MEM6810 Engineering Systems Modeling and Simulation
工程系统建模与仿真

Theory Analysis

Lecture 4: Random Variate Generation

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Introduction

- Random **variable** is a variable whose values are random and depend on a probability distribution.
  - E.g., normal, exponential, Poisson, etc.

- Random **variate** is a *particular* outcome (i.e. observed sample, realization) of a random variable.
  - E.g., 5 random variates (outcomes) from a $\mathcal{N}(0,1)$ random variable: $0.5377, 1.8339, -2.2588, 0.8622, 0.3188$.

- When simulating a system, we often need to generate random variates (e.g., interarrival time, service time) from all kinds of distributions (e.g., exponential distribution, arbitrary empirical distribution).

Introduction

- In practice:
  - Most simulation softwares have build-in functions to generate random variates from common distributions.
  - Most programming languages have implemented the common routines of random variate generation in the libraries.

- It is nevertheless worthwhile to understand how random variate generation occurs.
  - In case when build-in functions or libraries are unavailable.
  - To better understand the randomness in stochastic simulation.
  - Be alert to some inadequate random variate generator.

- To produce a sequence of random variates from a given distribution (of a random variable):
  1. Start with random variates from $\mathrm{Unif}(0, 1)$ (called **random numbers**).
  2. All random variates with given distribution are "transformed" from **random numbers**.

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- **Random numbers** are a sequence of **independent** random observations from **uniform** distribution on $[0, 1]$.
  - If $U \sim \text{Unif}(0, 1)$, then $\mathbb{E}[U] = \frac{1}{2}$, $\text{Var}(U) = \frac{1}{12}$, and its pdf is
    $$f(u) = \begin{cases} 1, & 0 \le u \le 1, \\ 0, & \text{otherwise.} \end{cases}$$
  - 10 random numbers generated in MATLAB: 0.8147, 0.9058, 0.1270, 0.9134, 0.6324, 0.0975, 0.2785, 0.5469, 0.9575, 0.9649.

- Statistical Properties
  - Uniformity: Each value on $[0, 1]$ has equal likelihood.
  - Independence: Implies no correlation between successive numbers.

- Uniformity

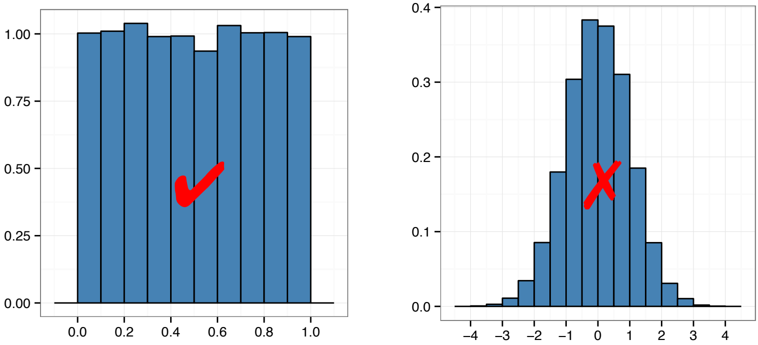
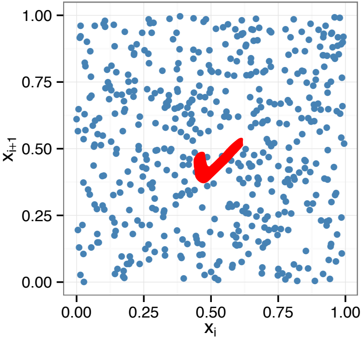


Figure: Empirical pdf (i.e., Scaled Histogram): Uniformity vs Nonuniformity (*from* *ZHANG Xiaowei*)

- Independence



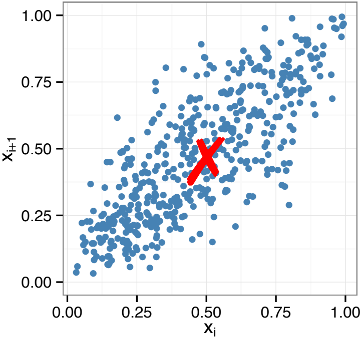


Figure: Scatter Plot: Uncorrelated vs Correlated (*from* *ZHANG Xiaowei*)

- A computer can NOT generate true randomness! It can only give us **pseudo-random** (伪随机) numbers.
- "Pseudo" means *false*
  - Generating random numbers by a known method removes true randomness.
  - The set of pseudo-random numbers can be repeated.
- Goal: To produce a sequence of numbers in $[0, 1]$ that imitates the ideal properties of random numbers.
  - Statistical properties are the most important.
  - True randomness is not the first priority.

