Monte Carlo integrations

Stat 580: Statistical Computing

- Theme: Black - White
- Printable version

Monte Carlo integration

- a numerical approximation for expectation
- often useful for multidimensional problems that require the estimation of $\mu = E\{h(\boldsymbol{X})\}$, where $\boldsymbol{X}$ is a random vector and h is a function
- simplest approach: approximate μ by $\hat{\mu}_m = \frac{1}{m}\sum_{i=1}^{m} h(\boldsymbol{X}_i)$ where $\boldsymbol{X}_1, \dots, \boldsymbol{X}_n$ are iid copies of $\boldsymbol{X}$
- properties:
  - $\hat{\mu}_m$ is consistent: by the Strong Law of Large Numbers, with probability 1, $\hat{\mu}_m \to \mu$ as $m \to \infty$
  - $\hat{\mu}_m$ is unbiased: $E(\hat{\mu}_m) = \mu = E\{h(\boldsymbol{X})\}$.
  - $\mathrm{Var}(\hat{\mu}_m) = \mathrm{Var}\{h(\boldsymbol{X})\}/m$ and can be estimated by
$$\widehat{\mathrm{Var}}\,(\hat{\mu}_m) = \frac{1}{m(m-1)}\sum_{i=1}^{m}\{h(\boldsymbol{X}_i) - \hat{\mu}_m\}^2.$$

Monte Carlo integration

- we will see methods:
  1. that are applicable when $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_m$ cannot be easily sampled
  2. that reduce $\mathrm{Var}(\hat{\mu}_m)$
- MC integration can be used to evaluate a "usual" integral $I = \int_{\mathcal{X}} H(x)dx$
  1. the idea is to "factorize" $H(x) = f(x)h(x)$ with $f(x)$ as a pdf with support $\supseteq \mathcal{X}$ (we take $h(x) = 0$ if $x \notin \mathcal{X}$.)
  2. approximate I by $\frac{1}{m}\sum_{i=1}^{m} h(X_i)$, where $X_1, \ldots, X_m$ are iid with pdf $f(x)$

Example

We want to compute

$$\int_{-\infty}^{\infty} \log|x| e^{-\frac{(x+1)^2}{8}} dx.$$

Set

$$f(x) = \frac{1}{\sqrt{8\pi}} e^{-\frac{(x+1)^2}{8}}$$

and

$$h(x) = \sqrt{8\pi} \log|x|.$$

Note that $f(x)$ is the pdf for $\mathcal{N}(-1, 4)$, so the integral can be approximated by $\frac{\sqrt{8\pi}}{n} \sum_{i=1}^{m} \log|X_i|$ with $\{X_i\}$ iid $\sim \mathcal{N}(-1, 4)$.

Importance sampling

Importance sampling

- Same setup: want to estimate
$$\mu = \int h(\boldsymbol{x}) f(\boldsymbol{x}) d\boldsymbol{x}, \quad f(\boldsymbol{x}) \text{ is a pdf.}$$
(the integral is taken over the region where the integrand is positive)
    - but it is difficult to sample from f

- Rewrite
$$\mu = \int h(\boldsymbol{x}) \frac{f(\boldsymbol{x})}{g(\boldsymbol{x})} g(\boldsymbol{x}) d\boldsymbol{x},$$
where g is a pdf such that $g(\boldsymbol{x}) > 0$ whenever $f(\boldsymbol{x}) > 0$.

- Let $\boldsymbol{X}$ have density $g(\boldsymbol{x})$.

- Then $\mu = E\{h(\boldsymbol{X}) w^*(\boldsymbol{X})\}$ with $w^*(\boldsymbol{X}) = \frac{f(\boldsymbol{X})}{g(\boldsymbol{X})}$.

Importance sampling

- Consider the following steps:
  1. Generate $\boldsymbol{X}_1, \ldots, \boldsymbol{X}_m$ iid $\sim g(\boldsymbol{x})$.
  2. Estimate μ by $\hat{\mu}_g = \frac{1}{m} \sum_{i=1}^{m} h(\boldsymbol{X}_i) w^*(\boldsymbol{X}_i)$.
- $\hat{\mu}_g$ is the importance sampling (IS) estimator of μ associated with g.
- $w^*(\boldsymbol{X}_i)$'s are referred to as importance ratios
- Note that $\hat{\mu}_g$ is a weighted sum of $h(\boldsymbol{X}_i)$.
- If $f = g$, then $\hat{\mu}_g$ is the ordinary MC estimator.

Example

We want to compute $\mu = E(U^5)$ where $U \sim \text{Unif}(0, 1)$.

