

# Statistical Models & Computing Methods

## Lecture 5: Advanced Monte Carlo



**Cheng Zhang**

School of Mathematical Sciences, Peking University

September 30, 2024

- ▶ While Monte Carlo estimation is attractive for high dimension integration, it may suffer from lots of problems, such as rare events, and irregular integrands, etc.
- ▶ In this lecture, we will discuss various methods to improve Monte Carlo approaches, with an emphasis on variance reduction techniques

- ▶ The simple Monte Carlo estimator of  $\int_a^b h(x)f(x)dx$  is

$$\hat{I}_n = \frac{1}{n} \sum_{i=1}^n h(x^{(i)})$$

where  $x^{(1)}, x^{(2)}, \dots, x^{(n)}$  are randomly sampled from  $f$

- ▶ A potential problem is the **mismatch** of the concentration of  $h(x)f(x)$  and  $f(x)$ . More specifically, if there is a region  $A$  of relatively small probability under  $f(x)$  that dominates the integral, we would not get enough data from the **important** region  $A$  by sampling from  $f(x)$
- ▶ Main idea: Get more data from  $A$ , and then correct the bias

- ▶ **Importance sampling** (IS) uses importance distribution  $q(x)$  to adapt to the true integrands  $h(x)f(x)$ , rather than the target distribution  $f(x)$
- ▶ By correcting for this bias, importance sampling can greatly reduce the variance in Monte Carlo estimation
- ▶ Unlike the rejection sampling, we do not need the envelop property
- ▶ The only requirement is that  $q(x) > 0$  whenever

$$h(x)f(x) \neq 0$$

- ▶ IS also applies when  $f(x)$  is not a probability density function

- Now we can rewrite  $I = \mathbb{E}_f(h(x)) = \int_{\mathcal{X}} h(x)f(x) dx$  as

$$\begin{aligned} I = \mathbb{E}_f(h(x)) &= \int_{\mathcal{X}} h(x)f(x) dx \\ &= \int_{\mathcal{X}} h(x)\frac{f(x)}{q(x)}q(x)dx \\ &= \int_{\mathcal{X}} (h(x)w(x))q(x) \\ &= \mathbb{E}_q(h(x)w(x)) \end{aligned}$$

where  $w(x) = \frac{f(x)}{q(x)}$  is the **importance weight** function

We can then approximate the original expectation as follows

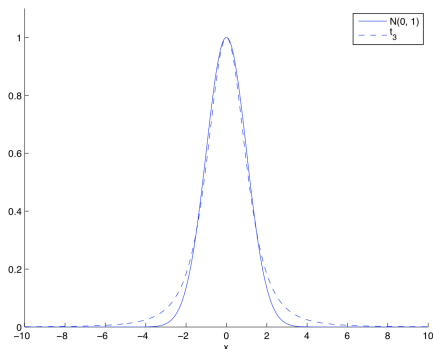
- ▶ Draw samples  $x^{(1)}, \dots, x^{(n)}$  from  $q(x)$
- ▶ Monte Carlo estimate

$$I_n^{\text{IS}} = \frac{1}{n} \sum_{i=1}^n h(x^{(i)})w(x^{(i)})$$

where  $w(x^{(i)}) = \frac{f(x^{(i)})}{q(x^{(i)})}$  are called importance ratios.

- ▶ Note that, now we only require sampling from  $q$  and do not require sampling from  $f$

- ▶ We want to approximate a  $\mathcal{N}(0, 1)$  distribution with  $t(3)$  distribution



- ▶ We generate 500 samples and estimated  $I = \mathbb{E}(x^2)$  as 0.97, which is close to the true value 1.

- Let  $t(x) = h(x)w(x)$ . Then  $\mathbb{E}_q(t(X)) = I, X \sim q$

$$\mathbb{E}(I_n^{\text{IS}}) = \frac{1}{n} \sum_{i=1}^n \mathbb{E}(t(x^{(i)})) = I$$

- Similarly, the variance is

$$\begin{aligned} \text{Var}_q(I_n^{\text{IS}}) &= \frac{1}{n} \text{Var}_q(t(X)) \\ &= \frac{1}{n} \int_{\mathcal{X}} \frac{(h(x)f(x))^2}{q(x)} dx - I^2 \end{aligned} \quad (1)$$

$$= \frac{1}{n} \int_{\mathcal{X}} \frac{(h(x)f(x) - Iq(x))^2}{q(x)} dx \quad (2)$$





