2 d\gamma(z) \leq c.$$

Therefore,

$$I_1 \leq c(\delta) 2^{-2l}.$$

To bound I_2 , we observe that

$$\begin{aligned} \left| Z^J(\delta)^{-\frac{1}{2}} - Z^{J,l}(\delta)^{-\frac{1}{2}} \right| & \leq C \max\{Z^J(\delta)^{-3}, Z^{J,l}(\delta)^{-3}\} |Z^J(\delta) - Z^{J,l}(\delta)|^2 \\ & \leq C |Z^J(\delta) - Z^{J,l}(\delta)|^2. \end{aligned}$$

From (4.7.5) and Lemma 4.6.1,

$$\begin{aligned} |Z^J(\delta) - Z^{J,l}(\delta)| &= \int_U |\exp(-\Phi^J(z, \delta)) - \exp(-\Phi^{J,l}(z, \delta))| d\gamma(z) \\ &\leq c(\delta)2^{-l}. \end{aligned}$$

Therefore,

$$I_2 \leq c(\delta)2^{-2l}.$$

Thus,

$$d_{\text{Hell}}(\gamma^{J,\delta}, \gamma^{J,l,\delta}) \leq \sqrt{I_1 + I_2} \leq c2^{-l}.$$

Together with $d_{\text{Hell}}(\gamma^\delta, \gamma^{J,\delta}) \leq cJ^{-q}$, we conclude the proof. $\square$

4.8 Appendix C

We prove Theorem 4.4.1 in this Appendix. To perform the error analysis of the MLMCMC approximation we decompose the error into three terms as follows.

Proposition 4.8.1. We have

$$\mathbb{E}^{\gamma^\delta}[\ell(P)] - E_L^{\text{MLMCMC}}[\ell(P)] = I_L + II_L + III_L \quad (4.8.1)$$

where

$$\begin{aligned} I_L &:= \mathbb{E}^{\gamma^\delta}[\ell(P)] - \mathbb{E}^{\gamma^L}[\ell(P)], \\ II_L &= \sum_{l=1}^L (\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}})[\ell(P) - \ell(P^{L'(l)})] + \mathbb{E}^{\gamma^0}[\ell(P) - \ell(P^{L'(0)})] \end{aligned}$$

and

$$III_L =$$

$$\begin{aligned}
& \sum_{l=1}^L \sum_{l'=1}^{L'(l)} \left[\mathbb{E}^{\gamma^l} [A_1^{ll'}] + \mathbb{E}^{\gamma^{l-1}} [A_2^{ll'}] + \mathbb{E}^{\gamma^l} [A_3^l] \cdot \mathbb{E}^{\gamma^{l-1}} [A_4^{ll'} + A_8^{ll'}] \right. \\
& \quad \left. + \mathbb{E}^{\gamma^{l-1}} [A_5^l] \cdot \mathbb{E}^{\gamma^l} [A_6^{ll'} + A_7^{ll'}] \right] \\
& + \sum_{l=1}^L \left[\mathbb{E}^{\gamma^l} [A_1^{l0}] + \mathbb{E}^{\gamma^{l-1}} [A_2^{l0}] + \mathbb{E}^{\gamma^l} [A_3^l] \cdot \mathbb{E}^{\gamma^{l-1}} [A_4^{l0} + A_8^{l0}] \right. \\
& \quad \left. + \mathbb{E}^{\gamma^{l-1}} [A_5^l] \cdot \mathbb{E}^{\gamma^l} [A_6^{l0} + A_7^{l0}] \right] \\
& + \sum_{l'=1}^{L'(0)} \mathbb{E}^{\gamma^0} [\ell(P^{l'} - P^{l'-1})] + \mathbb{E}^{\gamma^0} [\ell(P^0)] \\
& - E_L^{MLMCMC}[\ell(P)].
\end{aligned}$$

Proof From equation (3.4.4) we have

$$\mathbb{E}^{\gamma^\delta}[\ell(P)] - \mathbb{E}^{\gamma^L}[\ell(P)] = \mathbb{E}^{\gamma^\delta}[\ell(P)] - \sum_{l=1}^L \left(\mathbb{E}^{\gamma^l}[\ell(P)] - \mathbb{E}^{\gamma^{l-1}}[\ell(P)] \right) - \mathbb{E}^{\gamma^0}[\ell(P)]. \quad (4.8.2)$$

It follows that

$$\begin{aligned}
& \mathbb{E}^{\gamma^\delta}[\ell(P)] - \mathbb{E}^{\gamma^L}[\ell(P)] = \mathbb{E}^{\gamma^\delta}[\ell(P)] \\
& - \sum_{l=1}^L \left(\mathbb{E}^{\gamma^l}[\ell(P^{L'(l)})] - \mathbb{E}^{\gamma^{l-1}}[\ell(P^{L'(l)})] \right) - \mathbb{E}^{\gamma^0}[\ell(P^{L'(0)})] - II_L.
\end{aligned}$$

Rearranging and using (3.4.6) gives

$$\begin{aligned}
\mathbb{E}^{\gamma^\delta}[\ell(P)] & = I_L + II_L + \sum_{l=1}^L \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [\ell(P^{L'(l)})] + \mathbb{E}^{\gamma^0}[\ell(P^{L'(0)})] \\
& = I_L + II_L + \sum_{l=1}^L \sum_{l'=1}^{L'(l)} \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [\ell(P^{l'}) - \ell(P^{l'-1})] \\
& \quad + \sum_{l=1}^L (\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}}) [\ell(P^0)] \\
& \quad + \sum_{l'=1}^{L'(0)} \mathbb{E}^{\gamma^0} [\ell(P^{l'}) - \ell(P^{l'-1})] + \mathbb{E}^{\gamma^0}[\ell(P^0)].
\end{aligned}$$

We then get the conclusion. $\square$

To prove Theorem 4.4.1, we work under the following assumption of geometric ergodicity. Let $\mathcal{E}^{\bar{\gamma}, l}$ denote the expectation with respect to the probability space generated by the MCMC process with the acceptance probability defined in (4.4.1), with the initial sample $z^{(0)}$ distributed according to the probability measure $\bar{\gamma}$ defined in (4.4.4).

Assumption 4.8.2. Let C be a sufficiently large constant. For each l and l' in $\mathbb{N}$, we denote by

$$\mathcal{V}^{ll'}(z) = \exp \left(C \sum_{j=1}^{\infty} b_j |z_j| + \frac{1}{\varepsilon} \sum_{j > J_{l-1}} b_j |z_j| + \frac{1}{\varepsilon'} \sum_{j' > J_{l'-1}} b_{j'} |z_{j'}| \right) \quad (4.8.3)$$

where $\varepsilon = \sum_{j > J_{l-1}} b_j$ and $\varepsilon' = \sum_{j > J_{l'-1}} b_j$. Then if $g : U \rightarrow \mathbb{R}$ is a function such that $|g(z)| \leq \mathcal{V}^{ll'}(z)$ for every $z \in U$, there exists $C > 0$ independent of l and g such that for every $M \in \mathbb{N}$ we have

$$\left(\mathcal{E}^{\bar{\gamma}, l} \left[\left| \mathbb{E}^{\gamma^l}[g] - E_M^{\gamma^l}[g] \right| \right]^2 \right)^{1/2} \leq CM^{-1/2}.$$

Remark 4.8.3. We do not study geometric ergodicity in this thesis. However as in [33], geometric ergodicity for independent sampler can be shown which implies that Assumption 4.8.2 holds. For pCN sampler, if the spectral gap conditions in the paper by [29] holds, then Assumption 4.8.2 holds.

Remark 4.8.4. Assume that the expansion in (4.1.1) only has a finite number J of random variables z_j , i.e.

$$K(\cdot, z) = K_*(\cdot) + \exp \left(\bar{K}(\cdot) + \sum_{j=1}^J z_j \psi_j(\cdot) \right).$$

Then we can choose $\mathcal{V}^{ll'}$ as

$$\mathcal{V}^{ll'}(z) = \exp \left(11 \sum_{j=1}^J b_j |z_j| \right). \quad (4.8.4)$$

Proof of Theorem 4.4.1 We derive an error bound by estimating the three terms I_L , II_L and III_L in the error (4.8.1). Throughout we choose $J_l = 2^{\lceil l/q \rceil}$. For the first term I_L , from [51], we have

$$|(\mathbb{E}^{\gamma^\delta} - \mathbb{E}^{\gamma^L})[\ell(P)]| \leq 2 \left(\mathbb{E}^{\gamma^\delta}(\ell(P)^2) + \mathbb{E}^{\gamma^L}(\ell(P)^2) \right)^{1/2} d_{\text{Hell}}(\gamma^\delta, \gamma^L).$$

As the normalizing constant in (4.3.10) is uniformly (with respect to $J, l \in \mathbb{N}$) bounded from below away from zero, the expectations $\mathbb{E}^{\gamma^L}(\ell(P)^2)$ are uniformly bounded for all $L \in \mathbb{N}$. Then, there exists a constant $c > 0$ such that

$$\forall L \in \mathbb{N} : \quad |(\mathbb{E}^{\gamma^\delta} - \mathbb{E}^{\gamma^L})[\ell(P)]| \leq c2^{-L}.$$

For II_L , we note that

$$\begin{aligned} |II_L| &\leq \sum_{l=1}^L \left[2 \left(\mathbb{E}^{\gamma^l}(\ell(P - P^{L'(l)})^2) + \mathbb{E}^{\gamma^{l-1}}(\ell(P - P^{L'(l)})^2) \right)^{1/2} \cdot d_{\text{Hell}}(\gamma^l, \gamma^{l-1}) \right] \\ &\quad + c\mathbb{E}^\gamma[|\ell(P - P^{L'(0)})|]. \end{aligned}$$

From (4.7.2) we have that

$$\begin{aligned} \mathbb{E}^{\gamma^l}(\ell(P - P^{J_{L'(l)}})^2) &\leq c\mathbb{E}^\gamma(\ell(P - P^{L'(l)})^2) \leq c2^{-2L'(l)}, \\ \mathbb{E}^{\gamma^{l-1}}(\ell(P - P^{L'(l)})^2) &\leq c\mathbb{E}^\gamma(\ell(P - P^{J_{L'(l)}})^2) \leq c2^{-2L'(l)}, \end{aligned}$$

and

$$\mathbb{E}^\gamma[|\ell(P - P^{L'(l_0)})|] \leq c2^{-L'(0)}.$$

From Proposition 4.3.5, there exists a constant $c > 0$ such that for all $l \in \mathbb{N}$

$$d_{\text{Hell}}(\gamma^l, \gamma^{l-1}) \leq c2^{-l}.$$

Therefore

$$|II_L| \leq c \sum_{l=0}^L 2^{-(l+L'(l))}.$$

We now estimate III_L . Using inequalities $1 + x \leq \exp(x)$ and $x \leq \varepsilon \exp(x/\varepsilon)$ for $x, \varepsilon > 0$, we have from (4.3.11) that there exists a constant $C > 0$ such that, for every $z \in U$ and for every l, l', J for a positive constant c

$$\begin{aligned}
& |\ell(P^{J_{l'}, l'}(z) - P^{J_{l'-1}, l'-1}(z))| \\
& \leq C \exp\left(c \sum_{j=1}^{\infty} b_j |z_j|\right) \left(2^{-l'}(1 + \sum_{j=1}^{J_{l'}} b_j |z_j|) + \sum_{j=J_{l'-1}+1}^{\infty} b_j |z_j|\right) \\
& \leq C \exp\left(c \sum_{j=1}^{\infty} b_j |z_j|\right) \left(2^{-l'} \exp(\sum_{j=1}^{J_{l'}} b_j |z_j|) + \varepsilon' \exp(\frac{1}{\varepsilon'} \sum_{j>J_{l'-1}} b_j |z_j|)\right) \\
& \leq C 2^{-l'} \exp\left(c \sum_{j=1}^{\infty} b_j |z_j| + \sum_{j=1}^{J_{l'}} b_j |z_j| + \frac{1}{\varepsilon'} \sum_{j>J_{l'-1}} b_j |z_j|\right)
\end{aligned} \tag{4.8.5}$$

where $\varepsilon' = \sum_{j>J_{l'-1}} b_j \leq J_{l'-1}^{-q} \leq C 2^{-l'}$ is as in the definition of $\mathcal{V}^{ll'}$ in (4.8.3). Furthermore, for every $z \in U$,

$$\begin{aligned}
& |1 - \exp(\Phi^{J_l, l}(z, \delta) - \Phi^{J_{l-1}, l-1}(z, \delta))| \\
& \leq |\Phi^{J_l, l}(z, \delta) - \Phi^{J_{l-1}, l-1}(z, \delta)| (1 + \exp(\Phi^{J_l, l}(z, \delta) - \Phi^{J_{l-1}, l-1}(z, \delta))).
\end{aligned}$$

Therefore

$$|1 - \exp(\Phi^{J_l, l}(z, \delta) - \Phi^{J_{l-1}, l-1}(z, \delta))| I^l(z) \leq 2 |\Phi^{J_l, l}(z, \delta) - \Phi^{J_{l-1}, l-1}(z, \delta)|.$$

Thus, there exists a constant $C > 0$ such that for every $z \in U$ and for every $l, l', J \in \mathbb{N}$,

$$\begin{aligned}
& |1 - \exp(\Phi^{J_l, l}(z, \delta) - \Phi^{J_{l-1}, l-1}(z, \delta))| I^l(z) \\
& \leq C \exp\left(c \sum_{j=1}^{\infty} b_j |z_j|\right) \left(2^{-l}(1 + \sum_{j=1}^{J_l} b_j |z_j|) + \sum_{j=J_{l-1}+1}^{\infty} b_j |z_j|\right)
\end{aligned}$$

$$\begin{aligned}
&\leq C \exp \left(c \sum_{j=1}^{\infty} b_j |z_j| \right) \left(2^{-l} \exp \left(\sum_{j=1}^{J_l} b_j |z_j| \right) + \varepsilon \exp \left(\frac{1}{\varepsilon} \sum_{j>J_{l-1}} b_j |z_j| \right) \right) \\
&\leq C 2^{-l} \exp \left(c \sum_{j=1}^{\infty} b_j |z_j| + \sum_{j=1}^{J_l} b_j |z_j| + \frac{1}{\varepsilon} \sum_{j>J_{l-1}} b_j |z_j| \right). \tag{4.8.6}
\end{aligned}$$

where we defined $\varepsilon := \sum_{j>J_{l-1}} b_j \leq J_{l-1}^{-q} \leq C 2^{-l}$. We thus obtain a constant $c > 0$ such that, for every $z \in U$ and for every $l, l', J \in \mathbb{N}$,

$$\begin{aligned}
&|A_1^{ll'}(z)| \\
&= |1 - \exp(\Phi^{J_l, l}(z, \delta) - \Phi^{J_{l-1}, l-1}(z, \delta))| \left(\ell(P^{J_{l'}, l'}(z)) - \ell(P^{J_{l-1}, l'-1}(z)) \right) I^l(z) \\
&\leq c 2^{-(l+l')} \exp \left(c \sum_{j=1}^{\infty} b_j |z_j| + c \sum_{j=1}^{J_L} b_j |z_j| + \frac{1}{\varepsilon} \sum_{j>J_{l-1}} b_j |z_j| + \frac{1}{\varepsilon'} \sum_{j>J_{l'-1}} b_j |z_j| \right) \\
&\leq c 2^{-(l+l')} \mathcal{V}^{ll'}(z). \tag{4.8.7}
\end{aligned}$$

From Assumption 4.8.2, this implies the existence of a constant $C > 0$ such that, for every $l, l' \in \mathbb{N}$,

$$\mathbf{E}_L \left[\left| \mathbb{E}^{\gamma^l} [A_1^{ll'}] - E_{M_{ll'}}^{\gamma^l} [A_1^{ll'}] \right| \right] \leq C M_{ll'}^{-1/2} 2^{-(l+l')}.$$

Similarly, for every $z \in U$ we have $|A_2^{ll'}(z)| \leq 2^{-(l+l')} \mathcal{V}^{ll'}(z)$. Therefore, there is a constant $C > 0$ such that for every $z \in U$ and for every $l, l' \in \mathbb{N}$,

$$\mathbf{E}_L \left[\left| \mathbb{E}^{\gamma^l} [A_2^{ll'}] - E_{M_{ll'}}^{\gamma^l} [A_2^{ll'}] \right| \right] \leq C M_{ll'}^{-1/2} 2^{-(l+l')}.$$

To estimate the term $|\mathbb{E}^{\gamma^l} [A_3^l] \cdot \mathbb{E}^{\gamma^{l-1}} [A_4^{ll'}] - E_{M_{ll'}}^{\gamma^l} [A_3^l] \cdot E_{M_{ll'}}^{\gamma^{l-1}} [A_4^{ll'}]|$, we observe

$$\begin{aligned}
&\mathbf{E}_L \left[\left| \mathbb{E}^{\gamma^l} [A_3^l] \cdot \mathbb{E}^{\gamma^{l-1}} [A_4^{ll'}] - E_{M_{ll'}}^{\gamma^l} [A_3^l] \cdot E_{M_{ll'}}^{\gamma^{l-1}} [A_4^{ll'}] \right| \right] \\
&\leq \mathbf{E}_L \left[\left| \left(\mathbb{E}^{\gamma^l} [A_3^l] - E_{M_{ll'}}^{\gamma^l} [A_3^l] \right) \cdot \mathbb{E}^{\gamma^{l-1}} [A_4^{ll'}] \right| \right]
\end{aligned}$$

$$\begin{aligned}
& + \mathbf{E}_L \left[\left| \left(\mathbb{E}^{\gamma^{l-1}}[A_4^{l''}] - E_{M_{l''}}^{\gamma^{l-1}}[A_4^{l''}] \right) \cdot E_{M_{l''}}^{\gamma^l}[A_3^l] \right| \right] \\
& \leq \mathbf{E}_L \left[\left(\mathbb{E}^{\gamma^l}[A_3^l] - E_{M_{l''}}^{\gamma^l}[A_3^l] \right)^2 \right]^{1/2} \cdot \mathbb{E}^{\gamma^{l-1}}[|A_4^{l''}|] \\
& \quad + \mathbf{E}_L \left[\left(\mathbb{E}^{\gamma^{l-1}}[A_4^{l''}] - E_{M_{l''}}^{\gamma^{l-1}}[A_4^{l''}] \right)^2 \right]^{1/2} \cdot \mathbf{E}_L \left[E_{M_{l''}}^{\gamma^l}[A_3^l]^2 \right]^{1/2}.
\end{aligned}$$

From (4.8.5) and (4.8.6), for every $z \in U$ and for every $l \in \mathbb{N}$, $|A_3^l(z)| \leq c2^{-l}\mathcal{V}^{ll'}(z)$ and $|A_4^{l''}(z)| \leq c2^{-l'}\mathcal{V}^{ll'}(z)$. Assumption 4.8.2 then implies

$$\mathbf{E}_L \left[\left| \mathbb{E}^{\gamma^l}[A_3^l] \cdot \mathbb{E}^{\gamma^{l-1}}[A_4^{l''}] - E_{M_{l''}}^{\gamma^l}[A_3^l] \cdot E_{M_{l''}}^{\gamma^{l-1}}[A_4^{l''}] \right| \right] \leq cM_{ll}^{-1/2}2^{-(l+l')}.$$

We can estimate $E_L^{MLMCMC}[\ell(P)] - III_L$ similarly and obtain the same bound. We thus have

$$\begin{aligned}
\mathbf{E}_L[|III_L|] & \leq c \sum_{l=1}^L \sum_{l'=1}^{L'(l)} M_{ll'}^{-1/2} 2^{-(l+l')} + c \sum_{l=1}^L M_{l0}^{-1/2} 2^{-l} \\
& \quad + c \sum_{l'=0}^{L'(l_0)} M_{0l'}^{-1/2} 2^{-l'} + cM_{00}^{-1/2}.
\end{aligned} \tag{4.8.8}$$

We choose

$$\begin{aligned}
L'(l) &:= L - l, \quad \text{and} \quad M_{ll'} := 2^{2(L-(l+l'))} \quad \text{for} \quad l \geq 1, \quad l' \geq 1, \\
M_{l0} &= M_{0l} = 2^{2(L-l)}/L^2 \quad \text{and} \quad M_{00} = 2^{2L}/L^4.
\end{aligned} \tag{4.8.9}$$

We then have

$$\mathbf{E}_L[|III_L|] \leq c \sum_{l=0}^L (L-l)2^{-L} + cL^2 2^{-L} + cL^2 2^{-L} \leq CL^2 2^{-L}.$$

This bound is, up to logarithmic terms, of the same order as the discretization error of one instance of the forward problem on the finest mesh level L .

Next, we estimate the total number of degrees of freedom and floating point operations required for the MLMCMCFE method.

