Computer Simulation

Module 2: Calculus, Probability, and Statistics Primers

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Calculus Primer

Lesson Overview

Last Module: We gave a high-level overview on what simulation is.

This Time: This module will present various boot camps. Let's start with a Calculus lesson.

Dirty Little Secret: There's nothing new here if you've taken the prerequisites.

Calculus Primer

Goal: This section provides a brief review of various calculus tidbits that we'll be using later on.

First of all, let's suppose that $f(x)$ is a *function* that maps values of x from a certain *domain* X to a certain *range* Y, which we can denote by the shorthand $f : X \to Y$.

Example If $f(x) = x^2$, then the function takes x-values from the real line $\mathbb{R}$ to the nonnegative portion of the real line $\mathbb{R}^+$.

Definition We say that $f(x)$ is a *continuous* function if, for any x_0 and $x \in X$, we have $\lim_{x \to x_0} f(x) = f(x_0)$, where "lim" denotes a *limit* and $f(x)$ is assumed to exist for all $x \in X$.

Example The function $f(x) = 3x^2$ is continuous for all x. The function $f(x) = \lfloor x \rfloor$ (round down to the nearest integer, e.g., $\lfloor 3.4 \rfloor = 3$) has a "jump" discontinuity at any integer x. $\square$

Definition If $f(x)$ is continuous, then the *derivative* (slope) is

$$\frac{d}{dx} f(x) \equiv f'(x) \equiv \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

assuming it exists and is well-defined for any given x.

Some Old Friends

$$
\begin{aligned}
[x^k]' &= kx^{k-1}, \\
[e^x]' &= e^x, \\
[\sin(x)]' &= \cos(x), \\
[\cos(x)]' &= -\sin(x), \\
[\ell n(x)]' &= 1/x, \\
[\arctan(x)]' &= 1/(1+x^2).
\end{aligned}
$$

Theorem Some well-known properties of derivatives are:

$$[af(x)+b]' = af'(x),$$

$$[f(x)+g(x)]' = f'(x)+g'(x),$$

$$[f(x)g(x)]' = f'(x)g(x)+f(x)g'(x) \quad \text{(product rule)},$$

$$\left[\frac{f(x)}{g(x)}\right]' = \frac{g(x)f'(x)-f(x)g'(x)}{g^2(x)} \quad \text{(quotient rule)}^1,$$

$$[f(g(x))]' = f'(g(x))g'(x) \quad \text{(chain rule)}^2.$$

[1] Ho dee Hi minus Hi dee Ho over Ho Ho.
[2] www.youtube.com/watch?v=gGAiW5dOnKo

Example Suppose that $f(x) = x^2$ and $g(x) = \ell n(x)$. Then

$$[f(x)g(x)]' = \frac{d}{dx}x^2\ell n(x) = 2x\ell n(x) + x,$$

$$\left[\frac{f(x)}{g(x)}\right]' = \frac{d}{dx}\frac{x^2}{\ell n(x)} = \frac{2x\ell n(x) - x}{\ell n^2(x)},$$

$$[f(g(x))]' = 2g(x)g'(x) = \frac{2\ell n(x)}{x}. \quad \square$$

Remark The second derivative $f''(x) \equiv \frac{d}{dx} f'(x)$ and is the "slope of the slope." If $f(x)$ is "position," then $f'(x)$ can be regarded as "velocity," and as $f''(x)$ as "acceleration."

The minimum or maximum of $f(x)$ can only occur when the slope of $f(x)$ is zero, i.e., only when $f'(x) = 0$, say at $x = x_0$.

Then if $f''(x_0) < 0$, you get a max; if $f''(x_0) > 0$, you get a min; and if $f''(x_0) = 0$, you get a *point of inflection*.

Example Find x that minimizes $f(x) = e^{2x} + e^{-x}$. The min can only occur when $f'(x) = 2e^{2x} - e^{-x} = 0$. This occurs at $x_0 = -(1/3)\ell\text{n}(2)$. It's easy to show that $f''(x) > 0$ for all x; so x_0 is the min. $\square$

Summary

This Time: Some Calculus derivative memories. What's not to love?

