Control Variates

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Additive control variate: simplest setting

Simplest setting

- Suppose we observe $X \in \mathcal{X}$ and $Y \in \mathbb{R}$.
- (X, Y) have some unknown joint distribution.
- **Goal:** Estimate $\mathbb{E}Y$.
- Y is a simple estimator for $\mathbb{E}Y$.
- It's even unbiased.
- Can we use X to improve our estimate of Y?
- In particular, to reduce the variance of our estimate?

Suppose we have a regression function

- Suppose somehow we have a function f.
- And **we think** $f(X) \approx Y$. No guarantees.
- Suppose we also know $\mathbb{E}f(X)$.
- Can we use $f(X)$ to get a better estimate of $\mathbb{E}Y$?

A new unbiased estimator

- Consider the estimator
$$\hat{\mu} = \hat{\mu}(X, Y) = Y - f(X) + \mathbb{E}f(X).$$
- $\mathbb{E}\hat{\mu} = \mathbb{E}Y - \mathbb{E}f(X) + \mathbb{E}f(X) = \mathbb{E}Y$. ($\hat{\mu}$ is **unbiased** for $\mathbb{E}Y$)
- Variance is

$$\begin{aligned} \mathrm{Var}(\hat{\mu}) &= \mathrm{Var}(Y - f(X) + \mathbb{E}f(X)) \\ &= \mathrm{Var}(Y - f(X)) \quad \mathbb{E}f(X) \text{ is constant} \end{aligned}$$

- Did we improve over $\mathrm{Var}(Y)$?
- Sometimes yes and sometimes no...

A new unbiased estimator

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- Did we improve over $\mathrm{Var}(Y)$?
- Sometimes yes and sometimes no...

- How should we think about this estimator intuitively?
- We can think that we're starting our estimate of $\mathbb{E}Y$ with $\mathbb{E}f(X)$.
- Then we want to correct $\mathbb{E}f(X)$ by how much it's off by. Ideally that would be $\mathbb{E}(Y - f(X))$.
- We don't know $\mathbb{E}(Y - f(X))$, but $Y - f(X)$ is an unbiased estimate that we'll use instead.

Simple extreme cases

- f predicts Y perfectly: $f(X) = Y$

$$\begin{aligned} \hat{\mu} &= Y - f(X) + \mathbb{E}f(X) = \mathbb{E}f(X) \\ \text{Var}(\hat{\mu}) &= \text{Var}(Y - f(X)) = 0. \end{aligned}$$

- $f(X) = -Y$

$$\text{Var}(\hat{\mu}) = \text{Var}(Y - f(X)) = \text{Var}(2Y) = 4\text{Var}(Y).$$

  which is much worse than just using Y.

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- These cases are only possible if Y is some deterministic function of X.

Ideal case

- Suppose $f(x) = \mathbb{E}[Y \mid X = x]$.
- The best approximation for Y given $X = x$ (in MSE)
- Then

$$\text{Var}(\hat{\mu}) \quad = \quad \text{Var}(Y - \mathbb{E}[Y \mid X]).$$

- The projection-residual decomposition of variance gives:

$$\begin{aligned} \text{Var}(Y) &= \text{Var}(Y - \mathbb{E}[Y \mid X]) + \text{Var}(\mathbb{E}[Y \mid X]) \\ &= \text{Var}(\hat{\mu}) + \text{Var}(\mathbb{E}[Y \mid X]) \end{aligned}$$

- So $\hat{\mu}$ has smaller variance than Y by an amount $\text{Var}(\mathbb{E}[Y \mid X])$.
- This is the amount of variation in Y that we can account for with X.

Control variates

Definition

A **control variate** is a random variable with **known expectation** used to reduce the variance of an estimator. [Owe13, Sec 8.9].

- In the context described above, with

$$\hat{\mu} = Y - f(X) + \mathbb{E}f(X),$$

- $f(X)$ is called a **control variate**.
- Intuitively, to be effective in creating lower-variance estimators of $\mathbb{E}Y$, we need $f(X) \approx Y$,
  - but we'll make that more precise later.