For each proposal $s^{(k)}$, the number of degrees of freedom for computing $\Phi^l(s^{(k)})$ is $O(2^{dl})$. The expectation of the total number of degrees of freedom required for running the MLMCMC FE method at discretization level L is bounded by

$$\begin{aligned}
&\lesssim \sum_{l=1}^L \sum_{l'=0}^{L'(l)} M_{ll'} (2^{dl} + 2^{dl'}) + \sum_{l'=0}^{L'(0)} M_{0l'} 2^{dl'} \\
&= 2^{2L} \sum_{l=0}^L \sum_{l'=0}^{L'(l)} \left(2^{(d-2)l} \cdot 2^{-2l'} + 2^{-2l} \cdot 2^{(d-2)l'} \right) + 2^{2L} \sum_{l'=0}^{L'(0)} 2^{(d-2)l'} \\
&\lesssim 2^{2L} \left(\sum_{l=0}^L 2^{(d-2)l} + \sum_{l=0}^L 2^{-2l} \sum_{l'=0}^{L-l} 2^{(d-2)l'} + \sum_{l'=0}^L 2^{(d-2)l'} \right).
\end{aligned}$$

Therefore for $d = 2$, the number of degrees of freedom is bounded by

$$\lesssim 2^{2L} \left(L + \sum_{l=0}^L 2^{-2l} (L-l) \right) \lesssim L 2^{2L}.$$

For $d = 3$, it is bounded by

$$\lesssim 2^{2L} \left(2^L + \sum_{l=0}^L 2^{-2l} 2^{L-l} \right) \lesssim 2^{2L} \left(2^L + \sum_{l=0}^L 2^L 2^{-3l} \right) \lesssim 2^{3L}.$$

From Lemma 4.3.4, the number of iteration to solve the system in (4.3.5) is

$$j^*(s) \geq C (|\log h| + |\log K_{\min}(s)|) \sqrt{\frac{K_{\max}(s)}{K_{\min}(s)}}$$

where the finite element mesh is h . With the mesh size $h = 2^{-l}$ and the truncation level $J_l = \lceil 2^{l/q} \rceil$, the total work for performing one step of the MCMC process for solving the linear system for a sample $s \in U$ is bounded by

$$\lesssim l^{d-1} 2^{l/q+ld} + (K(s))^{1/2} (K_{\min}(s))^{-1/2} (1 + |\log K_{\min}(s)|) l^d 2^{ld}.$$

The expectation of the number of floating point operations to compute $\Phi^{J_l, l}(s^{(k)}; \delta)$ is bounded by

$$\lesssim l^{d-1} 2^{l/q+ld} + l^d 2^{ld} \lesssim l^{d-1} 2^{l/q+ld}.$$

Therefore, the expectation of the total number of floating point operations at each step is not larger than

$$\lesssim l^{d-1} 2^{l/q+ld} + l'^{d-1} 2^{l'/q+dl'}.$$

With the choice (4.8.9) for the number of MCMC steps the total number of floating point operations required to evaluate the MLMCMC estimator is bounded by

$$\begin{aligned} & \lesssim \sum_{l=0}^L \sum_{l'=0}^{L'(l)} M_{ll'} (l^{d-1} 2^{l/q+ld} + l'^{d-1} 2^{l'/q+dl'}) + \sum_{l'=0}^{L'(0)} M_{0l'} (l'^{d-1} 2^{l'/q+dl'}) \\ & \lesssim 2^{2L} \sum_{l=0}^L \sum_{l'=0}^{L'(l)} (l^{d-1} 2^{(d-2+1/q)l} 2^{-2l'} + l'^{d-1} 2^{(d-2+1/q)l'} 2^{-2l}) \\ & \quad + 2^{2L} \sum_{l'=0}^{L'(l_0)} l'^{d-1} 2^{(d-2+1/q)l'} \\ & \lesssim L^{d-1} 2^{2L} \left(\sum_{l=0}^L 2^{(d-2+1/q)l} + \sum_{l=0}^L 2^{(d-2+1/q)(L-l)} 2^{-2l} \right) \\ & \lesssim L^{d-1} 2^{(d+1/q)L}. \end{aligned}$$

□

Chapter 5

Bayesian Inverse Problems for Parabolic Problems with Uniform Prior

We consider Bayesian inverse problems for finding the coefficients of parabolic equations with uniform prior probability in this chapter. We set up the problem in Section 5.1 where we define the prior probability space that is similar to the prior probability space in Chapter 3. In Section 5.2, we prove the existence and well-posedness of the posterior measure. Section 5.3 considers the approximation of the posterior measure by solving the forward parabolic equation by Backward Euler (BE) method and Finite Elements (FE). We deduce explicit error for the approximation with respect to the Hellinger distance in terms of the finite number of terms chosen in the truncated coefficient, the FE mesh size and the time step size. We develop the Multilevel Markov Chain Monte Carlo (MLMCMC) in Section 5.4. We establish rigorously the convergence rate of the MLMCMC estimator. In Section 5.5, we present some numerical examples that illustrate the theo-

retical results. The appendices at the end of the chapter contain the long proofs of some results in the previous sections.

5.1 Problem Setting

We consider the parabolic equation with coefficient K as defined in Chapter 3. In particular, we consider a bounded polygonal domain D in $\mathbb{R}^d$, $d = 1, 2, 3$, and the time interval $[0, T]$, where $T > 0$. We recall the coefficient K defined in Chapter 3 as

$$K(x, z) = \bar{K}(x) + \sum_{j=1}^{\infty} z_j \psi_j(x), \quad x \in D, \quad (5.1.1)$$

where z_j are independently and uniformly distributed in $[-1, 1]$ and $\bar{K}$ and ψ_j belong to $L^\infty(D)$. To provide a uniform bound with respect to z , we consider the following assumptions on the coefficient:

Assumption 5.1.1. The functions $\bar{K}$ and ψ_j are in $L^\infty(D)$. In addition, there exists a constant $\kappa > 0$ such that

$$\sum_{j=1}^{\infty} \|\psi_j\|_{L^\infty(D)} \leq \frac{\kappa}{1 + \kappa} \bar{K}_{\min}$$

where $\bar{K}_{\min} = \operatorname{ess\,inf}_{x \in D} \bar{K}(x) > 0$.

Under this assumption, we can bound the coefficient by

$$K_{\min} := \frac{1}{1 + \kappa} \bar{K}_{\min} \leq K(x, z) \leq \bar{K}_{\max} + \frac{\kappa}{1 + \kappa} \bar{K}_{\min} := K_{\max} \quad (5.1.2)$$

where $\bar{K}_{\max} = \operatorname{ess\,sup}_{x \in D} \bar{K}(x)$, for all $z \in U$. As random variables z_j are assumed uniformly distributed in $[-1, 1]$ and are pairwise independent, we consider the prior probability space (U, Θ, γ) given by

$$U = [-1, 1]^{\mathbb{N}}, \quad \Theta = \bigotimes_{i=1}^{\infty} \mathcal{B}([-1, 1]) \quad \text{and} \quad \gamma = \bigotimes_{i=1}^{\infty} \frac{dz_i}{2} \quad (5.1.3)$$

where $\mathcal{B}([-1, 1])$ is the Borel σ -algebra in $[-1, 1]$, and dz_i denotes the Lebesgue measure in $\mathbb{R}$. We consider the forward parabolic problem

$$\begin{aligned} \frac{\partial P}{\partial t}(t, x, z) - \nabla \cdot (K(x, z) \nabla P(t, x, z)) &= f(t, x) \\ \text{for } x \in D, t \in (0, T) \end{aligned} \quad (5.1.4)$$

with the Dirichlet boundary condition $P|_{\partial D} = 0$ and the initial condition $P(0, x, z) = g(x)$. Here $g \in H$ with $H := L^2(D)$ and $f \in L^2((0, T); V')$ with $V := H_0^1(D)$. By $(\cdot, \cdot)$ we denote the inner product in H , extending to the duality pairing between V' and V by density. We show in the next lemma that the solution P of (5.1.4) is uniformly bounded in $L^2((0, T); V)$ with respect to $z \in U$.

Lemma 5.1.2. Under Assumption 5.1.1, there exists a $C > 0$ such that

$$\|P(z)\|_{L^2((0, T); V)} \leq C \left(\|f\|_{L^2((0, T); V')} + \|g\|_H \right), \quad \forall z \in U.$$

The proof follows the standard procedure. We present it in Section 5.6 for completeness.

Without further regularity, we cannot specify the pointwise V -value of P with respect to t . We may consider observations of the form

$$\mathcal{G}(z) = (\mathcal{O}_1(P(\cdot, z)), \dots, \mathcal{O}_N(P(\cdot, z))) \quad (5.1.5)$$

where

$$\mathcal{O}_i(P(t, \cdot, z)) = \frac{1}{|I_i|} \int_{I_i} \ell_i(P(t, \cdot, z)) dt$$

for $\ell_i \in V'$ and $I_i = [a_i, b_i] \subset [0, T]$. With this kind of observations, the theory in the later sections still hold and can be shown by the same argument. However, to get an explicit convergence error for the approximation of the posterior measure by FE and BE, further regularity is needed. In

particular, we need $P \in H^1((0, T); V) \subset C([0, T]; V)$. This allows pointwise V -value identification with respect to each $t \in [0, T]$. We therefore assume this regularity from the beginning. For this regularity to hold, we assume:

Assumption 5.1.3. The functions $\bar{K}, \psi_j \in W^{1,\infty}(D)$ and that there is a $s > 1$ such that

$$\|\psi_j\|_{W^{1,\infty}(D)} < \frac{C}{j^s}.$$

Further, $f \in H^1((0, T); V')$, $f(0, \cdot) \in H$ and $g \in H^2(D)$.

Lemma 5.1.4. Under Assumption 5.1.3, then there exist a $C > 0$ such that

$$\|P(z)\|_{H^1((0,T);V)} \leq C, \quad \forall z \in U.$$

The proof makes use of Lemma 5.1.2 which is done in Section 5.6. Thus with Assumption 5.1.3 and Lemma 5.1.4, we, from here on, consider observations

$$\mathcal{G}(z) = (\ell_1(P(\tau_1, \cdot, z)), \dots, \ell_N(P(\tau_N, \cdot, z)))$$

where $\ell_i \in V'$ for $i = 1, \dots, N$, and $\tau_i \in (0, T)$. We consider the noisy observation of $\mathcal{G}$

$$\delta = \mathcal{G}(z) + \vartheta$$

where ϑ follows the Gaussian distribution $\mathcal{N}(0, \Sigma)$ in $\mathbb{R}^N$; Σ is the $N \times N$ covariance matrix that is symmetric and positive definite. Our objective is to find the posterior probability measure $\gamma^\delta = \mathbb{P}(z|\delta)$. By Bayes' rule, we will show that

$$\frac{d\gamma^\delta}{d\gamma} \propto \exp(-\Phi(z, \delta)) \tag{5.1.6}$$

where

$$\Phi(z, \delta) = \frac{1}{2} |\delta - \mathcal{G}(z)|_\Sigma^2$$

is the misfit or potential function where $|\cdot|_{\Sigma}^2 = \langle \Sigma^{-\frac{1}{2}} \cdot, \Sigma^{-\frac{1}{2}} \cdot \rangle$, $\langle \cdot, \cdot \rangle$ denotes the inner product in $\mathbb{R}^N$. We denote by

$$Z(\delta) = \int_U \exp(-\Phi(z, \delta)) d\gamma(z)$$

the normalising constant of (5.1.6).

5.2 Existence and Well-posedness of the Posterior measure

We start off with the proof of the existence of the posterior measure.

Proposition 5.2.1. Under Assumption 5.1.1, the solution $P : U \rightarrow V$ is Lipschitz when viewed as a map from U to $H^1((0, T); V)$. That is, for any $z, z' \in U$, there is a $C > 0$ such that

$$\|P(z) - P(z')\|_{H^1((0, T); V)} \leq C \|z - z'\|_{\ell^\infty(\mathbb{N})}.$$

This implies the existence of the posterior measure γ^δ which is determined by

$$\frac{d\gamma^\delta}{d\gamma} \propto \exp(-\Phi(z, \delta)).$$

Proof From the forward problem (5.1.4), for $z, z' \in U$, we get

$$\begin{aligned} \frac{\partial(P(z) - P(z'))}{\partial t} - \nabla \cdot (K(z) \nabla (P(z) - P(z'))) \\ = \nabla \cdot ((K(z) - K(z')) \nabla P(z')). \end{aligned}$$

Thus

$$\int_0^T \left(\frac{\partial(P(z) - P(z'))}{\partial t}, (P(z) - P(z')) \right) dt$$

$$\begin{aligned}
& + \int_0^T \int_D K(z) \nabla(P(z) - P(z')) \cdot \nabla(P(z) - P(z')) dx dt \\
& = - \int_0^T \int_D (K(z) - K(z')) \nabla P(z') \cdot \nabla(P(z) - P(z')) dx dt.
\end{aligned}$$

With $P(0, \cdot, z) - P(0, \cdot, z') = 0$ and the coerciveness of K , we get

$$\begin{aligned}
& K_{\min} \|P(z) - P(z')\|_{L^2((0,T);V)}^2 \\
& \leq \|K(z) - K(z')\|_{L^\infty(D)} \|P(z')\|_{L^2((0,T);V)} \|P(z) - P(z')\|_{L^2((0,T);V)}.
\end{aligned}$$

From Lemma 5.1.2, we get

$$\|P(z) - P(z')\|_{L^2((0,T);V)} \leq C \|K(z) - K(z')\|_{L^\infty(D)} \leq C \|z - z'\|_{\ell^\infty(\mathbb{N})}.$$

Similarly, for the time derivative, we have

$$\begin{aligned}
& \frac{\partial}{\partial t} \frac{\partial(P(z) - P(z'))}{\partial t} - \nabla \cdot \left(K(z) \nabla \frac{\partial}{\partial t} (P(z) - P(z')) \right) \\
& = \nabla \cdot \left((K(z) - K(z')) \nabla \frac{\partial}{\partial t} P(z') \right).
\end{aligned}$$

The initial condition is now $\frac{\partial}{\partial t}(P(0, \cdot, z) - P(0, \cdot, z')) = \nabla \cdot ((K(\cdot, z) - K(\cdot, z')) \nabla g(\cdot))$. Hence,

$$\begin{aligned}
& K_{\min} \left\| \frac{\partial}{\partial t} (P(z) - P(z')) \right\|_{L^2((0,T);V)}^2 \\
& \leq \|K(z) - K(z')\|_{L^\infty(D)} \left\| \frac{\partial}{\partial t} P(z') \right\|_{L^2((0,T);V)} \left\| \frac{\partial}{\partial t} (P(z) - P(z')) \right\|_{L^2((0,T);V)} \\
& \quad + \frac{1}{2} \left\| \nabla \cdot ((K(z) - K(z')) \nabla g(x)) \right\|_H^2.
\end{aligned}$$

From Lemma 5.1.4, we get

$$\begin{aligned}
& \|P(z) - P(z')\|_{H^1((0,T);V)} \\
& \leq C \|z - z'\|_{\ell^\infty(\mathbb{N})} + C \left\| \nabla \cdot ((K(z) - K(z')) \nabla g(x)) \right\|_H \\
& \leq C \|z - z'\|_{\ell^\infty(\mathbb{N})}.
\end{aligned}$$

This means that P as a map from U to $H^1((0, T); V)$ is continuous, implying P as a map from U to $C([0, T]; V)$ is continuous and therefore measurable. Thus the forward functional $\mathcal{G}(z)$ is continuous, and is also a measurable map from U to $\mathbb{R}^N$. From Theorem 2.1 of [12], the posterior measure γ^δ is determined by (5.1.6). $\square$

We show the well-posedness of the posterior measure next.

Proposition 5.2.2. Under Assumption 5.1.3, if $|\delta|_\Sigma, |\delta'|_\Sigma < r$, where r is a constant, there exists a constant $C(r) > 0$ such that

$$d_{\text{Hell}}(\gamma^\delta, \gamma^{\delta'}) \leq C(r) |\delta - \delta'|_\Sigma.$$

Proof We follow the procedure in Proposition 4.3.2,

$$2d_{\text{Hell}}(\gamma^\delta, \gamma^{\delta'})^2 = I_1 + I_2 \quad (5.2.1)$$

where

$$\begin{aligned} I_1 &= 2Z(\delta)^{-1} \int_U \left(\exp \left(-\frac{1}{2} \Phi(z, \delta) \right) - \exp \left(-\frac{1}{2} \Phi(z, \delta') \right) \right)^2 d\gamma(z) \\ I_2 &= 2 \left| Z(\delta)^{-\frac{1}{2}} - Z(\delta')^{-\frac{1}{2}} \right|^2 \int_U \left(\exp \left(-\frac{1}{2} \Phi(z, \delta') \right) \right)^2 d\gamma(z). \end{aligned}$$

As P is uniformly bounded

$$|\mathcal{G}(z)|_\Sigma \leq C \max_{1 \leq i \leq N} \{\|\ell_i\|_{V'}\} \sup_{t \in (0, T)} \|P(t, \cdot, z)\|_V \leq C. \quad (5.2.2)$$

Thus,

$$|\Phi(z, \delta)| = \frac{1}{2} |\delta - \mathcal{G}(z)|_\Sigma^2 \leq |\delta|_\Sigma^2 + |\mathcal{G}(z)|_\Sigma^2 \leq C(r). \quad (5.2.3)$$

Thus the normalizing constant $Z(\delta)$ in (5.1.6) is bounded for all δ such that $|\delta| < r$, due to

$$Z(\delta) = \int_U \exp(-\Phi(z, \delta)) d\gamma(z) \geq \gamma(U) \exp(-C(r)) \geq C(r) > 0.$$

Using $0 < \exp(-x) \leq 1$ for all $x \geq 0$ and $1 - \exp(-x) \leq |x|$ for all $x \in \mathbb{R}$ together with equation (5.2.2) and $|\delta|_\Sigma, |\delta'|_\Sigma \leq r$, we get

$$\begin{aligned}
& \exp\left(-\frac{1}{2}\Phi(z, \delta)\right) - \exp\left(-\frac{1}{2}\Phi(z, \delta')\right) \\
&= \exp\left(-\frac{1}{2}\Phi(z, \delta)\right) \left[1 - \exp\left(-\frac{1}{2}(\Phi(z, \delta') - \Phi(z, \delta))\right)\right] \\
&\leq \frac{1}{2} |\Phi(z, \delta) - \Phi(z, \delta')| \\
&\leq \frac{1}{4} \left| |\delta - \mathcal{G}(z)|_\Sigma^2 - |\delta' - \mathcal{G}(z)|_\Sigma^2 \right| \\
&\leq \frac{1}{4} [|\delta|_\Sigma + |\delta'|_\Sigma + |2\mathcal{G}(z)|_\Sigma] |\delta - \delta'|_\Sigma \\
&\leq C(r) |\delta - \delta'|.
\end{aligned} \tag{5.2.4}$$

Returning to equation (5.2.1), we can bound I_1 using (5.2.3) and (5.2.4) to get

$$I_1 \leq C(r) |\delta - \delta'|^2.$$

To bound I_2 , we observe that

$$\begin{aligned}
\left| Z(\delta)^{-\frac{1}{2}} - Z(\delta')^{-\frac{1}{2}} \right| &\leq C \max\{Z(\delta)^{-3}, Z(\delta')^{-3}\} |Z(\delta) - Z(\delta')|^2 \\
&\leq C(r) |Z(\delta) - Z(\delta')|^2.
\end{aligned} \tag{5.2.5}$$

From (5.2.4),

$$\begin{aligned}
|Z(\delta) - Z(\delta')| &\leq \int_U |\exp(-\Phi(z, \delta)) - \exp(-\Phi(z, \delta'))| d\gamma(z) \\
&\leq C(r) |\delta - \delta'|.
\end{aligned} \tag{5.2.6}$$

Therefore,

$$I_2 \leq C(r) |\delta - \delta'|^2.$$

Combining I_1 and I_2 , we conclude that

$$d_{H_{ell}}(\gamma^\delta, \gamma^{\delta'}) \leq \sqrt{I_1 + I_2} \leq C(r) |\delta - \delta'|.$$

□

5.3 Approximation by BE and FE method

We consider the truncated coefficient K^J by taking only a finite number of terms in (5.1.1):

$$K^J(x, z) = \bar{K}(x) + \sum_{j=1}^J z_j \psi_j(x), \quad \text{for all } x \in D, z \in U. \quad (5.3.1)$$

We approximate the solution of the forward equation by the solution of the truncated equation

$$\begin{aligned} \frac{\partial P^J}{\partial t}(t, x, z) - \nabla \cdot (K^J(x, z) \nabla P^J(t, x, z)) &= f(t, x) \\ \text{for } x \in D, t \in (0, T) \end{aligned} \quad (5.3.2)$$

with the Dirichlet boundary condition $P^J|_{\partial D} = 0$ and the initial condition $P^J(0, x, z) = g(x)$. We define the approximated forward function

$$\mathcal{G}^J(z) = (\ell_1(P^J(\tau_1, \cdot, z)), \dots, \ell_N(P^J(\tau_N, \cdot, z))) \in \mathbb{R}^N.$$

Let

$$\Phi^J(z, \delta) = \frac{1}{2} |\delta - \mathcal{G}^J(z)|^2.$$

We consider the approximated posterior measure

$$\frac{d\gamma^{J,\delta}}{d\gamma} \propto \exp(-\Phi^J(z, \delta)).$$

We have the result.

Proposition 5.3.1. Under Assumption 5.1.3, the approximated posterior measure satisfies

$$d_{Hell}(\gamma^\delta, \gamma^{J,\delta}) \leq C J^{-q}.$$

We will prove this in Section 5.6.

