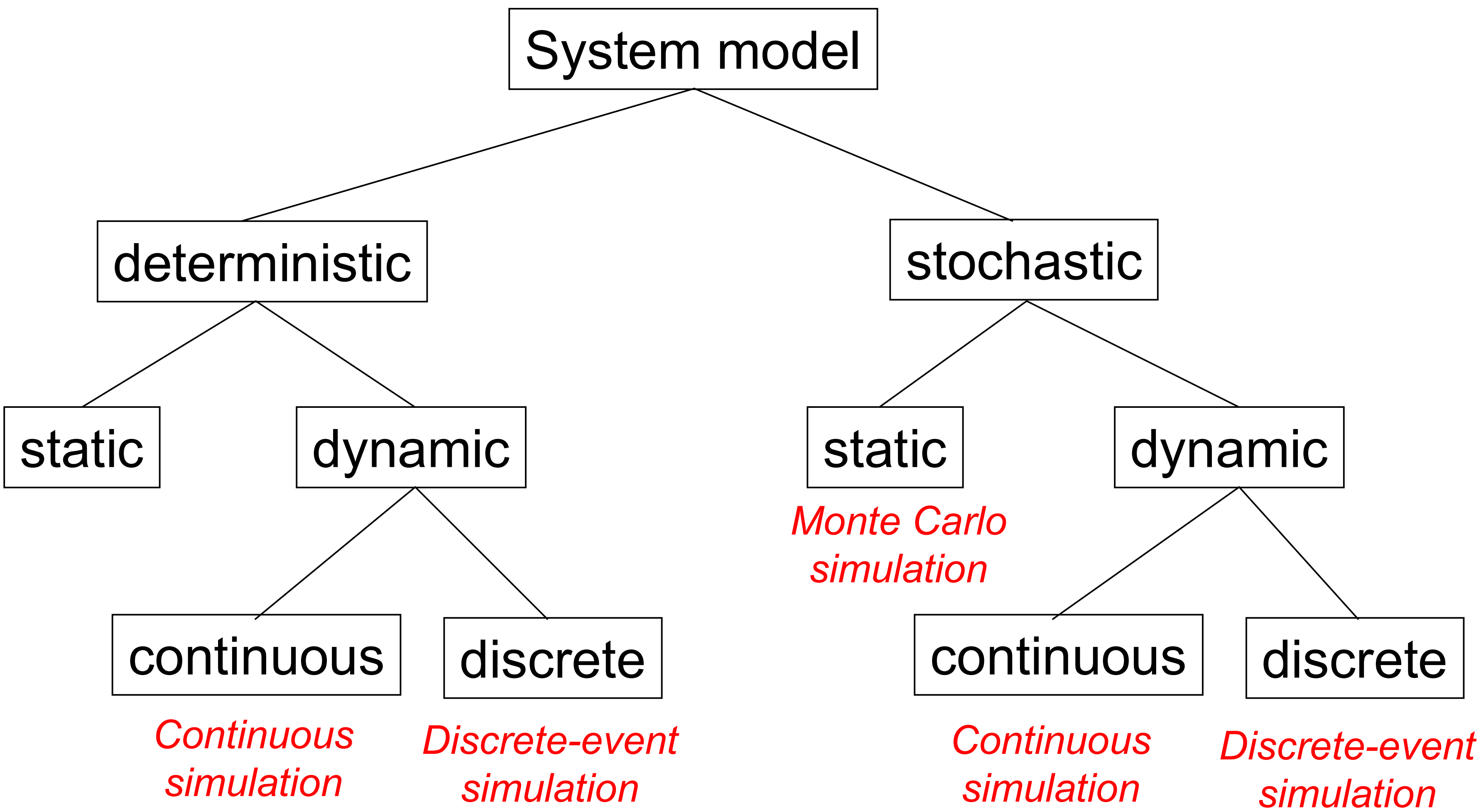
Types of Simulation Models

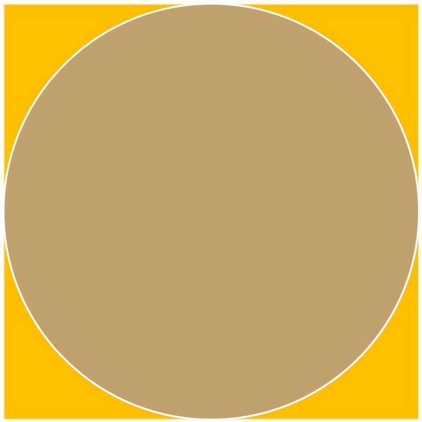


What is Monte Carlo Simulation ?