Control variate experiment

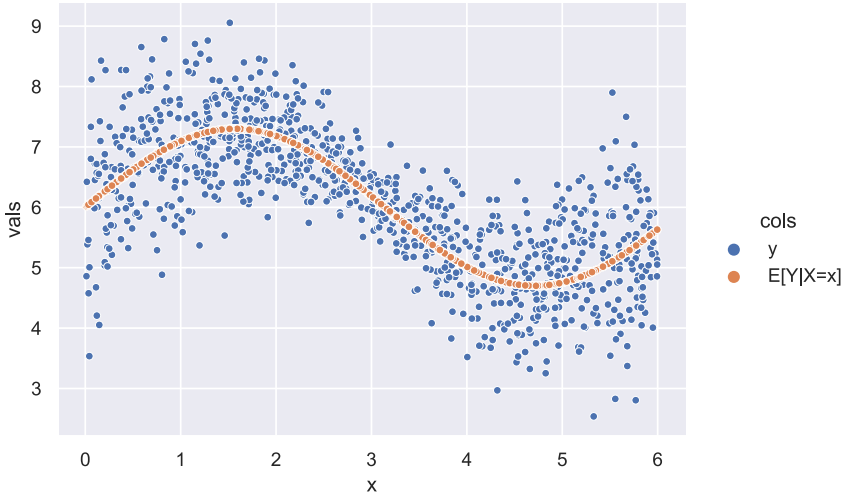
Control variate experiment

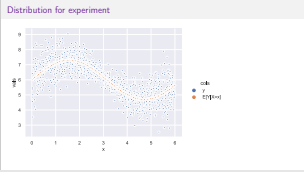
- Consider the following joint distribution of (X, Y):

$$\begin{aligned} X &\sim \text{Unif}[0,6] \\ Y \mid X &\sim \mathcal{N}\left(6 + 1.3\sin(X), \left[.3 + \frac{1}{4}|3 - X|\right]^2\right) \end{aligned}$$

- Goal: Estimate $\mathbb{E}Y$.

Distribution for experiment





- Note that the variance is much smaller around $x = 3$ than near $x = 0$ and $x = 6$.
- The objective is to estimate $\mathbb{E}Y$ given a sample of size $n = 1$, i.e. just one of those blue points.
- Can you roughly estimate, by eyeball, what $\mathrm{SD}(\mathbb{E}[Y \mid X])$ is? Looks to me roughly about 1. [In fact, it's 0.91.]
- Can you roughly estimate, by eyeball, what $\mathrm{SD}(Y)$ is? To me, it looks roughly like 2. [In fact, it's 1.18 – I was pretty off.]
- The hope is that with a control variate, we can eliminate a lot of the variance in Y that's due to $\mathbb{E}[Y \mid X]$. So we're hoping that our control-variate estimator will have variance in the ballpark of $\mathrm{Var}(Y) - \mathrm{Var}(\mathbb{E}[Y \mid X])$, which is about $(1.18)^2 - (.91)^2 = .55$. Of course, we can't get that low – that's what we would get if we knew $\mathbb{E}[Y \mid X = x]$. Perhaps we can come close with an estimate of $\mathbb{E}[Y \mid X = x]$

Getting our control variate

To get our control variate:

- Take a preliminary sample of size $n = 100$
- Fit a simple regression tree model to get $f(x)$
- Estimate $\mathbb{E}f(X)$ using the same preliminary sample, which we'll denote

$$\hat{\mathbb{E}}f(X) = \frac{1}{100}\sum_{i=1}^{100} f(X_i).$$

.