To apply the BE method, we partition $[0, T]$ by $0 = t_0 < t_1 < \dots < t_M = T$. We consider $t_m = mk$ for $m = 0, \dots, M$ where $k = \frac{T}{M}$ is the time step. We consider the finite element spaces we described in Chapter 3, Section 3.3, with mesh size $h_l = O(2^{-l})$. For ease of notations, we denote h_l by h . For $z \in U$, we solve the truncated forward parabolic problem by BE method.

We find a solution $P_m^{J,h,k}(z) \in V^l$ that satisfies

$$\begin{aligned} & \int_D \frac{P_m^{J,h,k}(x, z) - P_{m-1}^{J,h,k}(x, z)}{k} \phi(x) dx \\ & + \int_D K^J(x, z) \nabla P_m^{J,h,k}(x, z) \cdot \nabla \phi(x) dx = \int_D f(t_m, x) \phi(x) dx, \quad \forall \phi \in V^l \end{aligned} \quad (5.3.3)$$

with initial condition $P_0^{J,h,k}(x, z) = g^l(x)$ where $g^l(x)$ is an approximation of $g(x)$ in V^l . Assuming $g \in V \cap H^2(D)$ as in Assumption 5.1.3, we choose g^l so that $\|g - g^l\|_V \leq Ch$. For simplicity, we assume $\tau_i \in \{t_1, \dots, t_M\}$ $\forall i = 1, \dots, N$ and if $\tau_i = t_m$, denote $P_m^{J,h,k}$ by $P_{\tau_i}^{J,h,k}$. We define the approximated forward function

$$\mathcal{G}^{J,h,k}(z) = (\ell_1(P_{\tau_1}^{J,h,k}(\cdot, z)), \dots, \ell_N(P_{\tau_N}^{J,h,k}(\cdot, z))) \in \mathbb{R}^N.$$

Let

$$\Phi^{J,h,k}(z, \delta) = \frac{1}{2} |\delta - \mathcal{G}^{J,h,k}(z)|_{\Sigma}^2.$$

The approximated posterior measure is

$$\frac{d\gamma^{J,h,k,\delta}}{d\gamma} \propto \exp(-\Phi^{J,h,k}(z, \delta)), \quad (5.3.4)$$

with $Z^{J,h,k}(\delta) = \int_U \exp(-\Phi^{J,h,k}(z, \delta)) d\gamma(z)$ being the normalising constant.

We have the result

Proposition 5.3.2. Let D be a convex domain. Let f belong to $C([0, T]; H)$.

Under Assumption 5.1.3, the approximated posterior measure satisfies

$$d_{\text{Hell}}(\gamma^\delta, \gamma^{J,h,k,\delta}) \leq C(J^{-q} + h + k).$$

We will prove this in Section 5.7. As a quick remark, the effect for approximating the posterior probability measure by solving the forward equation by truncating the coefficient and solving the truncated equation using BE and FEM can be bounded as shown. This effect is observed in our numerical experiments when we are approximating the expectation with respect to the posterior probability measure by the expectation with respect to the approximated one.

5.4 Multilevel MCMC

We develop the MLMCMC for parabolic equation with uniform prior probability in this section. The method is quite similar to that presented in Chapter 3. We thus only touch upon the main points and present the convergence proof. We develop the method for approximating the posterior expectation for $\ell(P(T, \cdot, z))$ where $\ell \in V'$. However, the method works for other quantities of interest.

For conciseness, with the choice $J = \lceil 2^{l/q} \rceil$, $h_l = O(2^{-l})$ and $k = Th_l$, we denote $\gamma^{J, h_l, k, \delta}$ simply as γ^l , $P_m^{J, h_l, k}$ as P_m^l and $\Phi^{J, h_l, k}$ as Φ^l . As $T = t_M$ in Section 5.3, we denote by $P_M^{J, h_l, k}$ by P_T^l . We derive the MLMCMC estimator systematically as follows: We approximate the posterior measure first. This gives

$$\mathbb{E}^{\gamma^\delta}[\ell(P(T, \cdot, z))] \approx \mathbb{E}^{\gamma^L}[\ell(P(T, \cdot, z))].$$

We then expand the right hand side term into a telescopic sum,

$$\mathbb{E}^{\gamma^L}[\ell(P(T, \cdot, z))] = \sum_{l=1}^L \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [\ell(P(T, \cdot, z))] + \mathbb{E}^{\gamma^0}[\ell(P(T, \cdot, z))].$$

We then approximate the solution $P(T, \cdot, z)$ by $P_T^{L'(l)}$ at each level l where $L'(l)$ is a resolution level of approximation to be decided. We then have

$$\begin{aligned} \sum_{l=1}^L \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [\ell(P(T, \cdot, z))] + \mathbb{E}^{\gamma^0} [\ell(P(T, \cdot, z))] \\ \approx \sum_{l=1}^L \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [\ell(P_T^{L'(l)})] + \mathbb{E}^{\gamma^0} [\ell(P_T^{L'(0)})]. \end{aligned}$$

Similarly, writing $P_T^{L'(l)}$ as a telescopic sum, we get

$$\begin{aligned} \sum_{l=1}^L \sum_{l'=1}^{L'(l)} \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [\ell(P_T^{l'}) - \ell(P_T^{l'-1})] + \sum_{l=1}^L \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [\ell(P_T^0)] \\ + \sum_{l'=1}^{L'(0)} \mathbb{E}^{\gamma^0} [\ell(P_T^{l'}) - \ell(P_T^{l'-1})] + \mathbb{E}^{\gamma^0} [\ell(P_T^0)]. \quad (5.4.1) \end{aligned}$$

For each $l \geq 1$, we note that

$$\begin{aligned} \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [g] &= Z^l(\delta)^{-1} \int_U g(z) \exp(-\Phi^l(z, \delta)) d\gamma(z) \\ &\quad - Z^{l-1}(\delta)^{-1} \int_U g(z) \exp(-\Phi^{l-1}(z, \delta)) d\gamma(z) \end{aligned}$$

where $Z^l(\delta) = \int_U \exp(-\Phi^l(z, \delta)) d\gamma(z)$ is the normalizing constant. Adding and subtracting $Z^l(\delta)^{-1} \int_U g(z) \exp(-\Phi^{l-1}(z, \delta)) d\gamma(z)$, we get

$$\begin{aligned} \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [g] \\ = Z^l(\delta)^{-1} \int_U g(z) (1 - \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta))) \exp(-\Phi^l(z, \delta)) d\gamma(z) \\ + (Z^l(\delta)^{-1} - Z^{l-1}(\delta)^{-1}) \int_U g(z) \exp(-\Phi^{l-1}(z, \delta)) d\gamma(z). \end{aligned}$$

Rearranging,

$$\begin{aligned} \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [g] \\ = Z^l(\delta)^{-1} \int_U g(z) (1 - \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta))) \exp(-\Phi^l(z, \delta)) d\gamma(z) \\ + \left[Z^l(\delta)^{-1} (Z^{l-1}(\delta) - Z^l(\delta)) Z^{l-1}(\delta)^{-1} \int_U g(z) \exp(-\Phi^{l-1}(z, \delta)) d\gamma(z) \right]. \end{aligned}$$

We note that

$$\begin{aligned}
Z^l(\delta)^{-1}(Z^{l-1}(\delta) - Z^l(\delta)) \\
&= Z^l(\delta)^{-1} \int_U \exp(-\Phi^{l-1}(z, \delta)) - \exp(-\Phi^l(z, \delta)) d\gamma(z) \\
&= Z^l(\delta)^{-1} \int_U (\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) - 1) \exp(-\Phi^l(z, \delta)) d\gamma(z).
\end{aligned}$$

Therefore,

$$\begin{aligned}
(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}})[g] &= \mathbb{E}^{\gamma^l} \left[\left(1 - \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) \right) [g] \right] \\
&\quad + \mathbb{E}^{\gamma^l} [\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) - 1] \cdot \mathbb{E}^{\gamma^{l-1}}[g].
\end{aligned}$$

This implies that (5.4.1) can be written as

$$\begin{aligned}
&\sum_{l=1}^L \sum_{l'=1}^{L'(l)} \mathbb{E}^{\gamma^l} \left[\left(1 - \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) \right) (\ell(P_T^{l'}) - \ell(P_T^{l'-1})) \right] \\
&+ \sum_{l=1}^L \sum_{l'=1}^{L'(l)} \mathbb{E}^{\gamma^l} [\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) - 1] \cdot \mathbb{E}^{\gamma^{l-1}} [\ell(P_T^{l'}) - \ell(P_T^{l'-1})] \\
&+ \sum_{l=1}^L \mathbb{E}^{\gamma^l} \left[\left(1 - \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) \right) (\ell(P_T^0)) \right] \\
&+ \sum_{l=1}^L \mathbb{E}^{\gamma^l} [\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) - 1] \cdot \mathbb{E}^{\gamma^{l-1}} [\ell(P_T^0)] \\
&+ \sum_{l'=1}^{L'(0)} \mathbb{E}^{\gamma^0} [\ell(P_T^{l'}) - \ell(P_T^{l'-1})] + \mathbb{E}^{\gamma^0} [\ell(P_T^0)].
\end{aligned} \tag{5.4.2}$$

Approximating each expectation by the MCMC estimator, we get the MLMCMC estimator $E_L^{MLMCMC}[\ell(P(T, \cdot, z))]$, of $\mathbb{E}^{\gamma^\delta}[\ell(P(T, \cdot, z))]$,

$$\begin{aligned}
E_L^{MLMCMC}[\ell(P(T, \cdot, z))] = & \\
& \sum_{l=1}^L \sum_{l'=1}^{L'(l)} E_{M_{ll'}}^{\gamma^l} \left[\left(1 - \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) \right) (\ell(P_T^{l'}) - \ell(P_T^{l'-1})) \right] \\
& + \sum_{l=1}^L \sum_{l'=1}^{L'(l)} E_{M_{ll'}}^{\gamma^l} \left[\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) - 1 \right] \cdot E_{M_{ll'}}^{\gamma^{l-1}} \left[\ell(P_T^{l'}) - \ell(P_T^{l'-1}) \right] \\
& + \sum_{l=1}^L E_{M_{l0}}^{\gamma^l} \left[\left(1 - \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) \right) (\ell(P_T^0)) \right] \\
& + \sum_{l=1}^L E_{M_{l0}}^{\gamma^l} \left[\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) - 1 \right] \cdot E_{M_{l0}}^{\gamma^{l-1}} \left[\ell(P_T^0) \right] \\
& + \sum_{l=1}^L \sum_{l'=1}^{L'(0)} E_{M_{0l'}}^{\gamma^0} \left[\ell(P_T^{l'}) - \ell(P_T^{l'-1}) \right] + E_{M_{00}}^{\gamma^0} [\ell(P_T^0)].
\end{aligned} \tag{5.4.3}$$

where $E_{M_{ll'}}^{\gamma^l}$ represents the approximated expectation with respect to the posterior measure γ^l by MCMC with $M_{ll'}$ samples, with the acceptance probability

$$\alpha^l(z, s) = \min(1, \exp(\Phi^l(z, \delta) - \Phi^l(s, \delta))). \tag{5.4.4}$$

We choose the parameters

$$\begin{aligned}
L'(l) &= L - l, \quad M_{ll'} = 2^{2(L-(l+l'))} \quad \text{for } l \geq 1, \quad l' \geq 1, \\
M_{0l} &= M_{l0} = 2^{2L}/L^2, \quad M_{00} = 2^{2L}/L^4.
\end{aligned} \tag{5.4.5}$$

As in Chapter 3, let $C_l \subset \mathbb{R}^{J_l}$ be the Markov chain of an approximation level l with acceptance probability (5.4.4). Let $\mathcal{P}^{\gamma, J_l, l}$ denote the probability in the random space generated by this Markov chain with the initial state being distributed according to the prior measure γ . Let $\mathbf{C}_L = \{C_1, C_2, \dots, C_L\}$ be the probability space of all Markov chains for all approximated levels $l = 1, \dots, L$. We define the probability on $\mathbf{C}_L$ as

$$\mathbf{P}_L = \mathcal{P}^{\gamma, J_1, 1} \otimes \mathcal{P}^{\gamma, J_2, 2} \otimes \dots \otimes \mathcal{P}^{\gamma, J_L, L}.$$

Let $\mathbf{E}_L$ be the expectation in $\mathbf{C}_L$ with respect to $\mathbf{P}_L$. We have the following result.

Theorem 5.4.1. Assume that D is a convex domain and $f \in C([0, T]; H)$. For $d = 2, 3$, under Assumption 5.1.3, and with the parameter choices (5.4.5), there exists a constant $c(\delta) > 0$ such that for all $L \geq 1$

$$\mathbf{E}_L \left[\left| \mathbb{E}^{\gamma^\delta}[\ell(P(T, \cdot, z))] - E_L^{MLMCMC}[\ell(P(T, \cdot, z))] \right| \right] \leq C(\delta) L^2 2^{-L}. \quad (5.4.6)$$

Proof The proof is similar to that for the MLMCMC for elliptic equations with the uniform prior in [37]. The general idea is to break down the error into three parts; one is for approximating the posterior measure, one is for approximating the solution of the parabolic equation and the last is for using MCMC to estimate the expectation. To start, we express the error as

$$\begin{aligned} & \mathbb{E}^{\gamma^\delta}[\ell(P(T, \cdot, z))] - E_L^{MLMCMC}[\ell(P(T, \cdot, z))] \\ &= \mathbb{E}^{\gamma^\delta}[\ell(P(T, \cdot, z))] - \mathbb{E}^{\gamma^L}[\ell(P(T, \cdot, z))] \\ & \quad + \mathbb{E}^{\gamma^L}[\ell(P(T, \cdot, z))] - E_L^{MLMCMC}[\ell(P(T, \cdot, z))] \\ &= I_L + \sum_{l=1}^L \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [\ell(P(T, \cdot, z)) - \ell(P_T^{L'(l)})] \\ & \quad + \mathbb{E}^{\gamma^0}[\ell(P(T, \cdot, z)) - \ell(P_T^{L'(0)})] \\ & \quad + \sum_{l=1}^L \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [\ell(P_T^{L'(l)})] + \mathbb{E}^{\gamma^0}[\ell(P_T^{L'(0)})] - E_L^{MLMCMC}[\ell(P(T, \cdot, z))] \\ &= I_L + II_L + III_L \end{aligned}$$

where

$$\begin{aligned} I_L &= \mathbb{E}^{\gamma^\delta}[\ell(P(T, \cdot, z))] - \mathbb{E}^{\gamma^L}[\ell(P(T, \cdot, z))] \\ II_L &= \sum_{l=1}^L \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [\ell(P(T, \cdot, z)) - \ell(P_T^{L'(l)})] + \mathbb{E}^{\gamma^0}[\ell(P(T, \cdot, z)) - \ell(P_T^{L'(0)})] \end{aligned}$$

$$III_L = \sum_{l=1}^L \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) [\ell(P_T^{L'(l)})] + \mathbb{E}^{\gamma^0} [\ell(P_T^{L'(0)})] - E_L^{MLMCMC} [\ell(P(T, \cdot, z))].$$

We note that using (5.4.2) and (5.4.3) on III_L , we get

$$\begin{aligned} III_L &= \sum_{l=1}^L \sum_{l'=1}^{L'(l)} \left[\mathbb{E}^{\gamma^l} \left[\left(1 - \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) \right) (\ell(P_T^{l'}) - \ell(P_T^{l'-1})) \right] \right. \\ &\quad \left. - E_{M_{l'}}^{\gamma^l} \left[\left(1 - \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) \right) (\ell(P_T^{l'}) - \ell(P_T^{l'-1})) \right] \right] \\ &+ \sum_{l=1}^L \sum_{l'=1}^{L'(l)} \left[\mathbb{E}^{\gamma^l} \left[\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) - 1 \right] \cdot \mathbb{E}^{\gamma^{l-1}} \left[\ell(P_T^{l'}) - \ell(P_T^{l'-1}) \right] \right. \\ &\quad \left. - E_{M_{l'}}^{\gamma^l} \left[\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) - 1 \right] \cdot E_{M_{l'}}^{\gamma^{l-1}} \left[\ell(P_T^{l'}) - \ell(P_T^{l'-1}) \right] \right] \\ &+ \sum_{l=1}^L \left[\mathbb{E}^{\gamma^l} \left[\left(1 - \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) \right) (\ell(P_T^0)) \right] \right. \\ &\quad \left. - E_{M_{l_0}}^{\gamma^l} \left[\left(1 - \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) \right) (\ell(P_T^0)) \right] \right] \\ &+ \sum_{l=1}^L \left[\mathbb{E}^{\gamma^l} \left[\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) - 1 \right] \cdot \mathbb{E}^{\gamma^{l-1}} \left[\ell(P_T^0) \right] \right. \\ &\quad \left. - E_{M_{l_0}}^{\gamma^l} \left[\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) - 1 \right] \cdot E_{M_{l_0}}^{\gamma^{l-1}} \left[\ell(P_T^0) \right] \right] \\ &+ \sum_{l'=1}^{L'(0)} \left[\mathbb{E}^{\gamma^0} \left[\ell(P_T^{l'}) - \ell(P_T^{l'-1}) \right] - E_{M_{0l'}}^{\gamma^0} \left[\ell(P_T^{l'}) - \ell(P_T^{l'-1}) \right] \right] \\ &+ \mathbb{E}^{\gamma^0} [\ell(P_T^0)] - E_{M_{00}}^{\gamma^0} [\ell(P_T^0)]. \end{aligned}$$

Error term I_L is due to the approximation of the posterior γ^δ by γ^L . We estimate I_L by using the Hellinger distance of the two measures. From Proposition 5.3.2 with the choice $J = \lceil 2^{l/q} \rceil$, $h_l = 2^{-l}$ and $k = h_l$, we have

$$|I_L| \leq C d_{Hell}(\gamma^\delta, \gamma^L) \|\ell(P(T, \cdot, z))\|_{L^2(U, \gamma)} \leq C(\delta) 2^{-L}$$

which follows from the estimate in [51], Lemma 6.37. For the error term II_L , at each level $l \neq 0$, it represents the error due to the difference in posterior measure γ^l and γ^{l-1} followed by approximating the quantity of interest $\ell(P(T, \cdot, z))$ by $\ell(P_T^{L'(l)})$. When $l = 0$, it represents only the error from FE approximation of the solution. Like before, we can estimate the difference in the expectations with respect to γ^l and γ^{l-1} of a function by their Hellinger distance and the mean square norm of the function. That is, from [51],

$$\begin{aligned} & \left| \left(\mathbb{E}^{\gamma^l} - \mathbb{E}^{\gamma^{l-1}} \right) \left(\ell(P(T, \cdot, z)) - \ell(P_T^{L'(l)}) \right) \right| \\ & \leq Cd_{Hell}(\gamma^l, \gamma^{l-1}) \left\| \ell(P(T, \cdot, z)) - \ell(P_T^{L'(l)}) \right\|_{L^2(U, \gamma)} \\ & \leq Cd_{Hell}(\gamma^l, \gamma^{l-1}) \sup_{z \in U} \left\| P(T, \cdot, z) - P_T^{L'(l)} \right\|_V. \end{aligned}$$

Therefore, using the choice in equation (5.4.5),

$$II_L \leq C(\delta) \sum_{l=1}^L 2^{-(l+L'(l))} + 2^{-L'(0)} \leq C(\delta) L 2^{-L}.$$

Before bounding III_L , we recall two facts:

First, the MCMC algorithm produces an estimation of the expectation $\mathbb{E}^{\gamma^l}[g(z)]$, by $\frac{1}{M} \sum_{k=1}^M g(z^{(k)})$ where $z^{(k)}$ are the samples generated in the MCMC sampling, with a mean square error of

$$\left(\mathbf{E}_L \left[\left| \mathbb{E}^{\gamma^l}[g(z)] - \frac{1}{M} \sum_{k=1}^M g(z^{(k)}) \right|^2 \right] \right)^{\frac{1}{2}} \leq C \sup_{z \in U} |g(z)| M^{-\frac{1}{2}}.$$

Next,

$$\begin{aligned} & \sup_{z \in U} |1 - \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta))| \\ & \leq \sup_{z \in U} |\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)| (1 + \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta))) \end{aligned}$$

$$\begin{aligned}
&\leq C \sup_{z \in U} \frac{1}{2} |2|\delta|_{\Sigma} + |\mathcal{G}^l(z)| + |\mathcal{G}^{l-1}(z)| \|\mathcal{G}^l(z) - \mathcal{G}^{l-1}(z)\| \\
&\leq C \max_{0 \leq i \leq N} \{\|\ell_i\|_{V'}\} \max_{0 \leq i \leq N} \|P_{\tau_i}^l - P_{\tau_i}^{l-1}\|_V \\
&\leq C 2^{-l}
\end{aligned}$$

due to the uniform boundedness of $\Phi^l(z, \delta)$ with respect to z . Using these two facts and the Cauchy Schwarz inequality we can bound III_L by

$$\begin{aligned}
\mathbf{E}_L[|III_L|^2] &\leq CL \sum_{l=1}^L L'(l) \sum_{l'=1}^{L'(l)} M_{ll'}^{-1} 2^{-2(l+l')} + L \sum_{l=1}^L M_{l0}^{-1} 2^{-2l} + L'(0) \sum_{l'=1}^{L'(0)} M_{0l'}^{-1} 2^{-2l'} + M_{00}^{-1} \\
&\leq CL^4 2^{-2L}.
\end{aligned}$$

Combining all three terms, we conclude now that

$$\mathbf{E}_L \left[\left| \mathbb{E}^{\gamma^\delta}[\ell(P(T, \cdot, z))] - E_L^{MLMCMC}[\ell(P(T, \cdot, z))] \right| \right] \leq C(\delta) L^2 2^{-L}.$$

□

The logarithmic factor L^2 in the error bound may be reduced by increasing the sample numbers $M_{ll'}$. This can be done by choosing the sample numbers

$$M_{ll'} = (l + l')^a 2^{2(L-(l+l'))}$$

when $l \geq 1$ and $l' \geq 1$. The error due to the first two terms of (5.4.3) will then be bounded by an absolute multiple of $2^{-L} \sum_{l, l'=1}^L (l + l')^{-a/2}$. Table 5.1 collects the resulting asymptotic bounds, for some values of a .