Next Time: Saved by Zero! We'll give some numerical techniques to solve nonlinear equations.

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Saved By Zero! Solving Equations

Lesson Overview

Last Time: Talked about Calculus basics. At the end, we searched for the solution to a nonlinear equation (finding a zero).

This Time: Some formal ways to conduct the search.

This material will be used several times in the course… take my word for it!

Finding Zeroes

How might you find a 0 for a complicated nonlinear function, i.e., x such that $f(x) = 0$?

- Trial-and-error (not so great).
- Bisection (divide-and-conquer).
- Newton's method (or some variation)
- Fixed-point method (we'll do this later).

GTx

Example (from last lesson that has exact answer). Find the value of x that minimizes $f(x) = e^{2x} + e^{-x}$.

The minimum can only occur when $f'(x) = 2e^{2x} - e^{-x} = 0$.

After a little algebra, we find that this occurs at $x_0 = -(1/3)\ell n(2) \approx -0.231$.

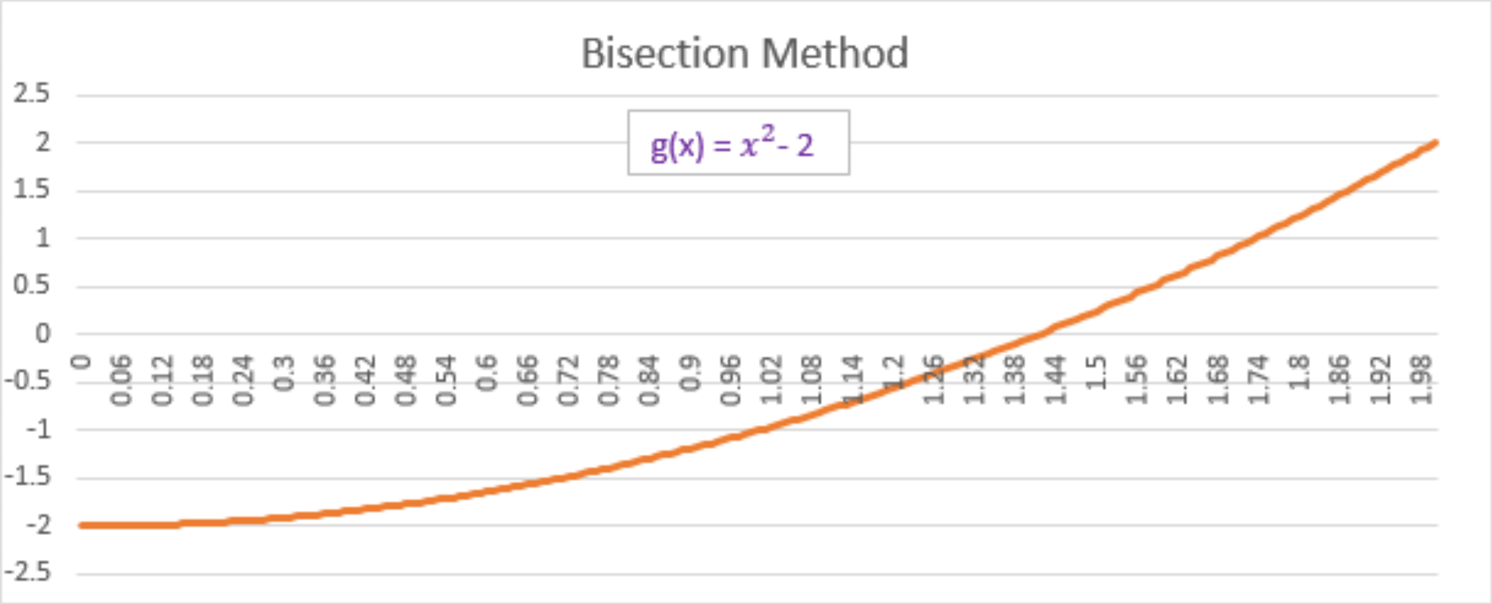
It's also easy to show that $f''(x) > 0$ for all x; and so x_0 yields a minimum. $\square$

Bisection: Suppose you can find x_1 and x_2 such that $g(x_1) < 0$ and $g(x_2) > 0$. (We'll follow similar logic if the inequalities are both reversed.) By the Intermediate Value Theorem (which you may remember), there must be a zero in $[x_1, x_2]$, that is, $x^\star \in [x_1, x_2]$ such that $g(x^\star) = 0$.

