

# FIT2086 Lecture 10

## Simulation Based Statistical Methods

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## 1 Simulation Based Methods

- Empirical Probabilities
- Generating Random Numbers

## 2 Bootstrap Methods

- The Bootstrap Algorithm
- Permutation Testing

# Revision from last week (1)

- Machine learning methods
- Cross validation for model selection
  - Withhold data to estimate prediction error
  - $K$ -fold CV divides data up into  $K$  equal sized groups
  - Train on  $K - 1$  folds, predict on the remaining fold
- Decision Trees
  - Split the data up by asking questions of the predictors
  - Number of leaves determines complexity of tree
  - Easy to interpret, flexible
- Methods for learning trees
  - Greedy growing of trees – find best split at each step
  - Backwards pruning of large tree
  - Use CV to select number of leaves in the tree

# Revision from last week (2)

- Trees have low bias, high variance
- One solution: random forests
  - Grow many trees with guided random search
  - Aggregate predictions from the trees
  - Stable, low variance, but loses interpretability
- $k$  nearest neighbours (kNN) methods
  - Assume individuals similar in predictors are similar in targets
  - Find  $k$  “most similar” individuals in data to new individual
  - Use their targets to predict target for new individual
- Use CV to select  $k$ , other tuning parameters

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# 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  $X_1, \dots, X_p \in \mathcal{X}$  from some population, find

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

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

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

- Or, let  $X_1 \sim \text{Poi}(\lambda_1)$  and  $X_2 \sim \text{Poi}(\lambda_2)$ ; 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  $X_1, \dots, X_p$  from their distribution  $m$  times
  - 2 Estimate the probability using the **empirical** probability

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

- 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  $\theta$  of success of this Bernoulli is

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

- Then

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

is the mean of our  $m$  Bernoulli RVs

- By weak law of large numbers

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

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

$$\mathbb{P}(Q > 1) = \int_1^\infty p(q) dq = 1 - \frac{2}{\sqrt{\pi}} \int_0^1 \exp(-t^4) dt = 0.3171$$

- 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 probabilities  $p$ , we need a very large  $m$ , at least 10 times greater than  $1/p$  to get a good estimate

# More generally

- We can find any statistic of  $X$  (variance, median, quantiles, etc.) to good accuracy if we have enough random samples
- Let  $\mathbf{x}$  be an R vector containing  $m$  samples drawn from  $p(x)$ ; then

$$\mathbb{E}[X] \approx \text{mean}(\mathbf{x});$$

and

$$\mathbb{V}[X] \approx \text{var}(\mathbf{x});$$

and

$$Q(p = 0.2) \approx \text{quantile}(\mathbf{x}, p=0.2);$$

and  $p(x)$  itself can be approximated by

$$\text{hist}(\mathbf{x}, \text{Probability}=\mathbf{T})$$

and so on, with better approximation as  $m$  grows.



# 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 Other Random Variables

- 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
- Some other methods for sampling RVs
  - Inverse CDF procedure
  - Metropolis-Hastings algorithm
  - Accept-Reject algorithms
  - Adaptive rejection sampling
  - Slice sampling
- To some degree, no need to worry as R/Python/Matlab have implementations of most standard RVs

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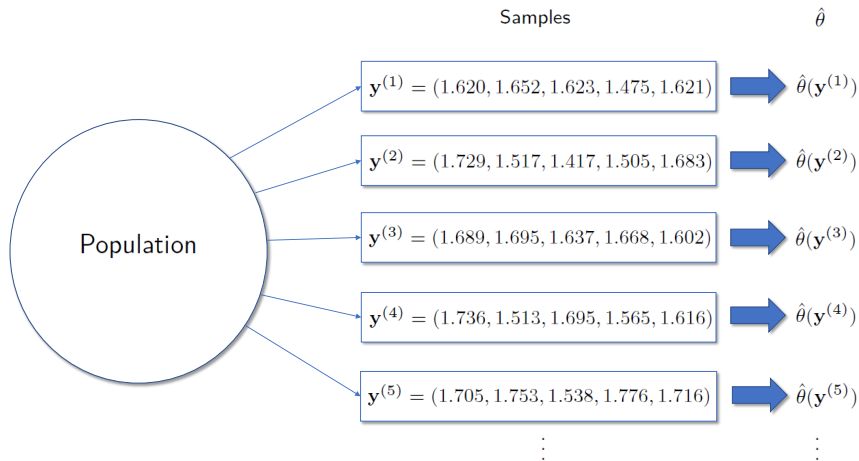
# Data Resampling Methods (1)