Remark 5.4.2. By carrying out a procedure similar to that in the proof of Theorem 4.4.1, we can show that the total number of degrees of freedom required by the MLMCMC method is $O(2^{L(d+1)})$. For solving a realization of the forward parabolic equation, using mesh size $O(2^{-L})$ and time step $O(2^{-L})$, we also need $O(2^{L(d+1)})$ total degrees of freedom. Thus, the number of degrees of freedom required by the MLMCMC method is optimal.

a	$M_{ll'}, l, l' > 1$	$M_{l0} = M_{0l}$	M_{00}	Total error
0	$2^{2(L-(l+l'))}$	$2^{2(L-l)}/L^2$	$2^{2L}/L^4$	$O(L^2 2^{-L})$
2	$(l+l')^2 2^{2(L-(l+l'))}$	$2^{2(L-l)}$	$2^{2L}/L^2$	$O(L \log L 2^{-L})$
3	$(l+l')^3 2^{2(L-(l+l'))}$	$l 2^{2(L-l)}$	$2^{2L}/L$	$O(L^{1/2} 2^{-L})$
4	$(l+l')^4 2^{2(L-(l+l'))}$	$l^2 2^{2(L-l)}$	$2^{2L}/(\log L^2)$	$O(\log L 2^{-L})$

Table 5.1: Relation of total error with different a

5.5 Numerical experiments

We perform numerical experiments in this section to verify the theory of the convergence established in the previous sections. We consider two dimensional parabolic equations with the periodic boundary condition. The theory remains the same for periodic boundary condition as for Dirichlet boundary condition. The reason for considering periodic boundary condition is that we can solve the forward equation by Fourier spectral method with very high accuracy to obtain a reference posterior expectation from which we compare the MLMCMC approximation to illustrate the theoretical error in Table 5.1. We consider the case of a single random parameter z as this allows for an accurate reference to be computed due to a high number of quadrature points required to obtain an accurate reference expectation, though our numerical MATLAB code works for an arbitrary number of random variables z . This means we illustrate the balancing between $M_{ll'}$, h_l and k in the theoretical results.

We consider the forward parabolic problem:

$$\begin{aligned} \frac{\partial P}{\partial t}(t, x, z) - \nabla \cdot (K(x, z) \nabla P(t, x, z)) &= f(t, x), \\ \text{for } x \in D = (0, 1) \times (0, 1), t \in [0, 1] \end{aligned} \quad (5.5.1)$$

where

$$\begin{aligned} K(x, z) &= 3 + z (\sin(2\pi x_1) + \sin(2\pi x_2)), \\ f(t, x) &= 200(\sin(2\pi x_1) + \sin(2\pi x_2))t, \end{aligned}$$

with periodic boundary condition and initial condition $P(0, x) = 0$. The random variable z is uniformly distributed in $[-1, 1]$. The observation functional is chosen to be

$$\mathcal{G}(z) = \int_D x_1 \frac{\partial P}{\partial x_1}(1, x, z) + x_2 \frac{\partial P}{\partial x_2}(1, x, z), \quad (5.5.2)$$

and the quantity of interest is

$$\ell(P(z)) = \int_D x_1^{1.5} \frac{\partial P}{\partial x_1}(1, x, z) + x_2^{1.5} \frac{\partial P}{\partial x_2}(1, x, z). \quad (5.5.3)$$

The reference solution that we use to compare with the MLMCMC experimental results is computed using Fourier Collocation, with 21×21 collocation nodes, to discretize the physical space, and implicit Runge Kutta method of order 12 with time step $\frac{1}{32}$ to discretize the time interval. To obtain a noisy observation data, a random input z was generated from $\mathcal{U}[-1, 1]$ to get a response $\mathcal{G}(z)$, which was then added by a random Gaussian noise generated from $\mathcal{N}(0, 1)$. The results are presented with MLMCMC error plotted against the finest mesh level h_L . The error is obtained by taking the arithmetic average of absolute errors from 64 independent runs of the MLMCMC when compared to the reference solution. In Figure 5.1, we plot the MLMCMC error for $a = 0$ in the choice of $M_{ll'}$ in Table 5.1. The

Figure 5.1: MLMCMC error for 2D parabolic equation with uniform prior probability, $a = 0$

gradient of the best fit straight line is 0.9916. This is in agreement with the theory.

In Figures 5.2 and 5.3, we plot the MLMCMC errors for $a = 2$ and 3 respectively. The gradient of the best fit straight line is 1.031 and 0.9818 respectively. These again are in agreement with the theory.

5.6 Appendix A

We prove Lemmas 5.1.2, 5.1.4 and Proposition 5.6.2 in this appendix.

Figure 5.2: MLMCMC error for 2D parabolic equation with uniform prior probability, $a = 2$

Proof of Lemma 5.1.2: From (5.1.4)

$$\int_0^T \left(\frac{\partial P}{\partial t}(z), P(z) \right) dt + \int_0^T \int_D K \nabla P(z) \cdot \nabla P(z) dx dt = \int_0^T \int_D f P(z) dx dt.$$

This implies

$$\begin{aligned} \frac{1}{2} \|P(T, \cdot, z)\|_H^2 - \frac{1}{2} \|P(0, \cdot, z)\|_H^2 + K_{\min} \|P(z)\|_{L^2((0,T);V)}^2 \\ \leq \|f\|_{L^2((0,T);V')} \|P(z)\|_{L^2((0,T);V)} \end{aligned}$$

where $K_{\min}$ is defined in equation (5.1.2). Thus

$$K_{\min} \|\nabla P(z)\|_{L^2((0,T);H)}^2 \leq \frac{1}{2K_{\min}} \|f\|_{L^2((0,T);V')}^2 + \frac{K_{\min}}{2} \|P(z)\|_{L^2((0,T);V)}^2 + \frac{1}{2} \|g\|_H^2,$$

so

$$\|P(z)\|_{L^2((0,T);V)}^2 \leq \frac{1}{K_{\min}^2} \|f\|_{L^2((0,T);V')}^2 + \frac{1}{K_{\min}} \|g\|_H^2,$$

Figure 5.3: MLMCMC error for 2D parabolic equation with uniform prior probability, $a = 3$

which implies

$$\|P(z)\|_{L^2((0,T);V)} \leq C \left(\|f\|_{L^2((0,T);V')} + \|g\|_H \right).$$

□

Proof of Lemma 5.1.4: Differentiating the forward parabolic equation (5.1.4) with respect to t , we get

$$\frac{\partial}{\partial t} \left(\frac{\partial P}{\partial t}(z) \right) - \nabla \cdot \left(K \nabla \left(\frac{\partial P}{\partial t}(z) \right) \right) = \frac{\partial f}{\partial t} \quad (5.6.1)$$

with the initial condition

$$\frac{\partial P}{\partial t}(0, x, z) = f(0, x) + \nabla \cdot (K(z) \nabla g(x))$$

which belongs to H due to the additional regularity in Assumption 5.1.3. As $\frac{\partial f}{\partial t} \in L^2((0, T); V')$ and the initial condition is compatible, (5.6.1) is well-posed with $\frac{\partial P}{\partial t}(z) \in L^2((0, T); V)$ so $P(z) \in H^1((0, T); V) \subset C([0, T]; V)$. □

We state the following lemma:

Lemma 5.6.1. Under Assumptions 5.1.3, there exists a constant $C > 0$ that depends on the initial condition g , the function f , and the final time T such that

$$\|P^J(z)\|_{H^1((0,T);V)} \leq C.$$

The proof is identical to that of Lemma 5.1.4.

We recall that $q = s - 1$ where s is the constant in Assumption 5.1.3. We first prove:

Proposition 5.6.2. Suppose that Assumption 5.1.3 holds, then there exists a constant $C > 0$, dependent on g , f and T such that for all $J \in \mathbb{N}$ and $z \in U$,

$$\|P(z) - P^J(z)\|_{H^1((0,T);V)} \leq CJ^{-q}$$

Proof Subtracting equation (5.3.2) from equation (5.1.4), we get

$$\frac{\partial}{\partial t}(P(z) - P^J(z)) - \nabla \cdot (K(z) \nabla (P(z) - P^J(z))) = \nabla \cdot ((K(z) - K^J(z)) \nabla P^J(z)).$$

Multiply by $P(z) - P^J(z)$ and integrating over D and $[0, T]$, we get

$$\begin{aligned} & \int_0^T \left(\frac{\partial}{\partial t}(P(z) - P^J(z)), (P(z) - P^J(z)) \right) dt \\ & + \int_0^T \int_D K(z) \nabla (P(z) - P^J(z)) \cdot \nabla (P(z) - P^J(z)) dx dt \\ & = - \int_0^T \int_D (K(z) - K^J(z)) \nabla P^J(z) \cdot \nabla (P(z) - P^J(z)) dx dt. \end{aligned}$$

Using the coerciveness of K , we have

$$\frac{1}{2} \|(P - P^J)(T, \cdot, z)\|_H^2 - \frac{1}{2} \|(P - P^J)(0, \cdot, z)\|_H^2$$

$$\begin{aligned}
& + K_{\min} \left\| \nabla(P(z) - P^J(z)) \right\|_{L^2((0,T);H)}^2 \\
& \leq \left\| K(z) - K^J(z) \right\|_{L^\infty(D)} \left\| \nabla P^J(z) \right\|_{L^2((0,T);H)} \left\| \nabla(P(z) - P^J(z)) \right\|_{L^2((0,T);H)} .
\end{aligned} \tag{5.6.2}$$

As $(P - P^J)(0, \cdot, z) = 0$,

$$\begin{aligned}
& K_{\min} \left\| P(z) - P^J(z) \right\|_{L^2((0,T);V)}^2 \\
& \leq \left\| K(z) - K^J(z) \right\|_{L^\infty(D)} \left\| P^J(z) \right\|_{L^2((0,T);V)} \left\| (P(z) - P^J(z)) \right\|_{L^2((0,T);V)} ,
\end{aligned}$$

implying

$$\left\| P(z) - P^J(z) \right\|_{L^2((0,T);V)} \leq \frac{1}{K_{\min}} \left\| K(z) - K^J(z) \right\|_{L^\infty(D)} \left\| P^J(z) \right\|_{L^2((0,T);V)} .$$

We note that

$$\begin{aligned}
\left\| K(z) - K^J(z) \right\|_{L^\infty(D)} &= \left\| \sum_{j>J} z_j \psi_j(x) \right\|_{L^\infty(D)} \\
&\leq \sup_{j>J} z_j \left\| \sum_{j>J} \psi_j(x) \right\|_{L^\infty(D)} \leq C J^{-q} .
\end{aligned}$$

Together with Lemma 5.6.1, we have

$$\left\| P(z) - P^J(z) \right\|_{L^2((0,T);V)} \leq C J^{-q} .$$

For the bound in $H^1((0,T);V)$, we follow the same procedure to get

$$\begin{aligned}
& \frac{1}{2} \left\| \frac{\partial}{\partial t}(P - P^J)(T, \cdot, z) \right\|_H^2 - \frac{1}{2} \left\| \frac{\partial}{\partial t}(P - P^J)(0, \cdot, z) \right\|_H^2 \\
& \quad + K_{\min} \left\| \nabla \frac{\partial}{\partial t}(P(z) - P^J(z)) \right\|_{L^2((0,T);H)}^2 \\
& \leq \left\| K(z) - K^J(z) \right\|_{L^\infty(D)} \left\| \nabla \frac{\partial P^J(z)}{\partial t} \right\|_{L^2((0,T);H)} \left\| \nabla \frac{\partial}{\partial t}(P(z) - P^J(z)) \right\|_{L^2((0,T);H)} .
\end{aligned} \tag{5.6.3}$$

We note that

$$\begin{aligned} \left(\frac{\partial}{\partial t} (P - P^J) \right) (0, \cdot, z) &= \nabla \cdot ((K(z) - K^J(z)) \nabla g(x)) \\ &= \nabla (K(z) - K^J(z)) \cdot \nabla g(x) + (K(z) - K^J(z)) \nabla \cdot \nabla g(x). \end{aligned}$$

It then follows from Assumption 5.1.3 that

$$\begin{aligned} \left\| \left(\frac{\partial}{\partial t} (P - P^J) \right) (0, \cdot, z) \right\|_H^2 &\leq \|K(z) - K^J(z)\|_{W^{1,\infty}(D)}^2 \|g\|_{H^1(D)}^2 \\ &\quad + \|(K(z) - K^J(z))\|_{L^\infty(D)}^2 \|g\|_{H^2(D)}^2 \end{aligned}$$

where

$$\begin{aligned} \|K(z) - K^J(z)\|_{W^{1,\infty}(D)} &= \left\| \sum_{j>J} z_j \psi_j(x) \right\|_{W^{1,\infty}(D)} \\ &\leq \sup_{j>J} z_j \left\| \sum_{j>J} \psi_j(x) \right\|_{W^{1,\infty}(D)} \\ &\leq C J^{-q}. \end{aligned}$$

Therefore

$$\left\| \left(\frac{\partial}{\partial t} (P - P^J) \right) (0, \cdot, z) \right\|_H^2 \leq C J^{-2q}.$$

From to (5.6.3), we get

$$\begin{aligned} &\left\| \nabla \frac{\partial}{\partial t} (P(z) - P^J(z)) \right\|_{L^2((0,T);H)} \\ &\leq \frac{1}{K_{\min}} \|K(z) - K^J(z)\|_{L^\infty(D)} \left\| \nabla \frac{\partial P^J(z)}{\partial t} \right\|_{L^2((0,T);H)} \\ &\quad + \frac{1}{K_{\min}^{1/2}} \left\| \left(\frac{\partial}{\partial t} (P - P^J) \right) (0, \cdot, z) \right\|_H, \end{aligned}$$

and using Lemma 5.6.1, we conclude that $\|P(z) - P^J(z)\|_{H^1((0,T);V)} \leq C J^{-q}$

□

We are now ready to prove Proposition 5.3.1.

Proof of Proposition 5.3.1: Following closely the proof of Proposition 5.2.2, we have

$$2d_{\text{Hell}}(\gamma^\delta, \gamma^{J,\delta})^2 \leq I_1 + I_2 \quad (5.6.4)$$

where

$$\begin{aligned} I_1 &= 2Z(\delta)^{-1} \int_U \left(\exp\left(-\frac{1}{2}\Phi(z, \delta)\right) - \exp\left(-\frac{1}{2}\Phi^J(z, \delta)\right) \right)^2 d\gamma(z) \\ I_2 &= 2 \left| Z(\delta)^{-\frac{1}{2}} - Z^J(\delta)^{-\frac{1}{2}} \right|^2 \int_U \left(\exp\left(-\frac{1}{2}\Phi^J(z, \delta)\right) \right)^2 d\gamma(z). \end{aligned}$$

We observe that,

$$\begin{aligned} & \exp\left(-\frac{1}{2}\Phi(z, \delta)\right) - \exp\left(-\frac{1}{2}\Phi^J(z, \delta)\right) \\ &= \exp\left(-\frac{1}{2}\Phi(z, \delta)\right) \left[1 - \exp\left(-\frac{1}{2}(\Phi^J(z, \delta) - \Phi(z, \delta))\right) \right] \\ &\leq \frac{1}{2} |\Phi(z, \delta) - \Phi^J(z, \delta)| \\ &= \frac{1}{4} \left| |\delta - \mathcal{G}(z)|_\Sigma^2 - |\delta - \mathcal{G}^J(z)|_\Sigma^2 \right| \\ &\leq \frac{1}{4} [2|\delta|_\Sigma + |\mathcal{G}^J(z)|_\Sigma + |\mathcal{G}(z)|_\Sigma] [|\mathcal{G}(z) - \mathcal{G}^J(z)|_\Sigma] \\ &\leq C(r) \max_{1 \leq i \leq N} \{\|\ell_i\|_{V'}\} \sup_{t \in (0, T)} \|(P - P^J)(t, \cdot, z)\|_V. \end{aligned} \quad (5.6.5)$$

From Proposition 5.6.2,

$$\left| \exp\left(-\frac{1}{2}\Phi(z, \delta)\right) - \exp\left(-\frac{1}{2}\Phi^J(z, \delta)\right) \right| \leq C(r)J^{-q}.$$

Recall that $Z(\delta) > C(r)$ shown in Proposition 5.2.2, hence

$$I_1 \leq C(r)J^{-2q}.$$

Next, we observe that

$$|\mathcal{G}^J(z)|_\Sigma \leq C \max_{1 \leq i \leq N} \{\|\ell_i\|_{V'}\} \sup_{t \in (0, T)} \|P^J(t, \cdot, z)\|_V \leq C$$

and

$$|\Phi^J(z, \delta)| = \frac{1}{2} |\delta - \mathcal{G}^J(z)|_\Sigma^2 \leq |\delta|_\Sigma^2 + |\mathcal{G}^J(z)|_\Sigma^2 \leq C(r).$$

To bound I_2 , we observe that

$$\begin{aligned} \left| Z(\delta)^{-\frac{1}{2}} - Z^J(\delta)^{-\frac{1}{2}} \right| &\leq C \max\{Z(\delta)^{-3}, Z^J(\delta)^{-3}\} |Z(\delta) - Z^J(\delta)|^2 \\ &\leq C(r) |Z(\delta) - Z^J(\delta)|^2. \end{aligned} \quad (5.6.6)$$

From (5.6.5),

$$\begin{aligned} |Z(\delta) - Z^J(\delta)| &= \int_U |\exp(-\Phi(z, \delta)) - \exp(-\Phi^J(z, \delta))| d\gamma(z) \\ &\leq C(r) J^{-q}. \end{aligned} \quad (5.6.7)$$

This implies that

$$I_2 \leq C(r) J^{-2q}.$$

Combining I_1 and I_2 ,

$$d_{\text{Hell}}(\gamma^\delta, \gamma^{J,\delta}) \leq \sqrt{I_1 + I_2} \leq C J^{-q}.$$

□

5.7 Appendix B

We prove Proposition 5.3.2 in this appendix. We state the following lemma which will be used in the next proposition.

Lemma 5.7.1. Assume that D is a convex domain. Suppose that $R_h : V \rightarrow V^l$ is the orthogonal projection that satisfies

$$\int_D K^J \nabla R_h \psi \cdot \nabla \phi dx = \int_D K^J \nabla \psi \cdot \nabla \phi dx, \quad \forall \psi \in V \text{ and } \forall \phi \in V^l$$

Then there exists $C > 0$ independent of h and J such that

$$\|R_h \psi - \psi\|_H \leq Ch \|\psi\|_V \quad \text{and} \quad \|R_h \psi - \psi\|_V \leq Ch \|\psi\|_{H^2(D)}$$

if $\psi \in H^2(D)$.

The proof is standard. We refer to Thom [52] Theorem 1.1.

Proposition 5.7.2. Let D be a convex domain. Let f belong to $C([0, T]; H)$. Under Assumption 5.1.3 and choosing $\|g - g^l\|_V \leq Ch$, let $P_m^{J,h,k}(z)$ be the solution of problem (5.3.3). Then there exists a constant $C > 0$ such that for all $z \in U$ and for all $m = 1, \dots, M$,

$$\|P(t_m, \cdot, z) - P_m^{J,h,k}(\cdot, z)\|_V \leq C(J^{-q} + h + k).$$

Proof First we estimate the error of the BE approximation in (5.3.3). This follows the standard procedure, see [52]. For completeness and for preparation for the more complicated estimate in Chapter 6, we present the full proof here.

