

# Introduction to the Bayesian Approach to Inverse Problems - Part 2: Algorithms

## Lecture 3

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## Contents

- The second half of this short course will focus on **algorithms in Bayesian inverse problems**, in particular algorithms for computing expectations with respect to the posterior distribution.
- The emphasis will be on **convergence properties** of the algorithms rather than implementation.
- The first lecture will focus on **standard Monte Carlo methods**: sampling methods based on independent and identically distributed (i.i.d.) samples.
- The second lecture will focus on **Markov chain Monte Carlo methods**: sampling methods based on correlated and approximate samples.

# Outline of first lecture

- 1 Bayesian Inverse Problems
- 2 Standard Monte Carlo Method
- 3 Convergence of Standard Monte Carlo Method
- 4 Multilevel Monte Carlo Method
- 5 Convergence of Multilevel Monte Carlo Method

# Bayesian Inverse Problems

Mathematical Formulation [Kaipio, Somersalo '04] [Stuart '10]

- We are interested in the following inverse problem: given observational data  $y \in \mathbb{R}^J$ , determine model parameter  $u \in \mathbb{R}^n$  such that

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

where  $\eta \sim N(0, \Gamma)$  represents observational noise.

- In the Bayesian approach, the solution to the inverse problem is the posterior distribution  $\mu^y$  on  $\mathbb{R}^n$ , given by

$$\frac{d\mu^y}{d\mu_0}(u) = \frac{1}{Z} \exp(-\Phi(u; y)),$$

where  $Z = \mathbb{E}_{\mu_0} \left( \exp(-\Phi(\cdot; y)) \right)$  and  $\Phi(u; y) = \frac{1}{2} \|y - \mathcal{G}(u)\|_{\Gamma}^2$ .

# Bayesian Inverse Problems

## Computing expectations

- We will here focus on computing the expected value of a quantity of interest  $\phi(u)$ ,  $\phi : \mathbb{R}^n \rightarrow \mathbb{R}$ , under the posterior distribution  $\mu^y$ .
- In most cases, we do not have a closed form expression for the posterior distribution  $\mu^y$ , since the normalising constant  $Z$  is not known explicitly.  
(Exception: forward map  $\mathcal{G}$  linear and prior  $\mu_0$  Gaussian  $\Rightarrow$  posterior  $\mu^y$  also Gaussian.)
- However, the prior distribution is known in closed form, and furthermore often has a simple structure (e.g. multivariate Gaussian or independent uniform).

# Bayesian Inverse Problems

## Computing Expectations

Using Bayes' Theorem, we can write  $\mathbb{E}_{\mu^y}[\phi]$  as

$$\begin{aligned}\mathbb{E}_{\mu^y}[\phi] &= \int_{\mathbb{R}^n} \phi(u) d\mu^y(u) \\ &= \int_{\mathbb{R}^n} \phi(u) \frac{d\mu^y}{d\mu_0}(u) d\mu_0(u) \\ &= \frac{1}{Z} \int_{\mathbb{R}^n} \phi(u) \exp[-\Phi(u; y)] d\mu_0(u) \\ &= \frac{\mathbb{E}_{\mu_0}[\phi \exp[-\Phi(\cdot; y)]]}{\mathbb{E}_{\mu_0}[\exp[-\Phi(\cdot; y)]]}.\end{aligned}$$

We have rewritten the posterior expectation as a ratio of two prior expectations.

We will now use Monte Carlo methods to estimate the two prior expectations.

# Standard Monte Carlo Method

## Sampling methods and random number generators

- The standard Monte Carlo method is a *sampling method*.
- To estimate  $\mathbb{E}_{\mu_0}[f]$ , for some  $f : \mathbb{R}^n \rightarrow \mathbb{R}$ , sampling methods use a sample average:

$$\mathbb{E}_{\mu_0}[f] = \int_{\mathbb{R}^n} f(u) d\mu_0(u) \approx \sum_{i=1}^N w_i f(u^{(i)}),$$

where the choice of samples  $\{u^{(i)}\}_{i=1}^N$  and weights  $\{w_i\}_{i=1}^N$  determines the sampling method.