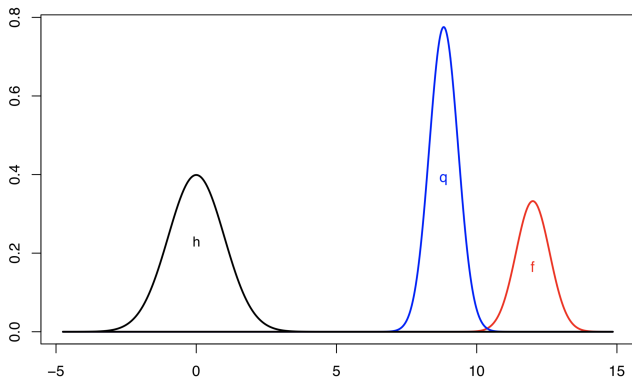
- ▶ Recall the convergence rate for Monte Carlo is

$$p \left( |\hat{I}_n - I| \leq \frac{\sigma}{\sqrt{n}\delta} \right) \geq 1 - \delta, \quad \forall \delta$$

For IS,  $\sigma = \sqrt{\text{Var}_q(t(X))}$ . A good importance distribution  $q(x)$  would make  $\text{Var}_q(t(X))$  small.

- ▶ What can we learn from equations (1) and (2)?
  - ▶ **Optimal choice:**  $q(x) \propto h(x)f(x)$
  - ▶  $q(x)$  near 0 can be **dangerous**
  - ▶ **Bounding**  $\frac{(h(x)f(x))^2}{q(x)}$  is useful theoretically





$$\text{Var}_q(t(X)) = 0$$

Gaussian  $h$  and  $f \Rightarrow$  Gaussian optimal  $q$  lies between.



- ▶ When  $f$  or/and  $q$  are unnormalized, we can estimate the expectation as follows

$$I = \frac{\int_{\mathcal{X}} h(x) f(x) dx}{\int_{\mathcal{X}} f(x) dx} = \frac{\int_{\mathcal{X}} h(x) \frac{f(x)}{q(x)} q^*(x) dx}{\int_{\mathcal{X}} \frac{f(x)}{q(x)} q^*(x) dx}$$

where  $q^*(x) = q(x)/c_q$

- ▶ Monte Carlo estimate

$$I_n^{\text{SNIS}} = \frac{\sum_{i=1}^n h(x^{(i)}) w(x^{(i)})}{\sum_{i=1}^n w(x^{(i)})}, \quad x^{(i)} \sim q(x)$$

- ▶ Requires a stronger condition:  $q(x) > 0$  whenever  $f(x) > 0$



- ▶ Unfortunately,  $I_n^{\text{SNIS}}$  is biased. However, the bias is asymptotically negligible.

$$\begin{aligned} I_n^{\text{SNIS}} &= \frac{1}{n} \sum_{i=1}^n h(x^{(i)}) f(x^{(i)}) / q(x^{(i)}) \bigg/ \frac{1}{n} \sum_{i=1}^n f(x^{(i)}) / q(x^{(i)}) \\ &\xrightarrow{p} \int_{\mathcal{X}} h(x) f(x) / q(x) q^*(x) dx \bigg/ \int_{\mathcal{X}} f(x) / q(x) q^*(x) dx \\ &= \int_{\mathcal{X}} h(x) f(x) dx \bigg/ \int_{\mathcal{X}} f(x) dx \\ &= I \end{aligned}$$



- ▶ We use delta method for the variance of SNIS, which is a ratio estimate

$$\text{Var}(I_n^{\text{SNIS}}) \approx \frac{\sigma_{q,\text{sn}}^2}{n} = \frac{\mathbb{E}_q(w(x)^2(h(x) - I)^2)}{n}$$

- ▶ We can rewrite the variance  $\sigma_{q,\text{sn}}^2$  as

$$\begin{aligned}\sigma_{q,\text{sn}}^2 &= \int_{\mathcal{X}} \frac{f(x)^2}{q(x)} (h(x) - I)^2 dx \\ &= \int_{\mathcal{X}} \frac{(h(x)f(x) - If(x))^2}{q(x)} dx\end{aligned}$$

- ▶ For comparison,  $\sigma_{q,\text{is}}^2 = \text{Var}_q(t(X)) = \int_{\mathcal{X}} \frac{(h(x)f(x) - If(x))^2}{q(x)} dx$
- ▶ No  $q$  can make  $\sigma_{q,\text{sn}}^2 = 0$  (unless  $h$  is constant)



