

# Statistical Computing with R – MATH 6382<sup>1,\*</sup>

## Set 5 (Monte Carlo Integration and Variance Reduction)

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<sup>1</sup>Based on textbook.

\* Last updated November 2, 2016

# *Numerical Integration*

# Integration

- The goal is to find the integral  $\int_a^b g(x)dx$  with possibly unbounded limits
- We know that  $\int_a^b 2xdx = b^2 - a^2$ , but we don't know a closed form for  $\int_a^b e^{-x^2} dx$

# 1. Newton-Cotes Integration

If  $a, b < \infty$ . The Newton-Cotes Integration of degree  $n$

$$\int_a^b g(x) dx \approx \sum_{j=0}^n w_j g(x_j)$$

where the nodal points  $x_j = a + j * h$ ,  $h = \frac{b - a}{n}$  and the weights are the solution of

$$\begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ x_0 & x_1 & x_2 & \cdots & x_n \\ x_0^2 & x_1^2 & x_2^2 & \cdots & x_n^2 \\ & & \vdots & & \\ x_0^n & x_1^n & x_2^n & \cdots & x_n^n \end{pmatrix} \begin{pmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_n \end{pmatrix} = (b - a) \begin{pmatrix} 1 \\ \frac{1}{2} \\ \frac{1}{3} \\ \vdots \\ \frac{1}{n+1} \end{pmatrix}$$

# 1. Newton-Cotes Integration

If  $a, b < \infty$ . The Newton-Cotes Integration of degree  $n$

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where the nodal points  $x_j = a + j * h$ ,  $h = \frac{b - a}{n}$  and the weights are the solution of

$$w_j = \int_a^b L_j(x) dx$$

where  $L_j(x) = \prod_{k=0, k \neq j}^n \frac{(x - x_k)}{(x_j - x_k)}$

# 1. Newton-Cotes Integration

- The **error** in the Newton-Cotes Integration of a function  $g \in C^{n+1}[a, b]$  of degree  $n$  is

$$\int_a^b g(x) dx - \sum_{j=0}^n w_j g(x_j) =$$

$$\frac{h^{n+2} g^{(n+1)}(\xi)}{n^{n+2} (n+1)!} \int_0^n t(t-1) \cdots (t-n) dt$$

if  $n$  is odd, where  $\xi \in (a, b)$ .

- Thus, Newton-Cotes has a precision of  $n$  if  $n$  is odd as it integrates polynomials of degrees up to  $n$  exactly.

# 1. Newton-Cotes Integration

- The **error** in the Newton-Cotes Integration of a function  $g \in C^{n+2}[a, b]$  of degree  $n$  is

$$\int_a^b g(x) dx - \sum_{j=0}^n w_j g(x_j) =$$

$$\frac{h^{n+3} g^{(n+2)}(\xi)}{n^{n+3} (n+2)!} \int_0^n t^2 (t-1) \cdots (t-n) dt$$

if  $n$  is even, where  $\xi \in (a, b)$ .

- Thus, Newton-Cotes has a precision of  $n+1$  if  $n$  is even as it integrates polynomials of degrees up to  $n+1$  exactly.

## 2. Gaussian Quadrature Integration

The Gaussian Quadrature (Gauss-"Polynomial") Integration of degree  $n$

$$\int_a^b g(x)\rho(x)dx \approx \sum_{j=0}^n w_j g(x_j)$$

where the nodal points  $x_0, x_1, \dots, x_n$  are the **zeros of an orthogonal polynomial**  $p_{n+1}(x)$  with weight function  $\rho(x)$ ; that is,

$$\int_a^b p_i(x)p_j(x)\rho(x)dx = 0 \text{ for } i \neq j$$

and the weights are

$$w_j = \int_a^b L_j(x)\rho(x)dx$$

where  $L_j(x) = \prod_{k=0, k \neq j}^n \frac{(x - x_k)}{(x_j - x_k)}$



## 2. Gaussian Quadrature Integration

The Gaussian Quadrature (Gauss-"Polynomial") Integration

$$\int_a^b g(x)\rho(x)dx$$

Gaussian Quad.	Polynomial	$\rho(\mathbf{x})$	$[a, b]$
Gauss-Legendre	Legendre	1	$[-1, 1]$
Gauss-Chebyshev	Chebyshev (first kind)	$\frac{1}{\sqrt{1-x^2}}$	$(-1, 1)$
Gauss-Chebyshev	Chebyshev (second kind)	$\sqrt{1-x^2}$	$[-1, 1]$
Gauss-Laguerre	Laguerre	$e^{-x}$	$[0, \infty)$
Gauss-Hermite	Hermite	$e^{-x^2}$	$(-\infty, \infty)$