Thus, take $x_3 = (x_1 + x_2)/2$. If $g(x_3) < 0$, then there must be a zero in $[x_3, x_2]$. Otherwise, if $g(x_3) > 0$, then there must be a zero in $[x_1, x_3]$. Either way, the length of the search interval decreases.

Continue in this same manner until the length of the search interval is as small as desired.

Exercise: Try this out for $g(x) = x^2 - 2$; and so approximate $\sqrt{2}$.



$x1 = 1$	$g(x1) = -1 < 0$	implication	
$x2 = 2$	$g(x2) = 2 > 0$	$x^* \varepsilon [1,2]$	
$x3 = 1.5$	$g(x3) = 0.25 > 0$	$x^* \varepsilon [1,1.5]$	
$x4 = 1.25$	$g(x4) = -0.438 < 0$	$x^* \varepsilon [1.25,1.5]$	
$x5 = 1.375$	$g(x5) = -0.109 < 0$	$x^* \varepsilon [1.375,1.5]$	
$x6 = 1.4375$	$g(x6) = 0.0664 > 0$	$x^* \varepsilon [1.375,1.4375]$	<--converging to 1.414...!

Newton's Method: Suppose you can find a reasonable first guess for the zero, say, x_i, where we start off at iteration $i = 0$. If $g(x)$ has a nice, well-behaved derivative (which doesn't happen to be too flat near the zero of $g(x)$), then iterate your guess as follows:

$$x_{i+1} = x_i - \frac{g(x_i)}{g'(x_i)}.$$

Keep going until things appear to converge.

This makes sense since for x_i and x_{i+1} close to each other and the zero $x^\star$, we have

$$g'(x_i) \approx \frac{g(x^\star) - g(x_i)}{x^\star - x_i}.$$

Exercise: Try Newton out for $g(x) = x^2 - 2$.

Note that the iteration step is to set

$$x_{i+1} = x_i - \frac{x_i^2 - 2}{2x_i} = \frac{x_i}{2} + \frac{1}{x_i}.$$

Let's start with a bad guess of $x_1 = 1$. Then

$$\begin{aligned}
x_2 &= \frac{x_1}{2} + \frac{1}{x_1} = \frac{1}{2} + 1 = 1.5 \\
x_3 &= \frac{x_2}{2} + \frac{1}{x_2} \approx \frac{1.5}{2} + \frac{1}{1.5} = 1.4167 \\
x_4 &= \frac{x_3}{2} + \frac{1}{x_3} \approx 1.4142 \quad \text{Wow!} \quad \square
\end{aligned}$$

Summary

We went over some basic techniques to solve nonlinear equations for zeroes.

Next Time: The battle of Leibniz vs. Newton — it’s integration time!

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Integration

Lesson Overview

Last Time: How do you find a zero of a complicated function?

This Time: What goes up must come down! A couple of lessons ago, we reviewed derivatives. Now integration.

Hopefully, you'll remember many old friends.

Integration

Definition The function $F(x)$ having derivative $f(x)$ is called the *antiderivative*. The antiderivative is denoted $F(x) = \int f(x)\,dx$; and this is also called the *indefinite integral* of $f(x)$.

Fundamental Theorem of Calculus: If $f(x)$ is continuous, then the area under the curve for $x \in [a, b]$ is denoted and given by the *definite integral* [3]

$$\int_a^b f(x)\,dx \equiv F(x)\Big|_a^b \equiv F(b) - F(a).$$

[3] "I'm *really* an integral!"

