

# Optimization and Simulation

## Drawing from distributions

Michel Bierlaire

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



# Outline

- 1 Discrete distributions
- 2 Continuous distributions
- 3 Transforming draws
- 4 Appendix

# Discrete distributions

- Let  $X$  be a discrete r.v. with pmf:

$$P(X = x_i) = p_i, \quad i = 0, \dots,$$

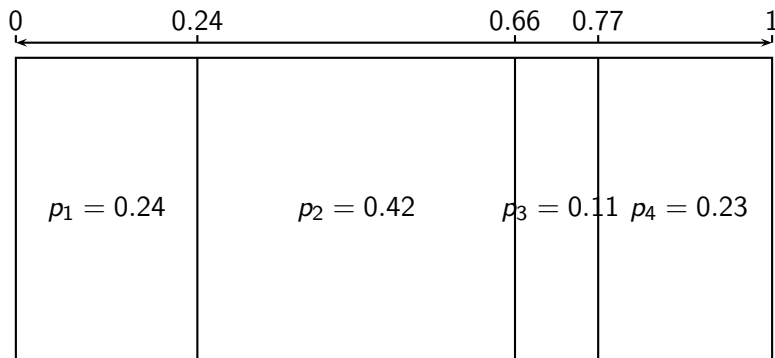
where  $\sum_i p_i = 1$ .

- The support can be finite or infinite.
- The following algorithm generates draws from this distribution

## Inverse transform method

- Let  $r$  be a draw from  $U(0, 1)$ .
- Initialize  $k = 0$ ,  $p = 0$ .
- $p = p + p_k$ .
- If  $r < p$ , set  $X = x_k$  and stop.
- Otherwise, set  $k = k + 1$  and go to step 3.

## Inverse Transform Method: illustration



# Discrete distributions

## Acceptance-rejection

- Attributed to von Neumann.
- Mostly useful with continuous distributions.
- We want to draw from  $X$  with pmf  $p_i$ .
- We know how to draw from  $Y$  with pmf  $q_i$ .

Define a constant  $c \geq 1$  such that

$$\frac{p_i}{q_i} \leq c \quad \forall i \text{ s.t. } p_i > 0.$$

## Algorithm

- 1 Draw  $y$  from  $Y$
- 2 Draw  $r$  from  $U(0, 1)$
- 3 If  $r < \frac{p_y}{cq_y}$ , return  $x = y$  and stop. Otherwise, start again.

# Acceptance-rejection: analysis

Probability to be accepted during a given iteration

$$\begin{aligned}
 P(Y = y, \text{accepted}) &= P(Y = y) P(\text{accepted} | Y = y) \\
 &= q_y \quad p_y / cq_y \\
 &= \frac{p_y}{c}
 \end{aligned}$$

Probability to be accepted

$$\begin{aligned}
 P(\text{accepted}) &= \sum_y P(\text{accepted} | Y = y) P(Y = y) \\
 &= \sum_y \frac{p_y}{cq_y} q_y \\
 &= 1/c.
 \end{aligned}$$

Probability to draw  $x$  at iteration  $n$

$$P(X = x | n) = \left(1 - \frac{1}{c}\right)^{n-1} \frac{p_x}{c}$$

# Acceptance-rejection: analysis

$$\begin{aligned}
 P(X = x) &= \sum_{n=1}^{+\infty} P(X = x|n) \\
 &= \sum_{n=1}^{+\infty} \left(1 - \frac{1}{c}\right)^{n-1} \frac{p_x}{c} \\
 &= c \frac{p_x}{c} \\
 &= p_x.
 \end{aligned}$$

Reminder: geometric series

$$\sum_{n=0}^{+\infty} x^n = \frac{1}{1-x}$$

# Acceptance-rejection: analysis

## Remarks

- Average number of iterations:  $c$
- The closer  $c$  is to 1, the closer the pmf of  $Y$  is to the pmf of  $X$ .