- Properties of a good random number generator (RNG):
  1. Pass statistical tests.
  2. Solid theoretical support.
  3. Fast.
  4. Sufficiently long cycle (period).
  5. Portable to different computers.
  6. Replicable.
- Techniques for RNG:
  - Linear Congruential Generator (LCG)
  - Combined LCG
  - Multiple Recursive Generator (MRG)

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- Linear Congruential Generator (LCG, 线性同余发生器) is a simple and early development of RNG.

1. Produce a sequence of integers $x_1, x_2, \ldots$ between 0 and $m-1$ by

$$x_{i+1} = (ax_i + c) \bmod m, \quad i = 0, 1, 2, \ldots.$$

   - The initial value x_0 is called the *seed* (种子), a is *multiplier* (乘子), c is *increment* (增量), and m is *modulus* (模数).

2. Transform x_i's to values between 0 and 1 by

$$u_i = \frac{x_i}{m}, \quad i = 0, 1, 2, \ldots.$$

   - Possible values of u_i: $\{0, \frac{1}{m}, \ldots, \frac{m-1}{m}\}$. (May not cover all!)

- The selection of the values for a, c, m, and x_0 drastically affects the statistical properties and the cycle length.

- Example: Use LCG with $x_0 = 27$, $a = 17$, $c = 43$, and $m = 100$.

$$
\begin{aligned}
x_0 &= 27 \\
x_1 &= (17 \times 27 + 43) \bmod 100 = 502 \bmod 100 = 2 \\
u_1 &= 2/100 = 0.02 \\
x_2 &= (17 \times 2 + 43) \bmod 100 = 77 \bmod 100 = 77 \\
u_2 &= 77/100 = 0.77 \\
x_3 &= (17 \times 77 + 43) \bmod 100 = 1352 \bmod 100 = 52 \\
u_3 &= 52/100 = 0.52 \\
x_4 &= (17 \times 52 + 43) \bmod 100 = 927 \bmod 100 = 27 \\
u_4 &= 27/100 = 0.27
\end{aligned}
$$

The cycle length is only 4!

- Try `https://xiaoweiz.shinyapps.io/randNumGen` for different parameters.

- An actual use of LCG (Lewis et al. 1969): $a = 7^5$, $c = 0$, $m = 2^{31} - 1 = 2{,}147{,}483{,}647$ (a prime number).
  - It adopts $u_i = \frac{x_i}{m+1}$.
  - It passes many of the standard statistical tests.
  - Cycle length $\approx 2^{31} - 2 \approx 2 \times 10^9$ (well over 2 billion).

- Note: By letting modulus m be a power of 2 (or close), the modulo operation can be conducted efficiently, since most digital computers use a binary representation of numbers.

- As computing power has increased, LCG is not adequate nowadays; more sophisticated RNGs are used in practice.

- Combined LCG: Combine J (≥ 2) LCG (with $c = 0$).
- For 32-bit computers, L'Ecuyer (1988) suggests combining $J = 2$ generators with $a_1 = 40{,}014$, $m_1 = 2{,}147{,}483{,}563$, $a_2 = 40{,}692$, and $m_2 = 2{,}147{,}483{,}399$.

