Modern Computational Statistics

Lecture 5: Advanced Monte Carlo

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- 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

What's Wrong with Simple Monte Carlo?

- 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 $x^{(1)}, x^{(2)}, \ldots, x^{(n)}$ 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 $w(x) = \dfrac{f(x)}{q(x)}$ is the importance weight function

We can then approximate the original expectation as follows

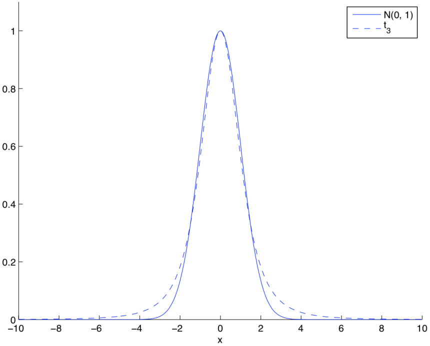
- Draw samples $x^{(1)}, \ldots, x^{(n)}$ from $q(x)$
- Monte Carlo estimate

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

  where $w(x^{(i)}) = \frac{f(x^{(i)})}{q(x^{(i)})}$ are called importance ratios.
- Note that, now we only require sampling from g and do not require sampling from f

Examples

- 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.

Mean and Variance of IS

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

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

- Similarly, the variance is

$$\begin{aligned}
\mathbb{V}\mathrm{ar}_q(I_n^{\mathrm{IS}}) &= \frac{1}{n}\mathbb{V}\mathrm{ar}_q(t(X)) \\
&= \frac{1}{n}\int_{\mathcal{X}} \frac{(h(x)f(x))^2}{q(x)}\, dx - I^2 \qquad (1) \\
&= \frac{1}{n}\int_{\mathcal{X}} \frac{(h(x)f(x) - Iq(x))^2}{q(x)}\, dx \qquad (2)
\end{aligned}$$

Variance Does Matter

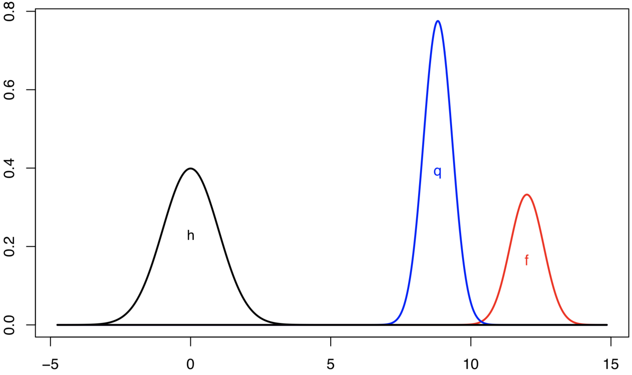
- Recall the convergence rate for Monte Carlo is

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

  For IS, $\sigma = \sqrt{\mathbb{V}\mathrm{ar}_q(t(X))}$. A good importance distribution $q(x)$ would make $\mathbb{V}\mathrm{ar}_q(t(X))$ 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

Examples



$\mathbb{V}\mathrm{ar}_q(t(X)) = 0$

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

Self-normalized Importance Sampling

- When f or/and q are unnormalized, we can esitmate 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

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

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

SNIS is Consistent

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

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

SNIS Variance

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

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

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

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

- For comparison, $\sigma_{q,\mathrm{is}}^2 = \mathbb{V}\mathrm{ar}_q(t(X)) = \int_{\mathcal{X}} \frac{(h(x)f(x) - I q(x))^2}{q(x)}\,dx$
- No q can make $\sigma_{q,\mathrm{sn}}^2 = 0$ (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

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

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

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

- 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 σ^2 and fixed weight $w_i \geq 0$

$$\mathbb{V}\mathrm{ar}\left(\frac{\sum_i w_i Y_i}{\sum_i w_i}\right) = \frac{\sum_i w_i^2 \sigma^2}{(\sum_i w_i)^2}$$

- 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.

Importance Sampling vs Rejection Sampling

- 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

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

Hessian and Gaussian

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

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

  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 $q_1, \ldots, q_K$, we can combine them into a mixture of distributions with probability $\alpha_1, \ldots, \alpha_K$, $\sum_i \alpha_i = 1$

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

- IS estimate $I_n^{\mathrm{IS}} = \frac{1}{n} \sum_{i=1}^{n} h(x^{(i)}) \frac{f(x^{(i)})}{\sum_{j=1}^{K} \alpha_j q_j(x^{(i)})}$
- 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

Variance Minimization

- 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 θ to minimize

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

$i.e.$, maximize

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

Cross Entropy

- Rewrite the negative cross entropy as

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

- Update θ to maximize the above

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

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

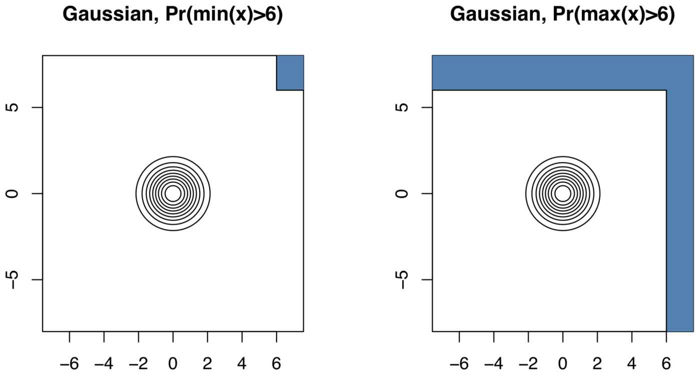
$$\theta^{(k+1)} = \frac{\sum_i H_i x^{(i)}}{\sum_i H_i}$$

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

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

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

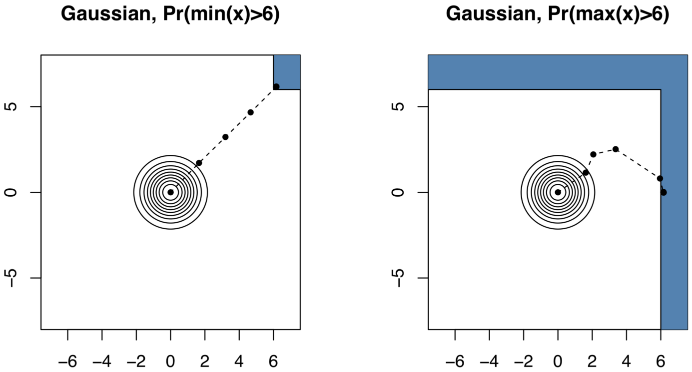
Example



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

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

Example



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

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

  where $\mathbb{E}(J_{\mathrm{MC}}) = J$. It is easy to show I_{CV} is unbiased, $\forall\lambda$
- We can choose λ to minimize the variance of I_{CV}

$$\hat{\lambda} = \frac{\mathbb{C}\mathrm{ov}(I_{\mathrm{MC}}, J_{\mathrm{MC}})}{\mathbb{V}\mathrm{ar}(J_{\mathrm{MC}})}$$

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

- Recall that IS estimator is

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

- 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

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

λ 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 $(x^{(1)}, y^{(1)}), \ldots, (x^{(n)}, y^{(n)})$ 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

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

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

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

follows from the conditional variance formula

Rao-Blackwellization for Rejection Sampling

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

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

- Rao-Blackwellization estimator

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

where

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