FIT2086 Lecture 11
Simulation Based Statistical Methods

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Outline

Revision from last week (1)

- Unsupervised Learning
- n individuals, q attributes
  - No "target"; instead, discover structure inherent in data
- Clustering
  - Model the population as K distinct sub-populations
  - Learn both K and the subpopulation parameters
- k-means clustering algorithm
  - Allocate individuals to closest clusters
  - Re-estimate cluster centres
  - Iterate until convergence

Revision from last week (2)

- Mixture modelling
  - Model population as a mixture of subpopulations (classes)
  - Each subpopulation characterised by distributions
  - "Soft" assignment of individuals to classes
  - Intrinsic classification
- Matrix completion
  - Missing entries in our data matrix
  - Try to estimate the values of the missing data
  - Applications: imputation, recommender systems
  - Mixture modelling approach, k-NN approaches

Outline

Simulation Based Statistical Methods (1)

- Statistics began as a discipline in early 1910s
- From 1910s through to 1970s, most focus was on what could be done by hand
- Most developed methods were easy/possible to do using pen and paper
- Limited scope of what could be done
- In 1970s, advent of cheap(ish) digital computers changed things

Simulation Based Statistical Methods (2)

- The idea of simulation based methods to solve problems pre-dates computers
- Example problem from 18th century: Buffon's needle
  - Named after Georges-Louis Leclerc, Comte De Buffon
  - Asked the question:
    "Suppose we have a floor made of parallel strips of wood, each the same width, and we drop a needle onto the floor. What is the probability that the needle will lie across a line between two strips?"
- Solving this problem analytically is difficult; requires knowledge of integral geometry
- But a simple solution exists that requires no special knowledge

Simulation Based Statistical Methods (3)

- Simulation solution to Buffon's needle problem
- Repeatedly drop a needle onto a floor made of parallel strips of wood, and record the proportion of times the needle lines across a line between the two strips
- By weak law of large numbers, if we repeat this sufficient times, we can estimate the probability with increasing accuracy
- This is an example of a Monte Carlo method
  - Why is it called this?

Convergence of Empirical Probabilities (1)

- Previous problem an example of the following general problem
- Given RVs $X_1, \ldots, X_p \in \mathcal{X}$ from some population, find

$$\mathbb{P}(\{X_1, \ldots, X_p\} \in Z)$$

  where $Z \subset \mathcal{X}$
- That is, find the probability that the RVs take on values in some set Z
- Very general problem statement

Convergence of Empirical Probabilities (2)

- For example, let $X_1, X_2 \sim N(0,1)$; what is

$$\mathbb{P}(\sqrt{|X_1|} + \sqrt{|X_2|} > 2)?$$

is a problem of the previous form with

$$Z = \{x_1, x_2 : \sqrt{|x_1|} + \sqrt{|x_1|} > 2\}$$

- Or, let $X_1 \sim \mathrm{Poi}(\lambda_1)$ and $X_2 \sim \mathrm{Poi}(\lambda_2)$; what is

$$\mathbb{P}(X_1 - X_2^{3/2} > 0)?$$

is another problem of previous form with

$$Z = \{x_1, x_2 : x_1 - x_2^{3/2} > 0\}$$

- These problems can be answered analytically, but it is hard

Convergence of Empirical Probabilities (3)

- Trivial to propose problems that cannot be solved analytically
- Simulation based approach always provides a solution
- Algorithm:
  1. Randomly generate $X_1, \ldots, X_p$ from their distribution m times
  2. Estimate the probability using the empirical probability

$$\mathbb{P}(X_1, \ldots, X_P \in Z) \approx \frac{1}{m} \sum_{i=1}^{m} I(X_1, \ldots, X_P \in Z)$$

- Here, $I(\cdot)$ is the indicator function
  - Returns a one if the condition is met
  - Returns a zero otherwise
- The larger m, the more accurate the probability

Convergence of Empirical Probabilities (4)

- Proof that this approach works is straightforward
- Indicator function $I(\cdot)$ transforms our RVs into Bernoulli RVs
- Probability θ of success of this Bernoulli is

$$\mathbb{P}(X_1, \ldots, X_P \in Z)$$

- Then

$$\frac{1}{m} \sum_{i=1}^{m} I(X_1, \ldots, X_P \in Z)$$

  is the mean of our m Bernoulli RVs
- By weak law of large numbers

$$\frac{1}{m} \sum_{i=1}^{m} I(X_1, \ldots, X_P \in Z) \rightarrow \theta$$

  as $m \rightarrow \infty$.