1. Select seed $x_{1,0}$ in the range $[1, m_1 - 1]$ for the first generator, and seed $x_{2,0}$ in the range $[1, m_2 - 1]$ for the second. Set $j = 0$.
2. Calculate
$$x_{1,j+1} = a_1 x_{1,j} \bmod m_1,$$
$$x_{2,j+1} = a_2 x_{2,j} \bmod m_2.$$
3. Let $x_{j+1} = (x_{1,j+1} - x_{2,j+1}) \bmod (m_1 - 1)$.
(*Remark*: $\bmod$ uses floored division, i.e., $y \bmod m = y - m\lfloor \frac{y}{m} \rfloor$.)
4. Return
$$u_{j+1} = \begin{cases} \frac{x_{j+1}}{m_1}, & \text{if } x_{j+1} > 0, \\ \frac{m_1 - 1}{m_1}, & \text{if } x_{j+1} = 0. \end{cases}$$
5. Set $j = j + 1$ and go to Step 2.

It has cycle length $(m_1 - 1)(m_2 - 1)/2 \approx 2 \times 10^{18}$.

- Multiple Recursive Generator (MRG): Extends LCG by using a higher-order recursion:

$$x_i = (a_1 x_{i-1} + a_2 x_{i-2} + \cdots + a_k x_{i-K}) \bmod m.$$

- A specific instance that has been widely implemented is `MRG32k3a`[†] (L'Ecuyer 1999), which is a *combined MRG* with $J = 2$ and $K = 3$.
  - It has cycle length $\approx 3 \times 10^{57}$, which is enormous.
  - If you could generate one billion (10^9) pseudo-random numbers per second, then it would take longer than the age of the universe to exhaust the period of `MRG32k3a`!

[†] `MRG32k3a` or its adaptation is one of the RNGs used in MATLAB, R, SAS, Arena, etc.

- Tests based on generated sequences of numbers.
  - *Frequency Test* for uniformity (discussed in next lecture)
    – Kolmogorov–Smirnov test (柯尔莫哥洛夫–斯米尔诺夫检验)
    – chi-square test (χ^2 test, 卡方检验)
  - *Autocorrelation Test* for independence.

- There are also some *theoretical tests* without actually generating any numbers, e.g., spectral test (谱检验).

- Fortunately, the well-known RNGs which are widely used in simulation softwares and languages have been extensively tested and validated.

- Be careful when the RNG at hand is not explicitly known or documented!
  - Even RNGs that have been used for years in popular commercial softwares (e.g., Excel, Visual Basic), have been found to be inadequate (L'Ecuyer 2001).

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- Assumption: RNG is available, i.e. we have a sequence of random numbers (i.e., $\mathrm{Unif}(0,1)$ random variates).
- Goal: Produce random variates from a given probability distribution (e.g. exponential, Poisson, etc.).
- Widely-used techniques†
  - Inverse-transform technique (generic)
  - Acceptance-rejection technique (generic)
  - Other ad-hoc methods for some specific distributions

† Methods introduced in this lecture are exact; there are also approximation methods such as MCMC.

- Let $F(x)$ be the CDF of X, i.e., $F(x) = \mathbb{P}(X \leq x)$.

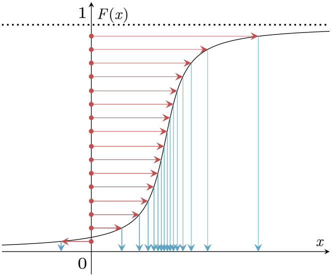


Figure: Continuous Random Variable

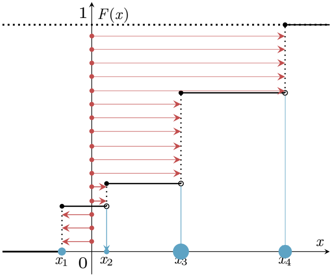


Figure: Discrete Random Variable

- Procedures
  1. Generate (as needed) random numbers (on vertical axis).
  2. Map inversely to points on horizontal axis, which are the desired random variates from $F(x)$.

