Goodness of Fit Tests

SYS-611: Simulation and Modeling

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Agenda

1. Review of Process Generators
2. Goodness of Fit Tests for Discrete Data
3. Goodness of Fit Tests for Continuous Data
4. Engineering Model Validation

Readings: J.V. Farr, “Review of Probability and Statistics,” Ch. 3 in *Simulation of Complex Systems and Enterprises,* Stevens Institute of Technology, 2007, pp. 39-47.

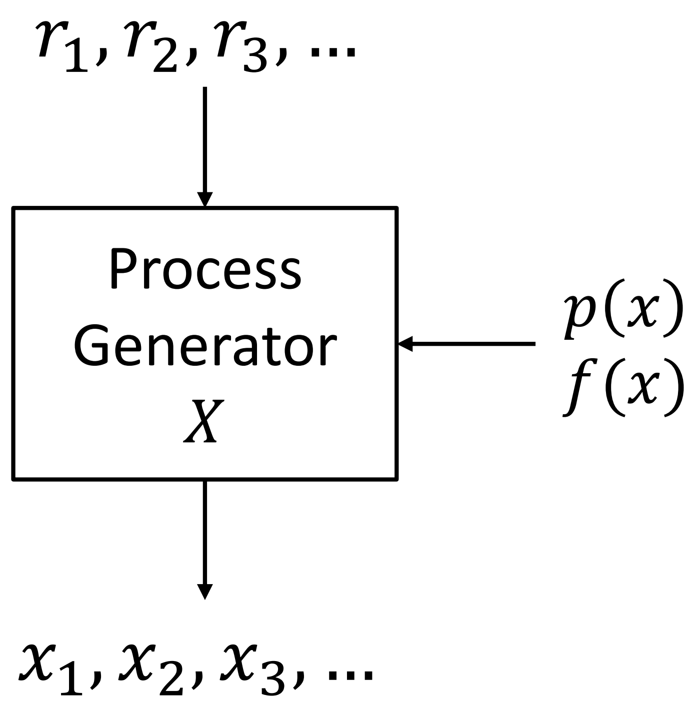
Optional: S.M. Ross, “Statistical Validation Techniques,” Ch. 9 in *Simulation*, McGraw-Hill, 2006, pp. 219-229.

G. Hazelrigg, “Thoughts on Model Validation for Engineering Design,” *Proceedings of the DETC’03*, Chicago, IL, 2003.

Review of Process Generators

Process Generator

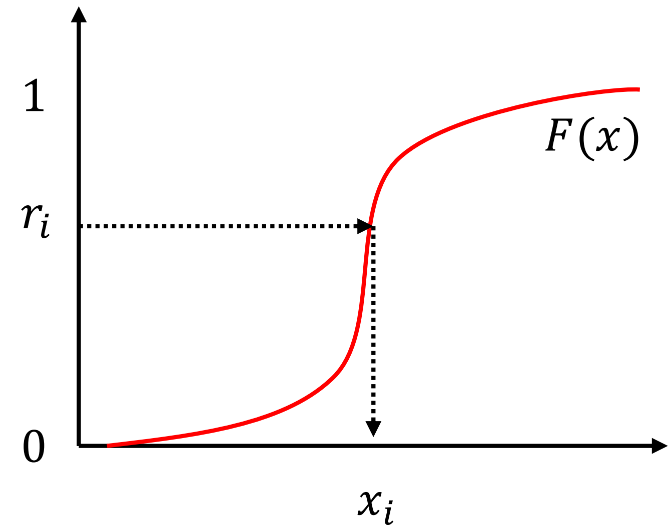
- Method to generate *simulated* random variables
- Requires a known probability distribution (PMF/PDF)
- Two classes of methods:
  - Inverse Transform
  - Accept-Reject



Inverse Transform Method

- Requires a known cumulative distribution function (CDF)
  - Must be able to describe the "inverse"
  - Visualized by tracing random y-axis to CDF