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# Continuous distributions

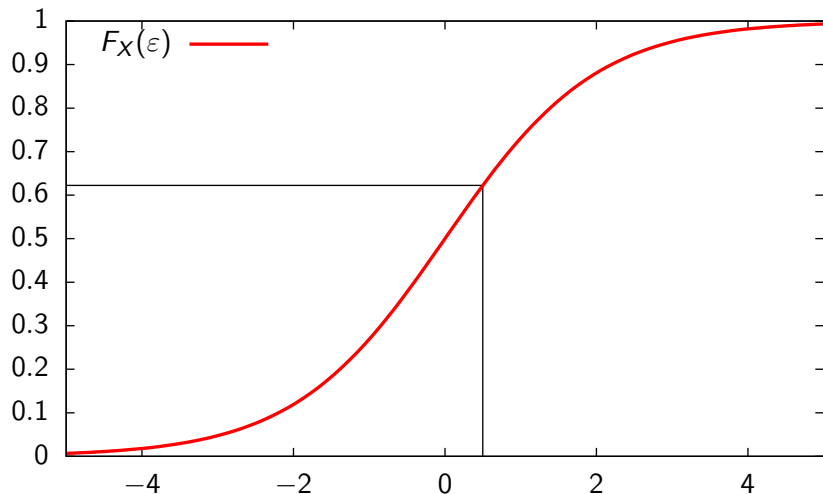
## Inverse Transform Method

- Let  $X$  be a continuous r.v. with CDF  $F_X(\varepsilon)$
- Draw  $r$  from a uniform  $U(0, 1)$
- Generate  $F_X^{-1}(r)$ .

## Motivation

- $F_X$  is monotonically increasing
- It implies that  $\varepsilon_1 \leq \varepsilon_2$  is equivalent to  $F_X(\varepsilon_1) \leq F_X(\varepsilon_2)$ .

# Inverse Transform Method



# Inverse Transform Method

## More formally

- Denote  $F_U(\varepsilon) = \varepsilon$  the CDF of the r.v.  $U(0, 1)$
- Let  $G$  be the distribution of the r.v.  $F_X^{-1}(U)$

$$\begin{aligned} G(\varepsilon) &= \Pr(F_X^{-1}(U) \leq \varepsilon) \\ &= \Pr(F_X(F_X^{-1}(U)) \leq F_X(\varepsilon)) \\ &= \Pr(U \leq F_X(\varepsilon)) \\ &= F_U(F_X(\varepsilon)) \\ &= F_X(\varepsilon) \end{aligned}$$

# Inverse Transform Method

Examples: let  $r$  be a draw from  $U(0, 1)$

Name	$F_X(\varepsilon)$	Draw
Exponential( $b$ )	$1 - e^{-\varepsilon/b}$	$-b \ln r$
Logistic( $\mu, \sigma$ )	$1 / (1 + \exp(-(\varepsilon - \mu) / \sigma))$	$\mu - \sigma \ln(\frac{1}{r} - 1)$
Power( $n, \sigma$ )	$(\varepsilon / \sigma)^n$	$\sigma r^{1/n}$

## Note

The CDF is not always available (e.g. normal distribution).

# Continuous distributions

## Rejection Method

- We want to draw from  $X$  with pdf  $f_X$ .
- We know how to draw from  $Y$  with pdf  $f_Y$ .

Define a constant  $c \geq 1$  such that

$$\frac{f_X(\varepsilon)}{f_Y(\varepsilon)} \leq c \quad \forall \varepsilon$$

## Algorithm

- 1 Draw  $y$  from  $Y$
- 2 Draw  $r$  from  $U(0, 1)$
- 3 If  $r < \frac{f_X(y)}{cf_Y(y)}$ , return  $x = y$  and stop. Otherwise, start again.

# Rejection Method: example

## Draw from a normal distribution

- Let  $\bar{X} \sim N(0, 1)$  and  $X = |\bar{X}|$
- Probability density function:  $f_X(\varepsilon) = \frac{2}{\sqrt{2\pi}} e^{-\varepsilon^2/2}$ ,  $0 < \varepsilon < +\infty$
- Consider an exponential r.v. with pdf  $f_Y(\varepsilon) = e^{-\varepsilon}$ ,  $0 < \varepsilon < +\infty$
- Then

$$\frac{f_X(\varepsilon)}{f_Y(\varepsilon)} = \frac{2}{\sqrt{2\pi}} e^{\varepsilon - \varepsilon^2/2}$$