- **Monte Carlo methods** are a widely used class of **computational algorithms** for simulating the behavior of various physical and mathematical systems, and for other computations.
- **Monte Carlo algorithm** is often used to find solutions to mathematical numerical problems (which may have many variables) that cannot easily be solved, (e.g. integral calculus, or other numerical methods)
- Determine some value using random numbers that could be very difficult to do by other means
- Ex: Evaluating an integral that has no closed analytical form

Monte Carlo Simulation

- Before any formal definitions, let's consider a simple example
  - Let's assume we don't know the formula for the area of a circle, but we do know the formula for the area of a square
  - We'd like to somehow find the area of a circle of a given radius (let's say 1)



Monte Carlo Simulation

- Let's generate a (Big) number of random points in the square
    - Test to see if each point is also in the circle
        - Since we know the circle has a radius of 1, we can put its center at the origin and any random point a distance <= 1 from the origin is within the circle
    - The ratio of points in the circle to total points generated should approximate the ratio of the area of circle to the area of the square

Monte Carlo Simulation

- "Informal" theory behind M.C.
  - Consider a random experiment with possible outcome C
  - Run the experiment N times, counting the number of C outcomes, N_C
  - The relative frequency of occurrence of C is the ratio N_C/N
  - As N → ∞, N_C/N converges to the probability of C, or

$$p(C) = \lim_{N \to \infty} \frac{N_C}{N}$$

Monte Carlo Simulation

- In Probability: we determines probability of an event based on the number of ways it may occur out of the total number of possible outcomes that gives the "true" probability of a given event
- Whereas empirical probability only gives an estimate (since we cannot actually have N be infinity)
- However, for complex situations this could be quite difficult to do

– When axiomatic probability is not practical, empirical probability (Monte Carlo simulation) can often be a good substitute

- Can also be used to verify axiomatic results

M.C. in Integration

- Another common problem – evaluating an integral
  - Many integrals have no closed form and can also be very difficult to evaluate with "traditional" numerical methods
  - How can we use Monte Carlo simulation to evaluate these?
  - Let's look at this in a somewhat simplified way (i.e. we will be light on the theory)

Monte Carlo Simulation

- A scheme employing random numbers which is used to solve certain stochastic or deterministic problems where the passage of time plays no substantive role.
- Common problem is the estimation of $\int_{\Omega} f(\mathbf{x})d\mathbf{x}$, where *f* is a function, **x** is a vector and Ω is domain of integration.
- Special case: Estimate $\int_a^b f(x)dx$ for scalar *x* and limits of integration *a*, *b*

Monte Carlo Simulation

Let X be a uniform random variable on the interval [a, b] with density

$$p(x) = \frac{1}{b-a}, \quad a \le x \le b$$

and let x_1, …, x_n be a random sample from X. Then

$$\begin{aligned}
\int_a^b f(x)dx &= \int_a^b \frac{f(x)}{p(x)} p(x)dx \\
&= (b-a)\int_a^b f(x)p(x)dx \\
&= (b-a)E[f(X)] \\
&\approx \frac{b-a}{n}\sum_{i=1}^{n} f(x_i)\,.
\end{aligned}$$

Monte Carlo Simulation

Example: Estimate $\int_0^b \sin(x)dx$.

We approximate this by

$$\frac{b}{n}\sum_{i=1}^{n}\sin(x_i)\ ,$$

where x_1, …, x_n are a sample from a uniform [0, b] random variable.