- In standard Monte Carlo,  $w_i = \frac{1}{N}$  and  $\{u^{(i)}\}_{i=1}^N$  is a sequence of independent and identically distributed (i.i.d.) random variables:  $\{u^{(i)}\}_{i=1}^N$  are mutually independent and  $u^{(i)} \sim \mu_0$ , for all  $1 \leq i \leq N$ .
- Since  $\mu_0$  is fully known and simple, i.i.d. samples from  $\mu_0$  can be generated on a computer using a (pseudo-)random number generator. For more details, see [Robert, Casella '99], [L'Ecuyer '11].

# Standard Monte Carlo Method

## Definition of Monte Carlo Estimator

- In the Bayesian inverse problem, we want to compute

$$\mathbb{E}_{\mu^y}[\phi] = \frac{\mathbb{E}_{\mu_0}[\phi \exp[-\Phi(\cdot; y)]]}{\mathbb{E}_{\mu_0}[\exp[-\Phi(\cdot; y)]]}.$$

- Using Monte Carlo, we approximate this by

$$\mathbb{E}_{\mu_0}[\phi \exp[-\Phi(\cdot; y)]] \approx \frac{1}{N} \sum_{i=1}^N \phi(u^{(i)}) \exp[-\Phi(u^{(i)}; y)],$$

$$\mathbb{E}_{\mu_0}[\exp[-\Phi(\cdot; y)]] \approx \frac{1}{N} \sum_{i=1}^N \exp[-\Phi(u^{(i)}; y)],$$

where  $\{u^{(i)}\}_{i=1}^N$  is an i.i.d. sequence distributed according to  $\mu_0$ .

(It is also possible to use different samples in the two estimators.)

# Standard Monte Carlo Method

## Definition of Monte Carlo Estimator

- In applications, it is usually not possible to evaluate  $\phi$  and  $\Phi$  exactly, since this involves the solution of the forward problem.
  - ▶ In the groundwater flow example, it involves the solution of a PDE.
- Denote by  $\phi_h$  and  $\Phi_h$  numerical approximations to  $\phi$  and  $\Phi$ , respectively, where  $h$  is the step length of the numerical method.
- The computable Monte Carlo ratio estimator of  $\mathbb{E}_{\mu^y}[\phi]$  is then

$$\mathbb{E}_{\mu^y}[\phi] \approx \frac{\frac{1}{N} \sum_{i=1}^N \phi_h(u^{(i)}) \exp[-\Phi_h(u^{(i)}; y)]}{\frac{1}{N} \sum_{i=1}^N \exp[-\Phi_h(u^{(i)}; y)]} := \frac{\widehat{Q}_{h,N}^{\text{MC}}}{\widehat{Z}_{h,N}^{\text{MC}}}.$$

- There are two sources of error in the Monte Carlo ratio estimator:
  - ▶ the **sampling error** due to using Monte Carlo,
  - ▶ the **discretisation error** due to the numerical approximation.

# Convergence of Standard Monte Carlo Method

Expected Value and Variance [Billingsley '95]

Consider a general Monte Carlo estimator  $\widehat{E}_{h,N}^{\text{MC}} = \frac{1}{N} \sum_{i=1}^N f_h(u^{(i)})$ , with  $\{u^{(i)}\}_{i=1}^N$  an i.i.d. sequence distributed as  $\mu_0$ .

**Lemma (Expected Value and Variance)**

$$\mathbb{E}[\widehat{E}_{h,N}^{\text{MC}}] = \mathbb{E}_{\mu_0}[f_h], \quad \mathbb{V}[\widehat{E}_{h,N}^{\text{MC}}] = \frac{\mathbb{V}_{\mu_0}[f_h]}{N}.$$