Friends of Mine

$$\int x^k\,dx = \frac{x^{k+1}}{k+1} + C,\; k \neq -1,$$

$$\int \frac{dx}{x} = \ell\text{n}|x| + C,$$

$$\int e^x\,dx = e^x + C,$$

$$\int \cos(x)\,dx = \sin(x) + C,$$

$$\int \frac{dx}{1+x^2} = \arctan(x) + C.$$

Example It is easy to see that

$$\int \frac{d\,\text{cabin}}{\text{cabin}} = \ell\text{n}|\text{cabin}| + C = \text{houseboat}. \quad \square$$

Theorem Some well-known properties of definite integrals are:

$$\int_a^a f(x)\,dx = 0,$$

$$\int_a^b f(x)\,dx = -\int_b^a f(x)\,dx,$$

$$\int_a^b f(x)\,dx = \int_a^c f(x)\,dx + \int_c^b f(x)\,dx.$$

Theorem Some other properties of general integrals are:

$$\int [f(x) + g(x)]\, dx = \int f(x)\, dx + \int g(x)\, dx,$$

$$\int f(x)g'(x)\, dx = f(x)g(x) - \int g(x)f'(x)\, dx \quad \text{(parts)}[4],$$

$$\int f(g(x))g'(x)\, dx = \int f(u)\, du \quad \text{(substitution rule)}[5].$$

[4] www.youtube.com/watch?v=OTzLVIc-O5E
[5] www.youtube.com/watch?v=eswQl-hcvU0

Example Using integration by parts with $f(x) = x$ and $g'(x) = e^{2x}$ and the chain rule, we have

$$\int_0^1 xe^{2x}\,dx = \left.\frac{xe^{2x}}{2}\right|_0^1 - \int_0^1 \frac{e^{2x}}{2}\,dx = \frac{e^2}{2} - \left.\frac{e^{2x}}{4}\right|_0^1 = \frac{e^2+1}{4}. \quad \square$$

Definition Derivatives of arbitrary order k can be written as $f^{(k)}(x)$ or $\frac{d^k}{dx^k} f(x)$. By convention, $f^{(0)}(x) = f(x)$.

The *Taylor series expansion* of $f(x)$ about a point a is given by

$$f(x) = \sum_{k=0}^{\infty} \frac{f^{(k)}(a)(x-a)^k}{k!}.$$

The *Maclaurin series* is simply Taylor expanded around $a = 0$.

Maclaurin Friends

$$\sin(x) = \sum_{k=0}^{\infty} \frac{(-1)^{k+1} x^{2k+1}}{(2k+1)!},$$

$$\cos(x) = \sum_{k=0}^{\infty} \frac{(-1)^{k} x^{2k}}{(2k)!},$$

$$e^x = \sum_{k=0}^{\infty} \frac{x^k}{k!}.$$

While We're at it...

$$\sum_{k=1}^{n} k = \frac{n(n+1)}{2},$$

$$\sum_{k=1}^{n} k^2 = \frac{n(n+1)(2n+1)}{6},$$

$$\sum_{k=0}^{\infty} p^k = \frac{1}{1-p} \text{ (for } -1 < p < 1).$$

Theorem Occasionally, we run into trouble when taking indeterminate ratios of the form $0/0$ or ∞/∞. In such cases, *L'Hôspital's Rule*[6] is useful: If the limits $\lim_{x\to a} f(x)$ and $\lim_{x\to a} g(x)$ both go to 0 or both go to ∞, then

$$\lim_{x\to a} \frac{f(x)}{g(x)} = \lim_{x\to a} \frac{f'(x)}{g'(x)}.$$

[6] This rule makes me sick.

Example L'Hôspital shows that

$$\lim_{x\to 0} \frac{\sin(x)}{x} = \lim_{x\to 0} \frac{\cos(x)}{1} = 1. \quad \square$$

Summary

We renewed acquaintances with some old integral friends.

Next Time: We'll look at some numerical integration techniques if those friends don't want to come out and play.

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Integration Computer Exercises

Lesson Overview

Last Time: A puntastic integration review.

This Time: Implement several numerical techniques that you might need to use if you can't find a nice, pretty closed-form solution to your integral.

One of these techniques incorporates simulation!