Monte Carlo Simulation

Example: Estimate $\int_0^b \sin(x)dx$.

	n = 10	n = 100	n = 1000	n = 2000
b = 1 (answer = 2)	1.753	2.032	1.994	1.999
b = 2 (answer = 0)	-0.898	-0.013	0.137	0.079

There is considerable variability in the quality of solution; accuracy of numerical integration sensitive to integrand and domain of integration

Two Types of Approaches

- Direct
  - Obtain an analytical expression
  - Inverse transform
    - Requires inverse of the distribution function
  - Composition & Convolution
    - For special forms of distribution functions
- Indirect
  - Acceptance-rejection

Acceptance-Rejection Method

By Von Neumann (1951), used when the direct approaches fail or inefficient.

A closed form for F(X) does not exist, so what we'll do is to add another distribution . For which we know "how to calculate the CDF and its inverse".

We pick a function t(x) that is larger than f(x) for all x. Technically we say that t(x) *majorizes* f(x).

Acceptance-Rejection Method

- Specify a function that majorizes the density

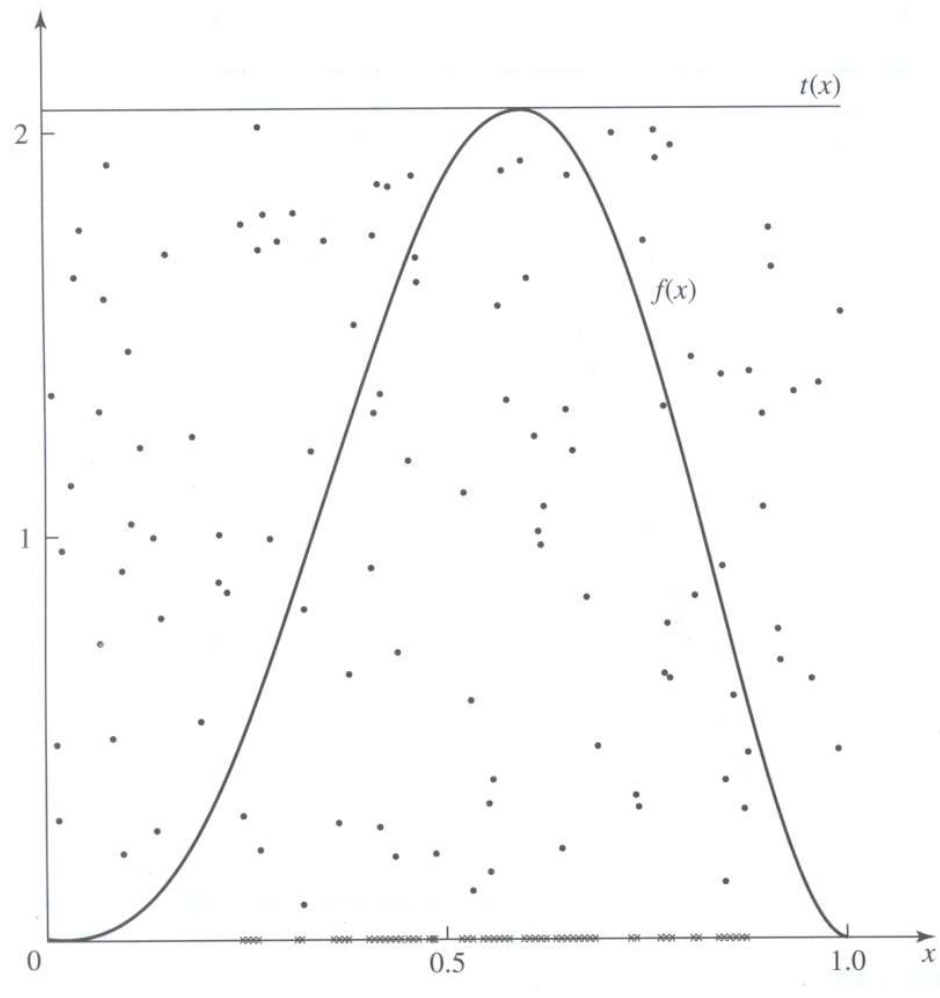
$$t(x) \geq f(x), \forall x$$

- *t(x) is clearly not a density fun.*
- New density function $$r(x) = t(x) \Big/ \int_{-\infty}^{\infty} t(x)dx$$
- Algorithm to generate a r.v. with density *f(x)*