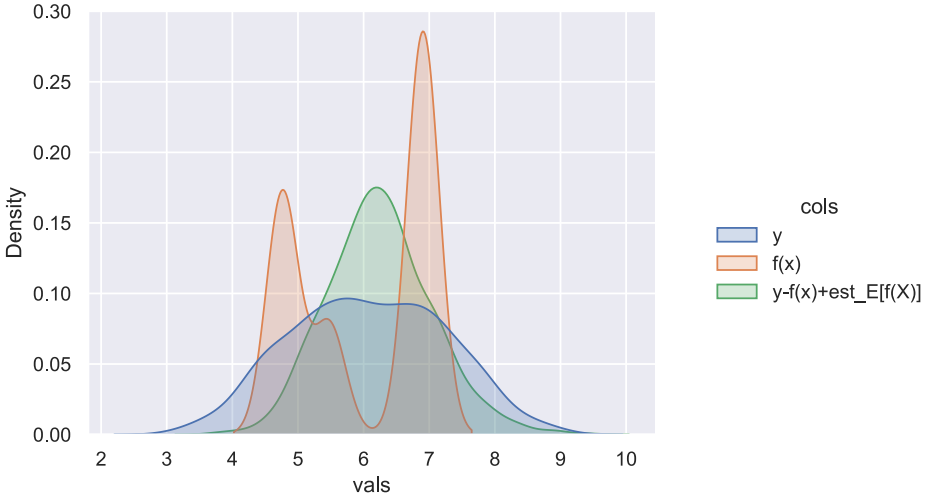
Distribution with our regression fit

Estimators for $\mathbb{E}Y$

Given (X, Y), a sample of size $n = 1$,
we'll consider the following estimators for $\mathbb{E}Y$:

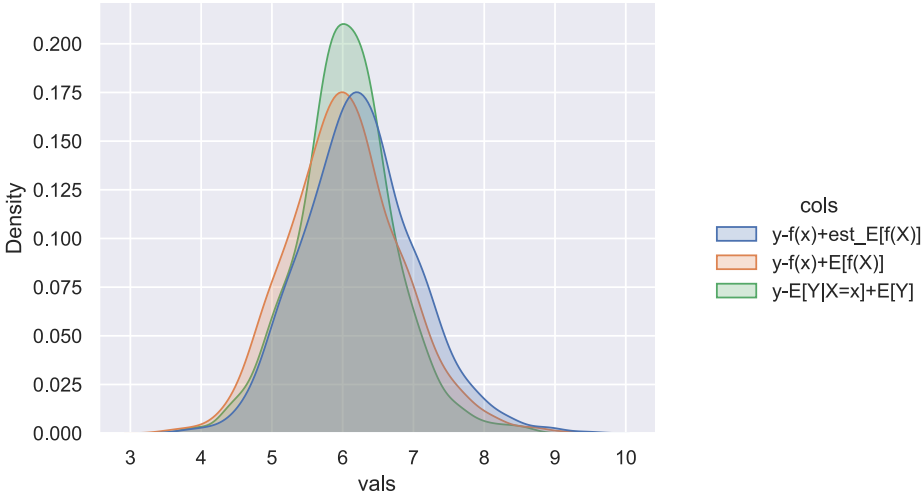
- Y (our baseline)
- $f(X)$ (benefits from the preliminary sample of size $n = 100$)
- $Y - f(X) + \hat{\mathbb{E}}[f(X)]$ (our estimate with a control variate)
- $Y - f(X) + \mathbb{E}[f(X)]$ (the actual $\mathbb{E}[f(X)]$ rather an estimate from the $n = 100$ sample)
- $Y - \mathbb{E}[Y \mid X = x] + \mathbb{E}Y$ (uses the the ideal control variate)

Estimator distributions

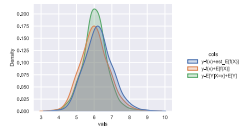


- These how the densities of the sampling distribution for three estimators of $\mathbb{E}Y$.
- The way to think about it is when we take our sample from the data generating distribution (here, just a sample of size $n = 1$), and then use that to instantiate our estimator, the estimator value we get is like being randomly drawn from one of the densities visualized above.
- Visually we can see that the control variate adjusted estimator has significantly lower variance than Y and $f(X)$.

Estimator compared to idealized estimators



Estimator compared to idealized estimators



- Visually, not a lot of difference when we replace $\hat{E}[f(X)]$ by $\mathbb{E}[f(X)]$. And that difference is dominated by the SD of the sampling distributions.
- There seems to be some improvement using $\mathbb{E}[Y \mid X = x]$, but doesn't seem to be huge.
- Next we'll look at numeric results.