- The formal definition of inverse function is
$$F^{-1}(y) := \min\{x : F(x) \geq y\}, \quad 0 < y < 1.$$

- If $U \sim \mathrm{Unif}(0,1)$, then $F^{-1}(U)$ has the same distribution as X, i.e.,
$$\mathbb{P}(F^{-1}(U) \leq x) = \mathbb{P}(U \leq F(x)) = F(x).$$

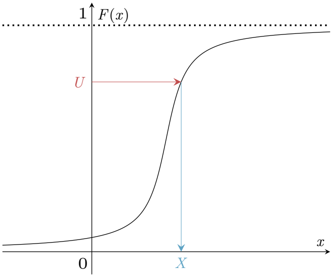


Figure: Continuous Random Variable

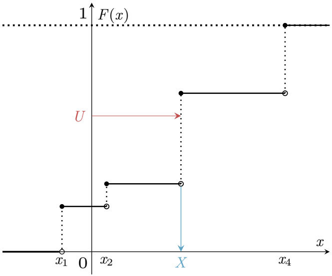


Figure: Discrete Random Variable

- The inverse-transform technique is useful when the CDF is so simple that its inverse function can be *analytically solved* or *easily computed*.
- It can be used to sample from various continuous distributions
  - uniform
  - exponential
  - triangular
  - Weibull
  - Cauchy
  - Pareto
- It can be used to sample from all (in principle) discrete distributions, e.g.,
  - discrete uniform
  - geometric
  - arbitrary empirical distribution

- Goal: Generate random variates from $X \sim \text{Unif}(a, b)$.
- Intuition: Since $X = a + (b-a)U$, we just need to:
  1. Generate random number u_i;
  2. Output $x_i = a + (b-a)u_i$ as the required random variates.
- For $X \sim \text{Unif}(a, b)$, the pdf and CDF are

$$f(x) = \begin{cases} \frac{1}{b-a}, & a \le x \le b, \\ 0, & \text{otherwise}, \end{cases} \quad F(x) = \begin{cases} 0, & x < a, \\ \frac{x-a}{b-a}, & a \le x \le b, \\ 1, & b < x. \end{cases}$$

- Solve the inverse function of $F(x)$,

$$F^{-1}(y) = a + (b-a)y, \quad 0 < y < 1.$$

- So, $F^{-1}(U) = a + (b-a)U$ has the same distribution as X.

- Goal: Generate random variates from $X \sim \mathrm{Exp}(\lambda)$.
- For $X \sim \mathrm{Exp}(\lambda)$, the pdf and CDF are

$$f(x) = \begin{cases} \lambda e^{-\lambda x}, & x \geq 0, \\ 0, & x < 0, \end{cases} \quad F(x) = \begin{cases} 1 - e^{-\lambda x}, & x \geq 0, \\ 0, & x < 0. \end{cases}$$

- Solve the inverse function of $F(x)$,

$$F^{-1}(y) = -\frac{1}{\lambda}\ln(1-y), \quad 0 < y < 1.$$

- So, $F^{-1}(U) = -\frac{1}{\lambda}\ln(1-U)$ has the same distribution as X.
- *Remark*: $1 - U \sim \mathrm{Unif}(0,1) \Longrightarrow -\frac{1}{\lambda}\ln(U)$ is sufficient.
- Numerical test for $\mathrm{Exp}(1)$ in Excel.
  1. Generate 200 random numbers.
  2. Obtain 200 random variates via the inverse function.

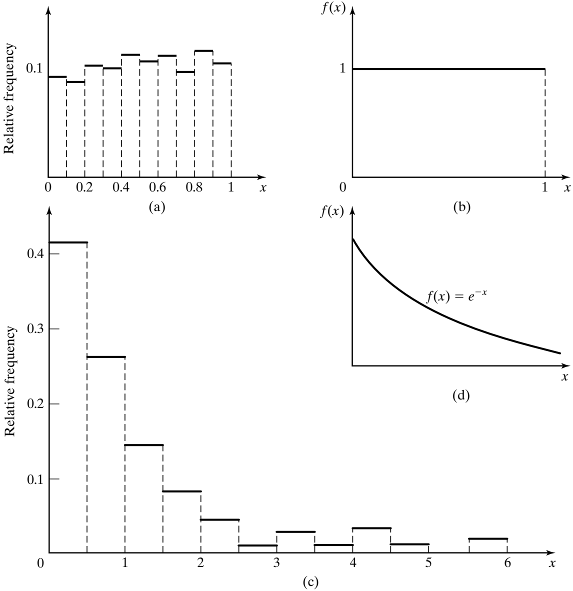


Figure:
(a) Empirical histogram of 200 generated uniform random numbers;
(b) Theoretical density of $\mathrm{Unif}(0, 1)$;

(c) Empirical histogram of 200 generated variates from $\mathrm{Exp}(1)$;
(d) Theoretical density of $\mathrm{Exp}(1)$.