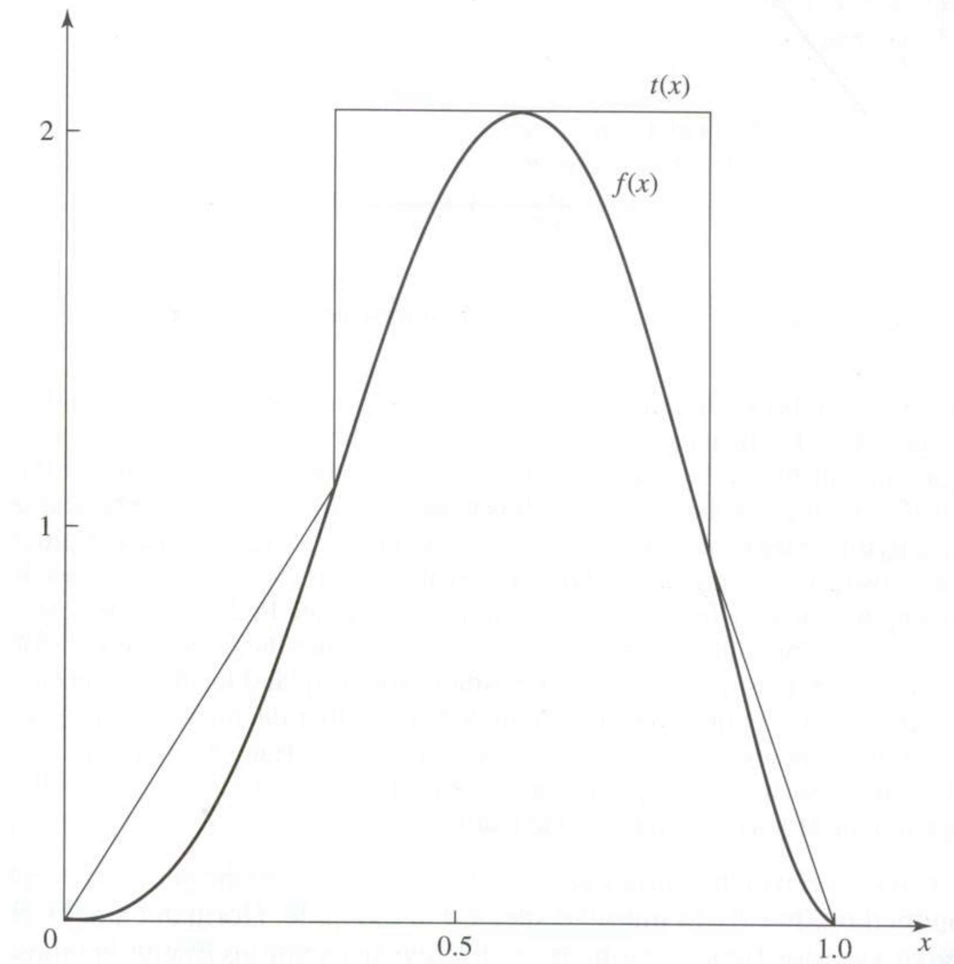
1. Generate Y with density r
2. Generate U independint of Y
3. If $U \leq f(Y)/t(Y)$, return $X = Y$.

   Otherwise go back to Step 1.