- The ratio takes its maximum at  $\varepsilon = 1$ , therefore

$$\frac{f_X(\varepsilon)}{f_Y(\varepsilon)} \leq \frac{f_X(1)}{f_Y(1)} = \sqrt{2e/\pi} \approx 1.315.$$

- Rejection method, with  $\frac{f_X(\varepsilon)}{cf_Y(\varepsilon)} = \frac{1}{\sqrt{e}} e^{\varepsilon - \varepsilon^2/2} = e^{\varepsilon - \frac{\varepsilon^2}{2} - \frac{1}{2}} = e^{-\frac{(\varepsilon-1)^2}{2}}$

# Rejection Method: example

Algorithm: draw from a normal

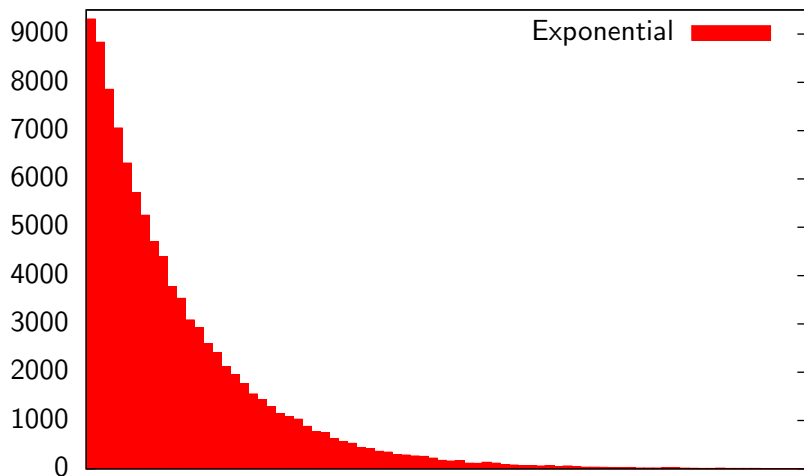
- 1 Draw  $r$  from  $U(0, 1)$
- 2 Let  $y = -\ln(1 - r)$  (draw from the exponential)
- 3 Draw  $s$  from  $U(0, 1)$
- 4 If  $s < e^{-\frac{(y-1)^2}{2}}$  return  $x = y$  and go to step 5. Otherwise, go to step 1.
- 5 Draw  $t$  from  $U(0, 1)$ .
- 6 If  $t \leq 0.5$ , return  $x$ . Otherwise, return  $-x$ .

Note

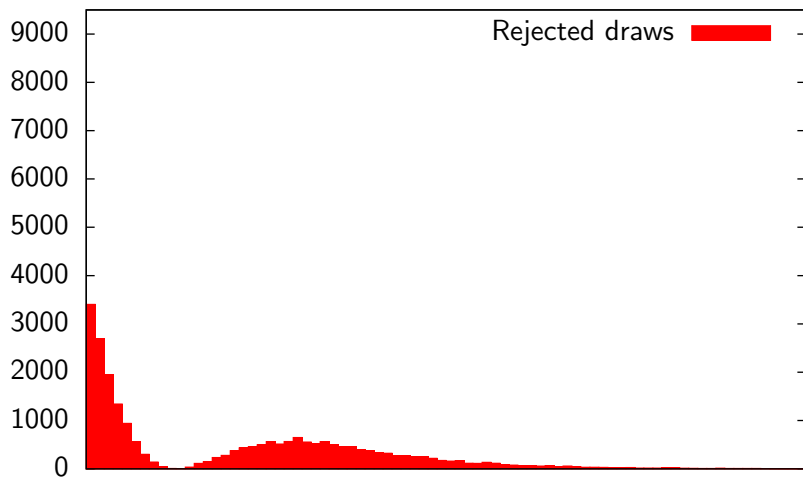
This procedure can be improved. See [Ross, 2006, Chapter 5].