Computer Exercise: Let's do some easy integration via *Riemann sums*. Simply approximate the area under the nice, continuous function $f(x)$ from a to b by adding up the areas of n adjacent rectangles of width $\Delta x = (b-a)/n$ and height $f(x_i)$, where $x_i = a + i\Delta x$ is the right-hand endpoint of the ith rectangle. Thus,

$$\int_a^b f(x)\,dx \approx \sum_{i=1}^{n} f(x_i)\Delta x = \frac{b-a}{n}\sum_{i=1}^{n} f\left(a + \frac{i(b-a)}{n}\right).$$

In fact, as $n \to \infty$, this result becomes an equality.

Try it out on $\int_0^1 \sin(\pi x/2)\,dx$ (which secretly equals $2/\pi$) for different values of n, and see for yourself.

Riemann (cont'd): Since I'm such a nice guy, I've made things easy for you. In this problem, I've thoughtfully taken $a = 0$ and $b = 1$, so that $\Delta x = 1/n$ and $x_i = i/n$, which simplifies the notation a bit. Then

$$\begin{aligned}\int_a^b f(x)\,dx &= \int_0^1 f(x)\,dx \\ &\approx \sum_{i=1}^{n} f(x_i)\Delta x \\ &= \frac{1}{n}\sum_{i=1}^{n} \sin\left(\frac{\pi i}{2n}\right).\end{aligned}$$

For $n = 100$, this calculates out to a value of 0.6416, which is pretty close to the true answer of $2/\pi \approx 0.6366$. $\square$

Computer Exercise, Trapezoid version: Same numerical integration via the Trapezoid Rule (which usually works a little better than Riemann). Now we have

$$\begin{aligned}\int_a^b f(x)\,dx &\approx \left[\frac{f(x_0)}{2} + \sum_{i=1}^{n-1} f(x_i) + \frac{f(x_n)}{2}\right]\Delta x \\ &= \frac{b-a}{n}\left[\frac{f(a)}{2} + \sum_{i=1}^{n-1} f\left(a + \frac{i(b-a)}{n}\right) + \frac{f(b)}{2}\right].\end{aligned}$$

Again try it out on $\int_0^1 \sin(\pi x/2)\,dx$.

Computer Exercise, Monte Carlo version: You will soon learn a Monte Carlo method to accomplish approximate integration. Just take my word for it for now. Let $U_1, U_2, \ldots, U_n$ denote a sequence of Unif(0,1) random numbers, which can be obtained from Excel using `RAND()`. It can be shown that

$$\int_a^b f(x)\,dx \;\approx\; \frac{b-a}{n}\sum_{i=1}^{n} f(a+(b-a)U_i),$$

with the result becoming an equality as $n \to \infty$.

Yet again try it out on $\int_0^1 \sin(\pi x/2)\,dx$.

Summary

Went over some easy numerical integration techniques. We snuck in a little simulation while we weren't looking.

Next Time: It is highly likely that we'll be starting our Probability Primer.

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Module 2: Calculus, Probability, and Statistics Primers

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Probability Basics

Lesson Overview

Last Time: We completed our Calculus Primer!

This Time: We'll start our review of Probability with some basics.

If you are a probability tyro, feel free to peruse the notes at your leisure; but pay attention to material that you don't remember so well.

Basics

Will assume that you know about sample spaces, events, and the definition of probability.

Definition: $P(A|B) \equiv P(A \cap B)/P(B)$ is the *conditional probability of A given B*.

Example: Toss a fair die. Let $A = \{1,2,3\}$ and $B = \{3,4,5,6\}$. Then

$$P(A|B) = \frac{P(A \cap B)}{P(B)} = \frac{1/6}{4/6} = 1/4. \quad \square$$

Definition: If $P(A \cap B) = P(A)P(B)$, then A and B are *independent* events.

Theorem: If A and B are independent, then $P(A|B) = P(A)$.

Example: Toss two dice. Let A = "Sum is 7" and B = "First die is 4". Then

$$P(A) = 1/6, \quad P(B) = 1/6, \quad \text{and}$$

$$P(A \cap B) = P((4,3)) = 1/36 = P(A)P(B).$$

So A and B are independent. $\square$

Definition: A *random variable* (RV) X is a function from the sample space Ω to the real line, i.e., $X : \Omega \to \mathbb{R}$.