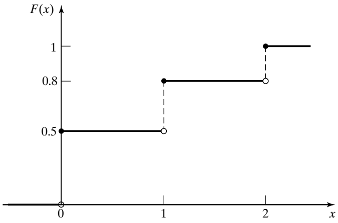
(*from Banks et al. (2010)*)

- Consider a discrete random variable X taking values 0, 1, 2 with probability 0.5, 0.3 and 0.2.

- The pmf and CDF are

$$p(x) = \begin{cases} 0.5, & x = 0, \\ 0.3, & x = 1, \\ 0.2, & x = 2, \end{cases} \qquad F(x) = \begin{cases} 0, & x < 0, \\ 0.5, & 0 \le x < 1, \\ 0.8, & 1 \le x < 2, \\ 1, & 2 \le x. \end{cases}$$

- Solve the inverse function. (Recall $F^{-1}(y) := \min\{x : F(x) \ge y\}$.)



$$F^{-1}(y) = \begin{cases} 0, & 0 < y \le 0.5, \\ 1, & 0.5 < y \le 0.8, \\ 2, & 0.8 < y < 1. \end{cases}$$

Try it in Excel.

- Why do we need another method when the inverse-transform technique is already generic?
  - The CDF of a desired distribution may not have an analytical form.
  - The inverse CDF may not exist in closed form and may be challenging to evaluate, e.g., beta, gamma, normal, etc.
  - Although you can solve the inverse transform via numerical methods anyway, the efficiency may be low.
- Acceptance-rejection technique is also useful for generating a *non-stationary Poisson process* (more details later).

- Goal: Generate random variates from $X \sim \mathrm{Unif}(1/4, 1)$ using acceptance-rejection technique.
  1. Generate a random number u (from $U \sim \mathrm{Unif}(0, 1)$).
  2. If $u \geq 1/4$, **accept** u, output u as the desired random variate; if $u < 1/4$, **reject** u, and return to Step 1.
  3. If another $\mathrm{Unif}(1/4, 1)$ random variate is needed, repeat the procedure from Step 1; stop otherwise.

- Important Observation 1: To produce one random variate using A-R technique, one may need to generate multiple random numbers.
  - Whereas there exists a one-to-one mapping for the inverse-transform method.

- Important Observation 2: The accepted values of U are conditioned values.
    - U itself does not have the desired distribution.
    - U conditioned on the event $\{U \geq 1/4\}$ does!

- For $1/4 \leq x \leq 1$,

$$\mathbb{P}\{U \leq x | U \geq 1/4\} = \frac{\mathbb{P}\{U \leq x \text{ and } U \geq 1/4\}}{\mathbb{P}\{U \geq 1/4\}} = \frac{x - 1/4}{3/4},$$

which is exactly the desired CDF of $X \sim \text{Unif}(1/4, 1)$.

- Suppose we want to generate random variates from X, whose density $f(x)$ has support $[a, b]$ and is upper bounded by M.

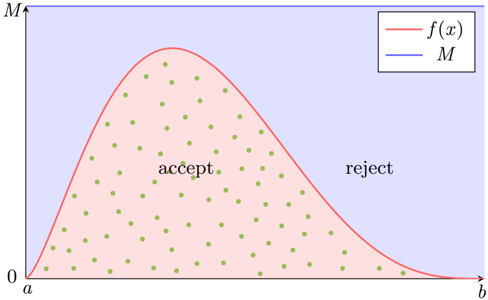


Figure: Bounded Support (*original image from ZHANG Xiaowei*)

1. Generate random variate pairs (y_1, z_1), (y_2, z_2), ..., from $\text{uniform}\{(y, z) : a \leq y \leq b,\ 0 \leq z \leq M\}$.
   - y_i from $Y \sim \text{Unif}(a, b)$, z_i from $Z \sim \text{Unif}(0, M)$
2. Accept the pair if $z_i < f(y_i)$ and output y_i as random variate from X with density $f(x)$.