## 2. Gaussian Quadrature Integration

- The **error** in the Gaussian Quadrature Integration of a function  $g \in C^{2n+2}[a, b]$  of degree  $n$  is

$$\int_a^b g(x)\rho(x)dx - \sum_{j=0}^n w_j g(x_j) = \frac{g^{(2n+2)}(\xi)}{(2n+2)!} \int_a^b p_{n+1}^2(x)\rho(x)dx$$

where  $\xi \in (a, b)$ .

- Thus, Gauss-Quadrature has a precision of  $2n + 1$  as it integrates polynomials of degrees up to  $2n + 1$  exactly.
- For Legendre polynomial,  $\int_{-1}^1 p_{n+1}^2(x)\rho(x)dx = \frac{2}{2n+3}$ .
- For Hermite polynomial,  $\int_{-\infty}^{\infty} p_{n+1}^2(x)\rho(x)dx = \sqrt{\pi}2^{n+1}(n+1)!$ .

## 2. Gaussian Quadrature Integration

To find

$$\int_1^3 e^{-x^2} dx$$

use either

- ① Gauss-Legendre with  $\rho(x) = 1$  and  $g(x) = e^{-(x+2)^2}$  as

$$\int_1^3 e^{-x^2} dx = \int_{-1}^1 e^{-(x+2)^2} * 1 dx$$

or

- ② Gauss-Hermite with  $\rho(x) = e^{-x^2}$  and  $g(x) = l_{(1,3)}(x)$  as

$$\int_1^3 e^{-x^2} dx = \int_{-\infty}^{\infty} l_{(1,3)}(x) * e^{-x^2} dx$$

# Adaptive Quadrature Integration in R

To find  $\int_a^b g(x)dx$  use

```
integrate(function(x) g(x), a, b)
```

Example: Find  $\int_0^1 2x dx$

```
> integrate(function(x) 2*x, 0, 1)
```

```
1 with absolute error < 1.1e-14
```

# *Monte Carlo Integration*

# Monte Carlo Integration

To find  $\int_0^1 g(x)dx$  we can estimate just  $\mathbf{E}(g(X)) = \int_0^1 g(x)dx$  with  $X \sim \text{unif}(0, 1)$  by generating  $x_1, \dots, x_n$  from  $\text{unif}(0, 1)$  and then use  $\frac{1}{n} \sum_{i=1}^n g(x_i)$  as estimate of  $\mathbf{E}(g(X))$ .

Recall (SLLN): (keep in mind  $Y = g(X)$ )

If  $Y, Y_1, Y_2, \dots$  are i.i.d.r.v.'s such that  $\mathbf{E} |Y| < \infty$ , then

$$\frac{1}{n} \sum_{i=1}^n Y_i \rightarrow \mathbf{E}(Y)$$

almost surely (with probability one).

# Monte Carlo Integration

Remark:

$$\int_a^b g(x) dx = (b-a) \int_0^1 g(y(b-a)+a) dy \approx (b-a) \frac{1}{n} \sum_{i=1}^n g(u_i(b-a)+a)$$

with  $u_1, \dots, u_n$  generated from *unif*(0, 1)

OR

$$\int_a^b g(x) dx = (b-a) \int_a^b g(x) \frac{1}{b-a} dx \approx (b-a) \frac{1}{n} \sum_{i=1}^n g(x_i)$$

with  $x_1, \dots, x_n$  generated from *unif*( $a, b$ )

# Monte Carlo Integration

Recall (CLT): (keep in mind  $Y = g(X)$ )

If  $Y, Y_1, Y_2, \dots$  are i.i.d.r.v.'s such that  $\mathbf{V}(Y) < \infty$ , then

$$\frac{\frac{1}{n} \sum_{i=1}^n Y_i - \mathbf{E}(Y)}{\sqrt{\mathbf{V}(Y)/n}} \rightarrow Z \text{ in distribution}$$

where  $Z \sim \text{norm}(0, 1)$ .

Note also, that  $\mathbf{E}(\frac{1}{n} \sum_{i=1}^n Y_i) = \mathbf{E}_X(g(X))$  so it is unbiased estimate.



