

# Optimization and Simulation

## Variance reduction

Michel Bierlaire

Transport and Mobility Laboratory  
School of Architecture, Civil and Environmental Engineering  
Ecole Polytechnique Fédérale de Lausanne



# Outline

- 1 Anthithetic draws
- 2 Control variates
- 3 Other techniques

## Example

Use simulation to compute

$$I = \int_0^1 e^x dx$$

We know the solution:  $e - 1 = 1.7183$

Simulation: consider draws two by two

- Let  $r_1, \dots, r_R$  be independent draws from  $U(0, 1)$ .
- Let  $s_1, \dots, s_R$  be independent draws from  $U(0, 1)$ .

$$I \approx \frac{1}{R} \sum_{i=1}^R \frac{e^{r_i} + e^{s_i}}{2}$$

- Use  $R = 10'000$  (that is, a total of 20'000 draws)
- Mean over  $R$  draws from  $(e^{r_i} + e^{s_i})/2$ : 1.720, variance: 0.123

## Example

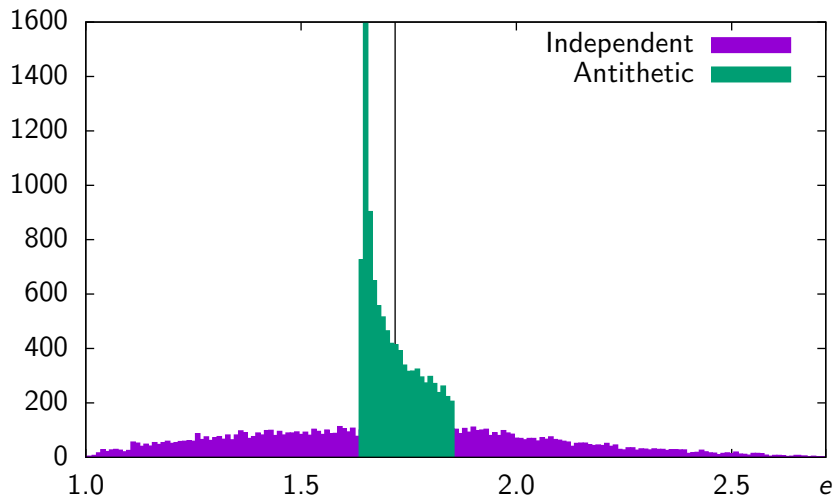
Now, use half the number of draws

- Idea: if  $X \sim U(0, 1)$ , then  $(1 - X) \sim U(0, 1)$
- Let  $r_1, \dots, r_R$  be independent draws from  $U(0, 1)$ .

$$I \approx \frac{1}{R} \sum_{i=1}^R \frac{e^{r_i} + e^{1-r_i}}{2}$$

- Use  $R = 10'000$
- Mean over  $R$  draws of  $(e^{r_i} + e^{1-r_i})/2$ : 1.7183, variance: **0.00388**
- Compared to: mean of  $(e^{r_i} + e^{s_i})/2$ : 1.720, variance: **0.123**

## Example



# Antithetic draws

- Let  $X_1$  and  $X_2$  i.i.d r.v. with mean  $\theta$
- Then

$$\text{Var}\left(\frac{X_1 + X_2}{2}\right) = \frac{1}{4} (\text{Var}(X_1) + \text{Var}(X_2) + 2 \text{Cov}(X_1, X_2))$$

- If  $X_1$  and  $X_2$  are independent, then  $\text{Cov}(X_1, X_2) = 0$ .
- If  $X_1$  and  $X_2$  are negatively correlated, then  $\text{Cov}(X_1, X_2) < 0$ , and the variance is reduced.

## Back to the example

### Independent draws

- $X_1 = e^U, X_2 = e^U$

$$\begin{aligned}
 \text{Var}(X_1) = \text{Var}(X_2) &= E[e^{2U}] - E[e^U]^2 \\
 &= \int_0^1 e^{2x} dx - (e - 1)^2 \\
 &= \frac{e^2 - 1}{2} - (e - 1)^2 \\
 &= 0.2420
 \end{aligned}$$

$$\text{Cov}(X_1, X_2) = 0$$

$$\text{Var}\left(\frac{X_1 + X_2}{2}\right) = \frac{1}{4} (0.2420 + 0.2420) = 0.1210$$

## Back to the example

### Antithetic draws

- $X_1 = e^U$ ,  $X_2 = e^{1-U}$

$$\text{Var}(X_1) = \text{Var}(X_2) = 0.2420$$

$$\begin{aligned} \text{Cov}(X_1, X_2) &= E[e^U e^{1-U}] - E[e^U]E[e^{1-U}] \\ &= e - (e-1)(e-1) \\ &= -0.2342 \end{aligned}$$

$$\text{Var}\left(\frac{X_1 + X_2}{2}\right) = \frac{1}{4} (0.2420 + 0.2420 - 2 \cdot 0.2342) = 0.0039$$



# Antithetic draws: generalization

- Suppose that

$$X_1 = h(U_1, \dots, U_m)$$

where  $U_1, \dots, U_m$  are i.i.d.  $U(0, 1)$ .

