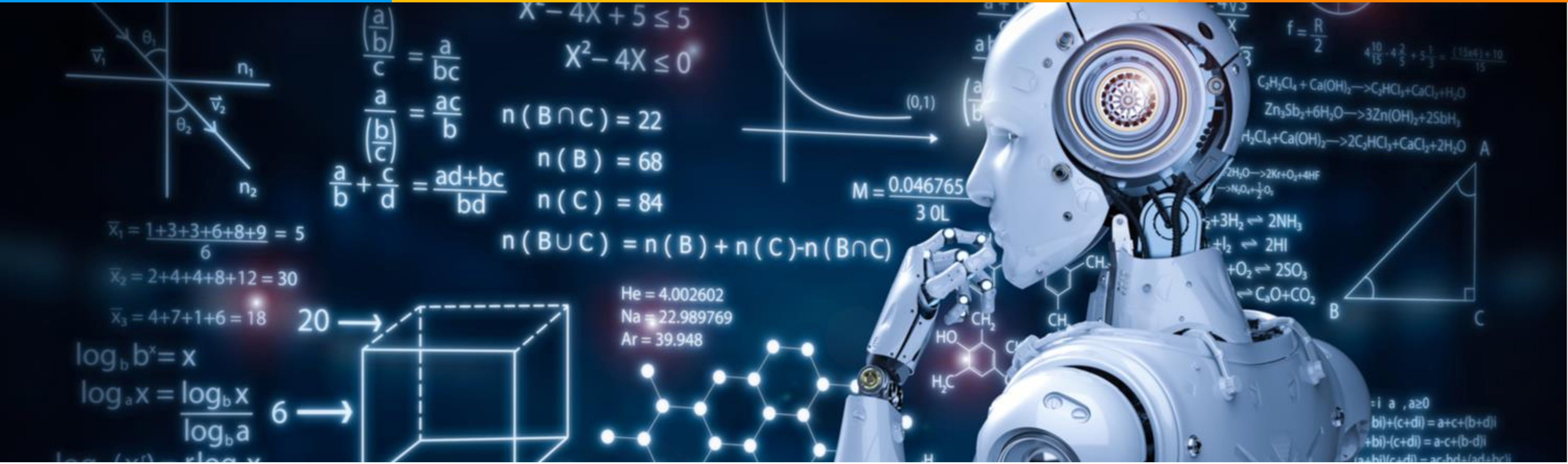
Duration: 60 min | Srikanth Shenoy | AML 5102 | M.E. AI & ML