$$r = F(x) \Rightarrow x = F^{-1}(r)$$



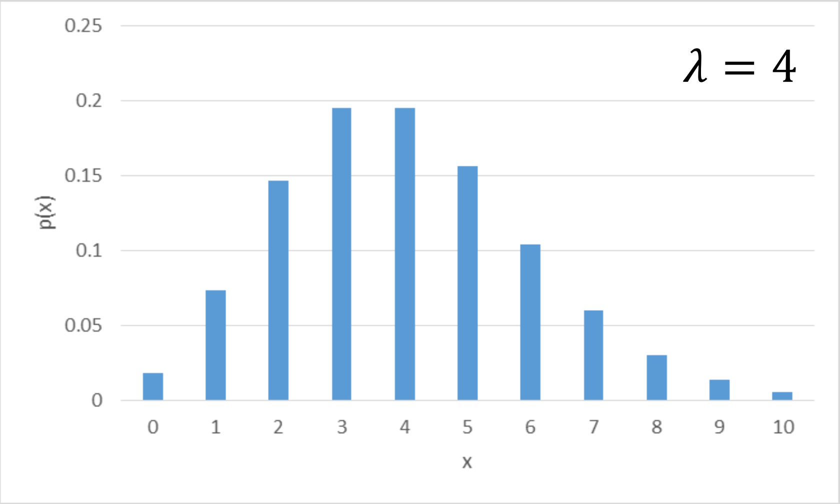
Poisson Generator

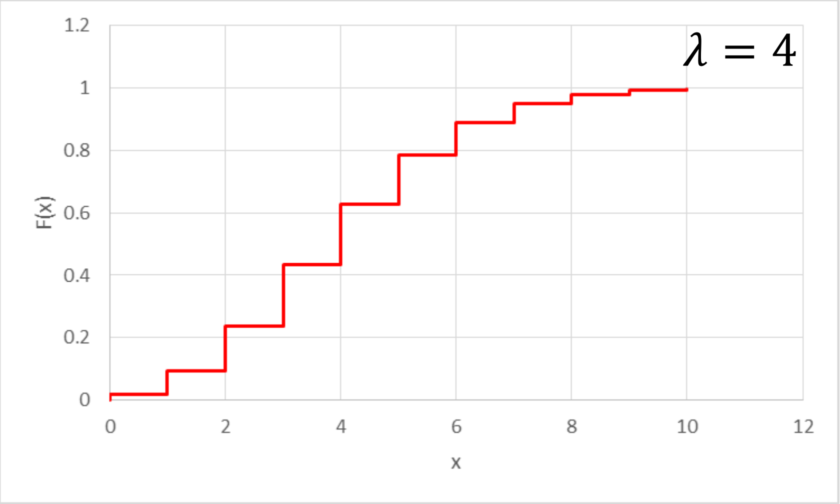
λ: mean event rate

$$p(x) = \frac{\lambda^x}{x!} e^{-\lambda}$$

$$F(x) = \sum_{i=0}^{x} \frac{\lambda^i}{i!} e^{-\lambda}$$

$$\Rightarrow x = \begin{cases} 0 & F(x) \le e^{-\lambda} \\ 1 & e^{-\lambda} < F(x) \le \sum_{i=0}^{1} \frac{\lambda^i}{i!} e^{-\lambda} \\ 2 & \sum_{i=0}^{1} \frac{\lambda^i}{i!} e^{-\lambda} < F(x) \le \sum_{i=0}^{2} \frac{\lambda^i}{i!} e^{-\lambda} \\ & \vdots \end{cases}$$