Experimental results

With 1,000,000 trials of samples of size $n = 1$; $\mathbb{E}Y = 6.0090$

estimator	mean	SD	SE	bias	RMSE
y	6.0085	1.1761	0.0012	-0.0005	1.1761
$f(x)$	5.9731	0.9825	0.0010	-0.0359	0.9831
$y - f(x) + \hat{\mathbb{E}}[f(X)]$	6.2169	0.8023	0.0008	0.2079	0.8288
$y - f(x) + \mathbb{E}[f(X)]$	6.0095	0.8023	0.0008	0.0005	0.8023
$y - \mathbb{E}[Y \mid X = x] + \mathbb{E}Y$	6.0099	0.7080	0.0007	0.0009	0.7080

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- The estimator $y - f(x) + \hat{\mathbb{E}}[f(X)]$ uses the small ($n = 100$) preliminary sample to determine both $f(x)$ and to get the estimate $\hat{\mathbb{E}}[f(X)]$. If we use the true value $\mathbb{E}[f(X)]$ in the estimator, the bias reduces significantly (from .21 to .00). However, the SD is so much larger than the bias, than the improvement in RMSE is relatively small.
- We certainly have more improvement from using the ideal control variate $\mathbb{E}[Y \mid X]$ over $f(X)$, but the majority of the RMSE improvement was already achieved by using $f(X)$.

Control Variates in Practice

In practice...

- In our previous experiment,
  - assumed we already had $f(x)$ before we got our sample
  - assumed we already knew or had an estimate for $\mathbb{E}[f(X)]$.
- Sometimes this is reasonable,
  - e.g. $f(x)$ can be from a previous experiment.
  - We can think of $f(x)$ as like a prior
- But often we only get a single sample, and we don't have an $f(x)$ to start with.

Practical setup for estimator with control variate

- $(X, Y), (X_1, Y_1), \ldots, (X_n, Y_n)$ i.i.d.
- Goal: Estimate $\mathbb{E}Y$.
- Parameterized functions: $f(x; \theta) : \mathcal{X} \to \mathbb{R}$, for $\theta \in \mathbb{R}^d$
- Fit θ using least squares:

$$\hat{\theta} = \arg\min_{\theta \in \mathbb{R}^d} \sum_{i=1}^{n} (f(X_i; \theta) - Y_i)^2$$

- Use $f(X; \hat{\theta})$ as control variate.

Estimate with control variate

- Consider the following estimator:

$$\hat{\mu} \quad = \quad \frac{1}{n}\sum_{i=1}^{n}\left(Y_i - f(X_i;\hat{\theta}) + \mathbb{E}_X\left[f(X;\hat{\theta})\right]\right)$$

- This is the mean of n control variate adjusted estimates of Y.
- $\mathbb{E}\hat{\mu} = \mathbb{E}Y$ and $\text{Var}(\hat{\mu}) = \frac{1}{n}\text{Var}\left(Y - f(X;\hat{\theta})\right)$.
- But how to get $\mathbb{E}_X\left[f(X,\hat{\theta})\right]$? (expectation only over X).

How to get $\mathbb{E}\left[f(X, \hat{\theta})\right]$?

- It's either easy, or it's hard.
- If we know $p(x)$ and/or we can sample from $p(x)$,
  - then we can get $\mathbb{E}\left[f(X, \hat{\theta})\right]$ to whatever precision we need.

Example (Survey from a voter file)

Suppose we have a "voter file", which has covariate information (X's) about 200M eligible voters. We survey 1000 individuals to get $(X_1, Y_1), \ldots, (X_n, Y_n)$, and we want to estimate $\mathbb{E}Y$. We fit $f(x, \hat{\theta})$ with this sample. Then estimate $\mathbb{E}f(X, \hat{\theta})$ using the full voter file.

- If all we know about $p(x)$ is from our sample $(X_1, Y_1), \ldots, (X_n, Y_n)$,
  - then it's going to be hard.

Can we estimate $\mathbb{E}\left[f(X,\hat{\theta})\right]$ from the sample?

- Estimate $\mathbb{E}_X\left[f(X;\hat{\theta})\right]$ as $\hat{\mathbb{E}}_X\left[f(X;\hat{\theta})\right] = \frac{1}{n}\sum_{i=1}^n f(X_i;\hat{\theta})$.
- If we plug this into our estimator, we get

$$\begin{aligned} & \frac{1}{n}\sum_{i=1}^n \left(Y_i - f(X_i;\hat{\theta}) + \hat{\mathbb{E}}_X\left[f(X;\hat{\theta})\right]\right) \\ = & \frac{1}{n}\sum_{i=1}^n \left(Y_i - f(X_i;\hat{\theta})\right) + \frac{1}{n}\sum_{i=1}^n f(X_i;\hat{\theta}) \\ = & \frac{1}{n}\sum_{i=1}^n Y_i \end{aligned}$$

- This leaves us back where we started.