Using triangle inequality, we get

$$\begin{aligned} & \|P(t_m, \cdot, z) - P_m^{J,h,k}(\cdot, z)\|_V \\ & \leq \|P(t_m, \cdot, z) - P^J(t_m, \cdot, z)\|_V + \|P^J(t_m, \cdot, z) - P_m^{J,h,k}(\cdot, z)\|_V. \end{aligned}$$

From Proposition 5.6.2, we have

$$\|P(t_m, \cdot, z) - P^J(t_m, \cdot, z)\|_V \leq CJ^{-q}.$$

Thus we estimate

$$\begin{aligned} & \|P_m^{J,h,k}(\cdot, z) - P^J(t_m, \cdot, z)\|_V \\ & \leq \|P_m^{J,h,k}(\cdot, z) - R_h P^J(t_m, \cdot, z)\|_V + \|R_h P^J(t_m, \cdot, z) - P^J(t_m, \cdot, z)\|_V \\ & = \|\theta^m\|_V + \|\varphi^m\|_V \end{aligned}$$

where

$$\theta^m = P_m^{J,h,k}(\cdot, z) - R_h P^J(t_m, \cdot, z) \quad \text{and} \quad \varphi^m = R_h P^J(t_m, \cdot, z) - P^J(t_m, \cdot, z).$$

We consider

$$\begin{aligned}
& \int_D \frac{\theta^m - \theta^{m-1}}{k} \phi dx + \int_D K^J(\cdot, z) \nabla \theta^m \cdot \nabla \phi dx \\
&= \int_D \frac{P_m^{J,h,k}(\cdot, z) - P_{m-1}^{J,h,k}(\cdot, z)}{k} \phi dx - \int_D \frac{R_h P^J(t_m, \cdot, z) - R_h P^J(t_{m-1}, \cdot, z)}{k} \phi dx \\
&+ \int_D K^J(\cdot, z) \nabla P_m^{J,h,k}(\cdot, z) \cdot \nabla \phi dx - \int_D K^J(\cdot, z) \nabla R_h P^J(t_m, \cdot, z) \cdot \nabla \phi dx.
\end{aligned}$$

By (5.3.3) and definition of R_h ,

$$\begin{aligned}
& \int_D \frac{\theta^m - \theta^{m-1}}{k} \phi dx + \int_D K^J(\cdot, z) \nabla \theta^m \cdot \nabla \phi dx \\
&= \int_D f(t_m, \cdot) \phi dx - \int_D \frac{R_h P^J(t_m, \cdot, z) - R_h P^J(t_{m-1}, \cdot, z)}{k} \phi dx \\
&\quad - \int_D K^J(\cdot, z) \nabla P^J(t_m, \cdot, z) \cdot \nabla \phi dx.
\end{aligned}$$

Adding and subtracting $\int_D \frac{\partial P^J}{\partial t}(t_m, \cdot, z) \phi dx$,

$$\begin{aligned}
& \int_D \frac{\theta^m - \theta^{m-1}}{k} \phi dx + \int_D K^J(\cdot, z) \nabla \theta^m \cdot \nabla \phi dx \\
&= \int_D f(t_m, \cdot) \phi dx \\
&\quad - \int_D \frac{R_h P^J(t_m, \cdot, z) - R_h P^J(t_{m-1}, \cdot, z)}{k} \phi dx + \int_D \frac{\partial P^J}{\partial t}(t_m, \cdot, z) \phi dx \\
&\quad - \int_D \frac{\partial P^J}{\partial t}(t_m, \cdot, z) \phi dx - \int_D K^J(\cdot, z) \nabla P^J(t_m, \cdot, z) \cdot \nabla \phi dx.
\end{aligned}$$

Using (5.3.2),

$$\begin{aligned}
& \int_D \frac{\theta^m - \theta^{m-1}}{k} \phi dx + \int_D K^J(\cdot, z) \nabla \theta^m \cdot \nabla \phi dx \\
&= \int_D f(t_m, \cdot) \phi dx \\
&\quad - \int_D \frac{R_h P^J(t_m, \cdot, z) - R_h P^J(t_{m-1}, \cdot, z)}{k} \phi dx + \int_D \frac{\partial P^J}{\partial t}(t_m, \cdot, z) \phi dx \\
&\quad - \int_D f(t_m, \cdot) \phi dx.
\end{aligned}$$

This implies that

$$\int_D \frac{\theta^m - \theta^{m-1}}{k} \phi dx + \int_D K^J(\cdot, z) \nabla \theta^m \cdot \nabla \phi dx = - \int_D \omega^m \phi dx \quad (5.7.1)$$

where $\omega^m = \frac{R_h P^J(t_m, \cdot, z) - R_h P^J(t_{m-1}, \cdot, z)}{k} - \frac{\partial P^J}{\partial t}(t_m, \cdot, z)$. We write $\omega^m = \omega_1^m + \omega_2^m$ where

$$\begin{aligned} \omega_1^m &= \frac{R_h P^J(t_m, \cdot, z) - R_h P^J(t_{m-1}, \cdot, z)}{k} - \frac{P^J(t_m, \cdot, z) - P^J(t_{m-1}, \cdot, z)}{k} \\ \omega_2^m &= \frac{P^J(t_m, \cdot, z) - P^J(t_{m-1}, \cdot, z)}{k} - \frac{\partial P^J}{\partial t}(t_m, \cdot, z). \end{aligned}$$

We note that

$$\begin{aligned} \int_D \nabla \theta^m \cdot \nabla \frac{\theta^m - \theta^{m-1}}{k} dx \\ = \frac{1}{2} \left[\frac{\|\nabla \theta^m\|_H^2 - \|\nabla \theta^{m-1}\|_H^2}{k} + k \left\| \nabla \left(\frac{\theta^m - \theta^{m-1}}{k} \right) \right\|_H^2 \right]. \end{aligned}$$

From (5.7.1), under Assumption 5.1.3, letting $\phi = \frac{\theta^m - \theta^{m-1}}{k}$,

$$\begin{aligned} \left\| \frac{\theta^m - \theta^{m-1}}{k} \right\|_H^2 + K_{\min} \int_D \nabla \theta^m \cdot \nabla \left(\frac{\theta^m - \theta^{m-1}}{k} \right) dx \\ \leq \int_D \omega^m \left(\frac{\theta^m - \theta^{m-1}}{k} \right) dx. \end{aligned}$$

Thus

$$\begin{aligned} \left\| \frac{\theta^m - \theta^{m-1}}{k} \right\|_H^2 + \frac{K_{\min}}{2} \left[\frac{\|\nabla \theta^m\|_H^2 - \|\nabla \theta^{m-1}\|_H^2}{k} + k \left\| \nabla \left(\frac{\theta^m - \theta^{m-1}}{k} \right) \right\|_H^2 \right] \\ \leq \frac{1}{2} \|\omega^m\|_H^2 + \frac{1}{2} \left\| \frac{\theta^m - \theta^{m-1}}{k} \right\|_H^2, \end{aligned}$$

which implies

$$\frac{K_{\min}}{2} \frac{\|\nabla \theta^m\|_H^2 - \|\nabla \theta^{m-1}\|_H^2}{k} \leq \frac{1}{2} \|\omega^m\|_H^2.$$

Thus

$$\|\theta^m\|_V^2 \leq Ck \|\omega^m\|_H^2 + \|\theta^{m-1}\|_V^2,$$

and recursively,

$$\|\theta^m\|_V^2 \leq Ck \sum_{i=1}^m \|\omega^i\|_H^2 + \|\theta^0\|_V^2.$$

Therefore

$$\|\theta^m\|_V^2 \leq Ck \sum_{i=1}^m \|\omega_1^i\|_H^2 + Ck \sum_{i=1}^m \|\omega_2^i\|_H^2 + \|\theta^0\|_V^2. \quad (5.7.2)$$

We observe that

$$\begin{aligned} |\omega_1^m| &= \left| (R_h - I) \frac{1}{k} \int_{t_{m-1}}^{t_m} P_t^J(s, \cdot, z) ds \right| \\ &= \left| \frac{1}{k} \int_{t_{m-1}}^{t_m} (R_h - I) P_t^J(s, \cdot, z) ds \right| \\ &\leq \frac{1}{k} \left[\int_{t_{m-1}}^{t_m} 1^2 dt \right]^{\frac{1}{2}} \left[\int_{t_{m-1}}^{t_m} [(R_h - I) P_t^J(s, \cdot, z)]^2 ds \right]^{\frac{1}{2}} \\ &\leq k^{-\frac{1}{2}} \left[\int_{t_{m-1}}^{t_m} [(R_h - I) P_t^J(s)]^2 ds \right]^{\frac{1}{2}}. \end{aligned}$$

Therefore

$$\begin{aligned} k \sum_{i=1}^m \|\omega_1^i\|_H^2 &\leq k \sum_{i=1}^m \int_D \left[k^{-1} \int_{t_{i-1}}^{t_i} [(R_h - I) P_t^J(s)]^2 ds \right] dx \\ &\leq \int_D \int_0^T [(R_h - I) P_t^J(s)]^2 ds dx. \end{aligned}$$

Using Lemma 5.7.1,

$$k \sum_{i=1}^m \|\omega_1^i\|_H^2 \leq Ch^2 \|P_t^J(z)\|_{L^2((0,T);V)}^2.$$

Next, we observe that

$$|\omega_2^m| = \left| -\frac{1}{k} \int_{t_{m-1}}^{t_m} (s - t_{m-1}) P_{tt}^J(s, \cdot, z) ds \right|$$

$$\begin{aligned}
&\leq \frac{1}{k} \left[\int_{t_{m-1}}^{t_m} (s - t_{m-1})^2 ds \right]^{\frac{1}{2}} \left[\int_{t_{m-1}}^{t_m} (P_{tt}^J(s, \cdot, z))^2 ds \right]^{\frac{1}{2}} \\
&\leq Ck^{\frac{1}{2}} \left[\int_{t_{m-1}}^{t_m} (P_{tt}^J(s, \cdot, z))^2 ds \right]^{\frac{1}{2}}.
\end{aligned}$$

This implies that

$$\begin{aligned}
k \sum_{i=1}^m \|\omega_2^i\|_H^2 &\leq k \sum_{i=1}^m \int_D \left[Ck \int_{t_{i-1}}^{t_i} (P_{tt}^J(s, \cdot, z))^2 ds \right] dx \\
&\leq Ck^2 \sum_{i=1}^m \int_{t_{i-1}}^{t_i} \|P_{tt}^J(s, \cdot, z)\|_H^2 ds \\
&\leq Ck^2 \|P_{tt}^J(z)\|_{L^2((0,T);H)}^2.
\end{aligned}$$

Lastly,

$$\begin{aligned}
\|\theta^0\|_V^2 &= \|P_0^J - R_h P^J(0, \cdot, z)\|_V^2 \\
&= \|g^l - R_h(g)\|_V^2 \\
&\leq \|g^l - g\|_V^2 + \|g - R_h(g)\|_V^2 \\
&\leq Ch^2 \|g\|_{H^2(D)}^2.
\end{aligned}$$

Putting all the error terms back into (5.7.2), we get

$$\|\theta^m\|_V \leq C(h + k) \left(\|P_t^J(z)\|_{L^2((0,T);V)} + \|P_{tt}^J(z)\|_{L^2((0,T);H)} + \|g\|_{H^2(D)} \right).$$

We show in Lemma 5.1.4 that P_t^J is uniformly bounded in $L^2((0,T);V)$ and P_{tt}^J is uniformly bounded in $L^2((0,T);H)$. For $H^2(D)$ regularity of $P^J(t, \cdot, z)$, we note that

$$-\Delta P^J(t, \cdot, z) = \frac{1}{K^J(\cdot, z)} \left(f - \frac{\partial P^J(t, \cdot, z)}{\partial t} + \nabla K^J(\cdot, z) \cdot \nabla P^J(t, \cdot, z) \right).$$

As D is convex, from [28],

$$\|P^J(t, \cdot, z)\|_{H^2(D)}$$

$$\begin{aligned}
&\leq c \left\| \frac{1}{K^J(\cdot, z)} \left(f(t, \cdot) - \frac{\partial P^J(t, \cdot, z)}{\partial t} + \nabla K^J(\cdot, z) \cdot \nabla P^J(t, \cdot, z) \right) \right\|_H \\
&\leq c \left(\|f(t, \cdot)\|_H + \left\| \frac{\partial P^J}{\partial t}(t, \cdot, z) \right\|_H + \|\nabla K^J(t, \cdot, z)\|_{L^\infty(D)} \|\nabla P^J(t, \cdot, z)\|_H \right).
\end{aligned}$$

Thus $P^J(t, \cdot, z)$ is uniformly bounded in $H^2(D)$. From Lemma 5.7.1,

$$\|\varphi^m\|_V \leq Ch \|P^J(t_m, \cdot, z)\|_{H^2(D)}.$$

Therefore

$$\begin{aligned}
&\|P_m^{J,h,k}(\cdot, z) - P^J(t_m, \cdot, z)\|_V \\
&\leq C(h+k) \\
&\left(\|P_t^J(z)\|_{L^2((0,T);V)} + \|P_{tt}^J(z)\|_{L^2((0,T);H)} + \sup_{t \in [0,T]} \|P^J(t, \cdot, z)\|_{H^2(D)} + \|g\|_{H^2(D)} \right).
\end{aligned} \tag{5.7.3}$$

Finally, with Proposition 5.6.2

$$\begin{aligned}
&\|P(t_m, \cdot, z) - P_m^{J,h,k}(\cdot, z)\|_V \\
&\leq \|P(t_m, \cdot, z) - P^J(t_m, \cdot, z)\|_V + \|P^J(t_m, \cdot, z) - P_m^{J,h,k}(\cdot, z)\|_V \\
&\leq C(J^{-q} + h + k).
\end{aligned}$$

□

We are now ready to prove Proposition 5.3.2

Proof of Proposition 5.3.2: We note that it is sufficient to prove that

$d_{Hell}(\gamma^{J,\delta}, \gamma^{J,h,k,\delta}) \leq C(h+k)$. We start with

$$2d_{Hell}(\gamma^{J,\delta}, \gamma^{J,h,k,\delta})^2 \leq I_1 + I_2 \tag{5.7.4}$$

where

$$I_1 = 2Z^J(\delta)^{-1} \int_U \left(\exp \left(-\frac{1}{2} \Phi^J(z, \delta) \right) - \exp \left(-\frac{1}{2} \Phi^{J,h,k}(z, \delta) \right) \right)^2 d\gamma(z)$$

$$I_2 = 2 \left| Z^J(\delta)^{-\frac{1}{2}} - Z^{J,h,k}(\delta)^{-\frac{1}{2}} \right|^2 \int_U \left(\exp \left(-\frac{1}{2} \Phi^{J,h,k}(z, \delta) \right) \right)^2 d\gamma(z).$$

Note that $P_{\tau_i}^{J,h,k}(z)$ are uniformly bounded in V from Lemma 5.1.4. Then,

$$|\mathcal{G}^{J,h,k}(z)|_{\Sigma} \leq C \max_{0 \leq i \leq N} \{ \|\ell_i\|_{V'} \|P_{\tau_i}^{J,h,k}(z)\|_V \} \leq C$$

which leads to $\Phi^{J,h,k}(z, \delta) \leq C$. This implies that $Z^{J,h,k}(\delta) > C > 0$.

Further, from equation (5.7.3)

$$\sup_{\tau_i \in (0, T)} \|P^J(\tau_i, \cdot, z) - P_{\tau_i}^{J,h,k}(z)\|_V \leq C(h + k).$$

Following 5.2.4, we see that

$$\begin{aligned} & \exp \left(-\frac{1}{2} \Phi^J(z, \delta) \right) - \exp \left(-\frac{1}{2} \Phi^{J,h,k}(z, \delta) \right) \\ &= \exp \left(-\frac{1}{2} \Phi^J(z, \delta) \right) \left[1 - \exp \left(-\frac{1}{2} (\Phi^{J,h,k}(z, \delta) - \Phi^J(z, \delta)) \right) \right] \\ &\leq \frac{1}{2} |\Phi^J(z, \delta) - \Phi^{J,h,k}(z, \delta)| \\ &= \frac{1}{4} \left| |\delta - \mathcal{G}^J(z)|_{\Sigma}^2 - |\delta - \mathcal{G}^{J,h,k}(z)|_{\Sigma}^2 \right| \\ &\leq \frac{1}{4} [2|\delta|_{\Sigma} + |\mathcal{G}^J(z)|_{\Sigma} + |\mathcal{G}^{J,h,k}(z)|_{\Sigma}] [|\mathcal{G}^J(z) - \mathcal{G}^{J,h,k}(z)|_{\Sigma}] \\ &\leq C(r) \max_{1 \leq i \leq N} \{ \|\ell_i\|_{V'} \} \sup_{\tau_i \in (0, T)} \|(P^J(\tau_i, \cdot, z) - P_{\tau_i}^{J,h,k}(z))\|_V \\ &\leq C(h + k) \end{aligned} \tag{5.7.5}$$

This implies that

$$I_1 \leq C(h + k)^2.$$

Similarly, following (5.2.5) and (5.2.6),

$$I_2 \leq C(h + k)^2.$$

Therefore

$$d_{Hell}(\gamma^{J,\delta}, \gamma^{J,h,k,\delta}) \leq \sqrt{I_1 + I_2} \leq C(h + k).$$

Together with $d_{Hell}(\gamma^{\delta}, \gamma^{J,\delta}) \leq CJ^{-q}$ from Proposition 5.3.1, we conclude the proof. $\square$

Chapter 6

Bayesian Inverse Problems for Parabolic Problems with Gaussian Prior

Bayesian inverse problems of parabolic equations with Gaussian prior probability is considered in this chapter. In Section 6.1, we set up the problem by introducing the coefficients of the log-normal form and defining the prior probability space. We show in Section 6.2 the existence and well-posedness of the posterior measure in terms of the Hellinger distance. In Section 6.3, we approximate the forward parabolic equation by taking only a finite number of terms in the coefficient and using Backward Euler (BE) and Finite Element (FE) method. From the approximated solution of the forward parabolic equation, we establish an approximation for the posterior measure with an explicit error with respect to the Hellinger distance. We develop the Multilevel Markov Chain Monte Carlo (MLMCMC) algorithm in Section 6.4 and establish rigorously the convergence rate of the MLMCMC estimator. In Section 6.5, we provide numerical results that support

the theoretical findings. The chapter concludes with some appendices.

6.1 Problem Setting

Let $D \subset \mathbb{R}^d$ be a bounded domain. Let $T > 0$. We consider a parabolic equation in the domain D and for time $t \in [0, T]$ with a coefficient which follows the log-normal form as in Chapter 4. First, we recall the definition of the log-normal coefficient in Chapter 4. Let $K_*, \bar{K} \in L^\infty(D)$ be non-negative functions and $\psi_j \in L^\infty(D)$ for $j = 1, 2, \dots$. Let $b_j = \|\psi_j\|_{L^\infty(D)}$. We assume that $\sum_{j=1}^\infty b_j$ is finite. Let the coefficient K be of the form

$$K(x, z) = K_*(x) + \exp(\bar{K}(x) + \sum_{j=1}^\infty z_j \psi_j(x)) \quad (6.1.1)$$

where $z = (z_1, z_2, \dots) \in \mathbb{R}^\mathbb{N}$. Note that if $\inf K_*(x) = 0$, then $K(x, z)$ can be arbitrarily close to 0. The random variables z_j follow the normal distribution in $\mathbb{R}$. In $\mathbb{R}^\mathbb{N}$, we define the σ algebra

$$\Theta = \bigotimes_{j=1}^\infty \mathcal{B}(\mathbb{R})$$

where $\mathcal{B}(\mathbb{R})$ is the Borel σ -algebra in $\mathbb{R}$. We equip $(\mathbb{R}^\mathbb{N}, \Theta)$ with the tensor product probability

$$\gamma = \bigotimes_{j=1}^\infty \mathcal{N}(0, 1).$$

For K to be well defined, we restrict our consideration to the subset of $\mathbb{R}^\mathbb{N}$

$$\Gamma = \{z = (z_1, z_2, \dots) \in \mathbb{R}^\mathbb{N} : \sum_{j=1}^\infty |z_j| b_j < \infty\}$$

which has γ measure 1. Let $V = H_0^1(D)$ and $H = L^2(D)$. Let $f \in L^2((0, T); V')$ and $g \in H$. For $z \in \Gamma$, we consider the parabolic problem

$$\frac{\partial P}{\partial t} - \nabla \cdot (K(x, z) \nabla P) = f, \quad P(0, x, z) = g. \quad (6.1.2)$$

We consider noisy observations of P . As we have elaborated in Chapter 5, the solution P of (6.1.2) belongs to $L^2((0, T); V) \cap H^1((0, T); V') \cap C([0, T]; H)$. When P belongs to these spaces, possible observations can be $l_i(P(\tau_i))$ where $l_i \in H'$ for $\tau_i \in (0, T)$, or $\frac{1}{|I_i|} \int_{I_i} \ell_i(P(t_i)) dt$ where $I_i \subset (0, T)$. The existence and well-posedness of the posterior probability measure can be established for these types of observations. However, to obtain an approximation for the posterior measure using truncation of expansion (6.1.1) and by solving the truncated forward equation by backward Euler and finite element method, we need regularity for the solution P . In particular, we will need that $P(z) \in H^1((0, T); V)$. For this regularity, it makes sense to identify the pointwise value of P in V for each $t \in (0, T)$. We therefore assume this regularity at the onset. We thus assume

Assumption 6.1.1. We assume $f \in H^1((0, T); V')$ with $f(0, \cdot) \in H$ and $g \in H^2(D)$. Further

$$K_*, \bar{K} \in W^{1,\infty}(D), \quad \psi_j \in W^{1,\infty}(D), \quad \|\psi_j\|_{W^{1,\infty}(D)} \leq \frac{C}{j^s}$$

for $s > 1$.