- Define

$$X_2 = h(1 - U_1, \dots, 1 - U_m)$$

- $X_2$  has the same distribution as  $X_1$
- If  $h$  is monotonic in each of its coordinates, then  $X_1$  and  $X_2$  are negatively correlated.
- If  $h$  is not monotonic, there is no guarantee that the variance will be reduced.

## Another example

$$I = \int_0^1 \left(x - \frac{1}{2}\right)^2 dx$$

- Antithetic draws:

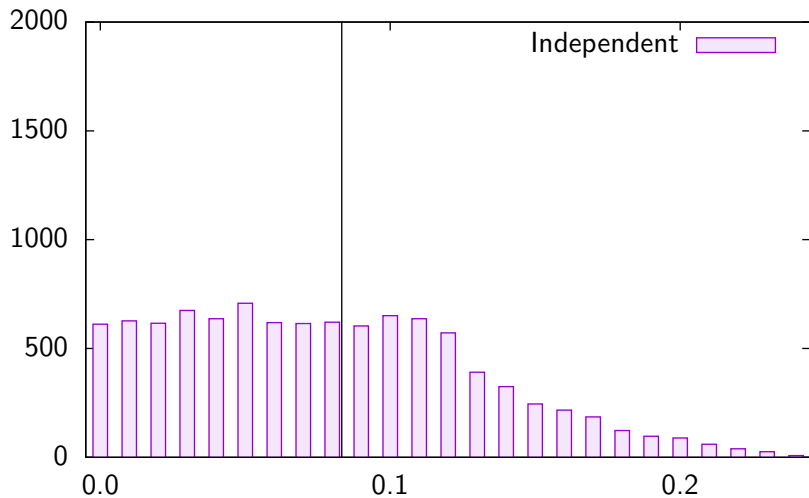
$$X_1 = \left(U - \frac{1}{2}\right)^2, \quad X_2 = \left((1 - U) - \frac{1}{2}\right)^2$$

- The covariance is positive:

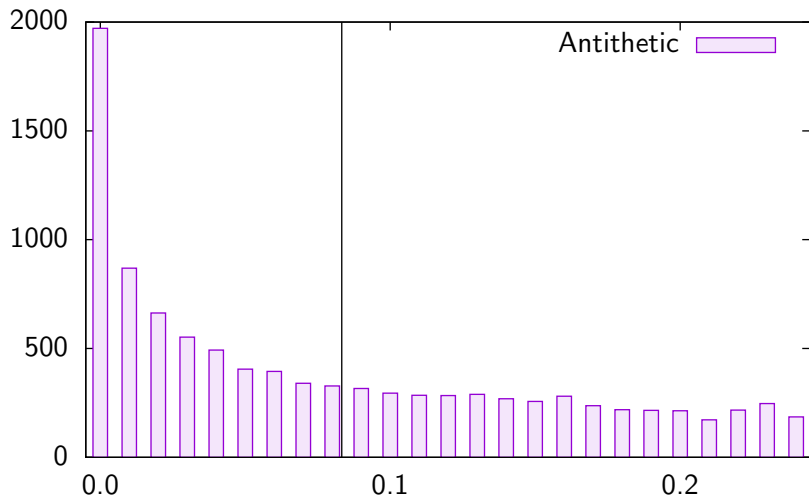
$$\text{Cov}(X_1, X_2) = \frac{1}{180} > 0.$$

- The variance will therefore be (slightly) increased!

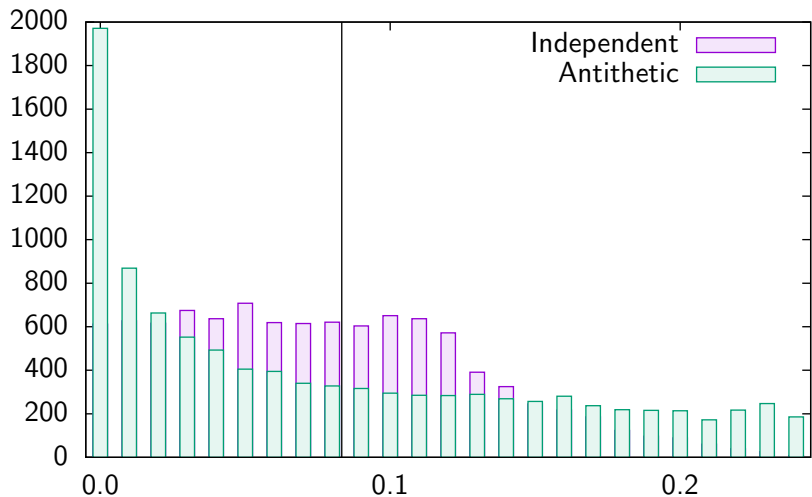
## Another example



## Another example



# Another example



# Outline

- 1 Anthitetic draws
- 2 Control variates**
- 3 Other techniques

# Control variates

- We use simulation to estimate  $\theta = E[X]$ , where  $X$  is an output of the simulation
- Let  $Y$  be another output of the simulation, such that we know  $E[Y] = \mu$
- We consider the quantity:

$$Z = X + c(Y - \mu).$$

- By construction,  $E[Z] = E[X]$
- Its variance is

$$\text{Var}(Z) = \text{Var}(X + cY) = \text{Var}(X) + c^2 \text{Var}(Y) + 2c \text{Cov}(X, Y)$$