Example:



Example: More Efficient



Ex. Beta Distribution

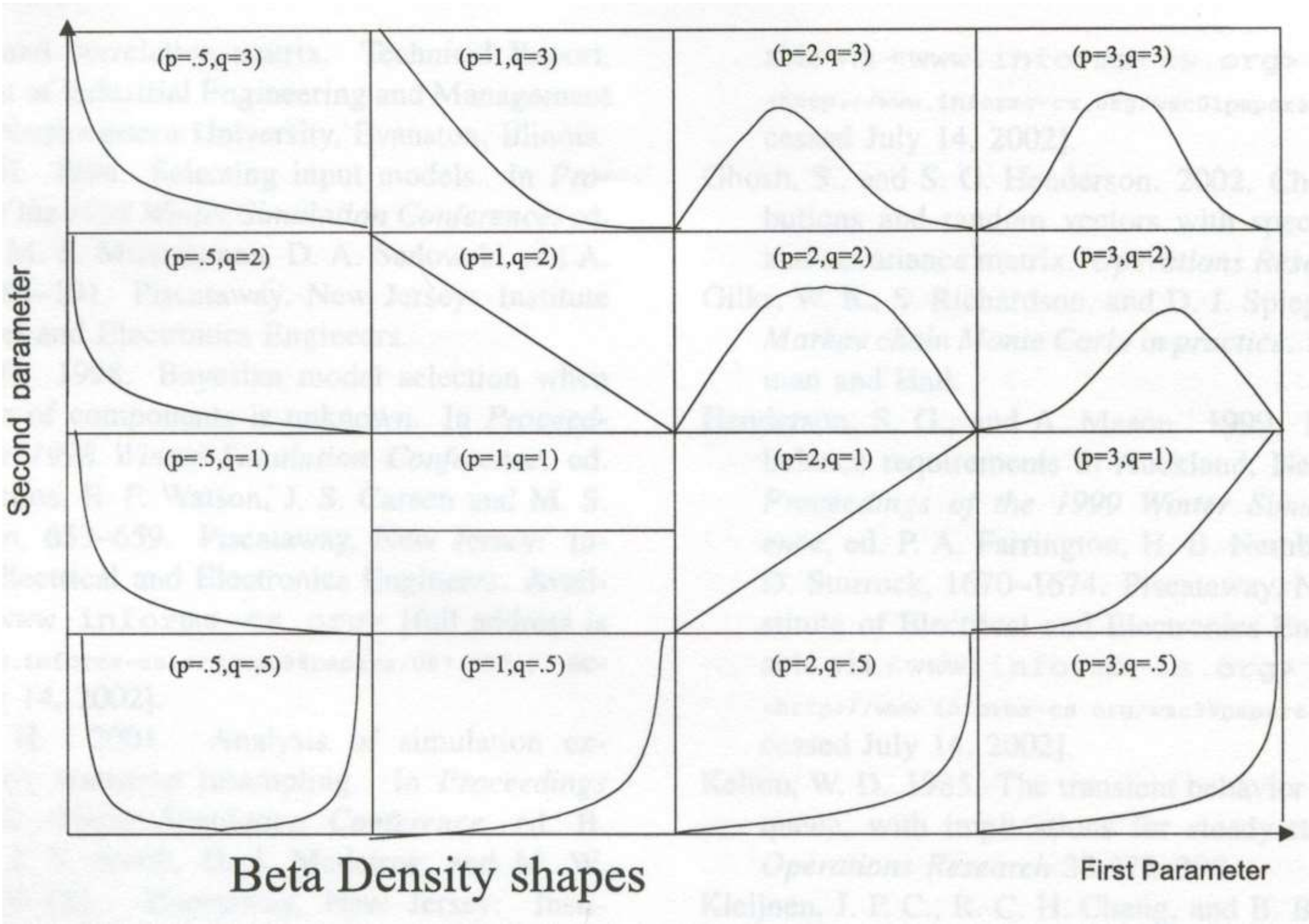
- Density

$$f(x) = \begin{cases} \dfrac{x^{\alpha_1 - 1}(1-x)^{\alpha_2 - 1}}{B(\alpha_1, \alpha_2)} & 0 < x < 1 \\ 0 & \text{otherwise} \end{cases}$$

$$B(\alpha_1, \alpha_2) = \int_0^1 t^{z_1 - 1}(1-t)^{z_2 - 1}\,dt$$

- No closed form CDF. No closed form inverse
- Must use numerical methods for inverse-transform method