Cross-fitting

- Simulate knowing $f(x)$ and $\mathbb{E}[f(X)]$ by cross-fitting.
- Randomly split data into two halves: $\mathcal{D}_1, \mathcal{D}_2$
- Fit $\hat{f}^{\mathcal{D}_1}$ on $\mathcal{D}_1$ and use $\hat{\mathbb{E}}^{\mathcal{D}_1}\hat{f}^{\mathcal{D}_1}(X) = \frac{1}{|\mathcal{D}_1|}\sum_{i\in\mathcal{D}_1}\hat{f}^{\mathcal{D}_1}(X_i)$ as mean estimate.
- Then $\hat{\mu}^{\mathcal{D}_2} = \hat{\mathbb{E}}^{\mathcal{D}_1}\hat{f}^{\mathcal{D}_1}(X) + \frac{1}{|\mathcal{D}_2|}\sum_{i\in\mathcal{D}_2}\left(Y_i - \hat{f}^{\mathcal{D}_1}(X_i)\right)$.
- and $\hat{\mu}^{\mathcal{D}_1} = \hat{\mathbb{E}}^{\mathcal{D}_2}\hat{f}^{\mathcal{D}_2}(X) + \frac{1}{|\mathcal{D}_1|}\sum_{i\in\mathcal{D}_1}\left(Y_i - \hat{f}^{\mathcal{D}_2}(X_i)\right)$
- Then define

$$\hat{\mu} = \frac{|\mathcal{D}_1|}{n}\hat{\mu}^{\mathcal{D}_1} + \frac{|\mathcal{D}_2|}{n}\hat{\mu}^{\mathcal{D}_2}.$$

- This is called **cross-estimation**.

$f(x)$ and $\mathbb{E}[f(X)]$ known: summary

- Conditions:
  - We know $f(x)$ and $\mathbb{E}[f(X)]$ before we get our sample.
  - We get a sample $(X, Y), (X_1, Y_1), \ldots, (X_n, Y_n)$
- Estimator:

$$\hat{\mu} = \mathbb{E}f(X) + \frac{1}{n}\sum_{i=1}^{n}(Y_i - f(X_i))$$

- $\mathbb{E}\hat{\mu} = \mathbb{E}Y$. (unbiased estimator)
- Interpretation: We start by estimating $\mathbb{E}Y$ using $\mathbb{E}f(X)$, and then correct it by the average residual, which is an unbiased estimator for $\mathbb{E}Y - \mathbb{E}f(X)$, the residual of $\mathbb{E}f(X)$ as an estimate for $\mathbb{E}Y$.

Unlimited samples from $p(x)$: summary

- Conditions:
  - We know $p(x)$ and/or can can get unlimited samples from it
  - We get a sample $(X, Y), (X_1, Y_1), \ldots, (X_n, Y_n)$
- Estimator:

$$\begin{aligned} \hat{\theta} &= \arg\min_{\theta \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} \Big(f(X_i; \hat{\theta}) - Y_i \Big)^2 \\ \hat{\mu} &= \hat{\mathbb{E}}_X f(X; \hat{\theta}) + \frac{1}{n} \sum_{i=1}^{n} \Big(Y_i - f(X_i; \hat{\theta}) \Big), \end{aligned}$$

where $\hat{\mathbb{E}}_X f(X; \hat{\theta}) = \frac{1}{N} \sum_{i=1}^{N} f(X_i; \hat{\theta})$, where $X_1, \ldots, X_N$ is a large i.i.d. sample from $p(x)$.

Optimal scaling to improve variance

Regression estimator with control variate

- The following estimator is also unbiased for $\mathbb{E}Y$, for any $\beta \in \mathbb{R}$:

$$\hat{\mu}_\beta = Y - \beta f(X) + \beta \mathbb{E} f(X).$$

- This is called a regression estimator of $\mathbb{E}Y$ in [Owe13, Ch 8.9].
- The variance is

$$\begin{aligned} \text{Var}\left(\hat{\mu}_\beta\right) &= \text{Var}\left(Y - \beta f(X)\right) \\ &= \text{Var}(Y) + \beta^2 \text{Var}\left(f(X)\right) - 2\beta \text{Cov}\left(Y, f(X)\right) \end{aligned}$$

- If we know $\text{Var}(Y)$, $\text{Var}(f(X))$, and $\text{Cov}(Y, f(X))$, then the β that minimizes the variance is

$$\beta_{\text{opt}} = \rho \frac{\text{SD}(Y)}{\text{SD}(f(X))},$$

where $\rho = \text{Corr}(Y, f(X))$.