# Monte Carlo Integration

It is good to build up a confidence interval for  $\mathbf{E}(g(X))$  with  $\sqrt{\mathbf{V}(Y)/n}$  estimated by the standard error

$$\hat{se}(\bar{Y}) = \sqrt{\frac{\hat{\mathbf{V}}(Y)}{n}} = \frac{1}{\sqrt{n}} \sqrt{\frac{1}{n} \sum_{i=1}^n (Y_i - \bar{Y})^2}$$

for sufficiently large  $n$ .

So,  $(1 - \alpha)100\%$  confidence interval is found by

$$\frac{1}{n} \sum_{i=1}^n Y_i \pm z_{\alpha/2} \hat{se}(\bar{Y})$$

# Monte Carlo Integration

Example: Estimate  $\int_1^3 e^{-x^2} dx$  and find 95% confidence interval for that integral. Remark:  $\int_1^3 e^{-x^2} dx = \sqrt{\pi}P(1 < X < 3)$  when  $X \sim N(0, \frac{1}{\sqrt{2}})$  and

```
sqrt(pi) * (pnorm(3, 0, 1/sqrt(2)) - pnorm(1, 0, 1/sqrt(2)))  
[1] 0.1393832
```

# Monte Carlo Integration

First method:

$$\int_1^3 e^{-x^2} dx = \int_1^3 (3-1) * e^{-x^2} \frac{1}{3-1} dx = \mathbf{E}_X((3-1) * e^{-X^2})$$

with  $X \sim \text{unif}(1, 3)$

```
n<-10000;CL<- .95
```

```
x<-runif(n,1,3)
```

```
y<-(3-1)*exp(-1*x^2)
```

```
mu1<-mean(y)
```

```
mu1
```

```
[1] 0.1363614
```

```
se1<-sd(y)/sqrt(n)
```

```
CI<-c(mu1-qnorm((1+CL)/2)*se1,mu1+qnorm((1+CL)/2)*se1)
```

```
CI
```

```
[1] 0.1326229 0.1401000
```

# Monte Carlo Integration

Second method:

$$\int_1^3 e^{-x^2} dx = \int_{-\infty}^{\infty} (\sqrt{\pi} I_{(1,3)}(x)) \frac{1}{\sqrt{\pi}} e^{-x^2} dx = \mathbf{E}_X(\sqrt{\pi} I_{(1,3)}(X))$$

with  $X \sim \text{norm}(0, \frac{1}{\sqrt{2}})$

```
n<-10000;CL<-.95
```

```
x<-rnorm(n, 0, 1/sqrt(2))
```

```
y<-sqrt(pi)*as.integer((x<3) & (x>1))
```

```
mu2<-mean(y)
```

```
mu2
```

```
[1] 0.1389604
```

```
se2<-sd(y)/sqrt(n)
```

```
CI<-c(mu2-qnorm((1+CL)/2)*se2, mu2+qnorm((1+CL)/2)*se2)
```

```
CI
```

```
[1] 0.1296219 0.1482988
```

# *Variance Reduction*

# Efficiency

If  $\hat{\theta}_1$  and  $\hat{\theta}_2$  are two estimators of a parameter  $\theta$  then  $\hat{\theta}_1$  is more efficient than  $\hat{\theta}_2$  if

$$\mathbf{V}(\hat{\theta}_1) < \mathbf{V}(\hat{\theta}_2)$$

and the amount of reduction in variance is measured by

$$(\mathbf{V}(\hat{\theta}_1) - \mathbf{V}(\hat{\theta}_2)) / \mathbf{V}(\hat{\theta}_1)$$

Note that computational efficiency is also implied.

Example: In the previous example  $\hat{\theta}_1 = 0.1363614$  and  $\hat{\theta}_2 = 0.1389604$  are two estimators of  $\int_1^3 e^{-x^2} dx$

The estimated amount of reduction in variance is

$$(se1^2 - se2^2) / se1^2$$

$$[1] \quad -5.31999$$

# *Variance Reduction–Antithetic Variables*

# Variance Reduction—Antithetic Variables

- If  $X$  and  $Y$  are negatively correlated ( $\text{Cov}(X, Y) < 0$ ) then

$$\mathbf{V}(X + Y) = \mathbf{V}(X) + \mathbf{V}(Y) + 2\text{Cov}(X, Y) < \mathbf{V}(X) + \mathbf{V}(Y)$$

- If  $U \sim \text{unif}(0, 1)$  then  $1 - U \sim \text{unif}(0, 1)$  and

$$\text{Cov}(U, 1 - U) = -\mathbf{V}(U) = -\frac{1}{12} < 0$$

- What about  $\text{Cov}\left(F_X^{-1}(U), F_X^{-1}(1 - U)\right)$ ?
- What about  $\text{Cov}\left(g(F_X^{-1}(U)), g(F_X^{-1}(1 - U))\right)$ ?