Exponential Generator

$\frac{1}{\lambda}$: mean inter-event time

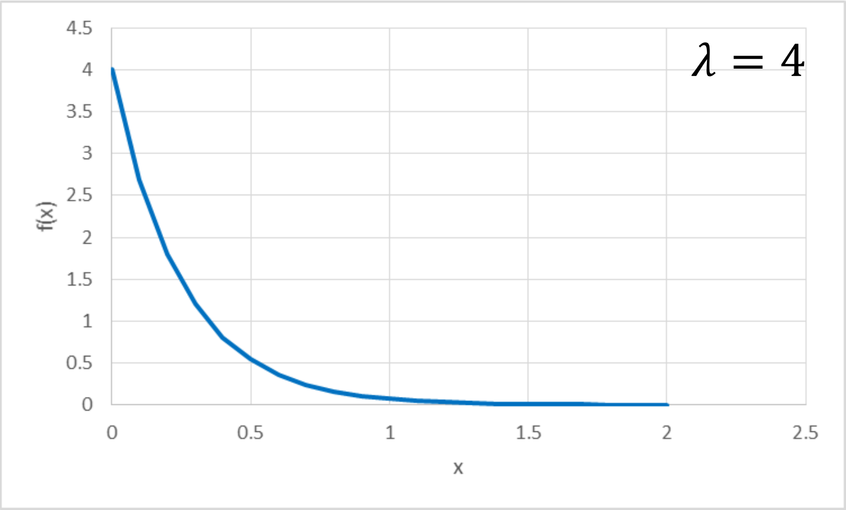
λ: mean event rate

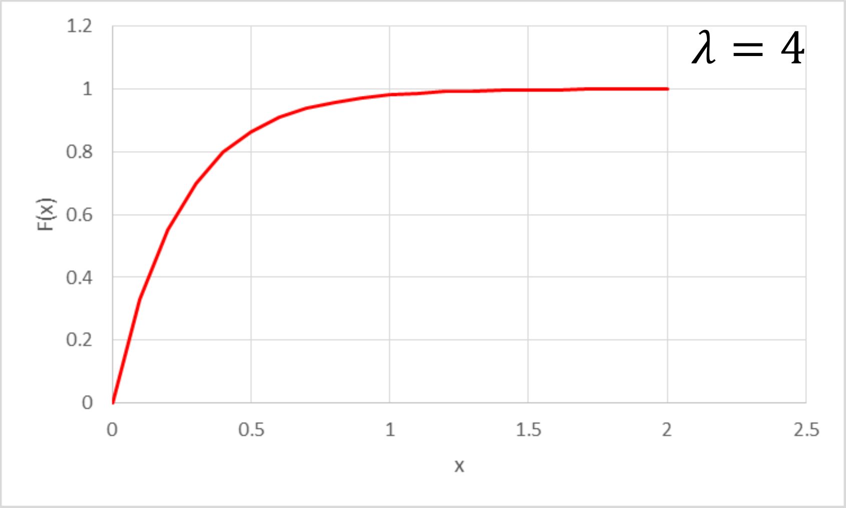
$$f(x) = \lambda e^{-\lambda x}$$

$$F(x) = \int_{i=0}^{x} \lambda e^{-\lambda i} di$$

$$= 1 - e^{-\lambda x}$$

$$\Rightarrow x = \frac{-\ln(1 - F(x))}{\lambda}$$





Goodness of Fit Tests for Discrete Data

Discrete Goodness of Fit Tests

A **Goodness of Fit** test checks if samples observed of a random variable come from a particular distribution

- Validate process generators with commonly-used distributions (e.g. Poisson, Binomial)
- **Pearson's Chi-squared (χ^2) Test**: requires large (>5) samples observed from most values
- **Fisher's Exact Test** (among others): handles small sample sizes but more complex

Pearson's Chi-squared (χ^2) Test

- **Pearson's chi-squared test** evaluates whether a set of samples follow a hypothesized distribution

  H_0: the data are consistent with a specified distribution

  H_a: the data are not consistent with a specified distribution

  - Should have 5+ observations for at least 80% of values
- Compares the following:
  - *Expected* or *theoretical* frequencies of categories
  - *Observed* or *actual* frequencies of categories

Dice Roller Data Set

- X: number of {3, 4, 5, 6} rolled in 10 dice
- Observed data (123 samples):

x_i	0	1	2	3	4	5	6	7	8	9	10
O_i	0	0	3	1	6	25	26	25	23	11	3

- Expected if $X \sim \text{binomial}(n = 10, p = 2/3)$:

$$E_i = N \cdot p(x_i), \qquad p(x) = \binom{10}{x}\left(1 - \frac{2}{3}\right)^{10-x}\left(\frac{2}{3}\right)^{x}$$

x_i	0	1	2	3	4	5	6	7	8	9	10
E_i	0.0	0.0	0.4	2.0	7.0	16.8	28.0	32.0	24.0	10.7	2.1

Combine for 5+ expected observations

Dice Roller Data Set

- X: number of {3, 4, 5, 6} rolled in 10 dice
- Observed data (123 samples):

x_i	0-4	5	6	7	8	9	10
O_i	10	25	26	25	23	11	3

- Expected if $X \sim \text{binomial}(n = 10, p = 2/3)$:

$$E_i = N \cdot p(x_i), \qquad p(x) = \binom{10}{x}\left(1 - \frac{2}{3}\right)^{10-x}\left(\frac{2}{3}\right)^{x}$$

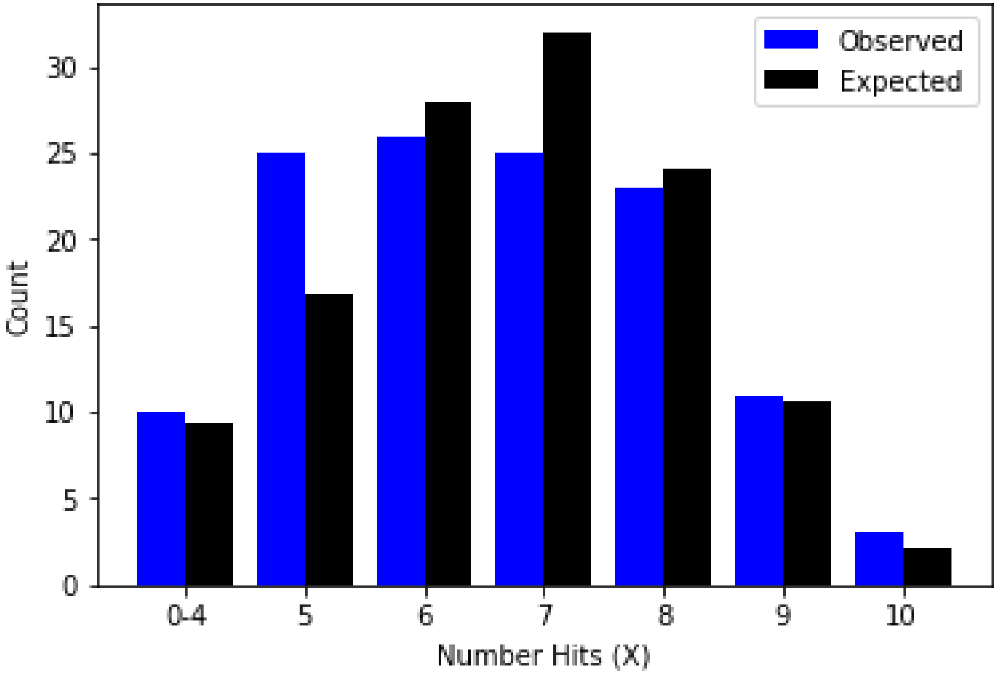
x_i	0-4	5	6	7	8	9	10
E_i	9.4	16.8	28.0	32.0	24.0	10.7	2.1