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where $\rho = \mathrm{Corr}(Y, f(X))$.

- Recall that the **variance of a sum** is

$$\mathrm{Var}\left(\sum_{i=1}^{n} X_i\right) = \sum_{i,j=1}^{n} \mathrm{Cov}\left(X_i, X_j\right) = \sum_{i=1}^{n} \mathrm{Var}\left(X_i\right) + 2\sum_{i \neq j} \mathrm{Cov}\left(X_i, X_j\right)$$

- Also that the **correlation** is defined as

$$\rho = \mathrm{Corr}\left(X, Y\right) = \frac{\mathrm{Cov}\left(X, Y\right)}{\sqrt{\mathrm{Var}(X)\mathrm{Var}(Y)}} = \frac{\mathrm{Cov}\left(X, Y\right)}{\mathrm{SD}(X)\mathrm{SD}(Y)}.$$

- Finding the optimum β is simple differential calculus:

$$\begin{aligned} 2\beta \mathrm{Var}\left(f(X)\right) - 2\mathrm{Cov}\left(Y, f(X)\right) &= 0 \\ \iff \beta &= \frac{\mathrm{Cov}\left(Y, f(X)\right)}{\mathrm{Var}\left(f(X)\right)} = \rho \frac{\mathrm{SD}(Y)}{\mathrm{SD}(f(X))} \end{aligned}$$

Optimal β and optimal variance

- The resulting variance is

$$\mathrm{Var}\left(\hat{\mu}_{\beta_{\mathsf{opt}}}\right) \quad = \quad (1-\rho^2)\mathrm{Var}(Y).$$

- In practical situations, we'll usually have to estimate $\mathrm{Var}(Y)$, $\mathrm{Var}(f(X))$, and $\mathrm{Cov}(Y, f(X))$ from our sample.
- Using $\hat{\beta}_{\mathsf{opt}}$ instead of β_{opt} will lead to a slight bias [Owe13, Ch 8.9].

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- Derivation is

$$\begin{aligned}
\mathrm{Var}\left(\hat{\mu}_{\beta_{\mathsf{opt}}}\right) &= \mathrm{Var}(Y) + \rho^2\mathrm{Var}(Y) - 2\rho\frac{\mathrm{SD}(Y)}{\mathrm{SD}(f(X))}\mathrm{Cov}(Y, f(X)) \\
&= \mathrm{Var}(Y) + \rho^2\mathrm{Var}(Y) - 2\rho\frac{\mathrm{Var}(Y)}{\mathrm{SD}(f(X))}\frac{\mathrm{Cov}(Y, f(X))}{\mathrm{SD}(Y)} \\
&= \mathrm{Var}(Y) + \rho^2\mathrm{Var}(Y) - 2\rho^2\mathrm{Var}(Y) \\
&= (1-\rho^2)\mathrm{Var}(Y)
\end{aligned}$$

- In the video I said that using $\hat{\beta}_{\mathsf{opt}}$ is the recommended approach. I was trying to capture Owen's statement that "In general $\mathbb{E}\left[\hat{\mu}_{\hat{\beta}_{\mathsf{opt}}}\right] \neq \mathbb{E}Y$, but this bias is usually small" [Owe13, Ch 8.9]. However, whether this approach improves things or not can be situation dependent. We only demonstrated improvement when the variances and covariance are known – when these are estimated, no guarantees. Besides introducing a bias, we may also inflate the variance, as we plug these random estimates into a ratio.

References

Resources

- A good reference for control variates is a section in Owen's book [Owe13, Ch 8.9].
- In general, most longer discussions of Monte Carlo methods get into control variates as a way to reduce variance.
- The short Wikipedia article is actually quite readable, and has its own useful list of references.

References I

[Owe13] Art B. Owen, *Monte carlo theory, methods and examples*, 2013.