

Weekly Report 4

Study notes for Monte-Carlo methods and
current progress for writing paper

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Outline

1 Introduction

2 Monte-Carlo study

- Importance sampling
- Metropolis-Hastings algorithm
- Gibbs sampling

3 Paper progress

4 Reference

Introduction

Monte-Carlo
study

Importance sampling

Metropolis-Hastings
algorithm

Gibbs sampling

Paper
progress

Reference



Outline

Introduction

Monte-Carlo study

Importance sampling
Metropolis-Hastings algorithm
Gibbs sampling

Paper progress

Reference

1 Introduction

2 Monte-Carlo study

- Importance sampling
- Metropolis-Hastings algorithm
- Gibbs sampling

3 Paper progress

4 Reference



Introduction

Introduction

Monte-Carlo study

Importance sampling
Metropolis-Hastings algorithm
Gibbs sampling

Paper progress

Reference

■ Recent works:

- Complete an new article
 - 1 **note20190215sp**: The first topic about stochastic optimization: from Monte-Carlo methods to Gibbs sampling [1].
- Progress on writing paper
 - 1 Have finished the framework of what we are planning for writing. (notes are attached to this slice).
 - 2 Generate more detail testing estimations.
 - 3 Propose a possible and slight revision for current work (Need to get more testing results).



Outline

Introduction

Monte-Carlo study

Importance sampling

Metropolis-Hastings algorithm

Gibbs sampling

Paper progress

Reference

1 Introduction

2 Monte-Carlo study

- Importance sampling
- Metropolis-Hastings algorithm
- Gibbs sampling

3 Paper progress

4 Reference



Monte-Carlo study

Importance sampling

Unbiased estimator for importance sampling

$$\overline{wf(x)} := \frac{1}{N} \sum_{i=1}^N w_i f(x_i), \quad (1)$$

$$s^2 := \frac{1}{N-1} \sum_{i=1}^N \left(w_i f(x_i) - \overline{wf(x)} \right)^2, \quad (2)$$

$$\text{SE}^2 := \frac{1}{N(N-1)} \sum_{i=1}^N \left(w_i f(x_i) - \overline{wf(x)} \right)^2, \quad (3)$$

- We use $w_i = \frac{q(x_i)}{p(x_i)}$ in importance sampling.
- We prove that (1) is an unbiased estimator for $\mathbb{E}_q[f(x)]$, however, (2) and (3) are unbiased estimators for larger standard deviation and stand error respectively.



Monte-Carlo study

Importance sampling

Introduction

Monte-Carlo study

Importance sampling

Metropolis-Hastings algorithm

Gibbs sampling

Paper progress

Reference

Unbiased estimator for importance sampling

$$\widetilde{wf(x)} = \frac{\sum_{i=1}^N w_i f(x_i)}{\sum_{i=1}^N w_i}, \quad (4)$$

$$\widetilde{SE}^2 = \frac{\sum_{i=1}^N w_i^2 \left(f(x_i) - \widetilde{wf(x)} \right)^2}{\left(\sum_{i=1}^N w_i \right)^2}. \quad (5)$$

- Prove that both of these two estimators are biased.
- $\widetilde{wf(x)}$ is an asymptotically unbiased estimator.



Monte-Carlo study

Importance sampling



Figure 1: Monte-Carlo simulation for importance sampling



Importance sampling

Introduction

Monte-Carlo
study

Importance sampling

Metropolis-Hastings
algorithm

Gibbs sampling

Paper
progress

Reference

- When we use a distribution which is close to the target distribution ($p \rightarrow q$), importance sampling is effective.
- When the distribution of the sampling is extremely different from the target distribution, the prediction would be in-precise.



Monte-Carlo study

Metropolis-Hastings algorithm

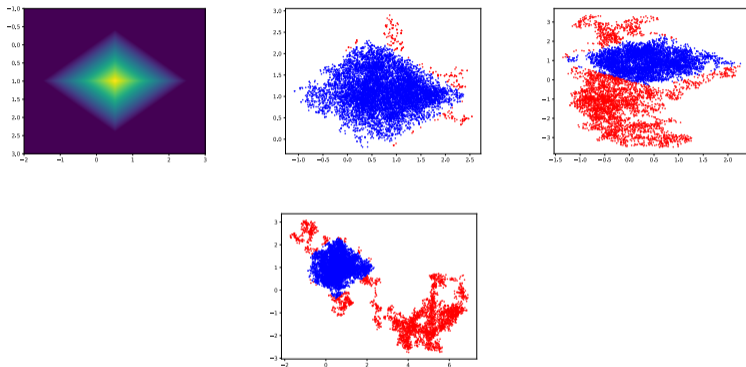


Figure 2: Distribution an using Metropolis sampling.

- Metropolis algorithm get bad performance if $p(x_k) = 0$ for current sample.



Monte-Carlo study

Metropolis-Hastings algorithm

Introduction

Monte-Carlo study

Importance sampling

Metropolis-Hastings algorithm

Gibbs sampling

Paper progress

Reference

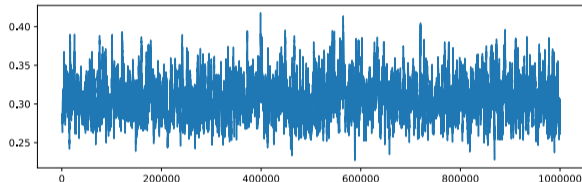
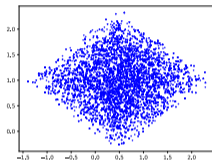


Figure 3: Improved Metropolis algorithm.

- Give a constraint that all cases that $p(x_{k+1}) = 0$ are not allowed. We could ensure that the sampling is restricted in the target domain.