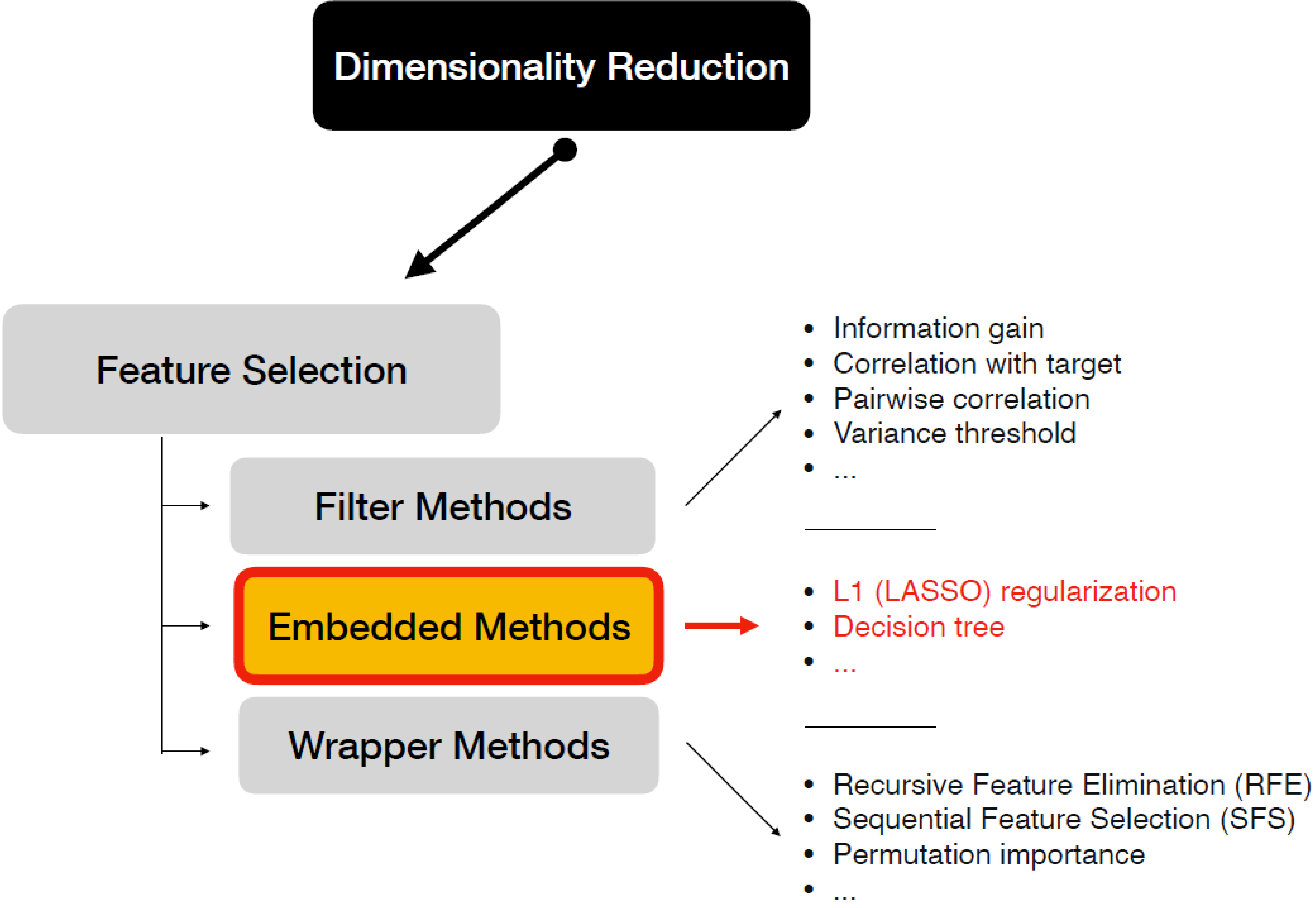


Lecture 28 & 29: Feature Selection Part 2

Recap

- Feature Selection
  - Unsupervised methods
  - Filter and wrapper methods

Feature Selection with Embedded (Intrinsic) methods

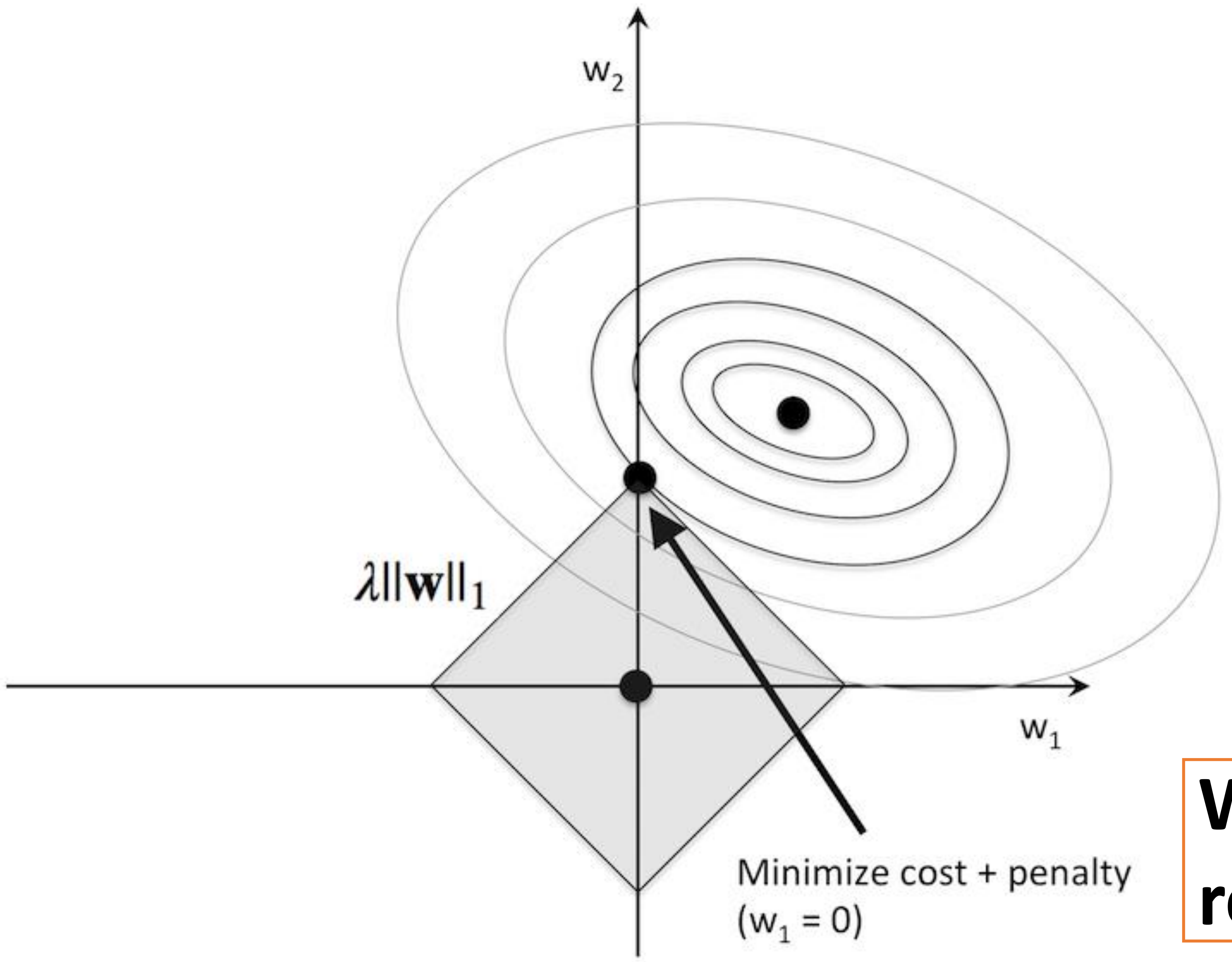

Dimensionality Reduction
Feature Selection
Filter Methods
Embedded Methods
Wrapper Methods
• Information gain
• Correlation with target
• Pairwise correlation
• Variance threshold
• ...
• L1 (LASSO) regularization
• Decision tree
• ...
• Recursive Feature Elimination (RFE)
• Sequential Feature Selection (SFS)
• Permutation importance
• ...

Embedded methods

- Always supervised
- No separate feature selection
- Feature Selection happens as part of model training
- E.g.:
  - LASSO
  - Feature Importance with Random Forest
- Returns coeff_ or feature_importances
- Other non parametric methods do not augur well

Feature Selection with LASSO

Cost function adjusted for L1 Regularization



$$\arg\min_w \nabla_w \mathcal{J} + \lambda \nabla_w \|w\|_1$$

$$\nabla_w \mathcal{J} = \frac{2}{m} X^T (Xw - y) \qquad \nabla_w \|w\|_1 = \mathbf{1}$$