If  $g$  is monotone then the last covariance is also negative.



# Variance Reduction—Antithetic Variables

- What about  $Cov\left(g(F_X^{-1}(U)), g(F_X^{-1}(1-U))\right)$ ?

If  $g$  is monotone then the last covariance is negative. Why?

- Note that  $h_1(s) = g(F_X^{-1}(s))$  and  $h_2(s) = -g(F_X^{-1}(1-s))$  are monotone in a similar fashion to  $g$ .
- Note that  $Y_1 = h_1(U)$  and  $Y_2 = -h_2(U)$  are identically distributed
- WTS:  $Cov(Y_1, Y_2) < 0$  or equivalently  $\mathbf{E}(Y_1 Y_2) < \mathbf{E}(Y_1)\mathbf{E}(Y_2)$  or equivalently  $\mathbf{E}(h_1(U)h_2(U)) > \mathbf{E}(h_1(U))\mathbf{E}(h_2(U))$

# Variance Reduction—Antithetic Variables

- Assume WLOG that  $h_1$  and  $h_2$  are increasing, then for any  $x$  and  $y \in \mathbb{R}$

$$(h_1(x) - h_1(y))(h_2(x) - h_2(y)) \geq 0$$

- Let  $U_1$  and  $U_2$  are i.i.d.r.v.'s then

$$\mathbf{E}((h_1(U_1) - h_1(U_2))(h_2(U_1) - h_2(U_2))) \geq 0$$

thus

$$\begin{aligned} \mathbf{E}((h_1(U_1)h_2(U_1) + h_1(U_2)h_2(U_2))) &\geq \\ \mathbf{E}(h_1(U_2)h_2(U_1) + h_1(U_1)h_2(U_2)) \end{aligned}$$

hence, by independence and identical distribution of  $U_1$  and  $U_2$

$$\mathbf{E}(h_1(U_1)h_2(U_1)) > \mathbf{E}(h_1(U_1))\mathbf{E}(h_2(U_1))$$

# Variance Reduction—Antithetic Variables

Application: If  $g(x)$  is monotone.

Using  $U_1, \dots, U_n \sim \text{unif}(0, 1)$  to find  $\hat{\theta}_{MC} = \frac{1}{n} \sum_{i=1}^n g(U_i)$  to estimate  $\theta = \int_0^1 g(x) dx$ , results in higher variance than using the antithetic estimator

$$\hat{\theta}_A = \frac{1}{n} \sum_{i=1}^{n/2} (g(U_i) + g(1 - U_i))$$

# Variance Reduction—Antithetic Variables

That is  $\hat{\theta}_A$  is more efficient than  $\hat{\theta}_{MC}$ . Since,

$$\begin{aligned}
 \mathbf{V}(\hat{\theta}_A) &= \frac{1}{n^2} \sum_{i=1}^{n/2} \mathbf{V}(g(U_i) + g(1 - U_i)) \text{ by independence} \\
 &= \frac{1}{2n} \mathbf{V}(g(U) + g(1 - U)) \text{ since identically distributed} \\
 &= \frac{1}{2n} [\mathbf{V}(g(U)) + \mathbf{V}(g(1 - U)) + 2\text{Cov}(g(U), g(1 - U))] \\
 &\leq \frac{1}{2n} [\mathbf{V}(g(U)) + \mathbf{V}(g(1 - U))] \\
 &\leq \frac{\mathbf{V}(g(U))}{n} = \mathbf{V}(\hat{\theta}_{MC})
 \end{aligned}$$

# Variance Reduction—Antithetic Variables

- Note that  $\mathbf{V}(\hat{\theta}_A) = \frac{1}{2n} \mathbf{V}(g(U) + g(1 - U))$
- What about  $\text{Cov}\left(g(F_X^{-1}(U_1), \dots, F_X^{-1}(U_n)), g(F_X^{-1}(1 - U_1), \dots, F_X^{-1}(1 - U_n))\right)$ ?
- If  $g$  is monotone then the last covariance is also negative. You can use induction on  $n$ .