Monte-Carlo study

Gibbs sampling

Introduction

Monte-Carlo study

Importance sampling
Metropolis-Hastings algorithm

Gibbs sampling

Paper progress

Reference

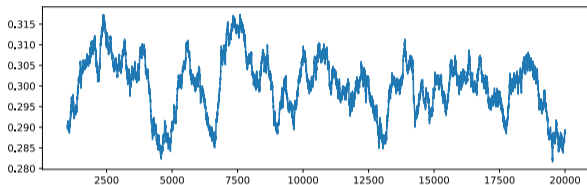
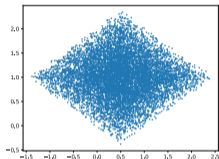


Figure 4: Improved Metropolis algorithm.

- Gibbs sampling is generally better than Metropolis-Hastings algorithm.
- Gibbs sampling could be use only when sampling under marginal distribution is easy to do.



Monte-Carlo study

Gibbs sampling

Introduction

Monte-Carlo study

Importance sampling
Metropolis-Hastings algorithm

Gibbs sampling

Paper progress

Reference

- Prove that if view MH algorithm and Gibbs sampling as AR_1 process, the standard error could be approximated by $SE \approx \frac{\sigma}{\sqrt{N}} \sqrt{\frac{1+\alpha}{1-\alpha}}$.
- The exact standard error should be represented as $SE^2 = \frac{1}{N} \left(\gamma(0) + 2 \sum_{i=1}^{N-1} \left(1 - \frac{i}{N}\right) \gamma(i) \right)$, where $\gamma(k)$ is the lag- k covariance.



Outline

1 Introduction

2 Monte-Carlo study

- Importance sampling
- Metropolis-Hastings algorithm
- Gibbs sampling

3 Paper progress

4 Reference

Introduction

Monte-Carlo study

Importance sampling
Metropolis-Hastings algorithm
Gibbs sampling

Paper progress

Reference



Paper progress

- The paper now follows like this structure: (this article will not be published on Github until the paper is reviewed.)
 - Introduction
 - Related works
 - Problem background
 - ▶ Industrial background
 - ▶ Data
 - ▶ Geosteering inverse problem
 - ▶ Challenges
 - Proposed method
 - ▶ Bayesian view of our problem
 - ▶ Proposed network
 - Train
 - Test
 - Testing results

Introduction

Monte-Carlo study

Importance sampling
Metropolis-Hastings algorithm
Gibbs sampling

Paper progress

Reference



Paper progress

Introduction

Monte-Carlo study

Importance sampling
Metropolis-Hastings algorithm
Gibbs sampling

Paper progress

Reference

- Reformulate our problem by Bayesian regularization.
- Bayesian regularization term is $\|\mathbf{x} - \mathbf{x}_0\|_2^2$, which could introduce the initial guess.

Reformulate the loss function by likelihood

$$p(\mathbf{x}|\mathbf{y}) \sim p(\mathbf{y}|\mathbf{x})p(\mathbf{x}) = \frac{1}{2\pi\sigma\sigma_0} e^{-\frac{1}{2\sigma^2}\|\mathbf{y}-\mathcal{F}(\mathbf{x})\|_2^2 - \frac{1}{2\sigma_0^2}\|\mathbf{x}-\mathbf{x}_0\|_2^2}. \quad (6)$$

$$\mathcal{L}(\mathbf{x}|\mathbf{y}) = \|\mathbf{y} - \mathcal{F}(\mathbf{x})\|_2^2 + \lambda \|\mathbf{x} - \mathbf{x}_0\|_2^2 + C. \quad (7)$$



Paper progress

Introduction

Monte-Carlo study

Importance sampling
Metropolis-Hastings algorithm
Gibbs sampling

Paper progress

Reference

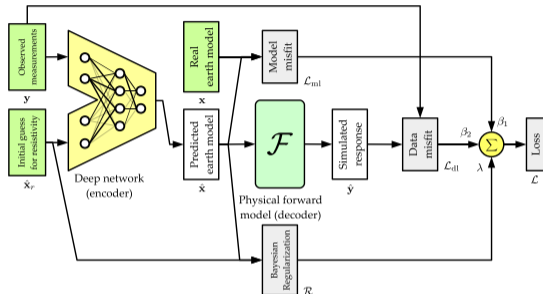


Figure 5: Improved Metropolis algorithm.

- Now we could add the Bayesian regularization to our network.
- This is a minor change, but may help us overcome the problem caused by undetermined solutions.
- Still need further tests to verify the effectiveness of this idea.



Paper progress

Introduction

Monte-Carlo study

Importance sampling
Metropolis-Hastings algorithm
Gibbs sampling

Paper progress

Reference

- Suggestions for adding more components to the paper.
 - 1 Use all predictions as the initial guess, to record the LMA optimization curves respectively. Use a fixed initial guess as a comparison. Then we could compare the two kinds of optimization curves and confirm that our network could help us accelerate the convergence of traditional methods.
 - 2 Predict some data with random noise.
 - 3 Show two more graphs to compare the model misfits and data misfits sample by sample.



Outline

1 Introduction

2 Monte-Carlo study

- Importance sampling
- Metropolis-Hastings algorithm
- Gibbs sampling

3 Paper progress

4 Reference

Introduction

Monte-Carlo study

Importance sampling

Metropolis-Hastings algorithm

Gibbs sampling

Paper progress

Reference



Reference I

Introduction

Monte-Carlo
study

Importance sampling

Metropolis-Hastings
algorithm

Gibbs sampling

Paper
progress

Reference



B. Walsh, "Markov chain monte carlo and gibbs sampling,"
<http://nitro.biosci.arizona.edu/courses/EEB596/handouts/Gibbs.pdf>, 2002.

Thank you for Listening

It's time for Q & A