Convergence of Empirical Probabilities (5)

- Example: Let $X \sim N(0,1)$, and find

$$\mathbb{P}(\sqrt{|X|} > 1)$$

- Let $Q = \sqrt{|X|}$; then the pdf of $Q = \sqrt{|X|}$ is

$$p(Q = q) = \left(\frac{2^3}{\pi}\right)^{\frac{1}{2}} q \exp\left(-\frac{q^4}{2}\right)$$

and

$$\mathbb{P}(Q > 1) = \int_1^\infty p(q)dq = 1 - \frac{2}{\sqrt{\pi}} \int_0^x \exp\left(-t^2\right) dt = 0.3171$$

- The integral can be evaluated using MATLAB/R as it is a standard integral (erf)

Convergence of Empirical Probabilities (6)

- To get an approximate answer using simulation is trivial

```
X = rnorm(m, 0, 1)
mean(sqrt(abs(X)) > 1)
```

- Results:
  - $m = 100$, estimate was 0.3300
  - $m = 1,000$, estimate was 0.3310
  - $m = 10,000$, estimate was 0.3179
  - $m = 100,000$, estimate was 0.3176
  - $m = 10^9$, estimate was 0.3172
- Recall exact probability is 0.3171

Convergence of Empirical Probabilities (7)

- In theory, for large enough m, one can always estimate any probability
- In practice, this simple approach may not always work well
- If m is the number of samples we have generated, then $1/m$ is the smallest non-zero probability we can estimate
  - This is the resolution of our estimate
- If the probability we are estimating is smaller than $1/m$, then we cannot estimate it well
- So for small probabilites p, we need a very large m, at least 10 times greater than $1/p$ to get a good estimate

Pseudo-Random Numbers (1)

- To use simulation we need to generate random numbers
- A computer is completely deterministic, so how to do that?
- We instead use pseudo random numbers
- A pseudo-random number generator is an algorithm that generates a sequence of numbers that
  - Are completely deterministic, assuming you know the process and the state of the algorithm
  - Are indistinguishable from true random numbers if you do not know the state

Pseudo-Random Numbers (2)

- The most important random numbers we need to generate are uniformly distributed
- The pdf for a uniformly distributed RV with support $(0, 1)$ is

$$p(X = x) = 1$$

- We can use uniformly distributed RVs to get RVs from any distribution
- Generating uniform RVs is a well studied problem
  - The SIMD-oriented Fast Mersenne Twister is cutting edge
  - It is fast, and has a period of up to $2^{2216091} - 1$ (before it repeats)

Pseudo-Random Numbers (3)

- Most uniform random number generators are based on

$$X_n \leftarrow f(X_{n-1}, X_{n-2}, \dots, X_0)$$

  where $f(\cdot)$ is a transition function.
- The initial choice of X_0 is called the seed
  - Usually chosen using the current time, or sometimes a "true" random number generator
- Given the same seed, the sequence of pseudo-random numbers will be identical
- This is a disadvantage, and an advantage
  - Disadvantage: good seeding is crucial
  - Advantage: your simulations can be exactly repeatable

Sampling Random Variables (1)

- Armed with the ability to generate uniform RVs, how to simulate from arbitrary distributions?
- For example, how to simulate RVs following a normal distribution?
- There are many, many algorithms to attack this problem; we will examine only one in detail
- The most straightforward is the inverse-CDF sampler
  - Easy to understand, very general
  - Often difficult to implement

Sampling Random Variables (2)

- Consider a RV X with pdf $p(X = x)$
- Recall the definition of the cumulative distribution function

$$\mathbb{P}(X \leq x) = \int_0^x p(x')dx'$$

  which is the probability that the RV X takes on a value less than or equal to x
- The inverse-CDF (quantile function) is then

$$Q(p) = \{x : \mathbb{P}(X \leq x) = p\}$$

  which finds the value x such that the probability that X is less than x is equal to p

Sampling Random Variables (3)

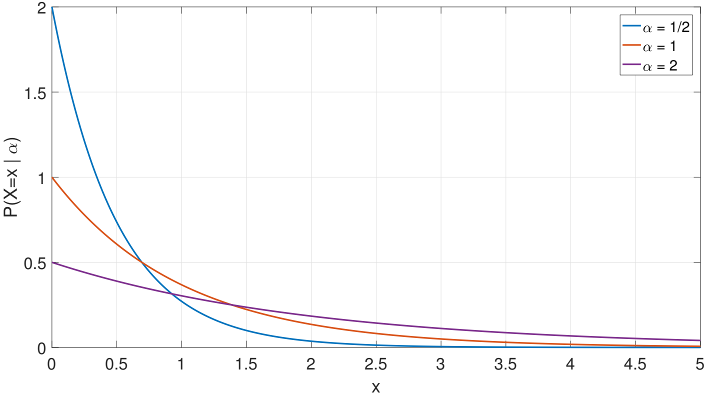
- Let $\mathrm{U}(a, b)$ denote a uniform distribution on (a, b)
- Given a target $p(X = x)$ and $Q(p)$, the inverse-CDF algorithm is:
  1. Generate $P \sim \mathrm{U}(0, 1)$
  2. Return $Y \leftarrow Q(P)$

- We first sample a uniformly distributed RV V from 0 to 1
- We then set Y equal to the value of x that satisfies $\mathbb{P}(X \leq x) = V$
- Then, Y will be randomly distributed as per our pdf $p(X = x)$
- Simple to understand, but efficiency depends on form of $Q(p)$