# Variance Reduction—Antithetic Variables

Example: Find the antithetic estimate of  $\int_1^3 e^{-x^2} dx$ .

```
n<-10000;CL<- .95
```

```
g<-function(x) (3-1)*exp(-1*x^2)
```

```
x<-runif(n/2,0,1)
```

```
u<-c(x,1-x)
```

```
u<-(3-1)*u+1
```

```
y<-g(u)
```

```
mu3<-mean(y)
```

```
mu3
```

```
[1] 0.1384035
```

```
se3<-sqrt(var(g(x)+g(1-x))/(2*n))
```

```
CI<-c(mu3-qnorm((1+CL)/2)*se3,mu3+qnorm((1+CL)/2)*se3)
```

```
CI
```

```
[1] 0.1368365 0.1399705
```

# Variance Reduction—Antithetic Variables

The standard error of the MC

```
> se1
```

```
[1] 0.001958881
```

```
> se2
```

```
[1] 0.004887449
```

The standard error of the antithetic

```
> se3
```

```
[1] 0.0007994974
```

and reduction in variance is

```
(se32-se12) / se32
```

```
[1] -5.00319
```

# *Variance Reduction–Control Variates*



## Variance Reduction—Control Variates

A  $\hat{\theta}_C$  estimates  $\theta = \mathbf{E}(g(X))$  via a control variate  $f(X)$  with a known  $\mu = \mathbf{E}(f(X))$  for some function  $f$ , is given by

$$\hat{\theta}_C = \frac{1}{n} \sum_{i=1}^n (g(X_i) + c(f(X_i) - \mu))$$

for some  $c$ , where  $X, X_1, \dots, X_n$  are i.i.d.r.v.

- It is unbiased estimator since

$$\begin{aligned} \mathbf{E}(\hat{\theta}_C) &= \frac{1}{n} \sum_{i=1}^n \mathbf{E}(g(X_i) + c(f(X_i) - \mu)) = \mathbf{E}(g(X)) + c\mathbf{E}((f(X) - \mu)) \\ &= \mathbf{E}(g(X)) \end{aligned}$$

- To make it efficient

$$\begin{aligned} n\mathbf{V}(\hat{\theta}_C) &= \mathbf{V}(g(X) + c(f(X) - \mu)) = \\ &= \mathbf{V}(g(X)) + c^2\mathbf{V}(f(X)) + 2c\text{Cov}(g(X), f(X)) \end{aligned}$$

# Variance Reduction—Control Variates

The quadratic function

$$h(c) := \mathbf{V}(g(X)) + c^2\mathbf{V}(f(X)) + 2c\mathit{Cov}(g(X), f(X))$$

attains its minimum at

$$c^* = -\frac{\mathit{Cov}(g(X), f(X))}{\mathbf{V}(f(X))}$$

and

$$\mathbf{V}(\hat{\theta}_{c^*}) = \underbrace{\frac{1}{n}\mathbf{V}(g(X))}_{\mathbf{V}(\hat{\theta}_{MC})} - \frac{1}{n} \frac{(\mathit{Cov}(g(X), f(X)))^2}{\mathbf{V}(f(X))} \leq \mathbf{V}(\hat{\theta}_{MC})$$

# Variance Reduction—Control Variates

and the reduction in variance is given by

$$\begin{aligned}\frac{\mathbf{V}(\hat{\theta}_{MC}) - \mathbf{V}(\hat{\theta}_{C^*})}{\mathbf{V}(\hat{\theta}_{MC})} &= \frac{(\text{Cov}(g(X), f(X)))^2}{\mathbf{V}(f(X))\mathbf{V}(g(X))} \\ &= (\text{Corr}(g(X), f(X)))^2\end{aligned}$$

so the higher the magnitude of correlation the higher is the reduction.

## Variance Reduction–Control Variates

Example: Find estimate of  $\int_1^3 e^{-x^2} dx$  using control variate.