Chi-squared (χ^2) Test Statistic

$$T = \sum_{i=1}^{n} \frac{(O_i - E_i)^2}{E_i}$$

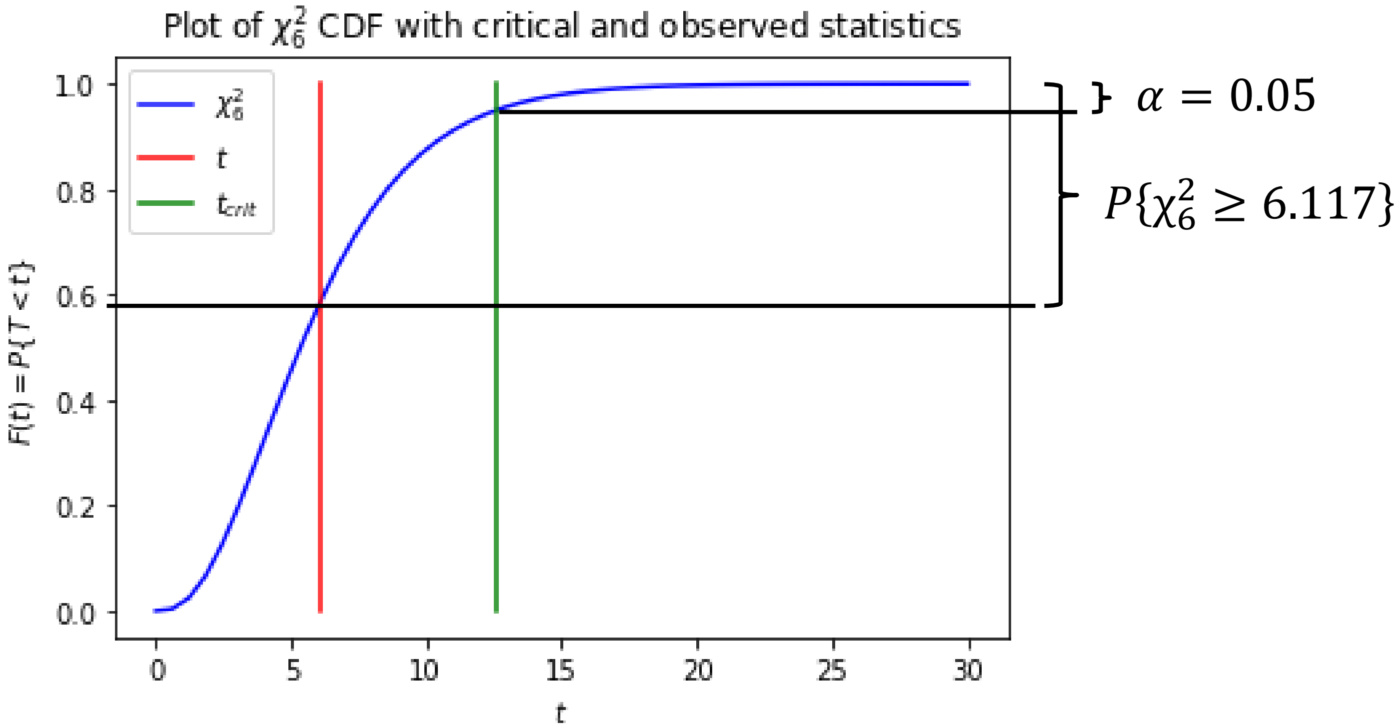
- N samples of n discrete values
- O_i observed samples for each value i
- E_i expected samples for each value i, $E_i = N * p(x_i)$
- p−value $= 1 - F_{\chi_k^2}(T)$
  - $F_{\chi_k^2}$: chi-squared CDF with $k = n - 1 - c$ degrees of freedom
  - c: number of distribution parameters estimated from samples
- Reject null hypothesis if p−value $< \alpha$ (bad distribution!)