Example: Exponential Distribution (1)

- A RV X is follows an exponential distribution with scale α if

$$p(X = x) = \left(\frac{1}{\alpha}\right) \exp\left(-\frac{x}{\alpha}\right)$$



- Frequently used distribution in many areas of statistics

Example: Exponential Distribution (2)

- The CDF for an exponential RV is

$$\mathbb{P}(X \leq x) = 1 - \exp\left(-\frac{x}{\alpha}\right)$$

- The inverse-CDF is then

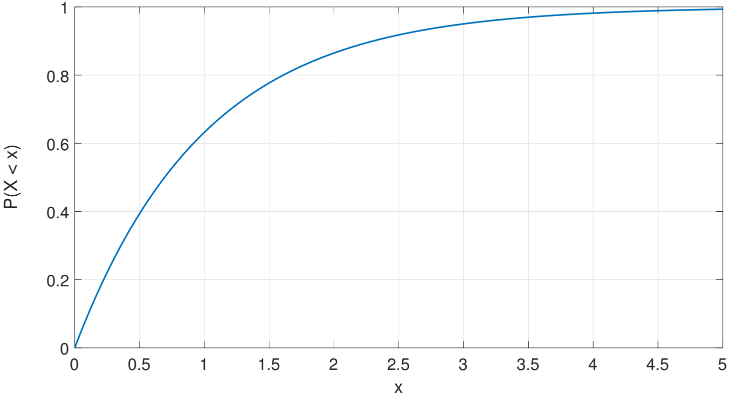
$$Q(p) = -\alpha \log(1 - p)$$

- So, if we follow the algorithm
  1. $V \sim \mathrm{U}(0, 1)$
  2. $X \leftarrow -\alpha \log(1 - V)$

  then $X \sim \mathrm{Exp}(\alpha)$

Example: Exponential Distribution (3)

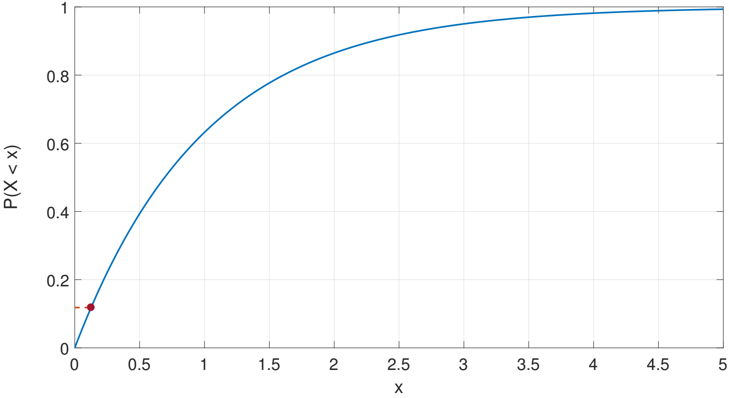
- CDF for exponential with $\alpha = 1$



- V :
- X :

Example: Exponential Distribution (4)

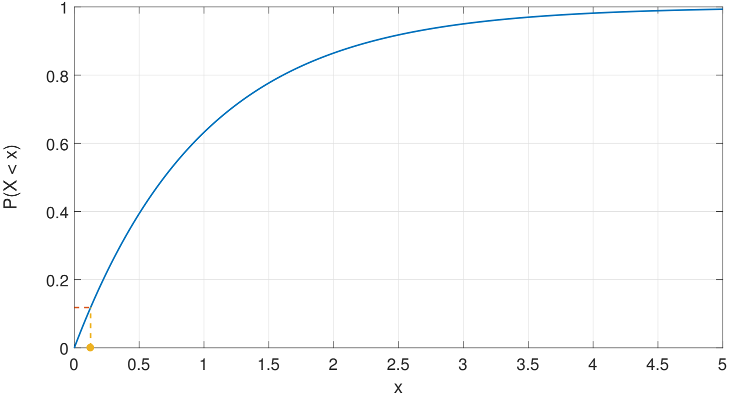
- CDF for exponential with $\alpha = 1$



- V : 0.1182
- X :

Example: Exponential Distribution (5)

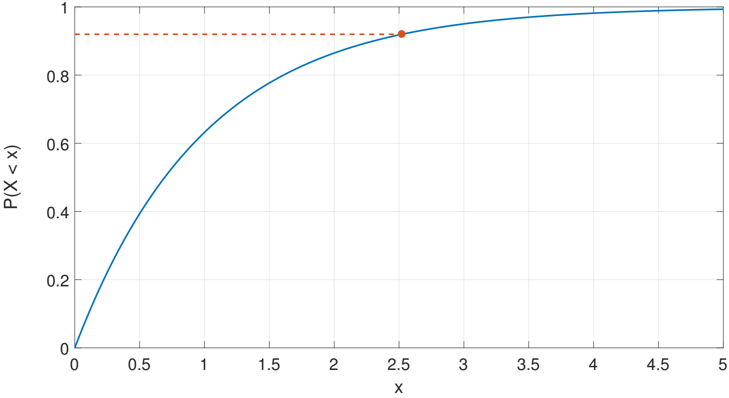
- CDF for exponential with $\alpha = 1$



- $V : 0.1182$
- $X : 0.1258$

Example: Exponential Distribution (6)