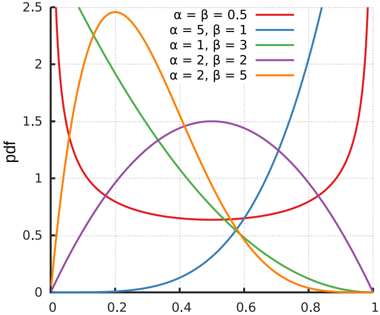
- Y conditioned on the event $\{Z < f(Y)\}$ has the same distribution as X, i.e., having density $f(x)$.
  - $(Y, Z) \sim \text{uniform}\{(y, z) : a \le y \le b,\ 0 \le z \le M\}$.

Proof.

$$\begin{aligned}
\mathbb{P}\{Y \le x | Z < f(Y)\} &= \frac{\mathbb{P}\{Y \le x, Z < f(Y)\}}{\mathbb{P}\{Z < f(Y)\}} \\
&= \frac{\int_a^x \int_0^{f(y)} f_{Y,Z}(y,z)\mathrm{d}z\mathrm{d}y}{\int_a^b \int_0^{f(y)} f_{Y,Z}(y,z)\mathrm{d}z\mathrm{d}y} \qquad \text{Note: } f_{Y,Z}(y,z) = \frac{1}{(b-a)M} \\
&= \frac{\int_a^x \int_0^{f(y)} \frac{1}{(b-a)M}\mathrm{d}z\mathrm{d}y}{\int_a^b \int_0^{f(y)} \frac{1}{(b-a)M}\mathrm{d}z\mathrm{d}y} = \frac{\int_a^x \int_0^{f(y)} \mathrm{d}z\mathrm{d}y}{\int_a^b \int_0^{f(y)} \mathrm{d}z\mathrm{d}y} \\
&= \frac{\int_a^x f(y)\mathrm{d}y}{\int_a^b f(y)\mathrm{d}y} = \frac{\mathbb{P}\{X \le x\}}{1} = \mathbb{P}\{X \le x\}. \qquad \blacksquare
\end{aligned}$$

- The acceptance rate is $\mathbb{P}\{Z < f(Y)\} = \frac{1}{(b-a)M}$.

- Goal: Generate random variates from $\mathrm{Beta}(\alpha, \beta)$, where the density is $f(x) = \frac{x^{\alpha-1}(1-x)^{\beta-1}}{B(\alpha, \beta)}$, $x \in [0, 1]$.



- If $\alpha > 1$ and $\beta > 1$, then $f(x)$ is maximized at $x = \frac{\alpha-1}{\alpha+\beta-2}$ and the maximum is $M = \frac{(\alpha-1)^{\alpha-1}(\beta-1)^{\beta-1}}{(\alpha+\beta-2)^{\alpha+\beta-2}B(\alpha, \beta)}$.
- The acceptance rate is $\frac{1}{(b-a)M} = \frac{1}{(1-0)M} = \frac{1}{M}$.

- Generate random variates from X, whose density $f(x)$ is upper bounded by $Mg(x)$, where $g(x)$ is *instrumental* density.

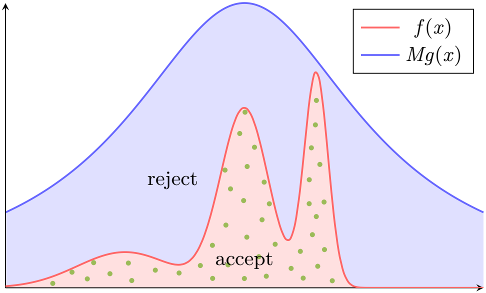


Figure: Unbounded Support (*original image from ZHANG Xiaowei*)

1. Generate random variate pairs (y_1, z_1), (y_2, z_2), ..., from $\text{uniform}\{(y, z) : y \in \text{support of } g(\cdot),\ 0 \le z \le Mg(y)\}$.
   - y_i from $Y \sim g(\cdot)$, z_i from $Z \sim \text{Unif}(0, Mg(y_i))$ **(why?)**
2. Accept the pair if $z_i < f(y_i)$ and output y_i as random variate from X with density $f(x)$.