- ▶ The optimal density for self-normalized importance sampling has the form (Hesterberg, 1988)

$$q(x) \propto |h(x) - I|f(x)$$

- ▶ Using this formula we find that

$$\sigma_{q,\text{sn}}^2 \geq (\mathbb{E}_f(|h(x) - I|))^2$$

which is zero only for constant  $h(x)$

- ▶ Note that the simple Monte Carlo has variance  $\sigma^2 = \mathbb{E}_f((h(x) - I)^2)$ , this means SNIS can not reduce the variance by

$$\frac{\sigma^2}{\sigma_{q,\text{sn}}^2} \leq \frac{\mathbb{E}_f((h(x) - I)^2)}{(\mathbb{E}_f(|h(x) - I|))^2}$$



- ▶ The importance weights in IS may be problematic, we would like to have a diagnostic to tell us when it happens.
- ▶ Unequal weighting raises variance (Kong, 1992). For IID  $Y_i$  with variance  $\sigma^2$  and fixed weight  $w_i \geq 0$

$$\text{Var} \left( \frac{\sum_i w_i Y_i}{\sum_i w_i} \right) = \frac{\sum_i w_i^2 \sigma^2}{(\sum_i w_i)^2}$$

- ▶ Write this as

$$\frac{\sigma^2}{n_e} \text{ where } n_e = \frac{(\sum_i w_i)^2}{\sum_i w_i^2}$$

- ▶  $n_e$  is the **effective sample size** and  $n_e \ll n$  if the weights are too imbalanced.



- ▶ Rejection Sampling requires bounded  $w(x) = f(x)/q(x)$
- ▶ We also have to know a bound for the envelop distribution
- ▶ Therefore, importance sampling is generally easier to implement
- ▶ IS and SNIS require us to keep track of weights
- ▶ Plain IS requires normalized  $p/q$
- ▶ Rejection sampling could be sample inefficient (due to rejections)





- ▶ Consider that  $f(x) = p(x; \theta_0)$  is from a family of distributions  $p_\theta(x)$ ,  $\theta \in \Theta$
- ▶ A simple importance sampling distribution would be  $q(x) = p(x; \theta)$  for some  $\theta \in \Theta$ .
- ▶ Suppose  $f(x)$  belongs to an exponential family

$$f(x) = g(x) \exp(\eta(\theta_0)^T T(x) - A(\theta_0))$$

- ▶ Use  $q(x) = g(x) \exp(\eta(\theta)^T T(x) - A(\theta))$ , the IS estimate is

$$I_n^{\text{IS}} = \exp(A(\theta) - A(\theta_0)) \cdot \frac{1}{n} \sum_{i=1}^n h(x^{(i)}) \exp((\eta(\theta_0) - \eta(\theta))^T T(x^{(i)}))$$



- ▶ Suppose that we find the mode  $x^*$  of  $k(x) = h(x)f(x)$
- ▶ We can use Taylor approximation

$$\log(k(x)) \approx \log(k(x^*)) - \frac{1}{2}(x - x^*)^T H^*(x - x^*)$$
$$k(x) \approx k(x^*) \exp\left(-\frac{1}{2}(x - x^*)^T H^*(x - x^*)\right)$$

which suggests  $q(x) = \mathcal{N}(x^*, (H^*)^{-1})$

- ▶ This requires positive definite  $H^*$
- ▶ Can be viewed as an IS version of the **Laplace approximation**



- ▶ Suppose we have  $K$  importance distributions  $q_1, \dots, q_K$ , we can combine them into a mixture of distributions with probability  $\alpha_1, \dots, \alpha_K$ ,  $\sum_i \alpha_i = 1$

$$q(x) = \sum_{i=1}^K \alpha_i q_i(x)$$

- ▶ IS estimate  $I_n^{\text{IS}} = \frac{1}{n} \sum_{i=1}^n h(x^{(i)}) \frac{f(x^{(i)})}{\sum_{j=1}^K \alpha_j q_j(x^{(i)})}$
- ▶ An alternative. Suppose  $x^{(i)}$  came from component  $j(i)$ , we could use

$$\frac{1}{n} \sum_{i=1}^n h(x^{(i)}) \frac{f(x^{(i)})}{q_{j(i)}(x^{(i)})}$$

**Remark:** This alternative is **faster** to compute, but has **higher** variance



- ▶ Designing importance distribution directly would be challenging. A better way would be to adapt some candidate distribution to our task through a learning process
- ▶ To do that, we first need to pick a family  $\mathcal{Q}$  of proposal distributions
- ▶ We have to choose a termination criterion, e.g., maximum steps, total number of observations, etc.
- ▶ Most importantly, we need a way to choose  $q_{k+1} \in \mathcal{Q}$  based on the observed information