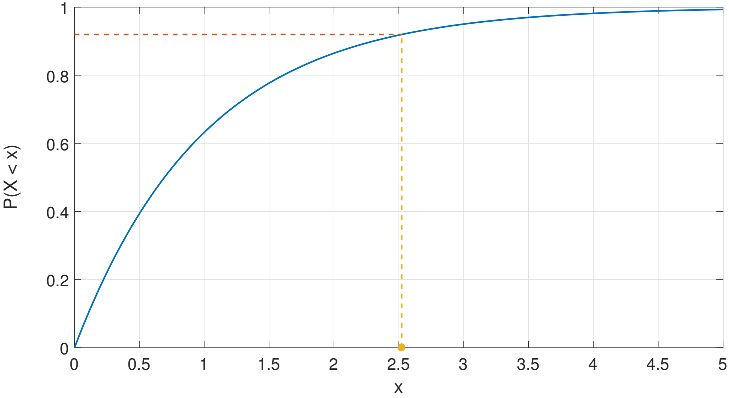
- CDF for exponential with $\alpha = 1$



- $V : 0.1182, 0.9197$
- $X : 0.1258$

Example: Exponential Distribution (7)

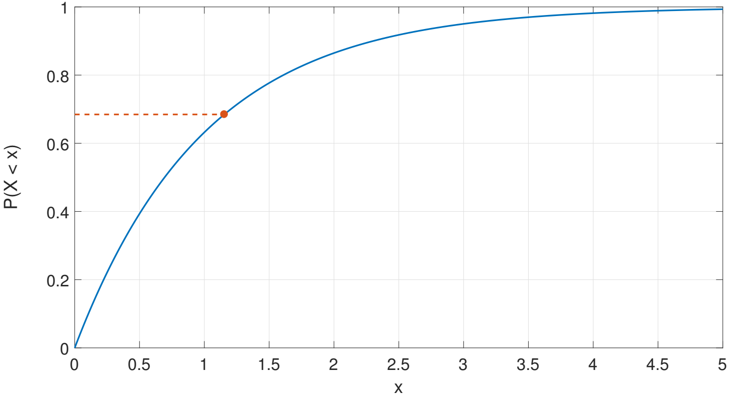
- CDF for exponential with $\alpha = 1$



- $V : 0.1182, 0.9197$
- $X : 0.1258, 2.5222$

Example: Exponential Distribution (8)

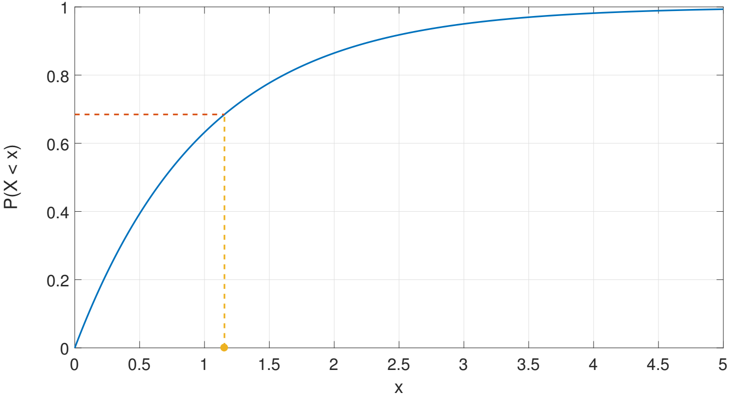
- CDF for exponential with $\alpha = 1$



- $V : 0.1182, 0.9197, 0.6846$
- $X : 0.1258, 2.5222$

Example: Exponential Distribution (9)

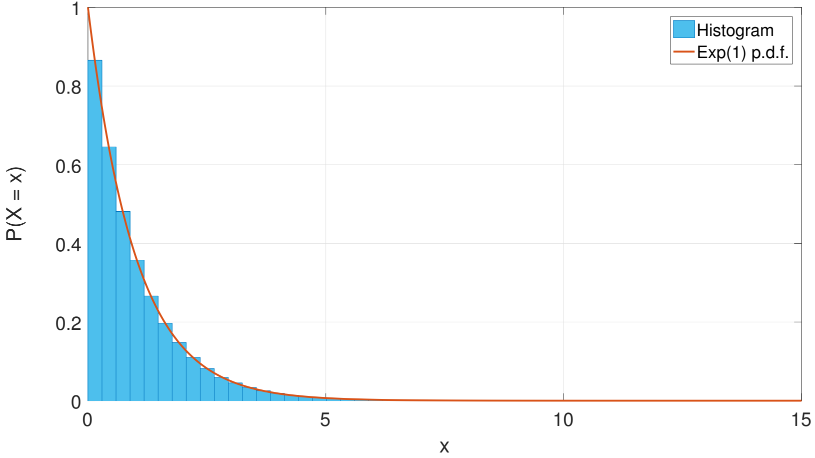
- CDF for exponential with $\alpha = 1$



- $V : 0.1182, 0.9197, 0.6846$
- $X : 0.1258, 2.5222, 1.1539$

Example: Exponential Distribution (10)