**Proof:** Since  $\{u^{(i)}\}_{i=1}^N$  is an i.i.d. sequence, we have

$$\mathbb{E}\left[\frac{1}{N} \sum_{i=1}^N f_h(u^{(i)})\right] = \frac{1}{N} \mathbb{E}\left[\sum_{i=1}^N f_h(u^{(i)})\right] = \frac{1}{N} \sum_{i=1}^N \mathbb{E}_{\mu_0}[f_h] = \mathbb{E}_{\mu_0}[f_h],$$

and

$$\mathbb{V}\left[\frac{1}{N} \sum_{i=1}^N f_h(u^{(i)})\right] = \frac{1}{N^2} \mathbb{V}\left[\sum_{i=1}^N f_h(u^{(i)})\right] = \frac{1}{N^2} \sum_{i=1}^N \mathbb{V}_{\mu_0}[f_h] = \frac{1}{N} \mathbb{V}_{\mu_0}[f_h].$$

# Convergence of Standard Monte Carlo Method

Central Limit Theorem [Billingsley '95]

## Theorem (Central Limit Theorem)

If  $\mathbb{V}_{\mu_0}[f_h] \in (0, \infty)$ , then as  $N \rightarrow \infty$  we have

$$\hat{E}_{h,N}^{\text{MC}} \xrightarrow{D} \mathcal{N}(\mathbb{E}_{\mu_0}[f_h], \frac{\mathbb{V}_{\mu_0}[f_h]}{N}).$$

Here,  $\xrightarrow{D}$  denotes convergence in distribution, i.e. point-wise convergence of the distribution function: with  $X \sim \mathcal{N}(\mathbb{E}_{\mu_0}[f_h], \frac{\mathbb{V}_{\mu_0}[f_h]}{N})$ ,

$$\Pr[\hat{E}_{h,N}^{\text{MC}} \leq x] \rightarrow \Pr[X \leq x], \quad \forall x \in \mathbb{R}.$$

The Central Limit Theorem crucially uses the fact that  $\hat{E}_{h,N}^{\text{MC}}$  is based on i.i.d. samples. If this is not the case, we require stronger assumptions and/or obtain a different limiting distribution.

# Convergence of Standard Monte Carlo Method

Strong Law of Large Numbers [Billingsley '95]

## Theorem (Strong Law of Large Numbers)

If  $\mathbb{E}_{\mu_0}[|f_h|] < \infty$ , then as  $N \rightarrow \infty$  we have

$$\hat{E}_{h,N}^{\text{MC}} \xrightarrow{a.s.} \mathbb{E}_{\mu_0}[f_h].$$

Here,  $\xrightarrow{a.s.}$  denotes almost sure convergence, i.e. convergence with probability 1:

$$\Pr[\hat{E}_{h,N}^{\text{MC}} \rightarrow \mathbb{E}_{\mu_0}[f_h]] = 1.$$

The Strong Law of Large Numbers crucially uses the fact that  $\hat{E}_{h,N}^{\text{MC}}$  is based on i.i.d. samples. If this is not the case, we may require stronger assumptions

# Convergence of Standard Monte Carlo Method

Mean Square Error [Billingsley '95]

A measure of **accuracy** of  $\hat{E}_{h,N}^{\text{MC}} = \frac{1}{N} \sum_{i=1}^N f_h(u^{(i)})$  as an estimator of  $\mathbb{E}_{\mu_0}[f]$  is given by the mean square error (MSE):

$$e(\hat{E}_{h,N}^{\text{MC}})^2 := \mathbb{E}[(\hat{E}_{h,N}^{\text{MC}} - \mathbb{E}_{\mu_0}[f])^2].$$

## Theorem (Mean Square Error)

$$e(\hat{E}_{h,N}^{\text{MC}})^2 = \underbrace{\frac{\mathbb{V}_{\mu_0}[f_h]}{N}}_{\text{sampling error}} + \underbrace{(\mathbb{E}_{\mu_0}[f_h - f])^2}_{\text{numerical error}}.$$