Dice Roller Statistic



x_i	O_i	E_i	$\frac{(O_i - E_i)^2}{E_i}$
0-4	10	9.4	0.036
5	25	16.8	4.005
6	26	28.0	0.142
7	25	32.0	1.529
8	23	24.0	0.041
9	11	10.7	0.011
10	3	2.1	0.352
		$T =$	6.117
		$k =$	7-1=6

Dice Roller Test



$$p\text{−value} = 1 - F_{\chi^2_6}(6.117) = 0.41$$

→ Cannot Reject H_0: data similar to binomial distribution

→ 41% chance of a more extreme statistic under H_0

Goodness of Fit Tests for Continuous Data

Continuous Goodness of Fit Tests

A **Goodness of Fit** test checks if samples observed of a random variable come from a particular distribution

- Validate process generators with commonly-used distributions (e.g. Normal, Exponential)
- **Chi-squared (χ^2) Test**: group continuous variables in bins (same as discrete case)
- **Kolmogorov-Smirnov Test:** compare observed CDF (discrete) with expected CDF (continuous)
- **Anderson-Darling Test:** variation of K-S test

Kolmogorov-Smirnov (K-S) Test

- **Kolmogorov-Smirnov (K-S) test** evaluates whether a set of samples follow a hypothesized *continuous* distribution

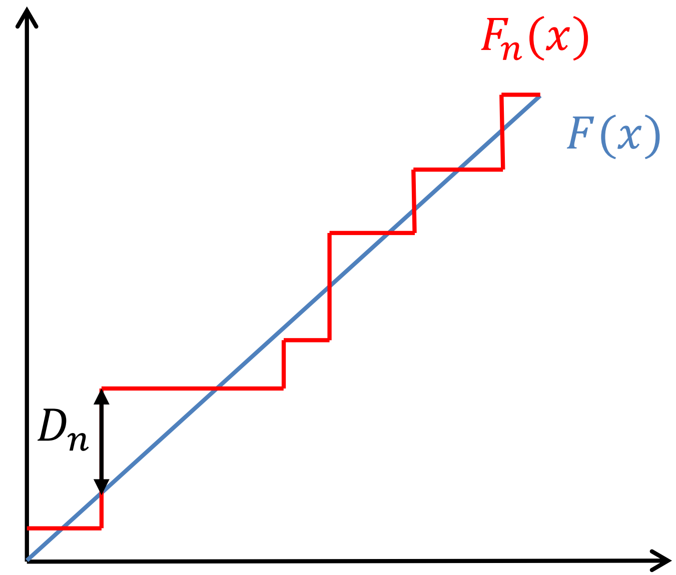
  H_0: the data are consistent with a specified distribution

  H_a: the data are not consistent with a specified distribution

- Compares the following:
  - *Expected* or *theoretical* CDF
  - *Observed* or *actual* CDF

K-S Test Statistic

- Test statistic D_n considers:
  - Largest vertical distance between observed and expected CDF
  - $F_n(x) = \frac{\text{\# samples} \leq \text{x}}{\text{\# samples}}$
  - $D_n = \max_{1 \leq i \leq N} \left(F(x_i) - F_n(x_{i-1}), F_n(x_i) - F(x_i) \right)$

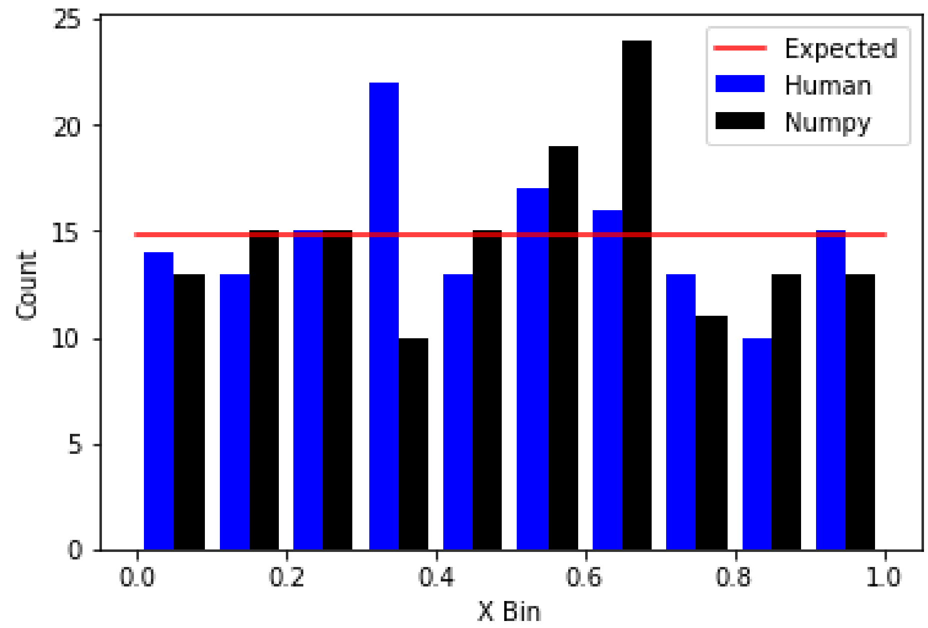


- Reject null hypothesis at significance level α if:

$P\{D_n \geq d_n\} = p{-}\text{value} < \alpha$ (use statistical software)