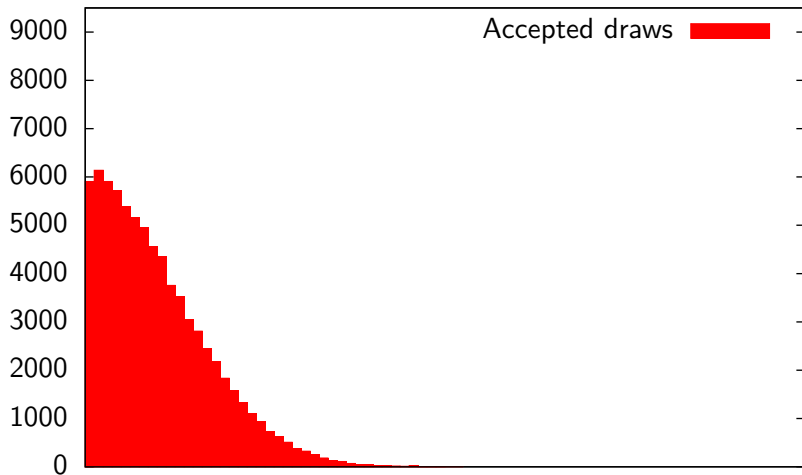
# Draws from the exponential



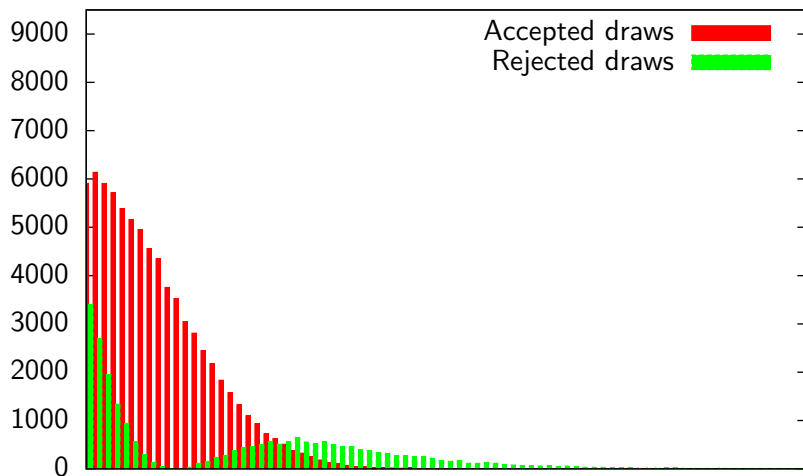
# Rejected draws



# Accepted draws



# Rejected and accepted draws



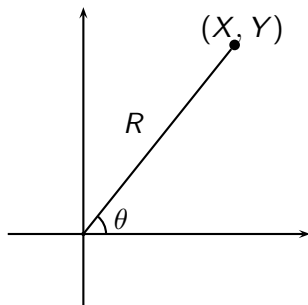
# The polar method

## Draw from a normal distribution

- Let  $X \sim N(0, 1)$  and  $Y \sim N(0, 1)$  independent
- pdf:

$$f(x, y) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \frac{1}{\sqrt{2\pi}} e^{-y^2/2} = \frac{1}{2\pi} e^{-(x^2+y^2)/2}.$$

- Let  $R$  and  $\theta$  such that  $R^2 = X^2 + Y^2$ , and  $\tan \theta = Y/X$ .



# The polar method

## Change of variables (reminder)

- Let  $A$  be a multivariate r.v. distributed with pdf  $f_A(a)$ .
- Consider the change of variables  $b = H(a)$  where  $H$  is bijective and differentiable
- Then  $B = H(A)$  is distributed with pdf

$$f_B(b) = f_A(H^{-1}(b)) \left| \det \left( \frac{dH^{-1}(b)}{db} \right) \right|.$$

Here:  $A = (X, Y)$ ,  $B = (R^2, \theta) = (T, \theta)$

$$H^{-1}(b) = \begin{pmatrix} T^{\frac{1}{2}} \cos \theta \\ T^{\frac{1}{2}} \sin \theta \end{pmatrix} \quad \frac{dH^{-1}(b)}{db} = \begin{pmatrix} \frac{1}{2} T^{-\frac{1}{2}} \cos \theta & -T^{\frac{1}{2}} \sin \theta \\ \frac{1}{2} T^{-\frac{1}{2}} \sin \theta & T^{\frac{1}{2}} \cos \theta \end{pmatrix}$$