We will denote by $q = s - 1$. For conciseness, we define by $b_j = \|\psi_j\|_{L^\infty(D)}$ and $\bar{b}_j = \|\psi_j\|_{W^{1,\infty}(D)}$. We define the prior probability space

$$U = \{z = (z_1, z_2, \dots) \in \mathbb{R}^\mathbb{N} : \sum_{j=1}^{\infty} |z_j| \bar{b}_j < \infty\}.$$

The set U has γ measure 1. The σ algebra Θ in U is defined as the restriction of the σ algebra $\otimes_{j=1}^{\infty} \mathcal{B}(\mathbb{R})$ in $\mathbb{R}^\mathbb{N}$ to U . The prior probability γ in U is defined as the restriction of the tensorized measure $\otimes_{j=1}^{\infty} \mathcal{N}(0, 1)$ to U . For $z \in U$, $K(z) \in W^{1,\infty}(D)$ and

$$\nabla K(z, x) = \nabla K_*(x) + \exp \left(\bar{K}(x) + \sum_{j=1}^{\infty} z_j \psi_j(x) \right) \left(\nabla \bar{K}(x) + \sum_{j=1}^{\infty} z_j \nabla \psi_j(x) \right).$$

We recall the upper and lower bounds $K_{\max}, K_{\min}$ in (4.1.4) (4.1.5). The time derivative of P satisfies the problem

$$\begin{aligned} \frac{\partial}{\partial t} \left(\frac{\partial P}{\partial t} \right) - \nabla \cdot (K \nabla \frac{\partial P}{\partial t}) &= \frac{\partial f}{\partial t}, \\ \frac{\partial P}{\partial t}(0) &= f(0, \cdot) + \nabla \cdot (K \nabla g). \end{aligned} \quad (6.1.3)$$

As $\frac{\partial f}{\partial t} \in L^2((0, T); V')$ and the initial condition $f(0, \cdot) + \nabla \cdot (K \nabla g) \in H$, problem (6.1.3) is well-posed. We thus have $P \in H^1((0, T); V)$. We consider observations ℓ_i as in Chapter 5. Let $N \in \mathbb{N}$. Let $\tau_i \in (0, T)$ ($i = 1, \dots, N$). Let $\ell_i \in V'$ for $i = 1, \dots, N$. We consider the forward function

$$\mathcal{G}(z) = (\ell_1(P(\tau_1, \cdot, z)), \dots, \ell_N(P(\tau_N, \cdot, z))) \in \mathbb{R}^N.$$

We consider the noisy observation of $\mathcal{G}$

$$\delta = \mathcal{G}(z) + \vartheta$$

where the noise ϑ follows the Gaussian distribution $\mathcal{N}(0, \Sigma)$ in $\mathbb{R}^N$; the $N \times N$ covariance matrix Σ is positive definite. Our purpose is to find the posterior probability measure $\gamma^\delta = \mathbb{P}(z|\delta)$. Let Φ be the misfit function

$$\Phi(z, \delta) = \frac{1}{2} |\delta - \mathcal{G}(z)|_\Sigma^2.$$

We will show that

$$\frac{d\gamma^\delta}{d\gamma} \propto \exp(-\Phi(z, \delta)), \quad (6.1.4)$$

and that γ^δ is well-posed with respect to δ . We denote

$Z(\delta) = \int_U \exp(-\Phi(z, \delta)) d\gamma(z)$ the normalising constant of (6.1.4).

6.2 Existence and Well-posedness of the Posterior measure

We have the following existence results.

Proposition 6.2.1. Under Assumption 6.1.1, the solution P is measurable when viewed as a map from U to $H^1((0, T); V)$. This implies the existence of the posterior measure γ^δ which is determined by

$$\frac{d\gamma^\delta}{d\gamma} \propto \exp(-\Phi(z, \delta)).$$

Proof First we show that P as a map from U to $H^1((0, T); V)$ is measurable. Let $z, z' \in U$. We then have

$$\frac{\partial}{\partial t}(P(z) - P(z')) - \nabla \cdot (K(z)\nabla(P(z) - P(z'))) = \nabla \cdot ((K(z) - K(z'))\nabla P(z))$$

with $P(0, \cdot, z) - P(0, \cdot, z') = 0$. Thus

$$\begin{aligned} & \int_0^T \left(\frac{\partial}{\partial t}(P(z) - P(z')), (P(z) - P(z')) \right) dt \\ & + \int_0^T \int_D K(z)\nabla(P(z) - P(z')) \cdot \nabla(P(z) - P(z')) dx dt \\ & = - \int_0^T \int_D (K(z) - K(z'))\nabla P(z) \cdot \nabla(P(z) - P(z')) dx dt. \end{aligned}$$

From this we have

$$\begin{aligned} & K_{\min}(z) \|P(z) - P(z')\|_{L^2((0, T); V)}^2 \\ & \leq \|K(z) - K(z')\|_{L^\infty(D)} \|P(z)\|_{L^2((0, T); V)} \|\nabla(P(z) - P(z'))\|_{L^2((0, T); V)} \end{aligned}$$

so

$$\|P(z) - P(z')\|_{L^2((0, T); V)} \leq \frac{1}{K_{\min}(z)} \|K(z) - K(z')\|_{L^\infty(D)} \|P(z)\|_{L^2((0, T); V)}. \quad (6.2.1)$$

Similarly, we have

$$\begin{aligned} & \frac{\partial}{\partial t} \frac{\partial}{\partial t}(P(z) - P(z')) - \nabla \cdot (K(z)\nabla \frac{\partial}{\partial t}(P(z) - P(z'))) \\ & = \nabla \cdot \left((K(z) - K(z'))\nabla \frac{\partial P(z)}{\partial t} \right). \end{aligned}$$

The initial condition is $\frac{\partial}{\partial t}(P(0, \cdot, z) - P(0, \cdot, z')) = \nabla \cdot ((K(z) - K(z'))\nabla g)$.

Thus

$$\begin{aligned} & K_{\min}(z) \left\| \frac{\partial}{\partial t}(P(z) - P(z')) \right\|_{L^2((0,T);V)}^2 \\ & \leq \|K(z) - K(z')\|_{L^\infty(D)} \left\| \nabla \frac{\partial P(z)}{\partial t} \right\|_{L^2((0,T);H)} \left\| \nabla \frac{\partial}{\partial t}(P(z) - P(z')) \right\|_{L^2((0,T);H)} \\ & \quad + \|\nabla \cdot (K(z) - K(z'))\nabla g\|_H^2. \end{aligned}$$

Therefore

$$\begin{aligned} & \left\| \frac{\partial}{\partial t}(P(z) - P(z')) \right\|_{L^2((0,T);V)} \\ & \leq \frac{1}{K_{\min}(z)} \|K(z) - K(z')\|_{L^\infty(D)} \left\| \nabla \frac{\partial P(z)}{\partial t} \right\|_{L^2((0,T);H)} \\ & \quad + \frac{1}{K_{\min}^{1/2}} \|\nabla \cdot (K(z) - K(z'))\nabla g\|_H. \quad (6.2.2) \end{aligned}$$

Assume that K only contains a finite number of J terms z_j for $j = 1, \dots, J$, i.e. $z \in \mathbb{R}^J$. Then equations (6.2.1) and (6.2.2) show that P as a map $\mathbb{R}^J \ni z \rightarrow H^1((0,T);V)$ is continuous. Thus as a map from $\mathbb{R}^J \ni z \rightarrow C([0,T];V)$ it is also continuous, and is measurable. Let $X \in \mathcal{B}(C([0,T];V))$. The preimage of $P^{-1}(X)$ in $\mathbb{R}^J$ belongs to $\mathcal{B}(\mathbb{R}^J)$.

Now for $z \in U$, we consider the truncated coefficient

$$K^J(x, z) = K_*(x) + \exp(\bar{K}(x) + \sum_{j=1}^J z_j \psi_j(x)).$$

We consider the truncated equation

$$\frac{\partial P^J}{\partial t}(z) - \nabla \cdot (K^J(z)\nabla P^J(z)) = f, \quad P^J(0, \cdot, z) = g.$$

Consider P^J as a map $U \ni z \rightarrow H^1((0,T);V)$, we then deduce that this map is measurable. From Lemma 6.6.2, we deduce that for $z \in U$,

$$\lim_{J \rightarrow \infty} \|P^J(z) - P(z)\|_{H^1((0,T);V)} = 0$$

so

$$\lim_{J \rightarrow \infty} \|P^J(z) - P(z)\|_{C([0,T];V)} = 0.$$

As P is a pointwise limit of a sequence of measurable maps, $P(z)$ as a map $U \ni z \rightarrow C([0, T]; V)$ is measurable. Therefore $\mathcal{G} : U \ni z \rightarrow \mathbb{R}^N$ is measurable. Thus (6.1.4) holds (see Theorem 2.1 of [12]). $\square$

Next, we show the well-posedness.

Proposition 6.2.2. The posterior probability measure γ^δ is determined from formula (6.1.4). It is well-posed; in particular, for $|\delta|, |\delta'| < r$, there is a constant $c(r)$ such that

$$d_{Hell}(\gamma^\delta, \gamma^{\delta'}) < c(r)|\delta - \delta'|. \quad (6.2.3)$$

Proof We show inequality (6.2.3). Similar to (5.2.1), we note that

$$2d_{Hell}(\gamma^\delta, \gamma^{\delta'})^2 \leq I_1 + I_2$$

where

$$I_1 = \frac{2}{Z(\delta)} \int_U \left(\exp(-\frac{1}{2}\Phi(z, \delta)) - \exp(-\frac{1}{2}\Phi(z, \delta')) \right)^2 d\gamma(z),$$

and

$$I_2 = 2|Z(\delta)^{-1/2} - Z(\delta')^{-1/2}|^2 \int_U \exp(-\frac{1}{2}\Phi(z, \delta)) d\gamma(z).$$

We have that

$$\left| \exp(-\frac{1}{2}\Phi(z, \delta)) - \exp(-\frac{1}{2}\Phi(z, \delta')) \right| \leq c(|\delta| + |\delta'| + |\mathcal{G}(z)|)|\delta - \delta'|.$$

From Lemma 6.6.1 in Section 6.6, we have that

$$\|P(\cdot, \cdot, z)\|_{C([0,T];V)} \leq c \exp\left(\sum_{j=1}^{\infty} |z_j|(b_j + \bar{b}_j)\right),$$

so

$$|\mathcal{G}(z)| \leq c \exp\left(\sum_{j=1}^{\infty} |z_j|(b_j + \bar{b}_j)\right).$$

Thus

$$\left| \exp\left(-\frac{1}{2}\Phi(z, \delta)\right) - \exp\left(-\frac{1}{2}\Phi(z, \delta')\right) \right| \leq c \exp\left(c \sum_{j=1}^{\infty} |z_j|(b_j + \bar{b}_j)\right) |\delta - \delta'|.$$

Therefore

$$I_1 \leq c |\delta - \delta'|^2 \int_U \exp\left(c \sum_{j=1}^{\infty} |z_j|(b_j + \bar{b}_j)\right) d\gamma(z) \leq c |\delta - \delta'|^2$$

due to Lemma 4.6.1. Similarly, we have

$$I_2 \leq c |\delta - \delta'|^2.$$

□

6.3 Approximation by BE and FE method

We consider the approximation of (6.1.2) by taking a finite number of terms in (6.1.1). Let

$$K^J(x, z) = K_*(x) + \exp(\bar{K}(x) + \sum_{j=1}^J z_j \psi_j(x)).$$

We consider the truncated forward equation

$$\frac{\partial P^J}{\partial t}(z) - \nabla \cdot (K^J(z) \nabla P^J(z)) = f, \quad P^J(0, \cdot, z) = g. \quad (6.3.1)$$

Under Assumption 6.1.1, we note that the equation for $\frac{\partial P^J}{\partial t}$

$$\begin{aligned} \frac{\partial}{\partial t} \frac{\partial P^J}{\partial t}(z) - \nabla \cdot (K^J(z) \nabla \frac{\partial P^J}{\partial t}(z)) &= \frac{\partial f}{\partial t} \\ \text{with } \frac{\partial P^J}{\partial t}(0, \cdot, z) &= f(0, \cdot) + \nabla \cdot (K^J(\cdot, z) \nabla g) \end{aligned}$$

is well posed as $\frac{\partial f}{\partial t} \in L^2((0, T); V')$ and $f(0, \cdot) + \nabla \cdot (K^J \nabla g) \in H$. Thus $P^J \in H^1((0, T); V)$. We consider the forward function

$$\mathcal{G}^J(z) = (\ell_1(P^J(\tau_1, \cdot, z)), \dots, \ell_N(P^J(\tau_N, \cdot, z))) \in \mathbb{R}^N.$$

Let

$$\Phi^J(z, \delta) = \frac{1}{2} |\delta - \mathcal{G}^J(z)|_{\Sigma}^2. \quad (6.3.2)$$

We define the measure

$$\frac{d\gamma^{J,\delta}}{d\gamma} \propto \exp(-\Phi^J(z, \delta)). \quad (6.3.3)$$

We have the following approximation

Proposition 6.3.1. The approximated posterior measure $\gamma^{J,\delta}$ satisfies

$$d_{Hell}(\gamma^\delta, \gamma^{J,\delta}) \leq cJ^{-q},$$

where $q = s - 1$.

We present the proof of this theorem in Section 6.6.

We then consider the backward Euler finite element method for solving the truncated equation (6.3.1). We consider a partition of $[0, T]$ by $0 = t_0 < t_1 < t_2 < \dots < t_M = T$ such that $t_j - t_{j-1} = k$ for all $j = 1, \dots, M$. We consider a general FE space $V^l \subset H_0^1(D)$ defined in Chapter 3, Section 3.3, with mesh size $h_l = O(2^{-l})$. As in Chapter 5, for notational simplicity, we denote h_l by h in the presentation below and in the proof in Section 6.7.

For $z \in U$, we consider the backward Euler finite element scheme: Find $P_m^{J,h,k}(z) \in V^l$ for $m = 1, \dots, M$ such that

$$\begin{aligned} \int_D \frac{P_m^{J,h,k}(x, z) - P_{m-1}^{J,h,k}(x, z)}{k} \phi dx + \int_D K^J(x, z) \nabla P_m^{J,h,k}(x, z) \cdot \nabla \phi(x) dx \\ = \int_D f(t_m, x) \phi(x) dx, \end{aligned} \quad (6.3.4)$$

$\forall \phi \in V^l$ with $P_0^{J,h,k} = g^l$ where g^l is an approximation of g in V^l . As $g \in H^2(D)$, we choose g^l so that $\|g - g^l\|_V \leq ch$. For simplicity, we assume that $\tau_i \in \{t_1, t_2, \dots, t_M\}$. If $\tau_i = t_m$, we denote $P_m^{J,h,k}$ by $P_{\tau_i}^{J,h,k}$. We define by

$$\mathcal{G}^{J,h,k}(z) = (\ell_1(P_{\tau_1}^{J,h,k}(z)), \dots, \ell_N(P_{\tau_N}^{J,h,k}(z))).$$

Let

$$\Phi^{J,h,k}(z, \delta) = \frac{1}{2} |\delta - \mathcal{G}^{J,h,k}(z)|_{\Sigma}^2.$$

We define the approximated measure

$$\frac{d\gamma^{J,h,k,\delta}}{d\gamma} \propto \exp(-\Phi^{J,h,k}(z, \delta)). \quad (6.3.5)$$

We then have the following result.

Proposition 6.3.2. Assume that D is a convex polygon and $f \in C([0, T], L^2(D))$ and $g \in V \cap H^2(D)$. Under Assumption 6.1.1 we have

$$d_{\text{Hell}}(\gamma^\delta, \gamma^{J,h,k,\delta}) \leq c(J^{-q} + h + k).$$

We prove this proposition in Section 6.7. As mentioned in the chapters before, this shows the corresponding error for approximating the posterior probability measure by solving the forward equation by truncating the coefficient and solving the truncated equation using BE and FEM. The effect of this approximation is observed numerically when we are approximating the expectation with respect to the posterior probability measure by the expectation with respect to the approximated posterior probability measure.

6.4 Multilevel MCMC

As in Chapter 5, we develop the method for approximating the posterior expectation of $\ell(P(T, \cdot, z))$. To develop the multilevel MCMC method, for

the FE mesh $h_l = O(2^{-l})$ we choose J and k so that the terms in the right hand side of the estimate in Proposition 6.3.2 are equivalent. In particular, we let $k = T2^{-l}$ and $J = \lceil 2^{l/q} \rceil$. We then denote the measure $\gamma^{J, h_l, k, \delta}$ by γ^l , solution $P_m^{J, h_l, k}$ by P_m^l and potential $\Phi^{J, h_l, k}$ by Φ^l . We denote $P_M^{J, h_l, k}$ which approximates $P(T, \cdot, z)$ by P_T^l . The multilevel MCMC method for the parabolic equation (6.1.2) is similar to that for elliptic problems in Chapter 4. Relying on the detailed derivation shown in Section 4.4, we shall only present the result.

We recall the definition of Chapter 4

$$\begin{aligned}
A_1^{ll'} &= (1 - \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)))Q(z)I^l(z), \\
A_2^{ll'} &= (\exp(\Phi^{l-1}(z, \delta) - \Phi^l(z, \delta)) - 1)Q(z)(1 - I^l(z)), \\
A_3^l &= (\exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta)) - 1)I^l(z), \\
A_4^{ll'} &= Q(z)I^l(z), \\
A_5^l &= (1 - \exp(\Phi^{l-1}(z, \delta) - \Phi^l(z, \delta)))(1 - I^l(z)), \\
A_6^{ll'} &= \exp(\Phi^l(z, \delta) - \Phi^{l-1}(z, \delta))Q(z)I^l(z), \\
A_7^{ll'} &= Q(z)(1 - I^l(z)), \\
A_8^{ll'} &= \exp(\Phi^{l-1}(z, \delta) - \Phi^l(z, \delta))Q(z)(1 - I^l(z)),
\end{aligned}$$

where

$$\begin{aligned}
Q &= \ell(P_T^{l'}) - \ell(P_T^{l'-1}) \quad \text{when } l' \neq 0 \text{ and} \\
Q &= \ell(P_T^0) \quad \text{when } l' = 0.
\end{aligned}$$

To approximate the posterior expectation of a quantity of interest, $\mathbb{E}^{\gamma^\delta}[\ell(P(T, \cdot, z))]$ where $\ell \in V'$, we define the MLMCMC estimator as

$$E_L^{MLMCMC}[\ell(P(T, \cdot, z))]$$

$$\begin{aligned}
&= \sum_{l=1}^L \sum_{l'=1}^{L'(l)} \left[E_{M_{ll'}}^{\gamma^l} [A_1^{ll'}] + E_{M_{ll'}}^{\gamma^{l-1}} [A_2^{ll'}] + E_{M_{ll'}}^{\gamma^l} [A_3^l] \cdot E_{M_{ll'}}^{\gamma^{l-1}} [A_4^{ll'} + A_8^{ll'}] \right. \\
&\quad \left. + E_{M_{ll'}}^{\gamma^{l-1}} [A_5^l] \cdot E_{M_{ll'}}^{\gamma^l} [A_6^{ll'} + A_7^{ll'}] \right] \\
&+ \sum_{l=1}^L \left[E_{M_{l0}}^{\gamma^l} [A_1^{l0}] + E_{M_{l0}}^{\gamma^{l-1}} [A_2^{l0}] + E_{M_{l0}}^{\gamma^l} [A_3^l] \cdot E_{M_{l0}}^{\gamma^{l-1}} [A_4^{l0} + A_8^{l0}] \right. \\
&\quad \left. + E_{M_{l0}}^{\gamma^{l-1}} [A_5^l] \cdot E_{M_{l0}}^{\gamma^l} [A_6^{l0} + A_7^{l0}] \right] \\
&+ \sum_{l'=1}^{L'(0)} E_{M_{0l'}}^{\gamma^0} [\ell(P_T^{l'} - P_T^{l'-1})] + E_{M_{00}}^{\gamma^0} [\ell(P_T^0)],
\end{aligned}$$

where $E_{M_{ll'}}^{\gamma^l}$ is the approximation of $\mathbb{E}^{\gamma^l}$ using MCMC with $M_{ll'}$ samples with the acceptance probability

$$\alpha^l(z, s) = 1 \wedge \exp(\Phi^l(z, \delta) - \Phi^l(s, \delta)).$$

With the parameter choices

$$\begin{aligned}
L'(l) &= L - l, \quad M_{ll'} = 2^{2(L-(l+l'))} \quad \text{for } l \geq 1, \quad l' \geq 1, \\
M_{0l} &= M_{l0} = 2^{2L}/L^2, \quad M_{00} = 2^{2L}/L^4,
\end{aligned} \tag{6.4.1}$$

we have the following convergence result.

Theorem 6.4.1. Suppose that the domain D is convex and that $f \in C([0, T]; H)$. Under Assumption 4.8.2 for $d = 2, 3$, with the choices

$$\begin{aligned}
L'(l) &= L - l, \quad M_{ll'} = 2^{2(L-(l+l'))} \quad \text{for } l \geq 1, \quad l' \geq 1, \\
M_{0l} &= M_{l0} = 2^{2L}/L^2, \quad M_{00} = 2^{2L}/L^4,
\end{aligned}$$

there exists a constant $C(\delta) > 0$ such that for every $L \in \mathbb{N}$

$$\mathbf{E}_L \left[\left| \mathbb{E}^{\gamma^\delta} [\ell(P(T, \cdot, z))] - E_L^{MLMCMC} [\ell(P(T, \cdot, z))] \right| \right] \leq C(\delta) L^2 2^{-L}. \tag{6.4.2}$$

The proof of this theorem is similar to that of Theorem 4.4.1. The logarithmic factor L^2 in the estimate of Theorem 6.4.1 can be reduced by

increasing the sample size of each Markov chain with the choice

$$M_{ll'} = (l + l')^a 2^{2(L-(l+l'))}$$

when $l \geq 1$ and $l' \geq 1$. We tabulate the resulting asymptotic bound in Table 5.1.