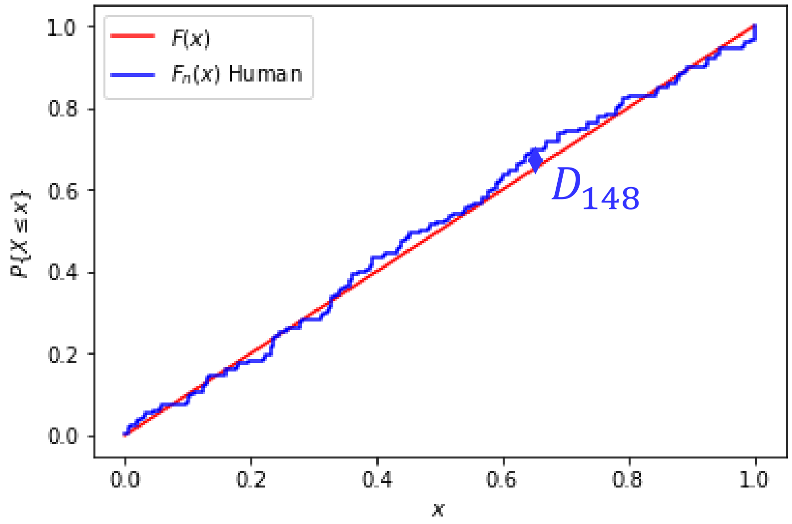
Human RNG Data

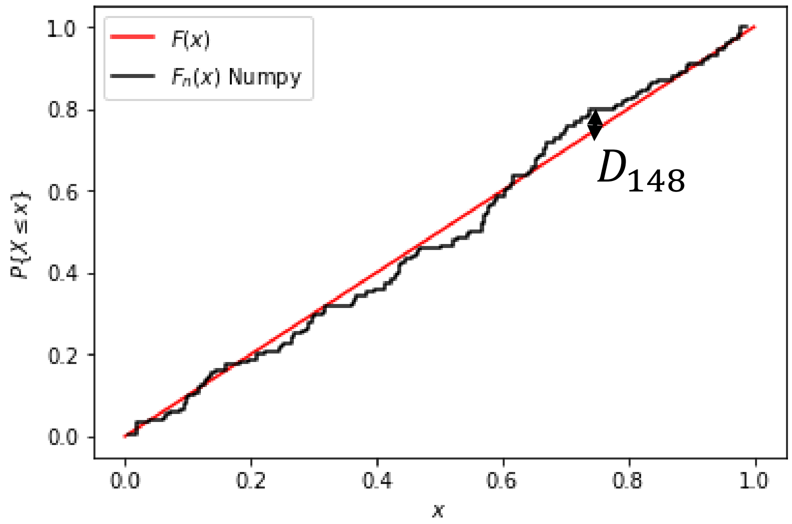
- Two U(0,1) sources with 148 samples:
  - Human samples
  - Numpy random.rand()
- Compare both with expected uniform (0,1) distribution
  - Examples use **`scipy.stats.kstest`**



Human RNG Statistic/Test

- Human samples
  - $D_{148} = 0.051$
  - $p-\text{value} = 0.84$
- Numpy samples:
  - $D_{148} = 0.067$
  - $p-\text{value} = 0.52$
- Both human and Numpy samples are similar to uniform (0,1) distributions!





Based on Hazelrigg (2003)

Engineering Model Validation

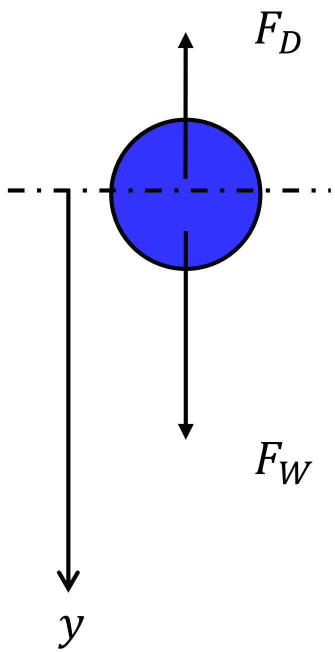
Scientific vs. Engineering

Based on Hazelrigg (2003)

- Science uses **models** to express causality
  - *Laws of nature* are “good” models that appear to be invariant and fixed over time and space
  - For example: $F = ma$
- Engineering uses **models** to represent physical artifacts and their behaviors
  - Necessary simplifications of reality, never perfect
  - Errors are dependent on the context

Example: Falling Object

Based on Hazelrigg (2003)



Natural Law

$$y = y_0 + \iint_{t_0}^{t} \frac{\sum F}{m} dt$$

Engineering Model

$$F_D = 0$$

$$F_W = mg$$

- No drag
- Earth surface

$$F_D = \frac{1}{2}\rho v^2 C_D A$$

$$F_W = G\frac{m_1 m_2}{r^2}$$

- Form drag
- Two-body gravity

Validity of engineering model is completely dependent on the application context

Use of Engineering Models

Based on Hazelrigg (2003)

- Not all engineering models must give **absolute measures** to be useful
- Models to inform decisions only need to **discriminate** between alternatives
  - Which is the better design to reduce drag?

vs.