- Histogram for 10^6 samples from our random number generator



Other Sampling Algorithms

- Inverse-CDF method is good because:
  - Every sample X is independent
  - We need to generate only one RV (V) per sample
- Inverse CDF method requires access to the inverse CDF
  $\Rightarrow$ not always possible
- Some other methods for sampling RVs
  - Metropolis-Hastings algorithm
  - Accept-Reject algorithms
  - Adaptive rejection sampling
  - Slice sampling
- These often have different disadvantages:
  - Samples exhibit correlation (no longer independent)
  - May be very slow, require many random number generations

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Outline

1. Simulation Based Methods
   - Empirical Probabilities
   - Generating Random Numbers

2. Bootstrap Methods
   - The Bootstrap Algorithm
   - Permutation Testing

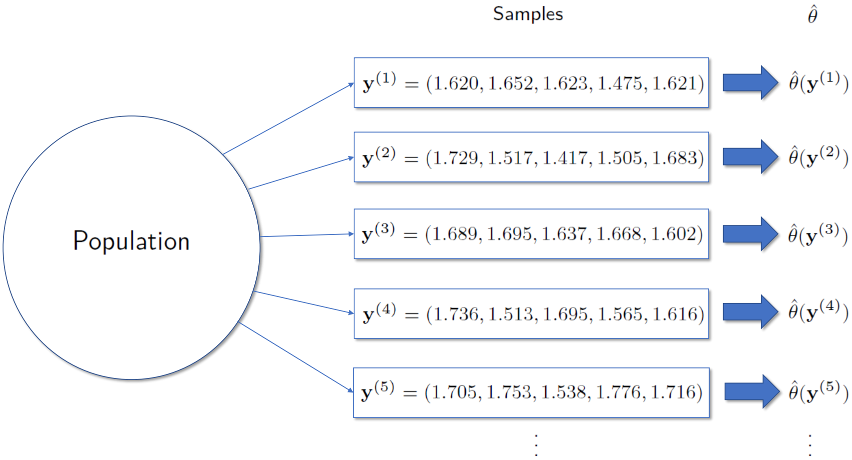
Data Resampling Methods (1)

- Bootstrap methods are one of the most widely used simulation based statistical methods
- They are part of the larger family of “resampling” methods
- We have already met one – cross validation
- In CV, we estimate prediction error on future data
- The bootstrap is about quantifying how variable our estimates are
    - Standard errors, confidence intervals, etc.

Data Resampling Methods (2)

- Recall the population-sample model of inference
- We have a (infinitely) large population
  - Characterised by some quantity θ
- We draw a *finite* sample of size n from our population
- Use this sample to estimate θ (call this $\hat{\theta}$)
- How much does this estimate vary if we draw a new sample from our population?

Data Resampling Methods (2)



Data Resampling Methods (3)

- In general, to analyse the behaviour of our estimate under repeated sampling, we need the sampling distribution
- This involves us specifying a population distribution we believe is appropriate
  - We must then derive the distribution of the estimate $\hat{\theta}$
- This can be difficult (or impossible), and relies on specific assumptions
- If $\hat{\theta}$ is equal to sample mean we need weaker assumptions
- But for general statistic, the problems remain

The Exact Bootstrap (1)

- In the 1970s several people proposed data resampling methods to solve this problem
- One of the most important is the bootstrap (Efron, 1970)
- The basic idea is that we should treat our sample as an estimate of our population
- We can then draw new samples from our this surrogate population
- Use this to define an empirical sampling distribution for statistic
- Relies on the fact that the as n increases, the sample probabilities are a consistent estimate of the population

The Exact Bootstrap (2)

- The bootstrap works by treating our sample as our population
- Form a distribution over all M possible combinations of data points you could form from the sample (with replacement)
- Let $\mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(M)}$ denote each of the combinations of data points you could form
- Compute our estimate of interest $\hat{\theta}$ for each combination
    - Call this quantity $\hat{\theta}^{(i)}$
- Let $\hat{\theta}$ denote the estimate from the original sample $\mathbf{y}$
    - We can then use the bootstrap distribution to estimate quantities such as bias

The Exact Bootstrap (3)

- For example, we can estimate the bias using:

$$\text{bias} = \frac{1}{M} \sum_{i=1}^{m} \hat{\theta} - \hat{\theta}^{(i)}$$

which is the average difference between the estimate on the original sample and the bootstrap estimates