Here, let  $U \sim \text{unif}(1, 3)$  and so  $g(x) = 2e^{-x^2}$ . Let the control variate be  $f(x) = x$  as it is easy to handle since  $\mu = \mathbf{E}(f(U)) = \mathbf{E}(U) = 2$  and  $\mathbf{V}(f(U)) = \mathbf{V}(U) = \frac{1}{3}$ . Then

$$\hat{\theta}_{C^*} = \frac{1}{n} \sum_{i=1}^n (g(U_i) + c^*(f(U_i) - \mu)) = \frac{1}{n} \sum_{i=1}^n (2e^{-U_i^2} + c^*(U_i - 2))$$

where

$$c^* = -\frac{\text{Cov}(g(U), f(U))}{\mathbf{V}(f(U))} =$$

$$-\frac{\mathbf{E}(2Ue^{-U^2}) - \mathbf{E}(2e^{-U^2})\mathbf{E}(U)}{1/3} = 6 \underbrace{\mathbf{E}(2e^{-U^2})}_{\text{estimated by } \hat{\theta}_{C^*}} - \frac{3}{2}(e^{-1} - e^{-9})$$

# Variance Reduction—Control Variates

Thus,

$$\hat{\theta}_{C^*} = \frac{\frac{1}{n} \sum_{i=1}^n \left( 2e^{-U_i^2} - \frac{3}{2}(e^{-1} - e^{-9})(U_i - 2) \right)}{1 - \frac{6}{n} \sum_{i=1}^n (U_i - 2)}$$

```
n<-10000;CL<-.95
x<-runif(n,1,3)
y<-mean(x)
z<-mean(2*exp(-1*x^2))
mu4<-(z-(3/2)*(exp(-1)-exp(-9))*(y-2))/(1-6*(y-2))
mu4
[1] 0.1379537
(cor(x,2*exp(-1*x^2)))^2
[1] 0.7138062
```

# Variance Reduction—Control Variates

```
n<-10000;CL<-.95
thetaC<-replicate(100,{
x<-runif(n,1,3)
y<-mean(x)
z<-mean(2*exp(-1*x^2))
mu4<-(z-(3/2)*(exp(-9)-exp(-1))*(y-2))/(1-6*(y-2))})
mu4<-mean(thetaC)
mu4
[1] 0.1393736
se4<-sd(thetaC)
se4
[1] 0.001039555
CI<-c(mu4-qnorm((1+CL)/2)*se4,mu4+qnorm((1+CL)/2)*se4)
CI
[1] 0.1373361 0.1414111
```

# Variance Reduction—Control Variates

The standard error of the MC

```
> se1
```

```
[1] 0.001958881
```

```
> se2
```

```
[1] 0.004887449
```

The standard error of the antithetic

```
> se3
```

```
[1] 0.0007994974
```

The standard error of the control variate

```
> se4
```

```
[1] 0.001039555
```

and reduction in variance is

```
(se12-se42) / se12
```

```
[1] 0.7183699
```

# *Variance Reduction–Importance Sampling*



# Variance Reduction–Importance Sampling

Since

$$\theta = \int_a^b g(x) dx = \int_a^b \frac{g(x)}{f(x)} f(x) dx = \mathbf{E}_f\left(\frac{g(X)}{f(X)}\right)$$

where  $f(x)$  is called the importance function (a pdf) then we can estimate it with

$$\hat{\theta}_I = \frac{1}{n} \sum_{i=1}^n \frac{g(X_i)}{f(X_i)}$$

where  $X_1, \dots, X_n$  are generated from  $f$ .

$\hat{\theta}_I$  is an unbiased estimator of  $\theta$ .

# Variance Reduction–Importance Sampling

How can we choose the importance function  $f$ ?

First, it must have a support coinciding with or including  $[a, b]$ ; yet, the bigger it is, the worse it will behave.

If  $[a, b] \subset [c, d]$  (the support of  $f$ ) then  $\int_c^d \frac{g(x)}{f(x)} I_{[a,b]}(x) f(x) dx$  will result in zeros when numbers falling outside the integration region are substituted in  $I_{[a,b]}(x)$ . Since that would be inefficient, then it is better to have the support of  $f$  coinciding with  $[a, b]$ .

# Variance Reduction–Importance Sampling

Second,  $\mathbf{V}(\hat{\theta}_I) = \frac{1}{n} \mathbf{V}_f\left(\frac{g(X)}{f(X)}\right)$  which is the smallest possible if  $\frac{g(x)}{f(x)}$  is nearly a constant as the variability in a constant is zero.

The minimum is reached at  $f(x) = \frac{|g(x)|}{\int_a^b |g(t)| dt}$  that is a pdf.

# Variance Reduction–Importance Sampling

Example: Find estimate of  $\int_1^3 e^{-x^2} dx$  using importance sampling.