- **Rational** decisions select the best alternative

Design Decisions

Based on Hazelrigg (2003)

- Must consider three things for design decisions:
  - **Alternatives**: various courses of action available
  - **Perceptions**: expectations of alternatives
  - **Preferences**: desirability of outcomes
- Only individuals make decisions
  - Act on behalf of own perceptions and preferences
  - Commit resources in the present
  - Seek preferred outcomes in the future

Models as Information Sources

Based on Hazelrigg (2003)

- **Model information quality** describes the probability a preferred choice leads to the most desirable outcome

- A model with **perfect information** guarantees the preferred choice has the best outcome
- **Valid models** produce high-quality information that leads to preferred choices/outcomes

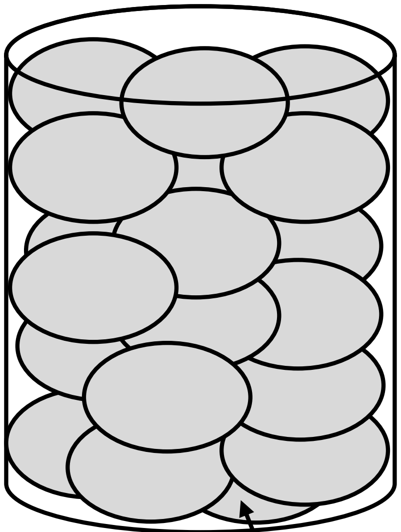
Guessing Game

Based on Hazelrigg (2003)

- **How many M&Ms are in the jar?**
- One guess per person, closest *without going over* wins the jar
- How can models provide information for this decision?
  - What are the alternatives?
  - What are your perceptions?
  - What are your preferences?

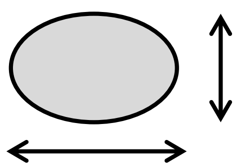
M&M Model

Based on Hazelrigg (2003)



$V = 1890 \pm 2\%\ \mathrm{mL}$ $\quad\mu = 0.55 \pm 20\%$

$V_c = \dfrac{\pi}{6} d^2 t$



$t = 0.6 \pm 10\%\ \mathrm{cm}$

$d = 1.4 \pm 10\%\ \mathrm{cm}$

$$N = \frac{V}{V_c}\mu = \frac{V}{\frac{\pi}{6} d^2 t}\mu$$

Volume of container:

$V \sim \mathrm{triangular}(1852, 1890, 1930)$

Diameter/thickness of M&M:

$d \sim \mathrm{triangular}(1.26, 1.4, 1.54)$

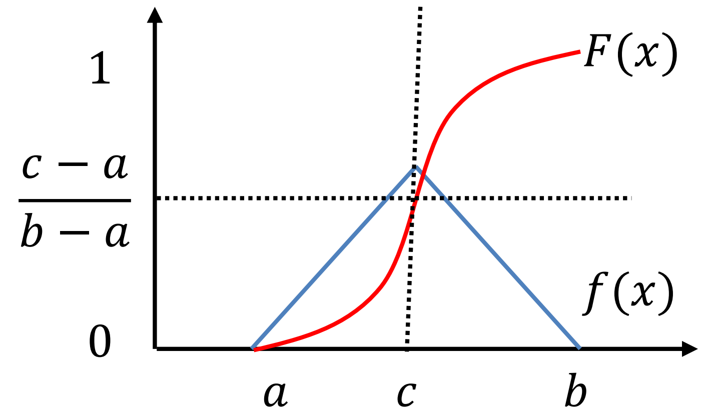
$t \sim \mathrm{triangular}(0.54, 0.6, 0.66)$

Packing factor:

$\mu \sim \mathrm{triangular}(0.44, 0.55, 0.66)$

Triangular Process Generators

$$f(x) = \begin{cases} \frac{2(x-a)}{(b-a)(c-a)} & a \le x \le c \\ \frac{2(b-x)}{(b-a)(b-c)} & c < x \le b \end{cases}$$