- Y conditioned on the event $\{Z < f(Y)\}$ has the same distribution as X, i.e., having density $f(x)$.
  - Let Θ denote $\{(y, z) : y \in \text{support of } g(\cdot),\ 0 \le z \le Mg(y)\}$.
  - $(Y, Z) \sim \text{uniform}\, \Theta$.

Proof.

$$\mathbb{P}\{Y \le x | Z < f(Y)\} = \frac{\mathbb{P}\{Y \le x, Z < f(Y)\}}{\mathbb{P}\{Z < f(Y)\}}$$

$$= \frac{\int_{-\infty}^{x} \int_0^{f(y)} f_{Y,Z}(y,z)\mathrm{d}z\mathrm{d}y}{\int_{-\infty}^{\infty} \int_0^{f(y)} f_{Y,Z}(y,z)\mathrm{d}z\mathrm{d}y}$$

Note: $f_{Y,Z}(y,z) = \frac{1}{\Theta \text{ area}}$

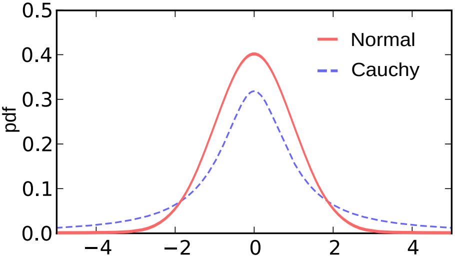
$$= \frac{\int_{-\infty}^{x} \int_0^{f(y)} \frac{1}{\Theta \text{ area}}\mathrm{d}z\mathrm{d}y}{\int_{-\infty}^{\infty} \int_0^{f(y)} \frac{1}{\Theta \text{ area}}\mathrm{d}z\mathrm{d}y} = \frac{\int_{-\infty}^{x} \int_0^{f(y)} \mathrm{d}z\mathrm{d}y}{\int_{-\infty}^{\infty} \int_0^{f(y)} \mathrm{d}z\mathrm{d}y}$$

$$= \frac{\int_{-\infty}^{x} f(y)\mathrm{d}y}{\int_{-\infty}^{\infty} f(y)\mathrm{d}y} = \frac{\mathbb{P}\{X \le x\}}{1} = \mathbb{P}\{X \le x\}.$$

■

- The acceptance rate is
$$\mathbb{P}\{Z < f(Y)\} = \frac{1}{\Theta \text{ area}} = \frac{1}{\int_{-\infty}^{\infty} Mg(y)\mathrm{d}y} = \frac{1}{M\int_{-\infty}^{\infty} g(y)\mathrm{d}y} = \frac{1}{M}.$$

- Goal: Generate random variates from $\mathcal{N}(0,1)$, where the density is $f(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}$, $x \in (-\infty, \infty)$.
- Use $\text{Cauchy}(0,1)$ density as instrumental density, which is $g(x) = \frac{1}{\pi(1+x^2)}$, $x \in (-\infty, \infty)$.



- It is easy to see that $\frac{f(x)}{g(x)} = \sqrt{\frac{\pi}{2}}(1+x^2)e^{-\frac{x^2}{2}}$ is maximized at $x = \pm 1$ and the maximum is $\sqrt{\frac{2\pi}{e}}$, which is the required M.
- The acceptance rate is $\frac{1}{M} = \sqrt{\frac{e}{2\pi}} \approx 0.6577$.

- Box–Muller method for $\mathcal{N}(0,1)$ random variates:
  1. Generate u_1 and u_2 independently from $\mathrm{Unif}(0,1)$.
  2. Let $z_1 = \sqrt{-2\ln u_1}\cos(2\pi u_2)$ and $z_2 = \sqrt{-2\ln u_1}\sin(2\pi u_2)$.