**Proof:** Since  $\mathbb{E}[\hat{E}_{h,N}^{\text{MC}}] = \mathbb{E}_{\mu_0}[f_h]$  and  $\mathbb{V}[\hat{E}_{h,N}^{\text{MC}}] = \frac{\mathbb{V}_{\mu_0}[f_h]}{N}$ , we have

$$\begin{aligned} e(\hat{E}_{h,N}^{\text{MC}})^2 &= \mathbb{E} \left[ (\hat{E}_{h,N}^{\text{MC}} - \mathbb{E}_{\mu_0}[f_h] + \mathbb{E}_{\mu_0}[f_h] - \mathbb{E}_{\mu_0}[f])^2 \right] \\ &= \mathbb{E} \left[ (\hat{E}_{h,N}^{\text{MC}} - \mathbb{E}_{\mu_0}[f_h])^2 \right] + \mathbb{E} \left[ (\mathbb{E}_{\mu_0}[f_h - f])^2 \right] \\ &= \frac{\mathbb{V}_{\mu_0}[f_h]}{N} + (\mathbb{E}_{\mu_0}[f_h - f])^2. \end{aligned}$$

# Convergence of Standard Monte Carlo Method

Mean Square Error of Monte Carlo ratio estimator [Scheichl, Stuart, ALT '16]

- Recall:  $\mathbb{E}_{\mu^y}[\phi] = \frac{\mathbb{E}_{\mu_0}[\phi \exp[-\Phi(\cdot; y)]]}{\mathbb{E}_{\mu_0}[\exp[-\Phi(\cdot; y)]]} =: \frac{Q}{Z} \approx \frac{\hat{Q}_{h,N}^{\text{MC}}}{\hat{Z}_{h,N}^{\text{MC}}}.$
- We know how to bound the MSEs of the individual estimators  $\hat{Q}_{h,N}^{\text{MC}}$  and  $\hat{Z}_{h,N}^{\text{MC}}$ . Can we bound the MSE of  $\hat{Q}_{h,N}^{\text{MC}}/\hat{Z}_{h,N}^{\text{MC}}?$
- Rearranging the MSE and applying the triangle inequality, we have

$$\begin{aligned} e\left(\frac{\hat{Q}_{h,N}^{\text{MC}}}{\hat{Z}_{h,N}^{\text{MC}}}\right)^2 &= \mathbb{E}\left[\left(\frac{Q}{Z} - \frac{\hat{Q}_{h,N}^{\text{MC}}}{\hat{Z}_{h,N}^{\text{MC}}}\right)^2\right] \\ &\leq \frac{2}{Z^2} \left( \mathbb{E}[(Q - \hat{Q}_{h,N}^{\text{MC}})^2] + \mathbb{E}\left[(\hat{Q}_{h,N}^{\text{MC}}/\hat{Z}_{h,N}^{\text{MC}})^2 (Z - \hat{Z}_{h,N}^{\text{MC}})^2\right] \right). \end{aligned}$$

# Convergence of Standard Monte Carlo Method

Mean Square Error of Monte Carlo ratio estimator [Scheichl, Stuart, ALT '16]

$$E\left(\frac{\widehat{Q}_{h,N}^{\text{MC}}}{\widehat{Z}_{h,N}^{\text{MC}}}\right)^2 \leq \frac{2}{Z^2} \left( E[(Q - \widehat{Q}_{h,N}^{\text{MC}})^2] + E[(\widehat{Q}_{h,N}^{\text{MC}}/\widehat{Z}_{h,N}^{\text{MC}})^2 (Z - \widehat{Z}_{h,N}^{\text{MC}})^2] \right)$$

## Theorem (Hölder's Inequality)

For any random variables  $X, Y$  and  $p, q \in [1, \infty]$ , with  $p^{-1} + q^{-1} = 1$ ,

$$E[|XY|] \leq E[|X|^p]^{1/p} E[|Y|^q]^{1/q}.$$

Here,  $E[|X|^\infty]^{1/\infty} := \text{ess sup } X$ .

If  $\text{ess sup}_{\{u^{(i)}\}_{i=1}^N} (\widehat{Q}_{h,N}^{\text{MC}}/\widehat{Z}_{h,N}^{\text{MC}})^2 \leq C$ , for a constant  $C$  independent of  $N$  and  $h$ , then the MSE of  $\widehat{Q}_{h,N}^{\text{MC}}/\widehat{Z}_{h,N}^{\text{MC}}$  can be bounded in terms of the individual MSEs of  $\widehat{Q}_{h,N}^{\text{MC}}$  and  $\widehat{Z}_{h,N}^{\text{MC}}$ .

