

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 μ^y on \mathbb{R}^n , given by

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

where $Z = \mathbb{E}_{\mu_0}(\exp(-\Phi(\cdot; y)))$ 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 μ^y .
- In most cases, we do not have a closed form expression for the posterior distribution μ^y , since the normalising constant Z is not known explicitly.
(Exception: forward map \mathcal{G} linear and prior μ_0 Gaussian \Rightarrow posterior μ^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 μ_0 is fully known and simple, i.i.d. samples from μ_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 μ_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 ϕ and Φ exactly, since this involves the solution of the forward problem.
 - ▶ In the groundwater flow example, it involves the solution of a PDE.
- Denote by ϕ_h and Φ_h numerical approximations to ϕ and Φ , 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

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

- 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 $\hat{E}_{h,N}^{\text{MC}} = \frac{1}{N} \sum_{i=1}^N f_h(u^{(i)})$, with $\{u^{(i)}\}_{i=1}^N$ an i.i.d. sequence distributed as μ_0 .

Lemma (Expected Value and Variance)

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

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

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

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

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

The **Central Limit Theorem** crucially uses the fact that $\widehat{E}_{h,N}^{\text{MC}}$ 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

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

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

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

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

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

Convergence of Standard Monte Carlo Method

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

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

Theorem (Hölder's Inequality)

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

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

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

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

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

To make $e(\widehat{E}_{h,N}^{\text{MC}})^2$, 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

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

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)

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

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

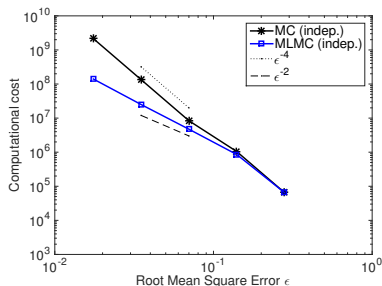
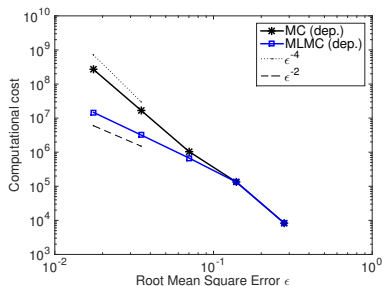
Thus,

- N_0 still needs to be large, **but** samples are much cheaper to obtain on coarse grid.
- N_ℓ ($\ell > 0$) 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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