# The polar method

$$H^{-1}(b) = \begin{pmatrix} T^{\frac{1}{2}} \cos \theta \\ T^{\frac{1}{2}} \sin \theta \end{pmatrix} \quad \frac{dH^{-1}(b)}{db} = \begin{pmatrix} \frac{1}{2} T^{-\frac{1}{2}} \cos \theta & -T^{\frac{1}{2}} \sin \theta \\ \frac{1}{2} T^{-\frac{1}{2}} \sin \theta & T^{\frac{1}{2}} \cos \theta \end{pmatrix}$$

Therefore,

$$\left| \det \left( \frac{dH^{-1}(b)}{db} \right) \right| = \frac{1}{2}.$$

and

$$f_B(T, \theta) = \frac{1}{2} \frac{1}{2\pi} e^{-T/2}, \quad 0 < T < +\infty, \quad 0 < \theta < 2\pi.$$

Product of

- an exponential with mean 2:  $\frac{1}{2} e^{-T/2}$
- a uniform on  $[0, 2\pi[$ :  $1/2\pi$

# The polar method

Therefore

- $R^2$  and  $\theta$  are independent
- $R^2$  is exponential with mean 2
- $\theta$  is uniform on  $(0, 2\pi)$

Algorithm

- 1 Let  $r_1$  and  $r_2$  be draws from  $U(0, 1)$ .
- 2 Let  $R^2 = -2 \ln r_1$  (draw from exponential of mean 2)
- 3 Let  $\theta = 2\pi r_2$  (draw from  $U(0, 2\pi)$ )
- 4 Let

$$\begin{aligned} X &= R \cos \theta = \sqrt{-2 \ln r_1} \cos(2\pi r_2) \\ Y &= R \sin \theta = \sqrt{-2 \ln r_1} \sin(2\pi r_2) \end{aligned}$$



# The polar method

## Issue

Time consuming to compute sine and cosine

## Solution

Generate directly the result of the sine and the cosine

- Draw a random point  $(s_1, s_2)$  in the circle of radius one centered at  $(0, 0)$ .
- **How?** Draw a random point in the square  $[-1, 1] \times [-1, 1]$  and reject points outside the circle
- Let  $(R, \theta)$  be the polar coordinates of this point.
- $R^2 \sim U(0, 1)$  and  $\theta \sim U(0, 2\pi)$  are independent

$$\begin{aligned}R^2 &= s_1^2 + s_2^2 \\ \cos \theta &= s_1/R \\ \sin \theta &= s_2/R\end{aligned}$$

# The polar method

## Original transformation

$$\begin{aligned} X &= R \cos \theta = \sqrt{-2 \ln r_1} \cos(2\pi r_2) \\ Y &= R \sin \theta = \sqrt{-2 \ln r_1} \sin(2\pi r_2) \end{aligned}$$

## Draw $(s_1, s_2)$ in the circle

$$\begin{aligned} t &= s_1^2 + s_2^2 \\ X &= R \cos \theta = \sqrt{-2 \ln t} \frac{s_1}{\sqrt{t}} = s_1 \sqrt{\frac{-2 \ln t}{t}} \\ Y &= R \sin \theta = \sqrt{-2 \ln t} \frac{s_2}{\sqrt{t}} = s_2 \sqrt{\frac{-2 \ln t}{t}} \end{aligned}$$

# The polar method

## Algorithm

- 1 Let  $r_1$  and  $r_2$  be draws from  $U(0, 1)$ .
- 2 Define  $s_1 = 2r_1 - 1$  and  $s_2 = 2r_2 - 1$  (draws from  $U(-1, 1)$ ).
- 3 Define  $t = s_1^2 + s_2^2$ .
- 4 If  $t > 1$ , reject the draws and go to step 1.
- 5 Return

$$x = s_1 \sqrt{\frac{-2 \ln t}{t}} \text{ and } y = s_2 \sqrt{\frac{-2 \ln t}{t}}.$$