- 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  $\theta$
- We draw a *finite* sample of size  $n$  from our population
- Use this sample to estimate  $\theta$  (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  $\mathbf{y}^{(1)}, \dots, \mathbf{y}^{(M)}$  the combinations of data points
  - These represent all the samples you could draw from this “population”
- 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  $\mathbf{y}$ 
  - If our data  $\mathbf{y}$  was the complete population, this would be our “population value” of  $\theta$
  - We can then use the bootstrap distribution to estimate quantities such as bias by comparing them against  $\hat{\theta}$

# 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 (our “population value”) 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  $\bar{Y}$

$(2, 2, 2)$		2
$(2, 2, 6)$		3.3333
$(2, 2, 3)$		2.3333
$(2, 6, 2)$		3.3333
$(2, 6, 6)$	$\xRightarrow{\bar{Y}}$	4.6667
$\vdots$		$\vdots$
$(3, 3, 2)$		2.6667
$(3, 3, 6)$		4
$(3, 3, 3)$		3

# 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  $\mathbf{y} = (y_1, \dots, y_n)$  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
- $\hat{\theta}^{(1)}, \dots, \hat{\theta}^{(m)}$  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 and Weight
- Example, forming a single bootstrap sample

Original Data			Bootstrap Sample			$I$
BP	Age	Weight	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				

$\Rightarrow$

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117	50	94.7	125	52	101.3	9
112	51	89.4	121	48	99.5	6
121	48	99.5	105	47	85.4	1
110	47	90.9	116	49	95.3	3
115	49	94.1	112	51	89.4	5
125	52	101.3	125	52	101.3	9

$\Rightarrow$

# Example: Bagging

- Bootstrapping can be used to improve prediction error
- The bagging (bootstrap aggregation algorithm) does just this
- Procedure:
  - Generate  $m$  bootstrap samples
  - For each bootstrap sample, fit a model
  - Predict onto new data by averaging over predictions from all  $m$  models
- Can improve prediction errors if model is low bias/high variance
  - Trees are a prime example
- Similar to random forests – inspired them, in fact

# 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  $\hat{\theta}^{(1)}, \dots, \hat{\theta}^{(m)}$ 
  - 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)

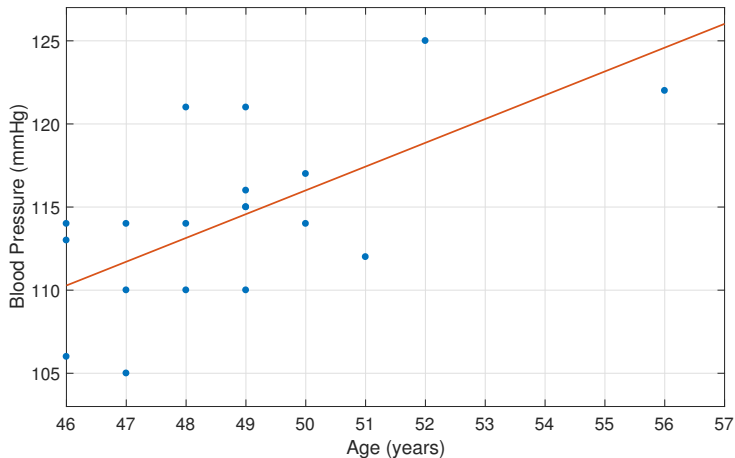
- Fit Age to BP using least-squares regression
  - $\hat{\beta} = 1.4310$
  - $p$ -value of association ( $t$ -test) = 0.00157
- $p$ -value was calculated under assumption population is normal
- To calculate a  $p$ -value using permutation test
  - Permute  $y$  (BP) values  $m$  times, then fit Age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

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

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

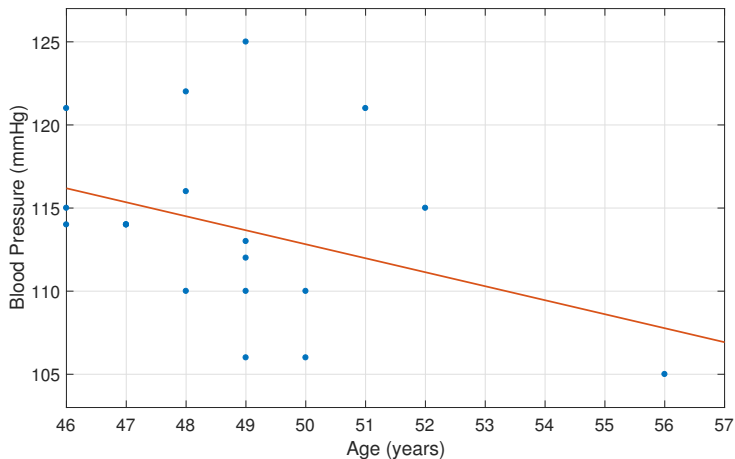
# Permutation Test: Example (3)