Example: Let X be the sum of two dice rolls. Then $X((4,6)) = 10$.

In addition,

$$P(X = x) = \begin{cases} 1/36 & \text{if } x = 2 \\ 2/36 & \text{if } x = 3 \\ \vdots & \\ 1/36 & \text{if } x = 12 \\ 0 & \text{otherwise} \end{cases}$$

Definition: If the number of possible values of a RV X is finite or countably infinite, then X is a *discrete* RV. Its *probability mass function* (pmf) is $f(x) \equiv P(X = x)$. Note that $\sum_x f(x) = 1$.

Example: Flip 2 coins. Let X be the number of heads.

$$f(x) = \begin{cases} 1/4 & \text{if } x = 0 \text{ or } 2 \\ 1/2 & \text{if } x = 1 \\ 0 & \text{otherwise} \end{cases} \qquad \square$$

Examples: Some well-known discrete RV's you may know: Bernoulli(p), Binomial(n, p), Geometric(p), Poisson(λ), etc.

Definition: A *continuous* RV is one with probability zero at every individual point, and for which there exists a *probability density function* (pdf) $f(x)$ such that $P(X \in A) = \int_A f(x)\,dx$ for every set A. Note that $\int_{\mathbb{R}} f(x)\,dx = 1$.

Example: Pick a random number between 3 and 7. Then

$$f(x) = \begin{cases} 1/4 & \text{if } 3 \le x \le 7 \\ 0 & \text{otherwise} \end{cases} \qquad \Box$$

Examples: Here are some well-known continuous RV's: Uniform(a, b), Exponential(λ), Normal(μ, σ^2), etc.

Notation: "~" means "is distributed as". For instance, $X \sim \mathrm{Unif}(0,1)$ means that X has the uniform distribution on [0,1].

Definition: For any RV X (discrete or continuous), the *cumulative distribution function* (cdf) is

$$F(x) \equiv P(X \leq x) = \begin{cases} \sum_{y \leq x} f(y) & \text{if } X \text{ is discrete} \\ \int_{-\infty}^{x} f(y)\,dy & \text{if } X \text{ is continuous} \end{cases}$$

Note that $\lim_{x \to -\infty} F(x) = 0$ and $\lim_{x \to \infty} F(x) = 1$. In addition, if X is continuous, then $\frac{d}{dx}F(x) = f(x)$.

Example: Flip 2 coins. Let X be the number of heads.

$$F(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1/4 & \text{if } 0 \le x < 1 \\ 3/4 & \text{if } 1 \le x < 2 \\ 1 & \text{if } x \ge 2 \end{cases} \qquad \square$$

Example: if $X \sim \text{Exp}(\lambda)$ (i.e., X is exponential with parameter λ), then $f(x) = \lambda e^{-\lambda x}$ and $F(x) = 1 - e^{-\lambda x}$, $x \ge 0$. $\square$

Summary

Started our review of Probability by touching on the basics.

Next Time: We'll finally formally simulate some random variables! About time, eh?

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Simulating Random Variables

Lesson Overview

Last Time: We started our Probability Primer!

This Time: We'll show how to simulate some easy random variables on the computer.

This is one of the main reasons that you're taking the course!

Example (Discrete Uniform): Consider a D.U. on $\{1, 2, \ldots, n\}$, i.e., $X = i$ with probability $1/n$ for $i = 1, 2, \ldots, n$. (Think of this as an n-sided dice toss for you Dungeons and Dragons fans.)

If $U \sim \mathrm{Unif}(0, 1)$, we can obtain a D.U. random variate simply by setting $X = \lceil nU \rceil$, where $\lceil \cdot \rceil$ is the "ceiling" (or "round up") function.