- We can estimate the variance using

$$\text{Var} = \left(\frac{1}{M-1} \right) \sum_{i=1}^{M} \left(\hat{\theta}^{(i)} - \frac{1}{M} \sum_{j=1}^{M} \hat{\theta}^{(j)} \right)^2$$

which is the empirical variance of our bootstrap samples of $\hat{\theta}$

- Confidence intervals can be obtained using percentiles of the bootstrap estimates

The Exact Bootstrap: Example (1)

- As an example, consider the sample

$$\mathbf{y} = (2, 6, 3)$$

- Compute the bootstrap distribution for the sample mean $\bar{Y}$

$$\begin{array}{ccc}
(2,2,2) & & 2 \\
(2,2,6) & & 3.3333 \\
(2,2,3) & & 2.3333 \\
(2,6,2) & & 3.3333 \\
(2,6,6) & \stackrel{\bar{Y}}{\Longrightarrow} & 4.6667 \\
\vdots & & \vdots \\
(3,3,2) & & 2.6667 \\
(3,3,6) & & 4 \\
(3,3,3) & & 3
\end{array}$$

The Exact Bootstrap: Example (1)

- Using this exact bootstrap distribution we find

$$\text{bias} = 0$$

and

$$\text{Var} = 1$$

- Note that we made no assumptions about the distribution of the population
  - The exact bootstrap distribution, and therefore estimates from bootstrap, become more accurate as n increases
- But the number of different bootstrap samples $M = n^n$
  $\Rightarrow$ the exact bootstrap rapidly becomes infeasible

The Bootstrap Algorithm (1)

- Let $\mathbf{y} = (y_1, \ldots, y_n)$ be a sample of size n from an unknown population
- Let $\hat{\theta}$ be the estimate of our statistic on the full sample $\mathbf{y}$
- The bootstrap algorithm: For $i = 1$ to m $(m \ll M)$
  1. Create a new sample of size n by sampling with replacement from $\mathbf{y}$
  2. Compute the estimate $\hat{\theta}^{(i)}$ of our statistic based on this new sample
- This is called a resampling procedure
- $\hat{\theta}^{(1)}, \ldots, \hat{\theta}^{(m)}$ is as estimate of bootstrap distribution
- The larger the m, the closer the bootstrap is to the exact bootstrap
  - Often works well even for values of $m = 1,000$

The Bootstrap Algorithm (2)

- The bootstrap is very general
- For example, imagine we have a linear regression model
- We can calculate the mean-squared prediction error on the data we used to fit the model
  - This will be optimistic, as we have used the training data twice
- It would be useful to get a confidence interval on this statistic
  - Will give us a range of plausible values of error for future data
- To do this using bootstrap
  - Resample m bootstrap samples
  - Fit models using these samples and calculate mean-squared error of our fit
  - Use set of different MSE values to get a confidence interval

Example: Supervised Learning

- Example: predicting `BP` (our y) using `Age`, `Weight`, `BSA`
- Example, forming a single bootstrap sample

Original Data

BP	Age	Weight
105	47	85.4
115	49	94.2
116	49	95.3
117	50	94.7
112	51	89.4
121	48	99.5
110	47	90.9
115	49	94.1
125	52	101.3

$\Longrightarrow$

Bootstrap Sample

BP	Age	Weight

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$\Longrightarrow$

Bootstrap Sample

BP	Age	Weight	I
115	49	94.1	8

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125	52	101.3	9
121	48	99.5	6
105	47	85.4	1
116	49	95.3	3
112	51	89.4	5
125	52	101.3	9

The Bootstrap

- Strengths of the bootstrap
  - Only assumption made is that our sample is representative of our population
  - Easy to code, easy to apply
  - Accuracy of estimates increases with increasing sample size
- Weaknesses of the bootstrap
  - Can be slow if estimates are slow to compute
  - For small n accuracy is not necessarily good
  - Might need large m to get "smooth" distribution
  - Cannot be applied to some problems without modifications, e.g., lasso

Permutation Tests (1)

- The bootstrap is usually used to estimate sampling statistics
  - Bias
  - Standard errors
  - Confidence intervals
- Another important statistic based on sampling distributions are p-values
- We can use another resampling technique called permutation tests to estimate these
- These are particular useful for testing hypotheses of association
  - E.g., supervised learning of y given predictors

Permutation Tests (2)

- Consider n pairs of targets y_i and predictor values x_i
  - Is y associated with x using a linear model?
- We want to test

$$H_0 : \beta = 0 \text{ vs } H_A : \beta \neq 0$$

- The usual procedure is to
  1. Specify a distribution for the population
  2. Calculate a test statistic (i.e., the least-squares estimate $\hat{\beta}$)
  3. See how likely our observed statistic would be under the null distribution
- The p-value depends crucially on
  - The choice of assumed distribution for the population
  - The ability to derive the null distribution for our statistic accurately (often CLT is used)

Permutation Tests (3)