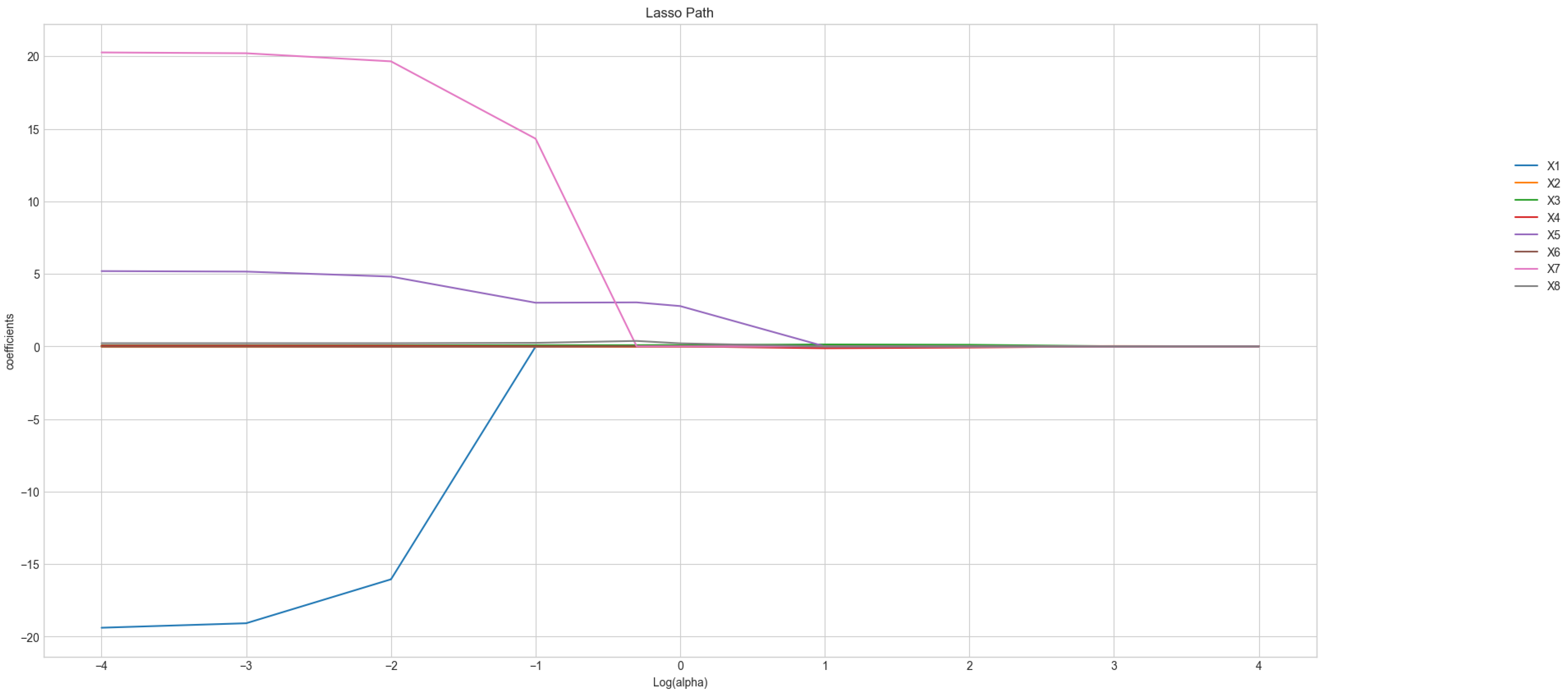
$$\mathbf{w} = \mathbf{w} - \eta \nabla_w \mathcal{J} \qquad \mathbf{w} = \mathbf{w} - \eta \nabla_w \mathcal{J} - \eta \lambda$$