For example, if $n = 10$ and we sample a Unif(0,1) random variable $U = 0.73$, then $X = \lceil 7.3 \rceil = 8$. $\square$

Example (Another Discrete Random Variable):

$$P(X = x) = \begin{cases} 0.25 & \text{if } x = -2 \\ 0.10 & \text{if } x = 3 \\ 0.65 & \text{if } x = 4.2 \\ 0 & \text{otherwise} \end{cases}$$

Can't use a die toss to simulate this random variable. Instead, use what's called the *inverse transform method*.

x	$f(x)$	$P(X \le x)$	Unif(0,1)'s
-2	0.25	0.25	$[0.00, 0.25]$
3	0.10	0.35	$(0.25, 0.35]$
4.2	0.65	1.00	$(0.35, 1.00)$

Sample $U \sim \text{Unif}(0, 1)$. Choose the corresponding x-value, i.e., $X = F^{-1}(U)$. For example, $U = 0.46$ means that $X = 4.2$. $\square$

Now we'll use the *inverse transform method* to generate a continuous random variable. We'll talk about the following result a little later…

Theorem: If X is a continuous random variable with cdf $F(x)$, then the random variable $F(X) \sim \text{Unif}(0,1)$.

This suggests a way to generate realizations of the RV X. Simply set $F(X) = U \sim \text{Unif}(0,1)$ and solve for $X = F^{-1}(U)$.

Example: Suppose $X \sim \text{Exp}(\lambda)$. Then $F(x) = 1 - e^{-\lambda x}$ for $x > 0$. Set $F(X) = 1 - e^{-\lambda X} = U$. Solve for X,

$$X = \frac{-1}{\lambda} \ell\text{n}(1-U) \sim \text{Exp}(\lambda). \quad \Box$$

Example (Generating Uniforms): The above RV generation examples required us to generate "practically" independent and identically distributed (iid) Unif(0,1) RV's.

If you don't like programming, you can use Excel function `RAND()` or something similar to generate Unif(0,1)'s.

Here's an algorithm to generate *pseudo-random numbers (PRN's)*, i.e., a series $R_1, R_2, \ldots$ of *deterministic* numbers that *appear* to be iid Unif(0,1). Pick a *seed* integer X_0, and calculate

$$X_i = 16807 X_{i-1} \bmod (2^{31} - 1), \quad i = 1, 2, \ldots.$$

Then set $R_i = X_i/(2^{31} - 1)$, $i = 1, 2, \ldots$.

Here's an easy FORTRAN implementation of the above algorithm (from Bratley, Fox, and Schrage).

```
FUNCTION UNIF(IX)
K1 = IX/127773     (this division truncates, e.g., 5/3 = 1.)
IX = 16807*(IX - K1*127773) - K1*2836     (update seed)
IF(IX.LT.0)IX = IX + 2147483647
UNIF = IX * 4.656612875E-10
RETURN
END
```

We input a positive integer IX and the function returns the PRN UNIF, as well as an updated IX that we can use again. □

Some Exercises: In the following, I'll assume that you can use Excel (or whatever) to simulate independent Unif(0,1) RV's. (We'll review independence in a little while.)

1. Make a histogram of $X_i = -\ell n(U_i)$, for $i = 1, 2, \ldots, 10000$, where the U_i's are independent Unif(0,1) RV's. What kind of distribution does it look like?

2. Suppose X_i and Y_i are independent Unif(0,1) RV's, $i = 1, 2, \ldots, 10000$. Let $Z_i = \sqrt{-2\ell n(X_i)}\,\sin(2\pi Y_i)$, and make a histogram of the Z_i's based on the 10000 replications.

3. Suppose X_i and Y_i are independent Unif(0,1) RV's, $i = 1, 2, \ldots, 10000$. Let $Z_i = X_i/(X_i - Y_i)$, and make a histogram of the Z_i's based on the 10000 replications. This may be somewhat interesting. It's possible to derive the distribution analytically, but it takes a lot of work.

Summary

This was a “starter” lecture on random variate generation – something to get you psyched up for what’s coming up!

Next Time: I know you’ve been expecting a nice lecture on expectations!

Summary Placeholder

- Talked about blah blah blah…
- This completes Module 2, which went over blah blah blah
- Coming up: Module 3 will blah blah blah