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. Monte-Carlo integration
5. Summary
6. Appendix

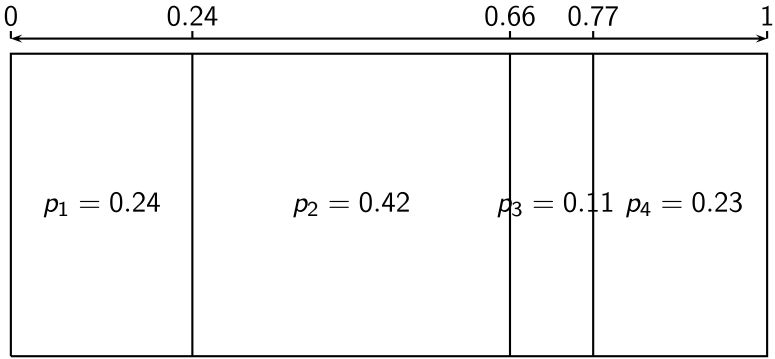
Discrete distributions

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

$$P(X = x_i) = p_i, \; i = 0, \ldots,$$

  where $\sum_i p_i = 1$.
- The support can be finite or infinite.
- We know how to draw from $U(0,1)$.
- How can we draw from X?

Inverse Transform Method: illustration



Discrete distributions

Inverse transform method

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

Discrete distributions

Acceptance-rejection

- Attributed to von Neumann.
- 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

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

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

$$\begin{array}{rcll} P(Y=y,\text{accepted}) & = & P(Y=y) & P(\text{accepted}|Y=y) \\ & = & q_y & p_y/cq_y \\ & = & \dfrac{p_y}{c} & \end{array}$$

Probability to be accepted

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

Probability to draw x at iteration n

$$P(X=x|n) \quad = \quad (1-\tfrac{1}{c})^{n-1}\tfrac{p_x}{c}$$

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

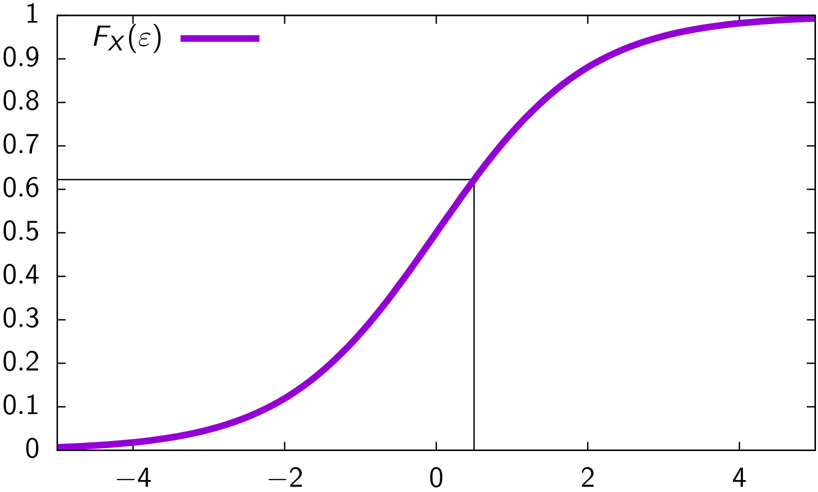
Inverse Transform Method

- 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(μ,σ)	$1/(1+\exp(-(\varepsilon-\mu)/\sigma))$	$\mu - \sigma \ln(\frac{1}{r} - 1)$
Power(n,σ)	$(\varepsilon/\sigma)^n$	$\sigma r^{1/n}$