Here we will compare several importance functions including

$$f_0(x) = \frac{1}{2}, \text{ for } 1 < x < 3 \text{ (MC Integration)}$$

$$f_1(x) = e^{-x}, \text{ for } 0 < x < \infty \text{ (Wider domain)}$$

$$f_2(x) = 2e^{-2x}, \text{ for } 0 < x < \infty \text{ (Wider domain)}$$

$$f_3(x) = .5e^{-.5x}, \text{ for } 0 < x < \infty \text{ (Wider domain)}$$

$$f_4(x) = \frac{1}{e^{-1}-e^{-3}} e^{-x}, \text{ for } 1 < x < 3$$

$$f_5(x) = \frac{15}{263} (1 - x^2 + x^4/2), \text{ for } 1 < x < 3$$

# Variance Reduction–Importance Sampling

```
n<-10000
g<-function(x) exp(-x^2)
x<-runif(n)
# f0
g_f<-g(2*x+1)/(1/2)
theta_0<-mean(g_f)
se_theta_0<-sd(g_f)/sqrt(n)
waste_0<-sum((g_f==0))/n
# f1
y<-1*log(1-x) # or directly rexp(n,1)
g_f<-as.integer((y>1)&(y<3))*g(y)/exp(-y)
theta_1<-mean(g_f)
se_theta_1<-sd(g_f)/sqrt(n)
waste_1<-sum((g_f==0))/n
```

# Variance Reduction–Importance Sampling

```
# f2
y<-.5*log(1-x) # or directly rexp(n,2)
g_f<-as.integer((y>1)&(y<3))*g(y)/(2*exp(-2*y))
theta_2<-mean(g_f)
se_theta_2<-sd(g_f)/sqrt(n)
waste_2<-sum((g_f==0))/n

# f3
y<-2*log(1-x) # or directly rexp(n,.5)
g_f<-as.integer((y>1)&(y<3))*g(y)/(.5*exp(-.5*y))
theta_3<-mean(g_f)
se_theta_3<-sd(g_f)/sqrt(n)
waste_3<-sum((g_f==0))/n
```

# Variance Reduction–Importance Sampling

```
# f4
c<-exp(-1)-exp(-3)
y<-1*log(exp(-1)-c*x)
g_f<-g(y)/((1/c)*exp(-1*y))
theta_4<-mean(g_f)
se_theta_4<-sd(g_f)/sqrt(n)
waste_4<-sum((g_f==0))/n

# f5
c<-15/263
InvF<-function(x){uniroot(function(y)
(c*(y-y^3/3+y^5/10-23/30)-x), lower=1, upper=3)$root}
xv<-as.array(x)
y<-apply(xv, 1, InvF)
g_f<-g(y)/(c*(1-y^2+y^4/2))
theta_5<-mean(g_f)
se_theta_5<-sd(g_f)/sqrt(n)
```

# Variance Reduction–Importance Sampling

```
waste_5<-sum((g_f==0))/n
result<-rbind(c(theta_0,theta_1,theta_2,theta_3,
theta_4,theta_5)
,c(se_theta_0,se_theta_1,se_theta_2,se_theta_3
,se_theta_4,se_theta_5)
,c(waste_0,waste_1,waste_2,waste_3,waste_4,waste_5))
result<-as.data.frame(result,row.names=c("theta"
,"se-theta","Waste"))
colnames(result)<-c("f0","f1","f2","f3","f4","f5")
result
```

	f0	f1	f2	f3	f4	f5
theta	0.139417213	0.137480914	0.138070629	0.141256850	0.140172414	0.124605248
se-theta	0.001922774	0.002727444	0.003787346	0.002919893	0.001033504	0.008143972
Waste	0.000000000	0.685200000	0.868600000	0.615200000	0.000000000	0.000000000