Beta Distribution Shapes



Beta(4,3) Example

- Density $f(x)=\begin{cases}60x^3(1-x)^2 & 0<x<1\\ 0 & \text{otherwise}\end{cases}$
- The distribution *F(x)* is a 6th degree polynomial, The inverse approach is not a good one.
- Try to find *t(x)*

  put *df/dx =0 to* find the max of the f, which will be a *x =0.6* , and *f(0.6)=2.0736*
- Put

$$t(x)=\begin{cases}2.0736 & 0<x<1\\ 0 & \text{otherwise}\end{cases}$$

- Then $r(x)=\dfrac{t(x)}{\int_{-\infty}^{\infty}t(x)dx}=\dfrac{2.0736}{\int_0^1 2.0736dx}=1$

Beta(4,3) Example

So *r(x)* is just *U(0,1)*

The algorithm:

1. *Generate Y having density of r(x) ; i.e. U(0,1)*
2. *Generate U ~ U(0,1), independent of Y*
3. *If* $U \le \frac{f(Y)}{t(Y)}$ *, return X=Y; Otherwise go to step 1*

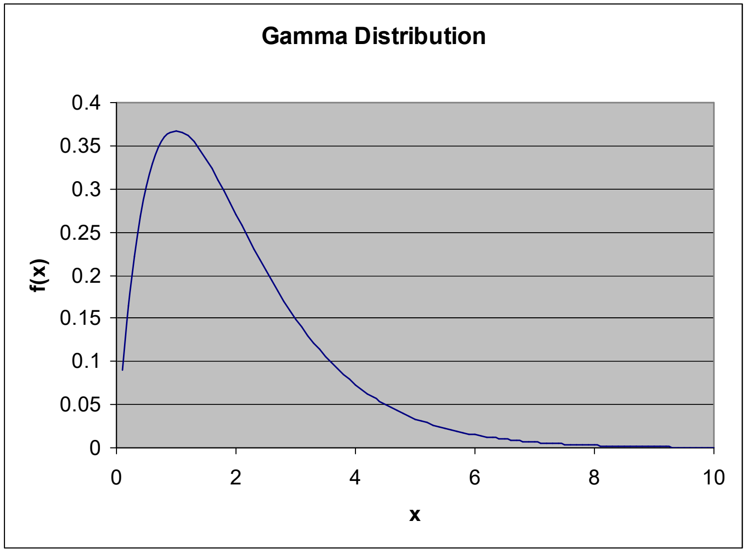
Acceptance – Rejection Technique for Gamma Dist.

A gamma(α,β) density

$$f(x) = \begin{cases} \dfrac{\beta^{-\alpha} x^{\alpha-1} e^{-x/\beta}}{\Gamma(\alpha)} & 0 < x \\ 0 & \text{otherwise} \end{cases}$$