- ▶ Suppose now we have a family of distributions (e.g., exponential family)  $q_\theta(x) = q(x; \theta)$ ,  $\theta \in \Theta$
- ▶ Recall that the variance of IS estimate is

$$\frac{1}{n} \int_{\mathcal{X}} \frac{(h(x)f(x))^2}{q(x)} dx - I^2, \quad \text{therefore, we would like}$$

$$\theta = \arg \min_{\theta \in \Theta} \int_{\mathcal{X}} \frac{(h(x)f(x))^2}{q_\theta(x)} dx$$

- ▶ Variance based update

$$\theta^{(k+1)} = \arg \min_{\theta \in \Theta} \frac{1}{n_k} \sum_{i=1}^{n_k} \frac{(h(x^{(i)})f(x^{(i)}))^2}{q_\theta(x^{(i)})^2}, \quad x^{(i)} \sim q_{\theta^{(k)}}$$

However, the optimization may be hard.



- ▶ Consider an exponential family

$$q_{\theta}(x) = g(x) \exp(\theta^T x - A(\theta))$$

- ▶ Now, replace variance by KL divergence

$$D_{KL}(k_* \| q_{\theta}) = \mathbb{E}_{k_*} \log \left( \frac{k_*(x)}{q_{\theta}(x)} \right)$$

- ▶ We seek  $\theta$  to minimize

$$D_{KL}(k_* \| q_{\theta}) = \mathbb{E}_{k_*} (\log(k_*(x)) - \log(q(x; \theta)))$$

*i.e.*, maximize

$$\mathbb{E}_{k_*} (\log(q(x; \theta)))$$



- Rewrite the negative cross entropy as

$$\begin{aligned}\mathbb{E}_{k_*}(\log(q(x; \theta))) &= \mathbb{E}_q \left( \frac{\log(q(x; \theta))k_*(x)}{q(x)} \right) \\ &= \frac{1}{I} \cdot \mathbb{E}_q \left( \frac{\log(q(x; \theta))h(x)f(x)}{q(x)} \right)\end{aligned}$$

- Update  $\theta$  to maximize the above

$$\begin{aligned}\theta^{(k+1)} &= \arg \max_{\theta} \frac{1}{n_k} \sum_{i=1}^{n_k} \frac{h(x^{(i)})f(x^{(i)})}{q(x^{(i)}; \theta^{(k)})} \log(q(x^{(i)}; \theta)) \\ &= \arg \max_{\theta} \frac{1}{n_k} \sum_{i=1}^k H_i \log(q(x^{(i)}; \theta)) \\ &= \arg \max_{\theta} \frac{1}{n_k} \sum_{i=1}^k H_i (\theta^T x^{(i)} - A(\theta))\end{aligned}$$



- ▶ The update often takes a simple moment matching form

$$\frac{\partial}{\partial \theta} A(\theta^{(k+1)}) = \frac{\sum_i H_i(x^{(i)})^T}{\sum_i H_i}$$

- ▶ Examples:

- ▶  $q_\theta = \mathcal{N}(\theta, I)$

$$\theta^{(k+1)} = \frac{\sum_i H_i x^{(i)}}{\sum_i H_i}$$

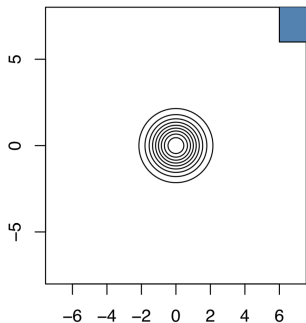
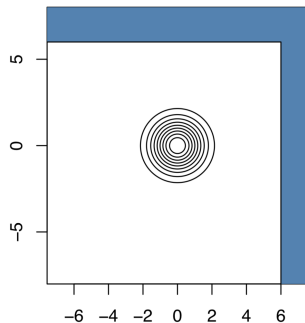
- ▶  $q_\theta = \mathcal{N}(\theta, \Sigma)$

$$\theta^{(k+1)} = \Sigma^{-1} \frac{\sum_i H_i x^{(i)}}{\sum_i H_i}$$

- ▶ Other exponential family updates are typically closed form functions of sample moments



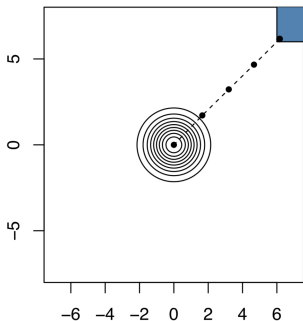
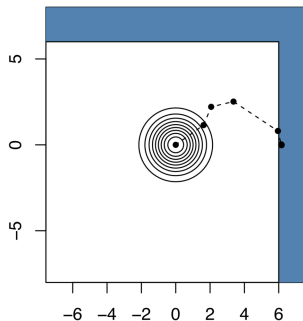