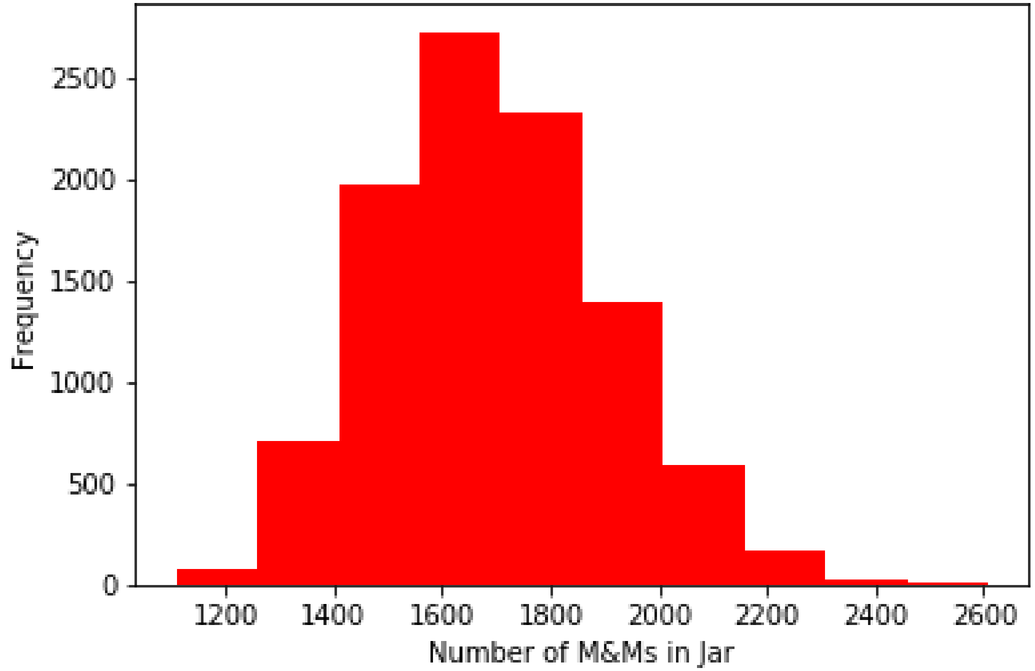
$$F(x) = \begin{cases} \frac{(x-a)^2}{(b-a)(c-a)} & a \le x \le c \\ 1 - \frac{(b-x)^2}{(b-a)(b-c)} & c < x \le b \end{cases}$$

$$x = F^{-1}(r) = \begin{cases} \sqrt{r(b-a)(c-a)} + a & r \le \frac{c-a}{b-a} \\ b - \sqrt{(1-r)(b-a)(b-c)} & r > \frac{c-a}{b-a} \end{cases}$$

(even easier in Python… `np.random.triangular(a,c,b)`)

Derived Distribution of N

- 10000 samples
- Mean: 1697
- Std. dev: 210.8
- Std. error: 2.1



Modeling Preference

- Derived state variable w shows whether a choice x wins the jar of M&Ms
  - Determined based on true number $N^\star$
  - Compare versus all others' choices $\boldsymbol{y}$

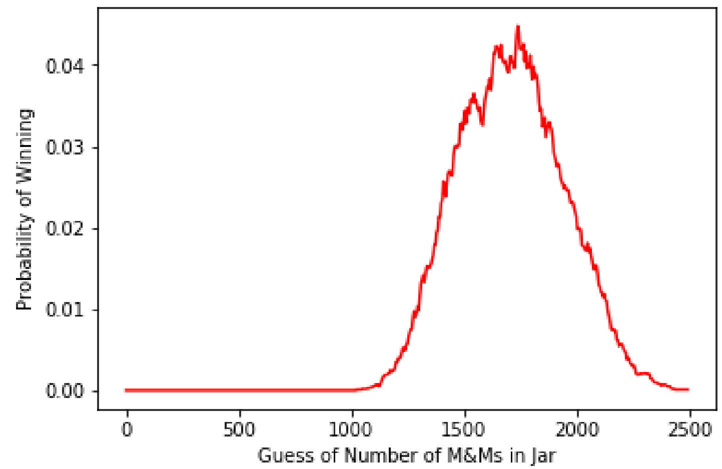
$$w(x, \boldsymbol{y}) = \begin{cases} 1 & if\ x \leq N^\star\ and\ x \geq j\ \forall\ j \in \boldsymbol{y}\text{: } j \leq N^\star \\ 0 & \text{otherwise} \end{cases}$$

- Model should estimate $p(w(x))$ from many trials
  - Find x to maximize probability of winning!
  - Try for 50 opponents…

Monte Carlo Simulation

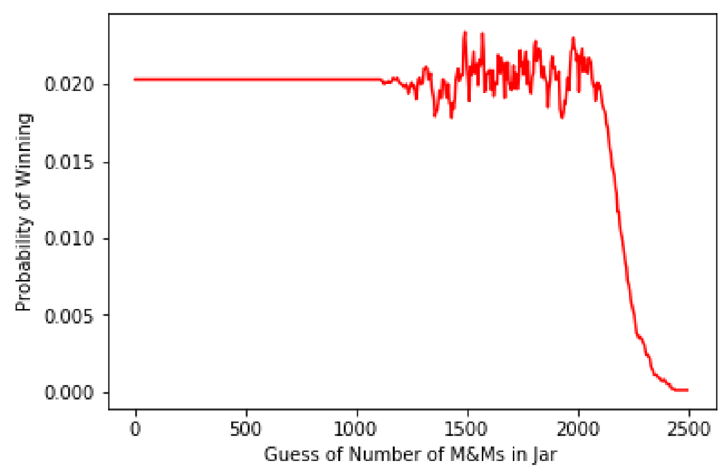
- Simple expectation of others' choices:

$$y \sim \text{triangular}(500{,}1600{,}2500)$$



- More advanced expectation of others' choices:

$$y \sim N$$



Committing Resources

- For question 7.1 on this week's assignment, take some time to do your own analysis…
  - "Le Parfait Super Terrines" 500ml jar, **overfilled** above max
  - Standard milk chocolate M&Ms
- Optional: submit your **one** final choice here:

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