where

$$\Gamma(\alpha) = \int_0^\infty y^{\alpha-1} e^{-1} dy$$

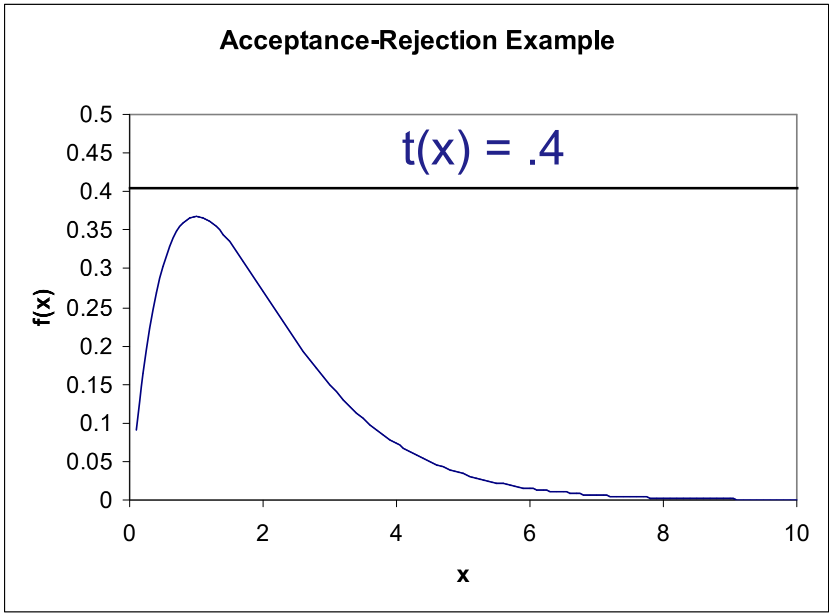


A closed form for F(X) does not exist,

Acceptance – Rejection Technique for Gamma Dist.

A gamma(2,1)

We pick a function t(x) that is larger than f(x) for all x.
t(x)=0.4



Acceptance-Rejection Gamma(2,1)

If we selected t(x) = .4 0 <= x <= 10

Now t(x) is not a density function, why?

since its integral from 0 to 10 doesn't add up to 1.

So let us define c: And r(x) = t(x)/c:

$$c = \int_0^\infty t(x)\,dx$$

$$= \int_0^{10} .4\,dx$$

$$= \Big|_0^{10} .4x$$

$$= 4$$

$$r(x) = .4/4$$

$$= .1$$

$$R(x) = \int_0^x .1dx'$$

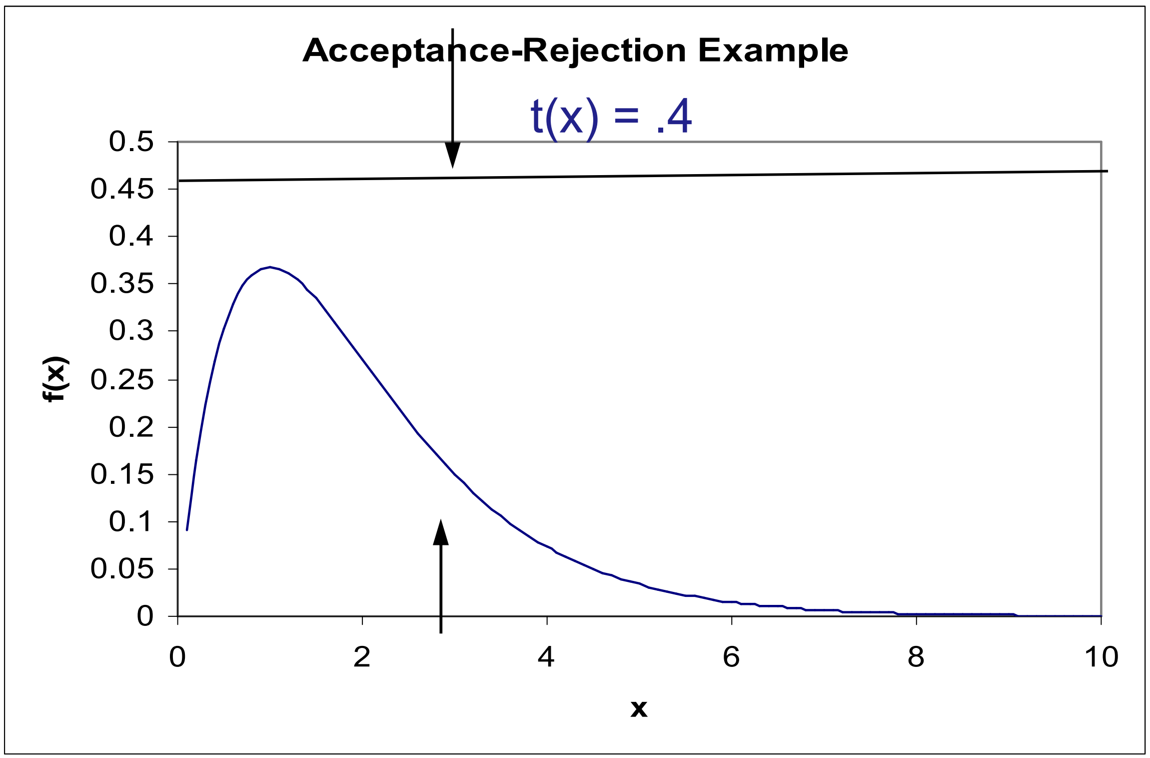
$$= .1x'$$

i.e. *r(x)* is a density fn.