# *Variance Reduction–Stratified Sampling*

# Variance Reduction—Stratified Sampling

To estimate  $\theta = \int_a^b g(x) \frac{1}{b-a} dx = \mathbf{E}(g(X))$

- 1 Stratify (split) the interval  $[a, b]$  into  $m$  sub-intervals  $\ell_j = [x_{j-1}, x_j]$  with  $x_j = a + j * h$  and  $h = \frac{b-a}{m}$  for  $j = 1, \dots, m$ .
- 2 Select a sub-interval  $I$  randomly and uniformly (with probability  $\frac{1}{m}$ ), say  $\ell_j$ , then  $\mathbf{E}(g(X)) = \mathbf{E}_I(\mathbf{E}(g(X)|I)) = \frac{1}{m} \sum_{j=1}^m \mathbf{E}(g(X)|I = \ell_j)$
- 3 For each  $j : j = 1, \dots, m$ , estimate  $\mathbf{E}(g(X)|I = \ell_j)$  by  $\hat{\theta}_{MC,j} = \frac{1}{n} \sum_{\{X_i \in \ell_j; i=1, \dots, n\}} g(X_i)$  which are independent for each  $j$  (if you use different randomly generated numbers  $X$ 's)
- 4 Estimate  $\theta$  by

$$\hat{\theta}_{S,m} = \frac{1}{m} \sum_{j=1}^m \hat{\theta}_{MC,j}$$

# Variance Reduction—Stratified Sampling

WTS:  $\mathbf{V}(\hat{\theta}_{S,m}) < \mathbf{V}(\hat{\theta}_{MC})$

$$\begin{aligned}\mathbf{V}(\hat{\theta}_{S,m}) &= \mathbf{V}\left(\frac{1}{m} \sum_{j=1}^m \hat{\theta}_{MC,j}\right) \\ &= \frac{1}{m^2} \sum_{j=1}^m \mathbf{V}(\hat{\theta}_{MC,j}) \text{ by independence} \\ &= \frac{1}{m^2} \sum_{j=1}^m \frac{\mathbf{V}(g(X)|I = \ell_j)}{n} \\ &= \frac{1}{mn} \mathbf{E}(\mathbf{V}(g(X)|I)) \\ &\leq \frac{1}{mn} \mathbf{V}(g(X)) = \mathbf{V}(\hat{\theta}_{MC}) \text{ since } mn \text{ data points are used}\end{aligned}$$

# Variance Reduction—Stratified Sampling

```
n<-10000;a<-1;b<-3
g<-function(x) { (b-a) *exp(-x^2) }
gx<-g(runif(n, a, b))
theta_MC<-mean(gx)
se_theta_MC<-sd(gx)/sqrt(n)
m<-4
L<-seq(a,b,length=m+1)
theta_MCJ<-c()
for (j in 1:m){
  theta_MCJ[j]<-mean(g(runif(n/m, L[j], L[j+1])))
}
theta_S<-mean(theta_MCJ)
c(theta_MC,theta_S)
[1] 0.1391709 0.1400730
```

# Variance Reduction—Stratified Sampling

```
n<-10000;a<-1;b<-3;m<-4;N<-1000
g<-function(x) { (b-a) *exp(-x^2) }
L<-seq(a,b,length=m+1)
Vtheta_S<-matrix(0,N,2)
for(i in 1:N){
  gx<-g(runif(n,a,b))
  Vtheta_S[i,1]<-mean(gx)
  theta_MCJ<-c()
  for (j in 1:m){
    theta_MCJ[j]<-mean(g(runif(n/m,L[j],L[j+1]))) }
  Vtheta_S[i,2]<-mean(theta_MCJ) }
apply(Vtheta_S,2,mean)
[1] 0.1393923 0.1393566
apply(Vtheta_S,2,sd)
[1] 0.0019811043 0.0008233142
```

# Variance Reduction—Stratified Sampling

```
n<-10000;a<-1;b<-3;N<-1000
g<-function(x) { (b-a) *exp(-x^2) }
Strat<-function(m) {
L<-seq(a,b,length=m+1)
Vtheta_S<-matrix(0,N,1)
for(i in 1:N){
  theta_MCJ<-c()
  for (j in 1:m){
    theta_MCJ[j]<-mean(g(runif(n/m,L[j],L[j+1]))) }
  Vtheta_S[i,1]<-mean(theta_MCJ) }
c(mean(Vtheta_S),sd(Vtheta_S)) }
result<-c()
for(m in
c(2,4,8,10)) {result<-c(result,c(m,Strat(m))) }
matrix(result,3,4)
```

# Variance Reduction—Stratified Sampling

	[, 1]	[, 2]	[, 3]	[, 4]
[1, ]	2.0000000000	4.0000000000	8.0000000000	1.000000e+01
[2, ]	0.139370017	0.1393186015	0.139409651	1.393670e-01
[3, ]	0.001497508	0.0007902412	0.000396519	3.229227e-04

# *End of Set 5*