- z_1 and z_2 are random variates from $\mathcal{N}(0,1)$ (independent).

- Intuition:
  - For two independent $\mathcal{N}(0,1)$ RVs Z_1 and Z_2,
  $$Z_1^2, Z_2^2 \sim \chi_1^2, \; Z_1^2 + Z_2^2 \sim \chi_2^2.$$
  - $X \sim \mathrm{Exp}(1/2) \iff X \sim \chi_2^2$.
  - $-2\ln u_1$ is a random variate from $\mathrm{Exp}(1/2)$ (and thus χ_2^2).
  - The angle is distributed uniformly around the circle.

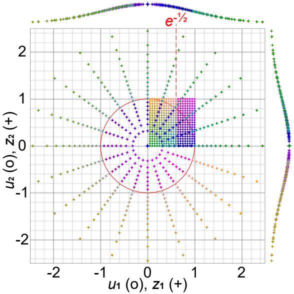


Figure: Box–Muller Method Visualisation
(image by Cmglee / CC BY 3.0)
Interactive Graph

- Rigorous proof.

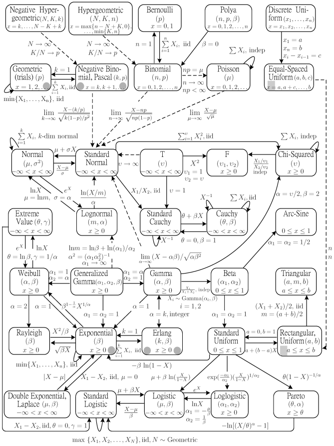


Figure: Relationships Among 35 Distributions (from Song (2005))

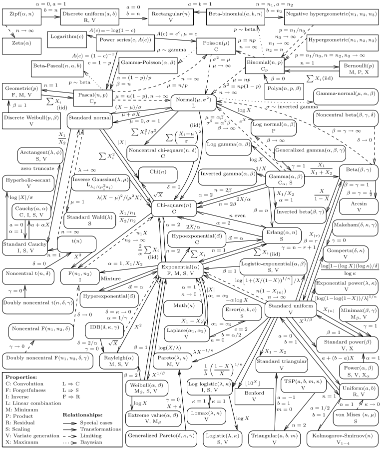


Figure: Relationships Among 76 Distributions (from Leemis & McQueston (2008))

- **Poisson process** with rate λ: Interarrival time distribution is exponential with rate λ (or mean $1/\lambda$), and

$$N(t+h) - N(t) \sim \text{Poisson}(\lambda h). \quad \text{(same as } N(h)\text{)}$$

- To generate Poisson process with rate λ, one only need to generate iid $\text{Exp}(\lambda)$ random variates.
  - s_i, the arrival time of the ith arrival, satisfies

$$s_i = s_{i-1} - (1/\lambda)\ln(u_i), \; i = 1, 2, \ldots.$$

- **Nonhomogeneous Poisson process** with rate (intensity) function $\lambda(t)$:

$$N(t+h) - N(t) \sim \text{Poisson}(m(t+h) - m(t)),$$

where $m(t) = \int_0^t \lambda(s)\mathrm{d}s$.

- To generate nonhomogeneous Poisson process with rate function $\lambda(t)$, one can use the acceptance-rejection method (which is also called *thinning* in this context).
- Idea behind thinning:
  - Generate a *stationary* Poisson arrival process at the fastest rate $\lambda^* = \max_t \lambda(t)$.
  - But "accept" only a portion of arrivals, thinning out just enough to get the desired time-varying rate.
- Algorithm:
  1. Set $t = 0$ and $i = 1$.
  2. Generate x from $\mathrm{Exp}(\lambda^*)$, and let $t \leftarrow t + x$ (this is the arrival time of the *stationary* Poisson process with rate λ^*).
  3. Generate random number u (from $\mathrm{Unif}(0, 1)$). If $u \leq \lambda(t)/\lambda^*$, then $s_i = t$ and $i \leftarrow i + 1$.
  4. Go to Step 2.