Acceptance – Rejection

The inverse transformation for R: X = 10Y.

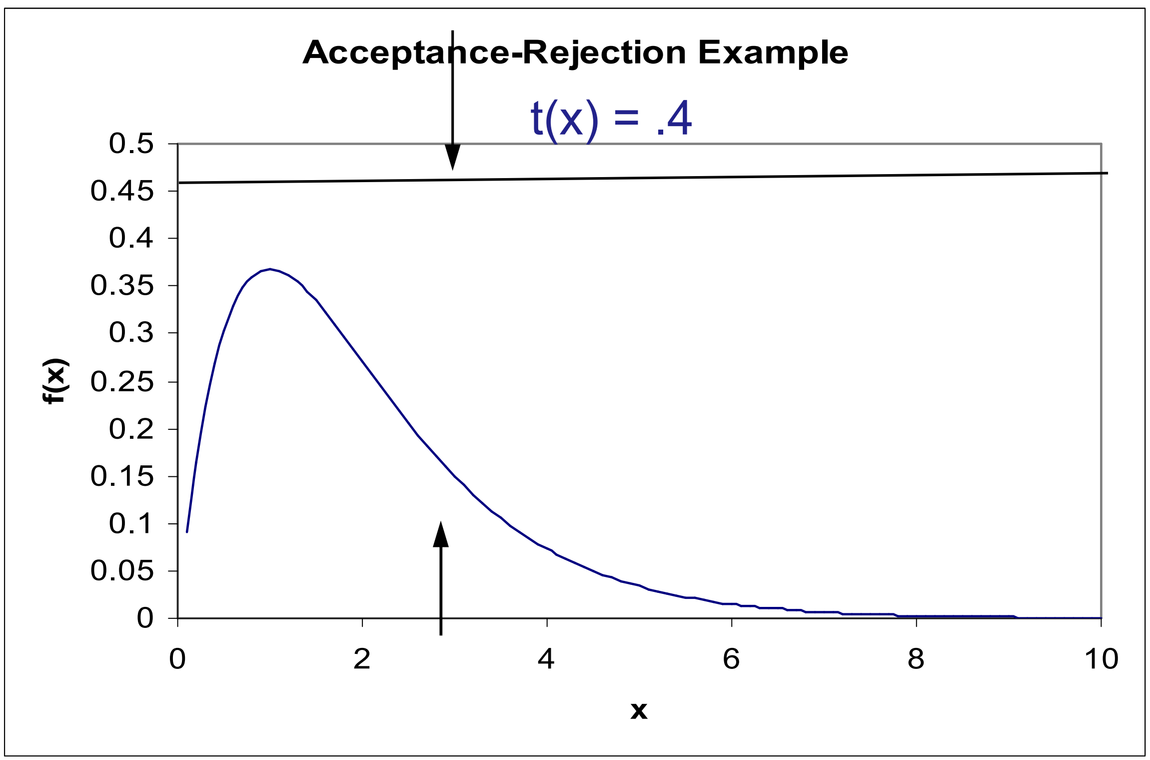
For a random number Y = 0.3,
This translates into an X of 3



If we threw darts that could land only on the line x = 3, then the probability that a dart hitting inside the distribution would be f(X=3)/t(X=3).

Acceptance – Rejection

f(X=.3)/t(X=.3)
= .15/.4
= .375



Generate U~U(0,1).

If U is less than .375, we will accept X= 3 as coming from a gamma(2,1) distribution.

Otherwise, we will start the process over by selecting a new R and new U.

Derived Distributions

- Several distributions are derived from the gamma and normal
- Can take advantage of knowing how to generate those two distributions