- the straightforward MC estimator: $\hat{\mu} = \frac{1}{m} \sum_{i=1}^{m} U_i^5$
  - oversample data U_i^5 near the origin and undersample the data near 1
  - $\text{Var}(\hat{\mu}) = 0.0631/m$
- Use IS to put more weights near 1:
  - use $g(x) = 5x^4$ for $0 < x < 1$
  - the IS estimator: $\hat{\mu}_g = \frac{1}{m} \sum_{i=1}^{m} X_i^5 w^*(X_i)$ where $w^*(X_i) = 1/(5X_i^4)$
  - $\text{Var}(\hat{\mu}_g) = 0.00794/m$ (verify!)
  - resulting a variance reduction of 98.74%!
- the IS can be used as a variance reduction technique!

Properties

1. $\hat{\mu}_g$ is unbiased for μ.
2. $\mathrm{Var}(\hat{\mu}_g) = \frac{1}{m}\mathrm{Var}\{h(\boldsymbol{X})w^*(\boldsymbol{X})\}$.

- To reduce the variance of $\hat{\mu}_g$, $g(\boldsymbol{x})$ should be in proportion to $h(\boldsymbol{x})f(\boldsymbol{x})$ as much as possible.

Properties

To show this, we need to reduce

$$E\left[\left\{h(\boldsymbol{X})\frac{f(\boldsymbol{X})}{g(\boldsymbol{X})}\right\}^2\right] = \mathrm{Var}(\hat{\mu}_g) + \mu^2.$$

We can use

$$E\left[\left\{h(\boldsymbol{X})\frac{f(\boldsymbol{X})}{g(\boldsymbol{X})}\right\}^2\right] \geq \left[E\left\{h(\boldsymbol{X})\frac{f(\boldsymbol{X})}{g(\boldsymbol{X})}\right\}\right]^2.$$

The equality holds if $h(\boldsymbol{x})\frac{f(\boldsymbol{x})}{g(\boldsymbol{x})}$ is a constant. That is, when $g(\boldsymbol{x}) \propto h(\boldsymbol{x})f(\boldsymbol{x})$. (Why is it called importance sampling?)

When f is only known up to a constant

- That means, $f(\boldsymbol{x}) = cq(\boldsymbol{x})$ with $c > 0$ unknown, then

$$\mu = \frac{E\{h(\boldsymbol{X})w^*(\boldsymbol{X})\}}{E\{w^*(\boldsymbol{X})\}}$$

  with $w^*(\boldsymbol{X}) = \frac{q(\boldsymbol{X})}{g(\boldsymbol{X})}$.

- In this case, standardized weights have to be used in IS:

  1. Generate $\boldsymbol{X}_1, \dots, \boldsymbol{X}_m$ iid from $g(\boldsymbol{x})$.
  2. Estimate μ by $\hat{\mu}_g = \frac{1}{m} \sum_{i=1}^m h(\boldsymbol{X}_i)w(\boldsymbol{X}_i)$ where $w(\boldsymbol{X}_i) = \frac{w^*(\boldsymbol{X}_i)}{\sum_{j=1}^m w^*(\boldsymbol{X}_j)/m}$.

Control variates

Control variates

- We still want to compute $\mu = E\{h(\boldsymbol{X})\}$.

- Suppose we know the exact value of $\theta = E\{c(\boldsymbol{Y})\}$, where c is a function of another random variable $\boldsymbol{Y}$.

- The simple MC estimators for μ and θ are, respectively,
$$\hat{\mu}_{\mathrm{MC}} = \frac{1}{n}\sum_{i=1}^{n} h(\boldsymbol{X}_i), \qquad \hat{\theta}_{\mathrm{MC}} = \frac{1}{n}\sum_{i=1}^{n} c(\boldsymbol{Y}_i).$$

- Of course, for θ, $\hat{\theta}_{\mathrm{MC}}$ is unnecessary. However, it can be helpful for the estimation of μ.

- How? Suppose $h(\boldsymbol{X})$ and $c(\boldsymbol{Y})$ are positively correlated. (If they are uncorrelated, this method is not useful.)

Control variates

- If we see $\hat{\theta}_{\text{MC}} > \theta$, then due to the positive correlation, $\hat{\mu}_{\text{MC}}$ is more likely to be $> \mu$.

- Then we can decrease the value of $\hat{\mu}_{\text{MC}}$ to obtain a better estimate.

- To be specific, suppose we can sample $(\boldsymbol{X}_1, \boldsymbol{Y}_1), \ldots, (\boldsymbol{X}_n, \boldsymbol{Y}_n)$ iid.

- The control variate estimator for μ is
$$\hat{\mu}_{\text{CV}} = \hat{\mu}_{\text{MC}} - b(\hat{\theta}_{\text{MC}} - \theta),$$
where b is a constant.

- $\hat{\mu}_{\text{CV}}$ is unbiased and consistent (as MC estimators are unbiased and consistent).