- The permutation test approach resamples the y values to approximate the (unknown) null distribution
- The permutation test algorithm: for $i = 1$ to m
  1. Randomly permute the values of the targets
  2. Calculate our association statistic of interest; call it $\hat{\theta}^{(i)}$
- Then we calculate the association statistic on our data
- And see how likely it would be to arise under our permutation distribution $\hat{\theta}^{(1)}, \ldots, \hat{\theta}^{(m)}$
  - This is our p-value of association
- The key idea is that permutations of the y's will not be associated with the predictors, so we can see how the estimates vary under our null distribution

Permutation Test: Example (1)

- Consider the following dataset (we examined in Lecture 6)

Pt	BP	Age	Weight	BSA	Dur	Pulse	Stress
1	105	47	85.4	1.75	5.1	63	33
2	115	49	94.2	2.10	3.8	70	14
3	116	49	95.3	1.98	8.2	72	10
4	117	50	94.7	2.01	5.8	73	99
5	112	51	89.4	1.89	7.0	72	95
6	121	48	99.5	2.25	9.3	71	10
7	121	49	99.8	2.25	2.5	69	42
8	110	47	90.9	1.90	6.2	66	8
9	110	49	89.2	1.83	7.1	69	62
10	114	48	92.7	2.07	5.6	64	35
11	114	47	94.4	2.07	5.3	74	90
12	115	49	94.1	1.98	5.6	71	21
13	114	50	91.6	2.05	10.2	68	47
14	106	45	87.1	1.92	5.6	67	80
15	125	52	101.3	2.19	10.0	76	98
16	114	46	94.5	1.98	7.4	69	95
17	106	46	87.0	1.87	3.6	62	18
18	113	46	94.5	1.90	4.3	70	12
19	110	48	90.5	1.88	9.0	71	99
20	122	56	95.7	2.09	7.0	75	99

- We want to model blood pressure using Age

Permutation Test: Example (2)

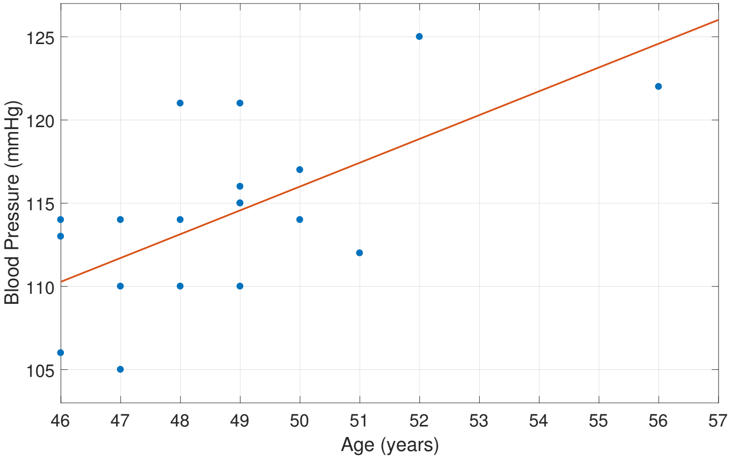
- Fit `Age` to `BP` using least-squares regression
  - $\hat{\beta} = 1.4310$
  - p-value of association (t-test) $= 0.00157$
- p-value was calculated under assumption population is normal
- To calculate a p-value using permutation test
  - Permute y (`BP`) values m times, then fit `Age` to `BP`
  - Store each permutation estimate as $\hat{\beta}^{(i)}$
- Calculate the p-value using

$$p \approx \frac{1}{m} \sum_{i=1}^{m} I\left(|\hat{\beta}^{(i)}| > |\hat{\beta}|\right)$$

i.e., the proportion of times the absolute value of estimate $\hat{\beta}$ obtained on our data exceeds the absolute value of the estimates obtained from our permutations

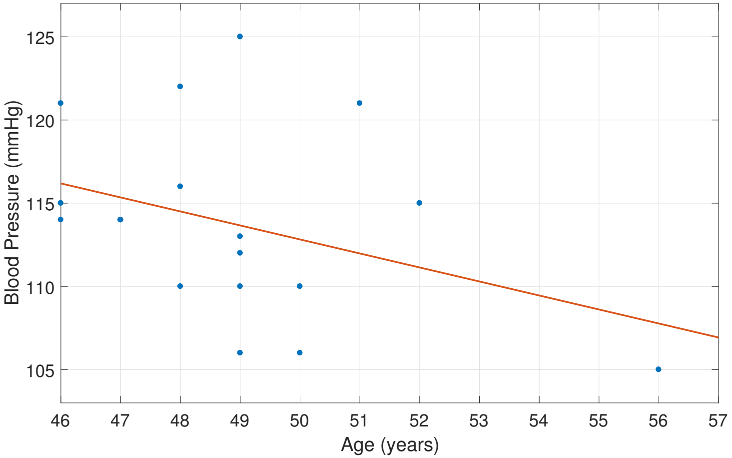
Permutation Test: Example (3)