# Transformations of standard normal

- If  $r$  is a draw from  $N(0, 1)$ , then

$$s = br + a$$

is a draw from  $N(a, b^2)$

- If  $r$  is a draw from  $N(a, b^2)$ , then

$$e^r$$

is a draw from a log normal  $LN(a, b^2)$  with mean

$$e^{a+(b^2/2)}$$

and variance

$$e^{2a+b^2}(e^{b^2} - 1)$$

# Multivariate normal

- If  $r_1, \dots, r_n$  are independent draws from  $N(0, 1)$ , and

$$r = \begin{pmatrix} r_1 \\ \vdots \\ r_n \end{pmatrix}$$

- then

$$s = a + Lr$$

is a vector of draws from the  $n$ -variate normal  $N(a, LL^T)$ , where

- $L$  is lower triangular, and
- $LL^T$  is the Cholesky factorization of the variance-covariance matrix

# Multivariate normal

Example:

$$L = \begin{pmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{pmatrix}$$

$$s_1 = l_{11}r_1$$

$$s_2 = l_{21}r_1 + l_{22}r_2$$

$$s_3 = l_{31}r_1 + l_{32}r_2 + l_{33}r_3$$

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# Transforming draws

## Method

- Consider draws from the following distributions:
  - normal:  $N(0, 1)$  (draws denoted by  $\xi$  below)
  - uniform:  $U(0, 1)$  (draws denoted by  $r$  below)
- Draws  $R$  from other distributions are obtained from nonlinear transforms.

## Lognormal(a,b)

$$f(x) = \frac{1}{xb\sqrt{2\pi}} \exp\left(\frac{-(\ln x - a)^2}{2b^2}\right) \quad R = e^{a+b\xi}$$



# Transforming draws

Cauchy(a,b)

$$f(x) = \left( \pi b \left( 1 + \left( \frac{x-a}{b} \right)^2 \right) \right)^{-1} \quad R = a + b \tan \left( \pi \left( r - \frac{1}{2} \right) \right)$$

$\chi^2(a)$  ( $a$  integer)

$$f(x) = \frac{x^{(a-2)/2} e^{-x/2}}{2^{a/2} \Gamma(a/2)} \quad R = \sum_{j=1}^a \xi_j^2$$

Erlang(a,b) ( $b$  integer)

$$f(x) = \frac{(x/a)^{b-1} e^{-x/a}}{a(b-1)!} \quad R = -a \sum_{j=1}^b \ln r_j$$

# Transforming draws

## Exponential(a)

$$F(x) = 1 - e^{-x/a} \quad R = -a \ln r$$

## Extreme Value(a,b)

$$F(x) = 1 - \exp\left(-e^{-(x-a)/b}\right) \quad R = a - b \ln(-\ln r)$$

## Logistic(a,b)

$$F(x) = \left(1 + e^{-(x-a)/b}\right)^{-1} \quad R = a + b \ln\left(\frac{r}{1-r}\right)$$

# Transforming draws

Pareto(a,b)

$$F(x) = 1 - \left(\frac{a}{x}\right)^b \quad R = a(1 - r)^{-1/b}$$

Standard symmetrical triangular distribution

$$f(x) = \begin{cases} 4x & \text{if } 0 \leq x \leq 1/2 \\ 4(1-x) & \text{if } 1/2 \leq x \leq 1 \end{cases} \quad R = \frac{r_1 + r_2}{2}$$

Weibull(a,b)

$$F(x) = 1 - e^{-\left(\frac{x}{a}\right)^b} \quad R = a(-\ln r)^{1/b}$$

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# Uniform distribution: $X \sim U(a, b)$

pdf

$$f_X(x) = \begin{cases} 1/(b-a) & \text{if } a \leq x \leq b, \\ 0 & \text{otherwise.} \end{cases}$$

CDF

$$F_X(x) = \begin{cases} 0 & \text{if } x \leq a, \\ (x-a)/(b-a) & \text{if } a \leq x \leq b, \\ 1 & \text{if } x \geq b. \end{cases}$$

Mean, median

$$(a+b)/2$$

Variance

$$(b-a)^2/12$$

# Normal distribution: $X \sim N(a, b)$

pdf

$$f_X(x) = \frac{1}{b\sqrt{2\pi}} \exp\left(-\frac{(x-a)^2}{2b^2}\right)$$

CDF

$$F_X(x) = \int_{-\infty}^x f_X(t) dt.$$

Mean, median

$a$

Variance

$b^2$

# Bibliography



Ross, S. M. (2006).

*Simulation.*

Academic Press, fourth edition.