- Find  $c$  such that  $\text{Var}(Z)$  is minimum

# Control variates

- First derivative:

$$2c \operatorname{Var}(Y) + 2 \operatorname{Cov}(X, Y)$$

- Zero if

$$c^* = -\frac{\operatorname{Cov}(X, Y)}{\operatorname{Var}(Y)}$$

- Second derivative:

$$2 \operatorname{Var}(Y) > 0$$

- We use

$$Z^* = X - \frac{\operatorname{Cov}(X, Y)}{\operatorname{Var}(Y)}(Y - \mu).$$

- Its variance

$$\operatorname{Var}(Z^*) = \operatorname{Var}(X) - \frac{\operatorname{Cov}(X, Y)^2}{\operatorname{Var}(Y)} \leq \operatorname{Var}(X)$$



# Control variates

In practice...

- $\text{Cov}(X, Y)$  and  $\text{Var}(Y)$  are usually not known.
- We can use their sample estimates:

$$\widehat{\text{Cov}}(X, Y) = \frac{1}{n-1} \sum_{r=1}^R (X_r - \bar{X})(Y_r - \bar{Y})$$

and

$$\widehat{\text{Var}}(Y) = \frac{1}{n-1} \sum_{r=1}^R (Y_r - \bar{Y})^2.$$

# Control variates

In practice...

- Alternatively, use linear regression

$$X = aY + b + \varepsilon$$

where  $\varepsilon \sim N(0, \sigma^2)$ .

- The least square estimators of  $a$  and  $b$  are

$$\hat{a} = \frac{\sum_{r=1}^R (X_r - \bar{X})(Y_r - \bar{Y})}{\sum_{r=1}^R (Y_r - \bar{Y})^2}$$

$$\hat{b} = \bar{X} - \hat{a}\bar{Y}.$$

- Therefore

$$c^* = -\hat{a}$$

# Control variates

- Moreover,

$$\begin{aligned}\hat{b} + \hat{a}\mu &= \bar{X} - \hat{a}\bar{Y} + \hat{a}\mu \\ &= \bar{X} - \hat{a}(\bar{Y} - \mu) \\ &= \bar{X} + c^*(\bar{Y} - \mu) \\ &= \hat{\theta}\end{aligned}$$

- Therefore, the control variate estimate  $\hat{\theta}$  of  $\theta$  is obtained by the estimated linear model, evaluated at  $\mu$ .

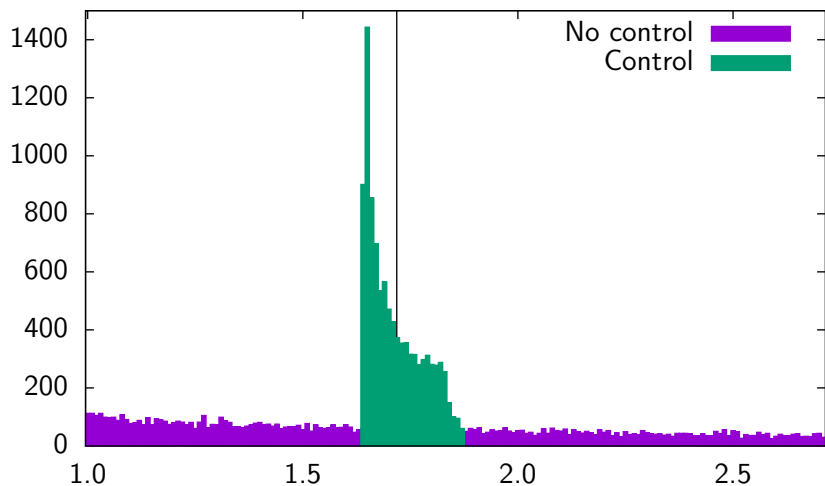
## Back to the example

- Use simulation to compute  $I = \int_0^1 e^x dx$
- $X = e^U$
- $Y = U$ ,  $E[Y] = 1/2$ ,  $\text{Var}(Y) = 1/12$
- $\text{Cov}(X, Y) = (3 - e)/2 \approx 0.14$
- Therefore, the best  $c$  is

$$c^* = -\frac{\text{Cov}(X, Y)}{\text{Var}(Y)} = -6(3 - e) \approx -1.69$$

- Test with  $R = 10'000$
- Result of the regression:  $\hat{a} = 1.6893$ ,  $\hat{b} = 0.8734$
- Estimate:  $\hat{b} + \hat{a}/2 = 1.7180$ , Variance: 0.003847 (compared to 0.24)

## Back to the example



# Outline

- 1 Anthitetic draws
- 2 Control variates
- 3 Other techniques

# Variance reductions techniques

## Other techniques

- Conditioning
- Stratified sampling
- Importance sampling
- Draw recycling

## In general

Correlation helps!