6.5 Numerical experiments

We present the numerical experiments to verify the theoretical results for MLMCMC for parabolic equation with log-normal coefficient. As in Chapter 5, we consider periodic boundary condition as this allows for establishing a very accurate reference solution to compare the MLMCMC results to. We consider both the independent sampler and the preconditioned Crank-Nicolson (pCN) sampler (see [51]) for the MCMC. We used Gauss Hermite quadrature points to estimate the posterior expectation. At each of the quadrature rule, the forward parabolic equation is solved using Fourier collocation and implicit Runge Kutta method.

We present the MLMCMC using independent sampler first. We consider the parametric forward equation

$$\begin{aligned} \frac{\partial P}{\partial t}(t, x, z) - \nabla \cdot (K(x, z) \nabla P(t, x, z)) &= f(t, x) \\ \text{for } x \in D = (0, 1) \times (0, 1), t \in (0, 1) \end{aligned} \quad (6.5.1)$$

where $K(x, z) = \exp(z(\sin(2\pi x_1) + \sin(2\pi x_2)))$ and $f(x, t) = 200(\sin(2\pi x_1) + \sin(2\pi x_2))$, with periodic boundary condition and initial condition $P(x, 0) = 0$. The observation functional is chosen to be

$$\mathcal{G}(z) = \int_D x_1 \frac{\partial P}{\partial x_1}(1, \cdot, z) + x_2 \frac{\partial P}{\partial x_2}(1, \cdot, z) dx \quad (6.5.2)$$

and the quantity of interest as

$$\ell(P(z)) = \int_D x_1^{1.5} \frac{\partial P}{\partial x_1}(1, \cdot, z) + x_2^{1.5} \frac{\partial P}{\partial x_2}(1, \cdot, z) dx. \quad (6.5.3)$$

To compute the reference solution, 1200 Gauss-Hermite quadrature points are used to estimate the expectation integral, 25×25 collocation points are used in Fourier Collocation and order 12 implicit Runge Kutta method with time step $\frac{1}{32}$ being used to solve the forward parabolic equation.

In Figure 6.1, we present the numerical result for a in Table 5.1 being 0. The error is computed as the average error of 64 runs of MLMCMC. We plot the error versus the finest mesh level h_L . The gradient of the best fit straight line is 0.8776. Similarly in Figures 6.2 and 6.3, we present the MLMCMC error for $a = 2$ and 4. The gradient of the best fit straight lines are 0.9306 and 0.9840 respectively. These results illustrates the theory. The slight difference in the gradient for $a = 0$ compare to $a = 2, 4$ shows the significance of the logarithmic factor in the convergence error shown in Table 5.1.

We now present the results for the MLMCMC method with the pCN sampler (see [51]) where a proposal is chosen from the current MCMC state $z^{(k)}$ as:

$$s^{(k)} = \sqrt{1 - \beta^2} z^{(k)} + \beta \xi,$$

where ξ is the standard normal variable. We consider several choices for β . We present the results for $\beta = \frac{1}{\sqrt{2}}$ first. In Figures 6.4 and 6.5, we plot the MLMCMC error versus the finest mesh level h_L for $a = 0$ and 2 respectively. The gradient of the best fit straight lines are 0.7947 and 1.0185.

Next, we present the results for $\beta = \frac{1}{\sqrt{10}}$. In Figures 6.6 and 6.7, we plot the MLMCMC error against finest mesh level h_L for $a = 0$ and 2 respectively. The gradient of the best fit straight lines are 0.6109 and 0.9285.

Figure 6.1: MLMCMC error for 2D parabolic equation with Gaussian prior probability using independence sampler, $a = 0$

In both cases, we observe that the choice of $a = 0$ under performs as compared to the choice of $a = 2$. This is due to the logarithmic factor in the error of the MLMCMC.

6.6 Appendix A

We prove Proposition 6.3.1 in this Appendix. First we show some lemmas.

Lemma 6.6.1. Under Assumption 6.1.1, there is a constant $c > 0$ such that $\forall z \in U$,

$$\|P(\cdot, \cdot, z)\|_{H^1((0,T);V)} \leq c \exp \left(\sum_{j=1}^{\infty} |z_j| (b_j + \bar{b}_j) \right).$$

Figure 6.2: MLMCMC error for 2D parabolic equation with Gaussian prior probability using independence sampler, $a = 2$

There is a constant $c > 0$ independent of J such that $\forall z \in U$

$$\|P^J(\cdot, \cdot, z)\|_{H^1((0,T);V)} \leq c \exp \left(\sum_{j=1}^{\infty} |z_j| (b_j + \bar{b}_j) \right).$$

Proof From (6.1.2) we have

$$\int_0^T \left(\frac{\partial P}{\partial t}(z), P(z) \right) dt + \int_0^T \int_D K(z) \nabla P(z) \cdot \nabla P(z) dx dt = \int_0^T \int_D f P(z) dx dt.$$

Thus

$$\begin{aligned} & \frac{1}{2} \|P(T, \cdot, z)\|_H^2 + K_{\min}(z) \|P(z)\|_{L^2((0,T);V)}^2 \\ & \leq \frac{1}{2K_{\min}(z)} \|f\|_{L^2((0,T);V')}^2 + \frac{K_{\min}(z)}{2} \|P(z)\|_{L^2((0,T);V)}^2 + \frac{1}{2} \|P(0, \cdot, z)\|_H^2. \end{aligned}$$

This implies

$$\frac{K_{\min}(z)}{2} \|P(z)\|_{L^2((0,T);V)}^2 \leq \frac{1}{2K_{\min}(z)} \|f\|_{L^2((0,T);V')}^2 + \frac{1}{2} \|g\|_H^2$$

Figure 6.3: MLMCMC error for 2D parabolic equation with Gaussian prior probability using independence sampler, $a = 4$

i.e.

$$\|P(z)\|_{L^2((0,T);V)}^2 \leq \frac{1}{K_{\min}^2(z)} \|f\|_{L^2((0,T);V')}^2 + \frac{1}{K_{\min}(z)} \|g\|_H^2.$$

Therefore, there is a constant $c > 0$ such that

$$\|P(z)\|_{L^2((0,T);V)} \leq c \left(\frac{1}{K_{\min}(z)} \|f\|_{L^2((0,T);V')} + \frac{1}{K_{\min}(z)^{1/2}} \|g\|_H \right).$$

Similarly, from (6.1.3), there is a constant $c > 0$ such that

$$\begin{aligned} & \left\| \frac{\partial P}{\partial t}(z) \right\|_{L^2((0,T);V)} \\ & \leq c \left(\frac{1}{K_{\min}(z)} \left\| \frac{\partial f}{\partial t} \right\|_{L^2((0,T);V')} + \frac{1}{K_{\min}(z)^{1/2}} (\|f(0, \cdot)\|_H + \|\nabla \cdot (K(z) \nabla g)\|_H) \right). \end{aligned}$$

We note that

$$\nabla \cdot (K(z) \nabla g) = \nabla K(z) \cdot \nabla g + K(z) \Delta g.$$

Figure 6.4: MLMCMC error for 2D parabolic equation with Gaussian prior probability using pCN sampler, $a = 0, \beta = \frac{1}{\sqrt{2}}$

From

$$\nabla K(z) = \nabla K_* + \exp(\bar{K}(x) + \sum_{j=1}^{\infty} z_j \psi_j)(\nabla \bar{K}(x) + \sum_{j=1}^{\infty} z_j \nabla \psi_j),$$

we have

$$\begin{aligned} \|\nabla K(z)\|_{L^\infty(D)} &\leq \|\nabla K_*\|_{L^\infty(D)} + c \exp\left(\sum_{j=1}^{\infty} |z_j| b_j\right) \left(1 + \sum_{j=1}^{\infty} z_j \bar{b}_j\right) \\ &\leq c(1 + \exp(\sum_{j=1}^{\infty} |z_j| (b_j + \bar{b}_j))). \end{aligned}$$

Thus

$$\|P(z)\|_{H^1((0,T);V)} \leq c(1 + \exp(\sum_{j=1}^{\infty} |z_j| (b_j + \bar{b}_j))).$$

The proof for $P^J(z)$ is similar. □

Figure 6.5: MLMCMC error for 2D parabolic equation with Gaussian prior probability using pCN sampler, $a = 2, \beta = \frac{1}{\sqrt{2}}$

Lemma 6.6.2. Under Assumption 6.1.1, there is a constant $c > 0$ such that

$$\|P(z) - P^J(z)\|_{H^1((0,T);V)} \leq c \left(\sum_{j>J} |z_j| (b_j + \bar{b}_j) \right) \exp \left(c \sum_{j=1}^{\infty} |z_j| (b_j + \bar{b}_j) \right).$$

Proof From (6.1.2)

$$\frac{\partial}{\partial t} (P(z) - P^J(z)) - \nabla \cdot (K(z) \nabla (P(z) - P^J(z))) = \nabla \cdot (K(z) - K^J(z)) \nabla P^J(z)$$

with $P(0, \cdot, z) - P^J(0, \cdot, z) = 0$. We therefore have that

$$\begin{aligned} & \int_0^T \left(\frac{\partial}{\partial t} (P(z) - P^J(z)), (P(z) - P^J(z)) \right) dt \\ & \quad + \int_0^T \int_D K \nabla (P(z) - P^J(z)) \cdot \nabla (P(z) - P^J(z)) dx dt \\ & = - \int_0^T \int_D (K(z) - K^J(z)) \nabla P^J(z) \cdot \nabla (P(z) - P^J(z)) dx dt. \quad (6.6.1) \end{aligned}$$

Figure 6.6: MLMCMC error for 2D parabolic equation with Gaussian prior probability using pCN sampler, $a = 0, \beta = \frac{1}{\sqrt{10}}$

Thus

$$\begin{aligned} & K_{\min}(z) \|P(z) - P^J(z)\|_{L^2((0,T);V)}^2 \\ & \leq \|K(z) - K^J(z)\|_{L^\infty(D)} \|\nabla P^J(z)\|_{L^2((0,T);H)} \|\nabla(P(z) - P^J(z))\|_{L^2((0,T);H)}. \end{aligned}$$

From this we have

$$\begin{aligned} \|P(z) - P^J(z)\|_{L^2((0,T);V)} & \leq \frac{1}{K_{\min}(z)} \|K(z) - K^J(z)\|_{L^\infty(D)} \|P^J(z)\|_{L^2((0,T);V)} \\ & \leq c \left(\sum_{j>J} |z_j| b_j \right) \left(\exp(c \sum_{j=1}^{\infty} |z_j| (b_j + \bar{b}_j)) \right). \end{aligned}$$

Similarly, we have from (6.1.3)

$$\begin{aligned} & \frac{\partial}{\partial t} \frac{\partial}{\partial t} (P(z) - P^J(z)) - \nabla \cdot (K \nabla \frac{\partial}{\partial t} (P(z) - P^J(z))) \\ & = \nabla \cdot (K(z) - K^J(z)) \nabla \frac{\partial P^J}{\partial t}(z), \end{aligned}$$

Figure 6.7: MLMCMC error for 2D parabolic equation with Gaussian prior probability using pCN sampler, $a = 2, \beta = \frac{1}{\sqrt{10}}$

with $\frac{\partial}{\partial t}(P(z) - P^J(z))(0, \cdot, z) = \nabla \cdot ((K(z) - K^J(z))\nabla g)$. We deduce

$$\begin{aligned}
& K_{\min}(z) \left\| \frac{\partial}{\partial t}(P(z) - P^J(z)) \right\|_{L^2((0,T);V)}^2 \\
& \leq \|K(z) - K^J(z)\|_{L^\infty(D)} \left\| \nabla \frac{\partial P^J}{\partial t}(z) \right\|_{L^2((0,T);H)} \left\| \nabla \frac{\partial}{\partial t}(P(z) - P^J(z)) \right\|_{L^2((0,T);H)} \\
& \quad + \|\nabla \cdot (K(z) - K^J(z))\nabla g\|_H^2.
\end{aligned}$$

We thus have

$$\begin{aligned}
& \left\| \frac{\partial}{\partial t}(P(z) - P^J(z)) \right\|_{L^2((0,T);V)} \\
& \leq \frac{1}{K_{\min}(z)} \|K(z) - K^J(z)\|_{L^\infty(D)} \left\| \nabla \frac{\partial P^J}{\partial t}(z) \right\|_{L^2((0,T);H)} \\
& \quad + \frac{1}{K_{\min}(z)^{1/2}} \|\nabla \cdot (K(z) - K^J(z))\nabla g\|_H.
\end{aligned}$$

Using inequality $|\exp(x) - \exp(y)| \leq |x - y| (\exp(x) + \exp(y))$, we have

$$\begin{aligned} & \|K(z) - K^J(z)\|_{L^\infty(D)} \\ & \leq \left\| \exp\left(\bar{K}(x) + \sum_{j=1}^{\infty} z_j \psi_j(x)\right) - \exp\left(\bar{K}(x) + \sum_{j=1}^J z_j \psi_j(x)\right) \right\|_{L^\infty(D)} \\ & \leq c \exp\left(\sum_{j=1}^{\infty} |z_j| b_j\right) \left(\sum_{j=1}^J |z_j| b_j\right). \end{aligned}$$

We note that

$$\begin{aligned} & \|\nabla K(z) - \nabla K^J(z)\|_{L^\infty(D)} \\ & \leq \left\| \exp\left(\bar{K}(x) + \sum_{j=1}^{\infty} z_j \psi_j(x)\right) \left(\nabla \bar{K}(x) + \sum_{j=1}^{\infty} z_j \nabla \psi_j(x)\right) \right. \\ & \quad \left. - \exp\left(\bar{K}(x) + \sum_{j=1}^J z_j \psi_j(x)\right) \left(\nabla \bar{K}(x) + \sum_{j=1}^J z_j \nabla \psi_j(x)\right) \right\|_{L^\infty(D)} \\ & \leq \left\| \exp\left(\bar{K}(x) + \sum_{j=1}^{\infty} z_j \psi_j(x)\right) - \exp\left(\bar{K}(x) + \sum_{j=1}^J z_j \psi_j(x)\right) \right\|_{L^\infty(D)} \\ & \quad \left\| \nabla \bar{K}(x) + \sum_{j=1}^J z_j \nabla \psi_j(x) \right\|_{L^\infty(D)} \\ & \quad + \left\| \exp\left(\bar{K}(x) + \sum_{j=1}^{\infty} z_j \psi_j(x)\right) \right\|_{L^\infty(D)} \left\| \sum_{j>J} z_j \nabla \psi_j(x) \right\|_{L^\infty(D)} \\ & \leq c \exp\left(\sum_{j=1}^{\infty} |z_j| b_j\right) \left(\sum_{j>J} |z_j| b_j\right) \left(1 + \sum_{j=1}^J |z_j| \bar{b}_j\right) \\ & \quad + c \exp\left(\sum_{j=1}^{\infty} |z_j| b_j\right) \left(\sum_{j>J} |z_j| \bar{b}_j\right) \\ & \leq c \exp\left(\sum_{j=1}^{\infty} |z_j| (b_j + \bar{b}_j)\right) \left(\sum_{j>J} |z_j| (b_j + \bar{b}_j)\right). \end{aligned}$$

From Lemma 6.6.1, we deduce that

$$\left\| \frac{\partial}{\partial t} (P(z) - P^J(z)) \right\|_{L^2((0,T);V)} \leq c \exp\left(c \sum_{j=1}^{\infty} |z_j| (b_j + \bar{b}_j)\right) \left(\sum_{j>J} |z_j| (b_j + \bar{b}_j)\right).$$

□

We now prove Proposition 6.3.1.

Proof of Proposition 6.3.1. From Lemma 6.6.1, we have that

$$|\mathcal{G}(z)| \leq c \exp\left(c \sum_{j=1}^{\infty} |z_j|(b_j + \bar{b}_j)\right), \quad |\mathcal{G}^J(z)| \leq c \exp\left(c \sum_{j=1}^{\infty} |z_j|(b_j + \bar{b}_j)\right)$$

for a constant $c > 0$. From Lemma 6.6.2, we have

$$|\mathcal{G}(z) - \mathcal{G}^J(z)| \leq c \left(\sum_{j>J} |z_j|(b_j + \bar{b}_j) \right) \exp\left(c \sum_{j=1}^{\infty} |z_j|(b_j + \bar{b}_j)\right).$$

Let $Z(\delta)$ and $Z^J(\delta)$ be the normalizing constants in (6.1.4) and (6.3.3) respectively. We first show that Z^J is uniformly bounded below from 0 uniformly with respect to J . From (6.3.2) and Lemma 6.6.1, we have that

$$|\Phi^J(z, \delta)| \leq c(\delta) \exp\left(\sum_{j=1}^J (b_j + \bar{b}_j)\right).$$

From Lemma 4.6.1, we have that

$$\int_U \Phi^J(z, \delta) d\gamma(z) < \Lambda$$

uniformly for all J . Fixing a constant $C > 0$, the γ measure of the set z such that $\Phi^J(z, \delta) > C$ is less than Λ/C so the γ measure of the set of z such that $\Phi^J(z, \delta) \leq C$ is more than $1 - \Lambda/C$ which is positive when C is sufficiently large. Thus

$$Z^J(\delta) = \int_U \exp(-\Phi^J(z, \delta)) d\gamma(z) > (1 - \Lambda/C) \exp(-C) > 0.$$

As in equation (5.2.1) of Chapter 5 we have

$$d_{\text{Hell}}(\gamma^\delta, \gamma^{J,\delta})^2 \leq I_1 + I_2,$$

where

$$I_1 = \frac{2}{Z(\delta)} \int_U \left(\exp\left(-\frac{1}{2}\Phi(z, \delta)\right) - \exp\left(-\frac{1}{2}\Phi^J(z, \delta)\right) \right)^2 d\gamma(z), \quad (6.6.2)$$

and

$$I_2 = 2|Z(\delta)^{-1/2} - Z^J(\delta)^{-1/2}|^2 \int_U \exp(-\Phi^J(z, \delta)) d\gamma(z). \quad (6.6.3)$$

We then have

$$\begin{aligned} \left| \exp(-\frac{1}{2}\Phi(z, \delta)) - \exp(-\frac{1}{2}\Phi^J(z, \delta)) \right| &\leq c(|\delta| + |\mathcal{G}(z)| + |\mathcal{G}^J(z)|) |\mathcal{G}(z) - \mathcal{G}^J(z)| \\ &\leq c(\delta) \exp \left(c \sum_{j=1}^{\infty} |z_j|(b_j + \bar{b}_j) \right) \left(\sum_{j>J} |z_j|(b_j + \bar{b}_j) \right). \end{aligned}$$

Thus

$$I_1 \leq c(\delta) \int_U \exp \left(c \sum_{j=1}^{\infty} |z_j|(b_j + \bar{b}_j) \right) \left(\sum_{j>J} |z_j|(b_j + \bar{b}_j) \right)^2.$$

The proof that the right hand side is bounded by cJ^{-2q} is similar to the result in Proposition 4.3.2 $\square$

6.7 Appendix B

We prove Proposition 6.3.2 in this appendix. First we note the following approximation for the approximating problem (6.3.4).