- If $b = 0$, then $\hat{\mu}_{\text{CV}} = \hat{\mu}_{\text{MC}}$.

- Given a control variate $c(\boldsymbol{Y})$, need to choose b (choosing $c(\boldsymbol{Y})$ is harder)

Choice of b

- How should we choose b?
  - for any given b,
    $$\mathrm{Var}(\hat{\mu}_{\mathrm{CV}}) = \mathrm{Var}(\hat{\mu}_{\mathrm{MC}}) + b^2\mathrm{Var}(\hat{\theta}_{\mathrm{MC}}) - 2b\mathrm{Cov}(\hat{\mu}_{\mathrm{MC}}, \hat{\theta}_{\mathrm{MC}}).$$
  - the minimum of $\mathrm{Var}(\hat{\mu}_{\mathrm{CV}})$ happens when $b = b^*$, where
    $$b^* = \frac{\mathrm{Cov}(\hat{\mu}_{\mathrm{MC}}, \hat{\theta}_{\mathrm{MC}})}{\mathrm{Var}(\hat{\theta}_{\mathrm{MC}})} = \frac{\mathrm{Cov}\{h(\boldsymbol{X}), c(\boldsymbol{Y})\}}{\mathrm{Var}\{c(\boldsymbol{Y})\}}.$$
  - in practice b^* is unknown, but we can estimate it.
  - plug b^* into $\mathrm{Var}(\hat{\mu}_{\mathrm{CV}})$ to get $\mathrm{Var}(\hat{\mu}_{\mathrm{CV}}^{\mathrm{opt}})$, and we can show the variance reduction factor is
    $$\frac{\mathrm{Var}(\hat{\mu}_{\mathrm{CV}}^{\mathrm{opt}})}{\mathrm{Var}(\hat{\mu}_{\mathrm{MC}})} = 1 - \rho^2,$$
    where ρ is the correlation coefficient between $h(\boldsymbol{X})$ and $c(\boldsymbol{Y})$.

Estimation of b^*

- the optimal b^* can be estimated by
$$\hat{b}_n = \frac{\widehat{\mathrm{Cov}}\,(\hat{\mu}_{\mathrm{MC}}, \hat{\theta}_{\mathrm{MC}})}{\widehat{\mathrm{Var}}\,(\hat{\theta}_{\mathrm{MC}})},$$
where
$$\widehat{\mathrm{Var}}\,(\hat{\theta}_{\mathrm{MC}}) = \frac{1}{n(n-1)} \sum_{i=1}^{n} \left\{c(\boldsymbol{Y}_i) - \hat{\theta}_{\mathrm{MC}}\right\}^2$$
and
$$\widehat{\mathrm{Cov}}\,(\hat{\mu}_{\mathrm{MC}}, \hat{\theta}_{\mathrm{MC}}) = \frac{1}{n(n-1)} \sum_{i=1}^{n} \{h(\boldsymbol{X}_i) - \hat{\mu}_{\mathrm{MC}}\}\{c(\boldsymbol{Y}_i) - \hat{\theta}_{\mathrm{MC}}\}.$$
- $\hat{b}_n$ is the slope of the least-squares regression line for $(h(\boldsymbol{X}_i), c(\boldsymbol{Y}_i))$, $i = 1, \dots, n$

General idea

- Overall, the general idea for the control variate method is to search $c(\boldsymbol{Y})$ such that
    1. $E\{c(\boldsymbol{Y})\}$ is known.
    2. the scatterplot of $(h(\boldsymbol{X}_i), c(\boldsymbol{Y}_i))$ shows strong correlation.
- In practice, $\hat{\mu}_{\text{MC}}$ and $\hat{\theta}_{\text{MC}}$ often depend on the same random variable; i.e., $\boldsymbol{Y}_i = \boldsymbol{X}_i$.
- It is possible to use more than one control variate; i.e.,
$$\hat{\mu}_{\text{CV}} = \hat{\mu}_{\text{MC}} - b_1(\hat{\theta}_{1,\text{MC}} - \theta_1) - b_2(\hat{\theta}_{2,\text{MC}} - \theta_2).$$

Example

Let $\mu = E(e^U)$ where $U \sim \text{Unif}(0, 1)$. Theoretical study of CV estimator with b^* (when $m = 1$):

- Use U as the control variate
- $E(U) = 1/2, \text{Cov}(e^U, U) = 1 - (e-1)/2 = 0.14086$ and $\text{Var}(U) = 1/12$
- the CV estimator: $\hat{\mu}_{CV} = e^U - b^*(U - 1/2)$, where $b^* = 12(0.14086)$
- $\text{Var}(\hat{\mu}_{CV}) = 0.0039$ (verify!)
- resulting a variance reduction of 98.4% when compared to $Var(e^U) = 0.242$