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

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

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

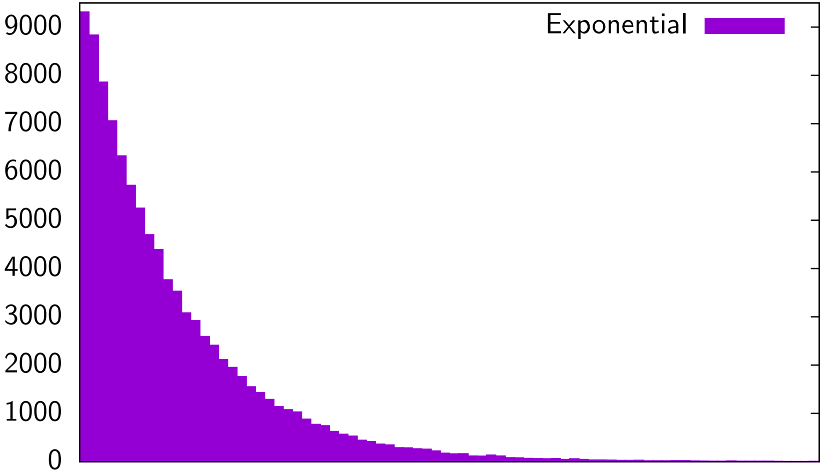
Algorithm: draw from a normal

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 $-x$.

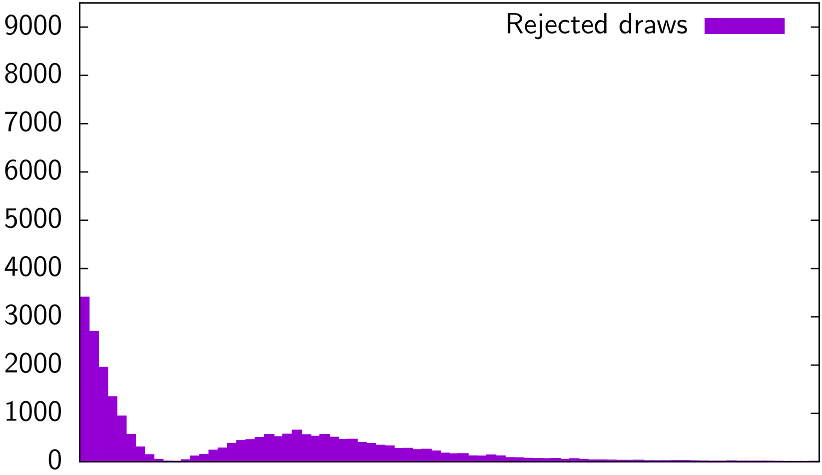
Note

This procedure can be improved. See [Ross, 2012, Chapter 5].