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



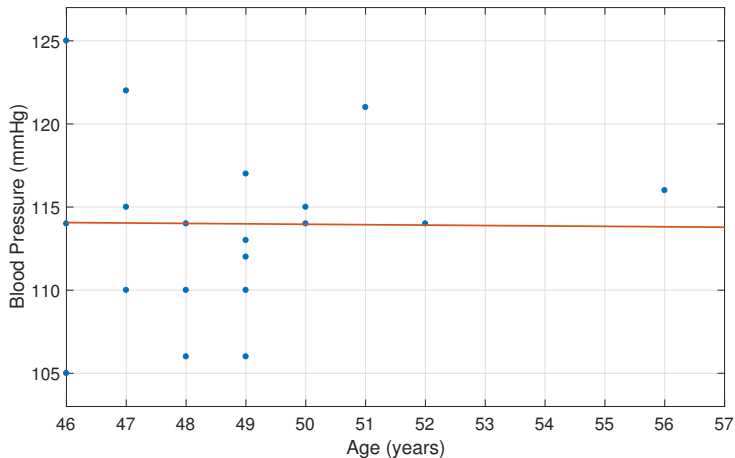
# Permutation Test: Example (4)

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



# Permutation Test: Example (5)

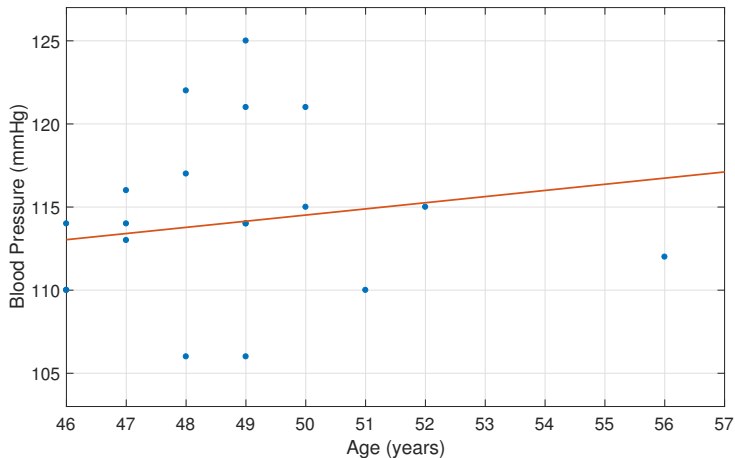
- Permutation:  $\hat{\beta} = -0.0253$





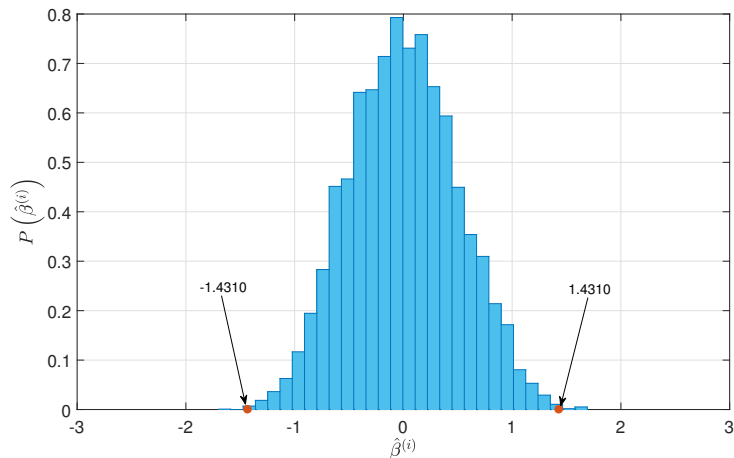
# Permutation Test: Example (6)

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



# Permutation Test: Example (7)

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



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

- 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

- 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: machine learning algorithms for unsupervised data discovery (clustering, mixture modelling, matrix completion)