For more details, see [Scheichl, Stuart, ALT '16].

# Multilevel Monte Carlo Method

## Motivation

The standard Monte Carlo estimator  $\hat{E}_{h,N}^{\text{MC}} = \frac{1}{N} \sum_{i=1}^N f_h(u^{(i)})$  of  $\mathbb{E}_{\mu_0}[f]$  has mean square error

$$e(\hat{E}_{h,N}^{\text{MC}})^2 = \frac{\mathbb{V}_{\mu_0}[f_h]}{N} + (\mathbb{E}_{\mu_0}[f_h] - f)^2.$$

To make  $e(\hat{E}_{h,N}^{\text{MC}})^2$ , small we need to

- choose a **large number of samples  $N$** ,
- choose a **small step length  $h$**  in our numerical approximation.

Since the cost of sampling methods grows as

$$\text{cost per sample} \times \text{number of samples}$$

the cost of standard Monte Carlo can be prohibitively large in applications.

# Multilevel Monte Carlo Method

Definition of Multilevel Monte Carlo Estimator [Giles, '08], [Heinrich '01]

The multilevel method works with a decreasing **sequence of step lengths**  $\{h_\ell\}_{\ell=0}^L$ , where  $h_L$  gives the most accurate numerical approximation.

Linearity of expectation gives us

$$\mathbb{E}_{\mu_0} [f_{h_L}] = \mathbb{E}_{\mu_0} [f_{h_0}] + \sum_{\ell=1}^L \mathbb{E}_{\mu_0} [f_{h_\ell} - f_{h_{\ell-1}}].$$

The **multilevel Monte Carlo (MLMC)** estimator

$$\widehat{E}_{\{M_\ell, N_\ell\}}^{\text{ML}} = \frac{1}{N_0} \sum_{i=1}^{N_0} f_{h_0}(u^{(i,0)}) + \sum_{\ell=1}^L \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} f_{h_\ell}(u^{(i,\ell)}) - f_{h_{\ell-1}}(u^{(i,\ell)}),$$

is a sum of  $L + 1$  independent MC estimators.

# Convergence of Multilevel Monte Carlo Method

Expected Value and Variance [Giles, '08]

$$\hat{E}_{\{M_\ell, N_\ell\}}^{\text{ML}} = \frac{1}{N_0} \sum_{i=1}^{N_0} f_{h_0}(u^{(i,0)}) + \sum_{\ell=1}^L \frac{1}{N_\ell} \sum_{i=1}^{N_\ell} f_{h_\ell}(u^{(i,\ell)}) - f_{h_{\ell-1}}(u^{(i,\ell)})$$

Lemma (Expected Value and Variance)

$$\mathbb{E}[\hat{E}_{\{M_\ell, N_\ell\}}^{\text{ML}}] = \mathbb{E}_{\mu_0}[f_{h_L}], \quad \mathbb{V}[\hat{E}_{\{M_\ell, N_\ell\}}^{\text{ML}}] = \frac{\mathbb{V}[f_{h_0}]}{N_0} + \sum_{\ell=1}^L \frac{\mathbb{V}[f_{h_\ell} - f_{h_{\ell-1}}]}{N_\ell}.$$

**Proof:** Uses the linearity of expectation and the fact the  $L + 1$  estimators are independent, together with results for standard Monte Carlo.

# Convergence of Multilevel Monte Carlo Method

Central Limit Theorem and Strong Law of Large Numbers [Billingsley '95]

## Theorem (Central Limit Theorem)

If  $\sigma_{\text{ML}}^2 := \mathbb{V}[f_{h_0}]N_0^{-1} + \sum_{\ell=1}^L \mathbb{V}[f_{h_\ell} - f_{h_{\ell-1}}]N_\ell^{-1} \in (0, \infty)$  and  $\{\mathbb{V}[f_{h_\ell} - f_{h_{\ell-1}}]\}_{\ell=1}^L$  satisfies a Lindeberg condition, then as  $\{N_\ell\}_{\ell=0}^L \rightarrow \infty$  we have

$$\hat{E}_{\{M_\ell, N_\ell\}}^{\text{ML}} \xrightarrow{D} \mathcal{N}(\mathbb{E}_{\mu_0}[f_{h_L}], \sigma_{\text{ML}}^2).$$

**Proof:** Requires Lindeberg condition to deal with sum of  $L + 1$  Monte Carlo estimators. For details, see [Collier et al '15] and [Billingsley '95].