Gaussian,  $\Pr(\min(x) > 6)$ Gaussian,  $\Pr(\max(x) > 6)$ 

$$\theta_1 = (0, 0)^T$$

Take  $K = 10$  steps with  $n = 1000$  each



Gaussian,  $\Pr(\min(x)>6)$ Gaussian,  $\Pr(\max(x)>6)$ 

For  $\min(x)$ ,  $\theta^{(k)}$  heads Northeast, which is OK.

For  $\max(x)$ ,  $\theta^{(k)}$  heads North or East, and miss the other part completely, leading to underestimates of  $I$  by about 1/2



- ▶ The control variate strategy improves estimation of an unknown integral by relating the estimate to some correlated estimator with known integral
- ▶ A general class of unbiased estimators

$$I_{CV} = I_{MC} - \lambda(J_{MC} - J)$$

where  $\mathbb{E}(J_{MC}) = J$ . It is easy to show  $I_{CV}$  is unbiased,  $\forall \lambda$

- ▶ We can choose  $\lambda$  to minimize the variance of  $I_{CV}$

$$\hat{\lambda} = \frac{\text{Cov}(I_{MC}, J_{MC})}{\text{Var}(J_{MC})}$$

where the related moments can be estimated using samples from corresponding distributions

- ▶ Recall that IS estimator is

$$I_n^{\text{IS}} = \frac{1}{n} \sum_{i=1}^n h(x^{(i)})w(x^{(i)})$$

- ▶ Note that  $h(x)w(x)$  and  $w(x)$  are correlated and  $\mathbb{E}w(x) = 1$ , we can use the control variate

$$\bar{w} = \frac{1}{n} \sum_{i=1}^n w(x^{(i)})$$

and the importance sampling control variate estimator is

$$I_n^{\text{ISCV}} = I_n^{\text{IS}} - \lambda(\bar{w} - 1)$$

$\lambda$  can be estimated from a regression of  $h(x)w(x)$  on  $w(x)$  as described before

- ▶ Consider estimation of  $I = \mathbb{E}(h(X, Y))$  using a random sample  $(x^{(1)}, y^{(1)}), \dots, (x^{(n)}, y^{(n)})$  drawn from  $f$
- ▶ Suppose the conditional expectation  $\mathbb{E}(h(X, Y)|Y)$  can be computed. Using  $\mathbb{E}(h(X, Y)) = \mathbb{E}(\mathbb{E}(h(X, Y)|Y))$ , the *Rao-Blackwellized estimator* can be defined as

$$I_n^{\text{RB}} = \frac{1}{n} \sum_{i=1}^n \mathbb{E}(h(X^{(i)}, Y^{(i)})|Y^{(i)} = y^{(i)})$$

- ▶ Rao-Blackwellized estimator gives smaller variance than the ordinary Monte Carlo estimator

$$\begin{aligned} \text{Var}(I_n^{\text{MC}}) &= \frac{1}{n} \text{Var}(\mathbb{E}(h(X, Y)|Y)) + \frac{1}{n} \mathbb{E}(\text{Var}(h(X, Y)|Y)) \\ &\geq \text{Var}(I_n^{\text{RB}}) \end{aligned}$$

follows from the conditional variance formula



- ▶ Suppose rejection sampling stops at a random time  $M$  with acceptance of the  $n$ th draw, yielding  $x^{(1)}, \dots, x^{(n)}$  from all  $M$  proposals  $y^{(1)}, \dots, y^{(M)}$
- ▶ The ordinary Monte Carlo estimator can be expressed as

$$I_n^{\text{MC}} = \frac{1}{n} \sum_{i=1}^M h(y^{(i)}) 1_{U_i \leq w(y^{(i)})}$$

- ▶ Rao-Blackwellization estimator

$$I_n^{\text{RB}} = \frac{1}{n} \sum_{i=1}^M h(y^{(i)}) t_i(Y)$$

where

$$t_i(Y) = \mathbb{E}(1_{U_i \leq w(y^{(i)})} | M, y^{(1)}, \dots, y^{(M)})$$



- ▶ Hesterberg, T. C. (1988). Advances in importance sampling. PhD thesis, Stanford University.
- ▶ Kong, A. (1992). A note on importance sampling using standardized weights. Technical Report 348, University of Chicago.