- Unpermutated data: $\hat{\beta} = 1.4310$



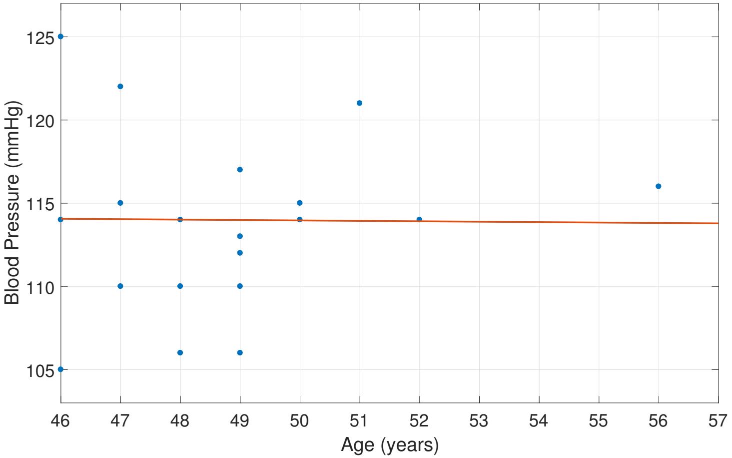
Permutation Test: Example (4)

- Permuation: $\hat{\beta} = -0.8418$



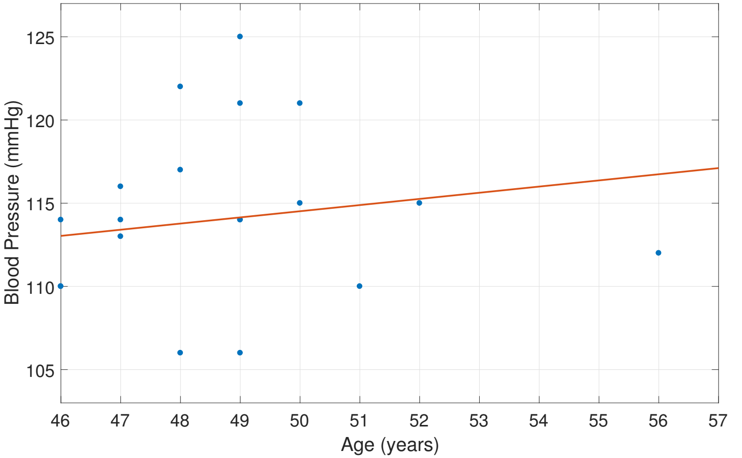
Permutation Test: Example (5)

- Permuation: $\hat{\beta} = -0.0253$



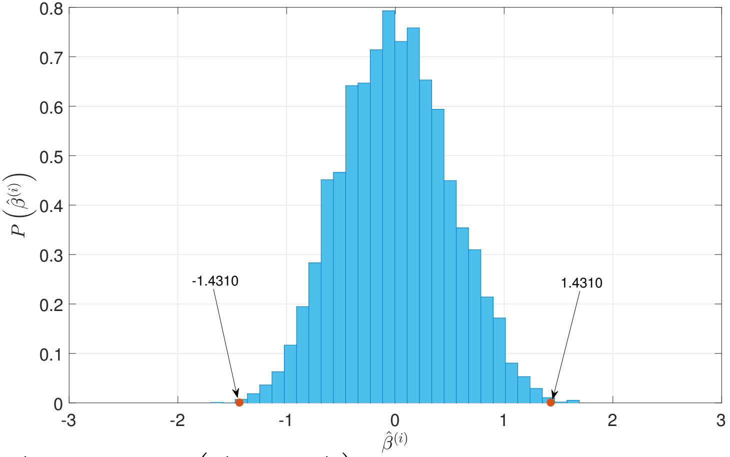
Permutation Test: Example (6)

- Permuation: $\hat{\beta} = 0.3704$



Permutation Test: Example (7)

- Distribution of $m = 10,000$ permutation samples



- $\hat{\beta} = 1.4310$, $\mathbb{P}\left(|\hat{\beta}^{(i)}| > |\hat{\beta}|\right) \approx 0.0013$, t-test $= 0.00157$

Permutation Tests

- Strengths of permutation tests:
  - Makes few assumptions about population distribution
  - Potentially more accurate p-values for non-normal models (logistic reg, etc.)
  - Easy to code, easy to apply
- Weaknesses of permutation tests:
  - Resolution is determined by m; smallest non-zero value is $1/m$
  - Can be slow to run if fitting model is very slow
  - Assumes that individuals in population are independent

Reading/Terms to Revise

- For those who want to know more about random number generation/sampling and bootstrap methods, I recommend the two books:
  - *An Introduction to the Bootstrap*, B. Efron and R. Tibshirani
  - *Monte Carlo Statistical Methods*, C. Robert
- Terms to know:
  - Simulation
  - Pseudo-random numbers
  - Bootstrap distribution
  - Bootstrap algorithm
  - Permutation test
- Next week: no new material – subject revision