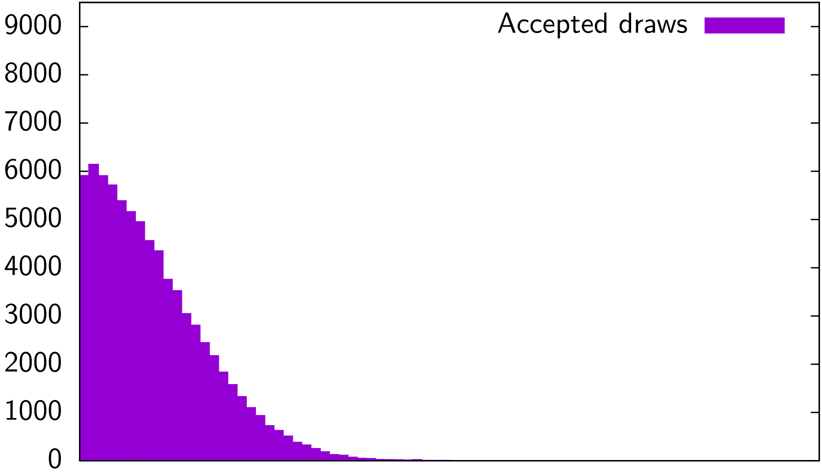
Draws from the exponential



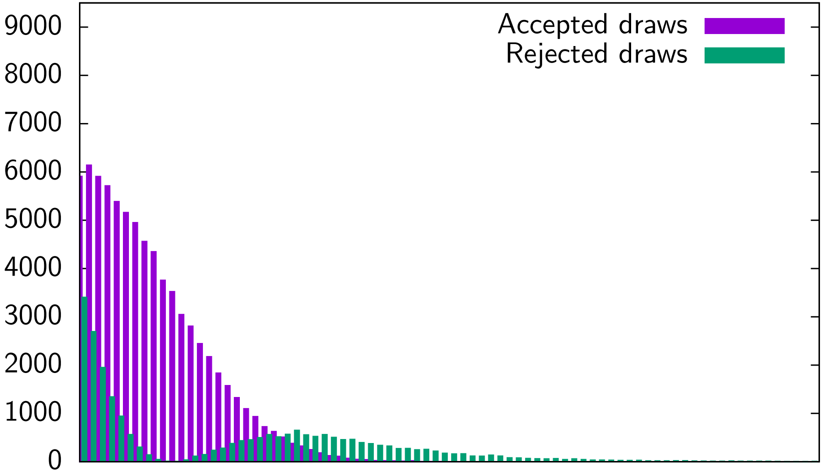
Rejected draws



Accepted draws



Rejected and accepted draws



Drawing from the standard normal distribution

- Accept/reject algorithm is not efficient
- Polar method: no rejection (see appendix)

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 $r_1,\ldots,r_n$ 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:

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

$$\begin{aligned} s_1 &= \ell_{11} r_1 \\ s_2 &= \ell_{21} r_1 + \ell_{22} r_2 \\ s_3 &= \ell_{31} r_1 + \ell_{32} r_2 + \ell_{33} r_3 \end{aligned}$$

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Transforming draws

Method

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

Lognormal(a,b)

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

Transforming draws

Cauchy(a,b)

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

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

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

Erlang(a,b) (b integer)

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

Transforming draws

Exponential(a)

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

Extreme Value(a,b)

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

Logistic(a,b)

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

Transforming draws

Pareto(a,b)

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

Standard symmetrical triangular distribution

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

Weibull(a,b)

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

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Monte-Carlo integration

Expectation

- X r.v. on $[a,b]$, $a \in \mathbb{R} \cup \{-\infty\}$, $b \in \mathbb{R} \cup \{+\infty\}$
- Expectation of X:

$$\mathrm{E}[X] = \int_a^b x f_X(x) dx.$$

- If $g : \mathbb{R} \to \mathbb{R}$ is a function, then

$$\mathrm{E}[g(X)] = \int_a^b g(x) f_X(x) dx.$$

Monte-Carlo integration

Simulation

$$\mathrm{E}[g(X)] \approx \frac{1}{R} \sum_{r=1}^{R} g(x_r).$$

Approximating the integral

$$\int_a^b g(x) f_X(x) dx = \lim_{R \to \infty} \frac{1}{R} \sum_{r=1}^{R} g(x_r).$$

so that

$$\int_a^b g(x) f_X(x) dx \approx \frac{1}{R} \sum_{r=1}^{R} g(x_r).$$

Monte-Carlo integration

Calculating $I = \int_a^b g(x) f_X(x) dx$

- Consider X with pdf f_X.
- Convenient choice: $X \sim U[0,1]$, as $f_U(x) = 1$, $\forall x$.
- Generate R draws x_r, $r = 1, \ldots, R$ from X;
- Calculate

$$I \approx \widehat{I} = \frac{1}{R} \sum_{r=1}^{R} g(x_r).$$

Monte-Carlo integration

Approximation error

- Sample variance:

$$V_R = \frac{1}{R-1} \sum_{r=1}^{R} (g(x_r) - \widehat{I})^2.$$

- By simulation: as

$$\mathrm{Var}[g(X)] = \mathrm{E}[g(X)^2] - \mathrm{E}[g(x)]^2,$$

  we have

$$V_R \approx \frac{1}{R} \sum_{r=1}^{R} g(x_r)^2 - \widehat{I}^2.$$

Monte-Carlo integration

Approximation error

95% confidence interval: $[\widehat{I} - 1.96 e_R \leq I \leq \widehat{I} + 1.96 e_R]$ where