## Theorem (Strong Law of Large Numbers)

If  $\mathbb{E}_{\mu_0}[|f_{h_\ell}|] < \infty$  for  $0 \leq \ell \leq L$ , then as  $\{N_\ell\}_{\ell=0}^L \rightarrow \infty$  we have

$$\hat{E}_{\{M_\ell, N_\ell\}}^{\text{ML}} \xrightarrow{\text{a.s.}} \mathbb{E}_{\mu_0}[f_{h_L}].$$

**Proof:** Follows from the linearity of a.s. convergence, together with results for standard Monte Carlo.

# Convergence of Multilevel Monte Carlo Method

Mean Square Error of Multilevel Monte Carlo [Giles, '08]

## Theorem (Mean Square Error)

$$e(\widehat{E}_{\{M_\ell, N_\ell\}}^{\text{ML}})^2 = \underbrace{\frac{\mathbb{V}[f_{h_0}]}{N_0} + \sum_{\ell=1}^L \frac{\mathbb{V}[f_{h_\ell} - f_{h_{\ell-1}}]}{N_\ell}}_{\text{sampling error}} + \underbrace{(\mathbb{E}_{\mu_0}[f_{h_L} - f])^2}_{\text{numerical error}}.$$

**Proof:** The derivation is identical to the standard Monte Carlo case.

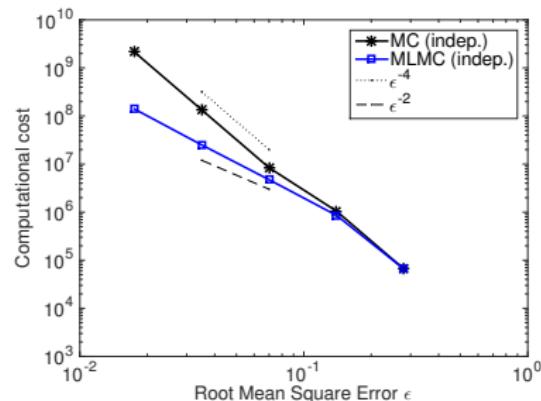
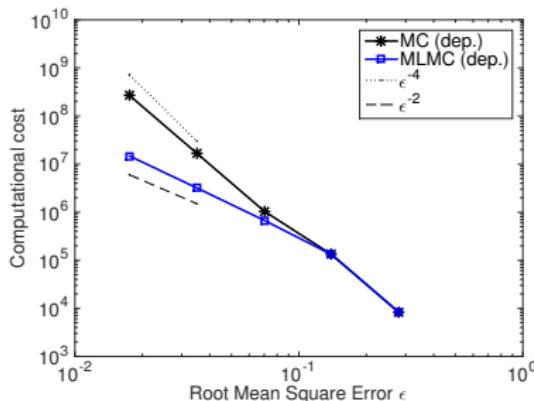
Thus,

- $N_0$  still needs to be large, **but** samples are much cheaper to obtain on coarse grid.
- $N_\ell$  ( $\ell > 0$ ) much smaller, **since**  $\mathbb{V}[f_{h_\ell} - f_{h_{\ell-1}}] \rightarrow 0$  as  $h_\ell \rightarrow 0$ .

# Convergence of Multilevel Monte Carlo Method

## Numerical Comparison: Mean Square Error

- We compute  $\mathbb{E}_{\mu^y}[\phi]$  for a typical model problem in groundwater flow, using a ratio of standard Monte Carlo and multilevel Monte Carlo estimators.
- Computational Cost is computed as number of FLOPS required.



[Scheichl, Stuart, ALT '16]

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