Lemma 6.7.1. Let D be a convex domain. Assume further that $f \in C([0, T]; H)$. Under Assumption 6.1.1, there is a constant $c > 0$ such that for all $m = 1, \dots, M$, $\forall z \in U$, the solution of problem (6.3.4) satisfies

$$\|P_m^{J,h,k}(z) - P^J(t_m, \cdot, z)\|_V \leq c \exp \left(c \sum_{j=1}^J |z_j|(b_j + \bar{b}_j) \right) (h+k) + c\|g - g^l\|_V.$$

Proof We follow the procedure in Chapter 5, Section 5.7. We start off with

$$\|P_m^{J,h,k}(\cdot, z) - P^J(t_m, \cdot, z)\|_V$$

$$\begin{aligned}
&\leq \|P_m^{J,h,k}(\cdot, z) - R_h P^J(t_m, \cdot, z)\|_V + \|R_h P^J(t_m, \cdot, z) - P^J(t_m, \cdot, z)\|_V \\
&= \|\theta^m\|_V + \|\varphi^m\|_V
\end{aligned}$$

where

$$\begin{aligned}
\theta^m &= P_m^{J,h,k}(\cdot, z) - R_h P^J(t_m, \cdot, z) \\
\varphi^m &= R_h P^J(t_m, \cdot, z) - P^J(t_m, \cdot, z)
\end{aligned}$$

and that $R_h : V \rightarrow V^l$ is the orthogonal projection satisfying

$$\int_D K^J(\cdot, z) \nabla(R_h \psi) \cdot \nabla \phi dx = \int_D K^J(\cdot, z) \nabla \psi \cdot \nabla \phi dx$$

$\forall \psi \in V$ and $\forall \phi \in V^l$. Further, we have from equation (5.7.2)

$$\|\theta^m\|_V^2 \leq Ck \sum_{i=1}^m \|\omega_1^i\|_H^2 + Ck \sum_{i=1}^m \|\omega_2^i\|_H^2 + \|\theta^0\|_V^2 \quad (6.7.1)$$

where

$$\begin{aligned}
\omega_1^m &= \frac{R_h P^J(t_m, \cdot, z) - R_h P^J(t_{m-1}, \cdot, z)}{k} - \frac{P^J(t_m, \cdot, z) - P^J(t_{m-1}, \cdot, z)}{k} \\
\omega_2^m &= \frac{P^J(t_m, \cdot, z) - P^J(t_{m-1}, \cdot, z)}{k} - \frac{\partial P^J}{\partial t}(t_m, \cdot, z).
\end{aligned}$$

We have

$$\omega_1^m = (R_h - I) \frac{1}{k} \int_{t_{m-1}}^{t_m} P_t^J(s, \cdot, z) ds = \frac{1}{k} \int_{t_{m-1}}^{t_m} (R_h - I) P_t^J(s, \cdot, z) ds.$$

From the duality argument in the proof of Theorem 1.1 of Thomee [52], we have

$$\|(R_h - I) P_t^J(t, \cdot, z)\|_H \leq ch \exp \left(c \sum_{j=1}^{\infty} |z_j| (b_j + \bar{b}_j) \right) \|P_t^J(t, \cdot, z)\|_V.$$

We have

$$k\omega_1^m = \int_{t_{m-1}}^{t_m} (R_h - I) P_t^J(s, \cdot, z) ds.$$

Thus

$$\begin{aligned} k^2 \|\omega_1^m\|_H^2 &\leq c \exp \left(c \sum_{j=1}^{\infty} |z_j| (b_j + \bar{b}_j) \right) h^2 \left(\int_{t_{m-1}}^{t_m} \|P_t^J(s, \cdot, z)\|_V ds \right)^2 \\ &\leq c \exp \left(c \sum_{j=1}^{\infty} |z_j| (b_j + \bar{b}_j) \right) h^2 k \int_{t_{m-1}}^{t_m} \|P_t^J(s, \cdot, z)\|_V^2 ds. \end{aligned}$$

Thus for all $m = 1, \dots, M$

$$k \sum_{i=1}^m \|\omega_1^i\|_H^2 \leq c \exp \left(c \sum_{j=1}^{\infty} |z_j| (b_j + \bar{b}_j) \right) h^2 \int_0^T \|P_t^J(s, \cdot, z)\|_V^2 ds.$$

For ω_2^m , we have

$$k\omega_2^m = - \int_{t_{m-1}}^{t_m} (s - t_{m-1}) P_{tt}^J(s, \cdot, z) ds$$

so

$$k^2 \|\omega_2^m\|^2 \leq k^2 \left(\int_{t_{m-1}}^{t_m} \|P_{tt}^J(s, \cdot, z)\|_H ds \right)^2,$$

i.e.

$$\|\omega_2^m\|_H^2 \leq \left(\int_{t_{m-1}}^{t_m} \|P_{tt}^J(s, \cdot, z)\|_H ds \right)^2 \leq k \int_{t_{m-1}}^{t_m} \|P_{tt}^J(s, \cdot, z)\|_H^2 ds.$$

Thus

$$k \sum_{i=1}^m \|\omega_2^i\|_H^2 \leq ck^2 \int_0^T \|P_{tt}^J(s, \cdot, z)\|_H^2 ds.$$

Using Lemma 6.6.1 for P^J where we consider z with only the first J components being nonzero, we have that

$$\|P_t^J(z)\|_{L^2((0,T);V)} \leq c \exp \left(c \sum_{j=1}^J |z_j| (b_j + \bar{b}_j) \right).$$

From (6.1.3), we have $\frac{dP^J}{dt}(z) \in C([0, T]; H)$ and

$$\left\| \frac{\partial P^J}{\partial t}(z) \right\|_{C([0,T];H)} \leq c \left(\left\| \frac{\partial P^J}{\partial t}(z) \right\|_{L^2([0,T];V)} + \left\| \frac{\partial P^J}{\partial t}(z) \right\|_{H^1((0,T);V')} \right).$$

Thus

$$\left\| \frac{\partial P^J}{\partial t}(z) \right\|_{C([0,T];H)} \leq c \exp(c \sum_{j=1}^{\infty} |z_j| (b_j + \bar{b}_j)). \quad (6.7.2)$$

From (6.1.2),

$$-\Delta P^J(z) = \frac{1}{K^J(z)} (f - \frac{\partial P^J}{\partial t}(z) + \nabla K^J(z) \cdot \nabla P^J(z)).$$

As D is convex domain, there is a constant c which only depends on the domain D such that

$$\begin{aligned} & \|P^J(t, \cdot, z)\|_{H^2(D)} \\ & \leq \frac{c}{K_{\min}^J(z)} \left(\|f(t, \cdot)\|_H + \left\| \frac{\partial P^J}{\partial t}(t, \cdot, z) \right\|_H + \|\nabla K^J(t, \cdot, z)\|_{L^\infty(D)} \|\nabla P^J(t, \cdot, z)\|_H \right) \end{aligned}$$

(see, e.g., [28]). From Lemma 6.6.1, we have

$$\sup_{t \in [0, T]} \|\nabla P^J(t, \cdot, z)\|_H \leq c \exp(c \sum_{j=1}^{\infty} |z_j| (b_j + \bar{b}_j)).$$

From (6.7.2),

$$\sup_{t \in [0, T]} \left\| \frac{\partial P^J}{\partial t}(t, \cdot, z) \right\|_H \leq c \exp(c \sum_{j=1}^{\infty} |z_j| (b_j + \bar{b}_j)).$$

Thus

$$\|P^J(t, \cdot, z)\|_{H^2(D)} \leq c \exp \left(c \sum_{j=1}^{\infty} |z_j| (b_j + \bar{b}_j) \right).$$

We further have $\varphi^m = (R_h - I)P^J(t_m, \cdot, z)$ so

$$\|\varphi^m\|_V \leq ch \|P^J(t_m, \cdot, z)\|_{H^2(D)}.$$

Therefore for all $m = 1, \dots, M$

$$\begin{aligned} & \|P_m^{J,h,k}(z) - P^J(t_m, \cdot, z)\|_V \\ & \leq c \exp(c \sum_{j=1}^{\infty} |z_j| b_j) (h + k). \end{aligned}$$

$$\left(\|P_t^J(z)\|_{L^2((0,T);V)} + \|P_{tt}^J(z)\|_{L^2((0,T);H)} + \sup_{t \in (0,T)} \|P^J(t, \cdot, z)\|_{H^2(D)} \right) + \|g - g^L\|_V.$$

Hence, there is a constant $c > 0$ such that $\forall z \in U$

$$\|P_m^{J,h,k}(z) - P^J(t_m, \cdot, z)\|_V \leq c \exp \left(c \sum_{j=1}^{\infty} |z_j|(b_j + \bar{b}_j) \right) (h+k) + \|g - g^L\|_V.$$

We are now ready to prove Proposition 6.3.2.

Proof of Proposition 6.3.2: We note that it is sufficient to show that $d_{Hell}(\gamma^{J,\delta}, \gamma^{J,h,k,\delta}) \leq C(h+k)$. From Lemma 6.6.1 and 6.7.1, when choosing g^l such that $\|g - g^l\|_V \leq ch$, we have

$$\|P_{\tau_i}^{J,h,k}(z)\|_V \leq c \exp \left(c \sum_{j=1}^J |z_j|(b_j + \bar{b}_j) \right)$$

so

$$|\mathcal{G}^{J,h,k}(z)| \leq c \exp \left(c \sum_{j=1}^{\infty} |z_j|(b_j + \bar{b}_j) \right).$$

We have further from Lemma 6.7.1 that $\forall z \in U$

$$|\ell_i(P^J(\tau_i, \cdot, z)) - \ell_i(P_{\tau_i}^{J,h,k}(\cdot, z))| \leq c \exp \left(c \sum_{j=1}^J |z_j|(b_j + \bar{b}_j) \right) (h+k).$$

Thus

$$|\mathcal{G}^J(z) - \mathcal{G}^{J,h,k}(z)| \leq c \exp \left(c \sum_{j=1}^J |z_j|(b_j + \bar{b}_j) \right) (h+k).$$

We proceed as in the proof of Proposition 5.3.2 in Chapter 5. Let $Z^J(\delta)$ and $Z^{J,h,k}(\delta)$ be the normalizing constants in (6.3.1) and (6.3.5) respectively. We have

$$2d_{Hell}(\gamma^{J,\delta}, \gamma^{J,h,k,\delta})^2 \leq I_1 + I_2,$$

where

$$I_1 = \frac{2}{Z^J(\delta)} \int_U \left(\exp\left(-\frac{1}{2}\Phi^J(z, \delta)\right) - \exp\left(-\frac{1}{2}\Phi^{J,h,k}(z, \delta)\right) \right)^2 d\gamma(z), \quad (6.7.3)$$

and

$$I_2 = 2|Z^J(\delta)^{-1/2} - Z^{J,h,k}(\delta)^{-1/2}|^2 \int_U \exp(-\frac{1}{2}\Phi^{J,h,k}(z, \delta)) d\gamma(z). \quad (6.7.4)$$

A similar proof to that for $Z^J(\delta)$ above shows that $Z^{J,h,k}(\delta)$ is uniformly bounded below from 0 for all J, h and k . We then have

$$\begin{aligned} & \left| \exp(-\frac{1}{2}\Phi^J(z, \delta)) - \exp(-\frac{1}{2}\Phi^{J,h,k}(z, \delta)) \right| \\ & \leq c(|\delta| + |\mathcal{G}^J(z)| + |\mathcal{G}^{J,h,k}(z)|) |\mathcal{G}^J(z) - \mathcal{G}^{J,h,k}(z)| \\ & \leq c \exp\left(c \sum_{j=1}^J |z_j|(b_j + \bar{b}_j)\right) (h + k). \end{aligned}$$

Using the first inequality of Lemma 4.6.1 we have

$$I_1 \leq c \exp\left(c \sum_{j=1}^J (b_j + \bar{b}_j)^2 + c \sum_{j=1}^J (b_j + \bar{b}_j)\right) (h + k)^2 \leq c(h + k)^2.$$

Similarly, we have $I_2 \leq c(h + k)^2$, implying that $d_{Hell}(\gamma^{J,\delta}, \gamma^{J,h,k,\delta}) \leq c(h + k)^2$. Together with $d_{Hell}(\gamma^\delta, \gamma^{J,\delta}) \leq cJ^{-q}$, we get the conclusion. $\square$

References

- [1] R. J. Adler. *The geometry of random fields*, volume 62 of *Classics in Applied Mathematics*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2010. Reprint of the 1981 original [MR0611857].
- [2] G. Allaire. Homogenization and two-scale convergence. *SIAM J. Math. Anal.*, 23(6):1482–1518, 1992.
- [3] G. Allaire and M. Briane. Multiscale convergence and reiterated homogenization. *Proc. Roy. Soc. Edinburgh Sect. A*, 126(2):297–342, 1996.
- [4] N. Bakhvalov and G. Panasenko. *Homogenisation: averaging processes in periodic media*, volume 36 of *Mathematics and its Applications (Soviet Series)*. Kluwer Academic Publishers Group, Dordrecht, 1989. Mathematical problems in the mechanics of composite materials, Translated from the Russian by D. Leutes.
- [5] A. Bensoussan, J.-L. Lions, and G. Papanicolaou. *Asymptotic analysis*

- for periodic structures, volume 5 of *Studies in Mathematics and its Applications*. North-Holland Publishing Co., Amsterdam, 1978.
- [6] A. Beskos, A. Jasra, K. Law, R. Tempone, and Y. Zhou. Multilevel sequential Monte Carlo samplers. *Stochastic Process. Appl.*, 127(5):1417–1440, 2017.
- [7] H.-J. Bungartz and M. Griebel. Sparse grids. *Acta Numer.*, 13:1–123, 2004.
- [8] J. Charrier. Strong and weak error estimates for elliptic partial differential equations with random coefficients. *SIAM J. Numer. Anal.*, 50(1):216–246, 2012.
- [9] E. T. Chung, Y. Efendiev, B. Jin, W. T. Leung, and M. Vasilyeva. Generalized multiscale inversion for heterogeneous problems. *arXiv:1707.08194*, 2017.
- [10] P. Ciarlet. *The finite element method for elliptic problems*. North-Holland Publishing Co., Amsterdam, 1978.
- [11] A. Cohen. *Numerical analysis of wavelet methods*, volume 32 of *Studies in Mathematics and its Applications*. North-Holland Publishing Co., Amsterdam, 2003.
- [12] S. L. Cotter, M. Dashti, J. C. Robinson, and A. M. Stuart. Bayesian inverse problems for functions and applications to fluid mechanics. *Inverse Problems*, 25(11):115008, 43, 2009.
- [13] W. Dahmen. Wavelet and multiscale methods for operator equations. In *Acta numerica, 1997*, volume 6 of *Acta Numer.*, pages 55–228. Cambridge Univ. Press, Cambridge, 1997.

- [14] M. Dashti and A.M.Stuart. The bayesian approach to inverse problems. In R. Ghanem, D. Higdon, and H. Owhadi, editors, *Handbook of Uncertainty Quantification*, pages 311–428. Springer, 2017.
- [15] M. Dashti and A. M. Stuart. The bayesian approach to inverse problems. Technical Report 1302.6989v4, ArXiv.
- [16] M. Dashti and A. M. Stuart. Uncertainty quantification and weak approximation of an elliptic inverse problem. *SIAM J. Numer. Anal.*, 49(6):2524–2542, 2011.
- [17] P. Del Moral, A. Jasra, K. J. H. Law, and Y. Zhou. Multilevel sequential Monte Carlo samplers for normalizing constants. *ACM Trans. Model. Comput. Simul.*, 27(3):Art. 20, 22, 2017.
- [18] C. R. Dietrich and G. N. Newsam. Fast and exact simulation of stationary Gaussian processes through circulant embedding of the covariance matrix. *SIAM J. Sci. Comput.*, 18(4):1088–1107, 1997.
- [19] T. J. Dodwell, C. Ketelsen, R. Scheichl, and A. L. Teckentrup. A hierarchical multilevel Markov chain Monte Carlo algorithm with applications to uncertainty quantification in subsurface flow. *SIAM/ASA J. Uncertain. Quantif.*, 3(1):1075–1108, 2015.
- [20] Y. Efendiev, T. Hou, and W. Luo. Preconditioning Markov chain Monte Carlo simulations using coarse-scale models. *SIAM J. Sci. Comput.*, 28(2):776–803, 2006.
- [21] H. W. Engl, M. Hanke, and A. Neubauer. *Regularization of inverse problems*, volume 375 of *Mathematics and its Applications*. Kluwer Academic Publishers Group, Dordrecht, 1996.

-
- [22] C. Frederick and B. Engquist. Numerical methods for multiscale inverse problems. Technical Report 1401.2431v3, ArXiv.
 - [23] J. Galvis and M. Sarkis. Approximating infinity-dimensional stochastic Darcy's equations without uniform ellipticity. *SIAM J. Numer. Anal.*, 47(5):3624–3651, 2009.
 - [24] C. J. Gittelsohn. Stochastic Galerkin discretization of the log-normal isotropic diffusion problem. *Mathematical Models and Methods in Applied Sciences*, 20(2):237–263, 2010.
 - [25] C. J. Gittelsohn. Stochastic Galerkin discretization of the log-normal isotropic diffusion problem. *Mathematical Models and Methods in Applied Sciences*, 20(2):237–263, 2010.
 - [26] I. G. Graham, F. Y. Kuo, D. Nuyens, R. Scheichl, and I. H. Sloan. Quasi-Monte Carlo methods for elliptic PDEs with random coefficients and applications. *J. Comput. Phys.*, 230(10):3668–3694, 2011.
 - [27] M. Griebel and P. Oswald. Tensor product type subspace splittings and multilevel iterative methods for anisotropic problems. *Adv. Comput. Math.*, 4(1-2):171–206, 1995.
 - [28] P. Grisvard. *Elliptic problems in nonsmooth domains*, volume 24 of *Monographs and Studies in Mathematics*. Pitman (Advanced Publishing Program), Boston, MA, 1985.
 - [29] M. Hairer, A. M. Stuart, and S. J. Vollmer. Spectral gaps for a Metropolis-Hastings algorithm in infinite dimensions. *Ann. Appl. Probab.*, 24(6):2455–2490, 2014.

- [30] J. S. Hesthaven, S. Gottlieb, and D. Gottlieb. *Spectral methods for time-dependent problems*, volume 21 of *Cambridge Monographs on Applied and Computational Mathematics*. Cambridge University Press, Cambridge, 2007.
- [31] V. Hoang and C. Schwab. Convergence rate analysis of mcmc-fem for Bayesian inversion of log-normal diffusion problems. 2016.
- [32] V. H. Hoang. Bayesian inverse problems in measure spaces with application to Burgers and Hamilton-Jacobi equations with white noise forcing. *Inverse Problems*, 28(2):025009, 29, 2012.
- [33] V. H. Hoang, J. H. Quek, and C. Schwab. In preparation. 2018.
- [34] V. H. Hoang and C. Schwab. Convergence rate analysis of mcmc-fem for bayesian inversion of log-normal diffusion problems. *Preprint*.
- [35] V. H. Hoang and C. Schwab. High-dimensional finite elements for elliptic problems with multiple scales. *Multiscale Model. Simul.*, 3(1):168–194, 2004/05.
- [36] V. H. Hoang and C. Schwab. Analytic regularity and polynomial approximation of stochastic, parametric elliptic multiscale pdes. *Analysis and Applications*, 11:1350001, 2013.
- [37] V. H. Hoang, C. Schwab, and A. Stuart. Complexity analysis of accelerated MCMC methods for Bayesian inversion. *Inverse Problems*, 29(8), 2013.
- [38] V. Isakov. *Inverse problems for partial differential equations*, volume 127 of *Applied Mathematical Sciences*. Springer, Cham, third edition, 2017.

- [39] A. Jasra, K. J. H. Law, and Y. Zhou. Forward and inverse uncertainty quantification using multilevel Monte Carlo algorithms for an elliptic nonlocal equation. *Int. J. Uncertain. Quantif.*, 6(6):501–514, 2016.
- [40] L. Jiang and N. Ou. Multiscale model reduction method for Bayesian inverse problems of subsurface flow. *J. Comput. Appl. Math.*, 319:188–209, 2017.
- [41] L. Jiang and N. Ou. Bayesian inference using intermediate distribution based on coarse multiscale model for time fractional diffusion equations. *Multiscale Model. Simul.*, 16(1):327–355, 2018.
- [42] V. V. Jikov, S. M. Kozlov, and O. A. Oleumik. *Homogenization of differential operators and integral functionals*. Springer-Verlag, Berlin, 1994. Translated from the Russian by G. A. Yosifian [G. A. Iosifyan].
- [43] J. Kaipio and E. Somersalo. *Statistical and computational inverse problems*, volume 160 of *Applied Mathematical Sciences*. Springer-Verlag, New York, 2005.
- [44] W. McLean. *Strongly Elliptic Systems and Boundary Integral Equations*. Cambridge University Press, 2000.
- [45] G. Nguetseng. A general convergence result for a functional related to the theory of homogenization. *SIAM J. Math. Anal.*, 20(3):608–623, 1989.
- [46] J. Nolen, G. A. Pavliotis, and A. M. Stuart. Multiscale modeling and inverse problems. In *Numerical analysis of multiscale problems*, volume 83 of *Lect. Notes Comput. Sci. Eng.*, pages 1–34. Springer, Heidelberg, 2012.

-
- [47] R. Scheichl, A. M. Stuart, and A. L. Teckentrup. Quasi-Monte Carlo and multilevel Monte Carlo methods for computing posterior expectations in elliptic inverse problems. *SIAM/ASA J. Uncertain. Quantif.*, 5(1):493–518, 2017.
 - [48] C. Schillings and C. Schwab. Sparse, adaptive Smolyak quadratures for Bayesian inverse problems. *Inverse Problems*, 29(6):065011, 28, 2013.
 - [49] C. Schillings and A. M. Stuart. Analysis of the ensemble Kalman filter for inverse problems. *SIAM J. Numer. Anal.*, 55(3):1264–1290, 2017.
 - [50] C. Schwab and C. J. Gittelson. Sparse tensor discretizations of high-dimensional parametric and stochastic PDEs. *Acta Numerica*, 20:291–467, 2011.
 - [51] A. M. Stuart. Inverse problems: A Bayesian perspective. *Acta Numerica*, 2010.
 - [52] V. Thomée. *Galerkin finite element methods for parabolic problems*, volume 25 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, second edition, 2006.
 - [53] T. von Petersdorff and C. Schwab. Numerical solution of parabolic equations in high dimensions. *M2AN Math. Model. Numer. Anal.*, 38(1):93–127, 2004.
 - [54] J. Wloka. *Partial differential equations*. Cambridge University Press, Cambridge, 1987. Translated from the German by C. B. Thomas and M. J. Thomas.

- [55] Y. Yamasaki. *Measures on infinite-dimensional spaces*, volume 5 of *Series in Pure Mathematics*. World Scientific Publishing Co., Singapore, 1985.