$$e_R = \sqrt{\frac{V_R}{R}}.$$

Monte-Carlo integration

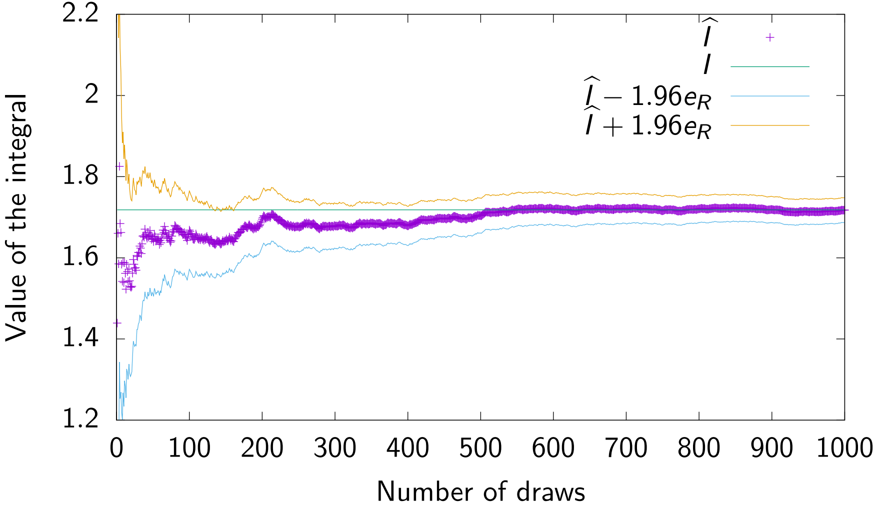
Example

$$\int_0^1 e^x dx = e - 1 = 1.7183$$

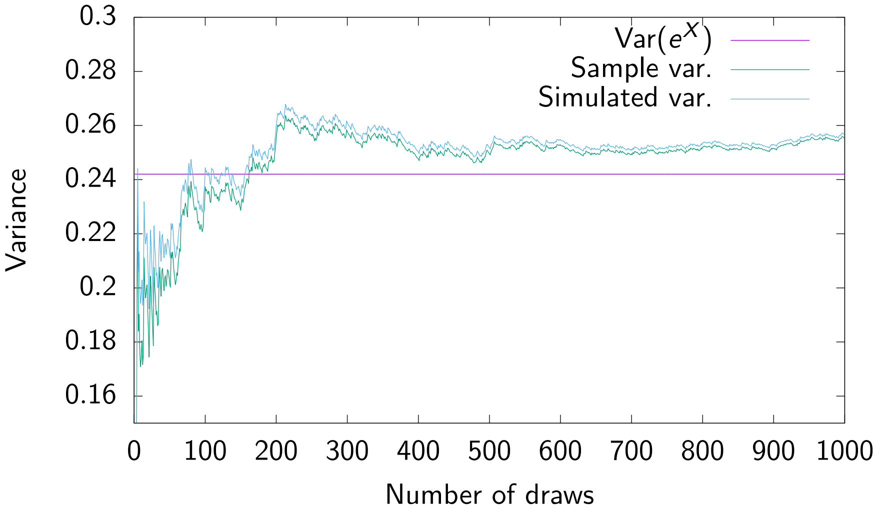
- Random variable X uniformly distributed ($f_X(\varepsilon) = 1$)
- $g(X) = e^X$
- $\text{Var}(e^X) = \frac{e^2-1}{2} - (e-1)^2 = 0.2420$

R	10	100	1000
$\widehat{I}$	1.8270	1.7707	1.7287
Sample variance	0.1607	0.2125	0.2385
Simulated variance	0.1742	0.2197	0.2398

Monte-Carlo integration



Monte-Carlo integration



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Summary

- Draws from uniform distribution: available in any programming language
- Inverse transform method: requires the pmf or the CDF.
- Accept-reject: needs a “similar” r.v. easy to draw from.
- Transforming uniform and normal draws.
- First application: Monte-Carlo integration.

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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

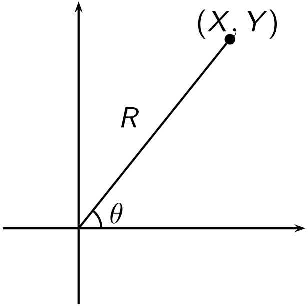
The polar method

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 θ 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

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

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 θ are independent
- R^2 is exponential with mean 2
- θ 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

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

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, θ) 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

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

Draw (s_1, s_2) in the circle

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

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

Bibliography

Ross, S. M. (2012).
Simulation.
Elsevier, fifth edition.