Without regularization

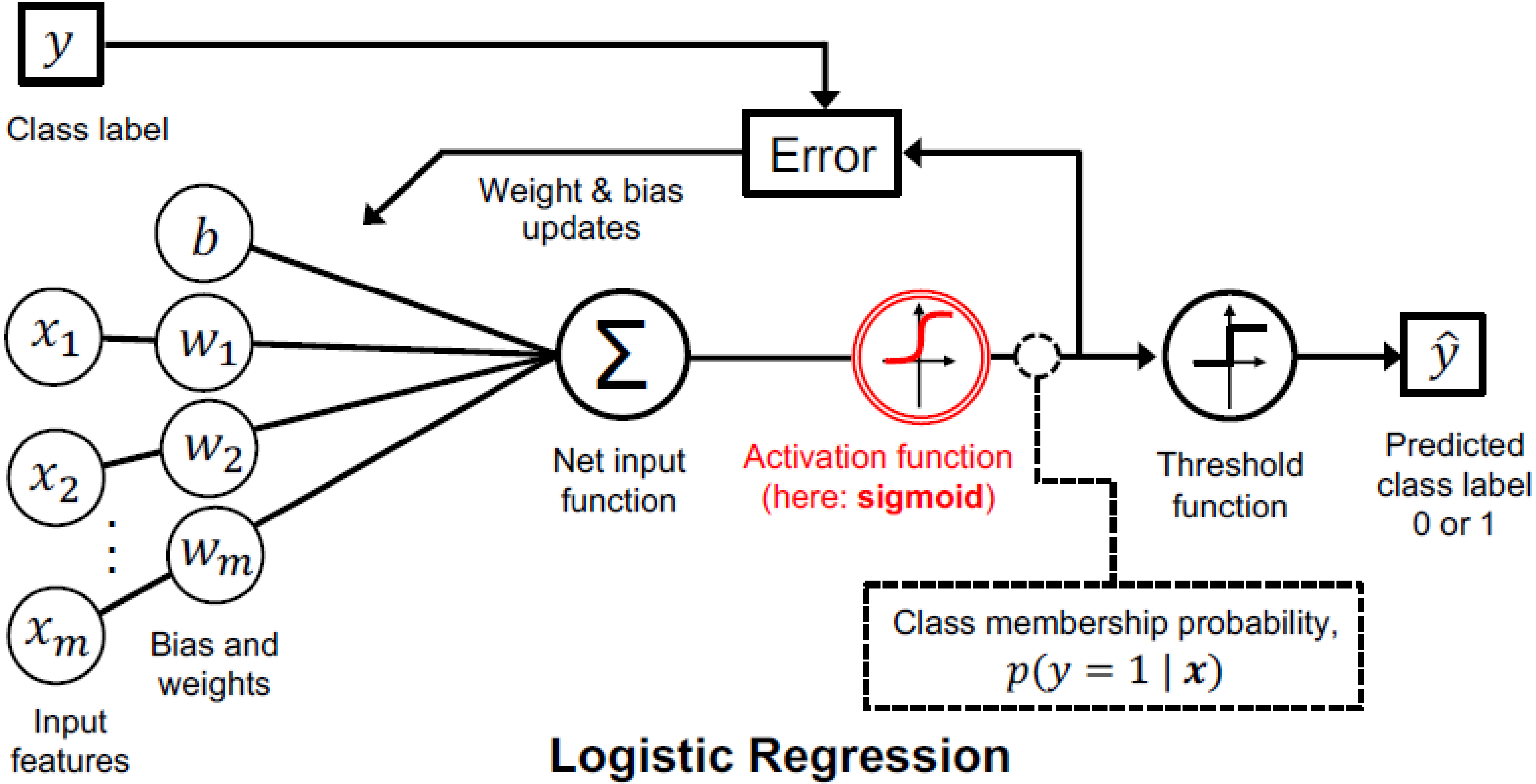
$$\mathbf{w} = (\mathbf{w} - \eta \lambda) - \eta \nabla_w \mathcal{J}$$

A FIXED small number keeps getting subtracting from a small w. Net effect w becomes 0

Lasso path



$$\arg\min_{w} \nabla_w \mathcal{J} + \lambda \nabla_w \|w\|_1$$



Logistic Regression

$$-\sum_{i=1} \left[y^{(i)} \log\left(\sigma\left(z^{(i)}\right)\right) + \left(1-y^{(i)}\right) \log\left(1-\sigma\left(z^{(i)}\right)\right)\right] + \lambda \|w\|_1$$

Feature Selection with Decision Tree & Random Forest

Sample Tree:

- 2 Features : X1 & X2
- 2 Classes : Class1 & Class2
- Impurity Metric : Gini

- A feature is important if
  - If used many times for splitting
  - Each split on the feature is high in the tree
  - Split produces lot of decrease in impurity at each node

Sample Tree:

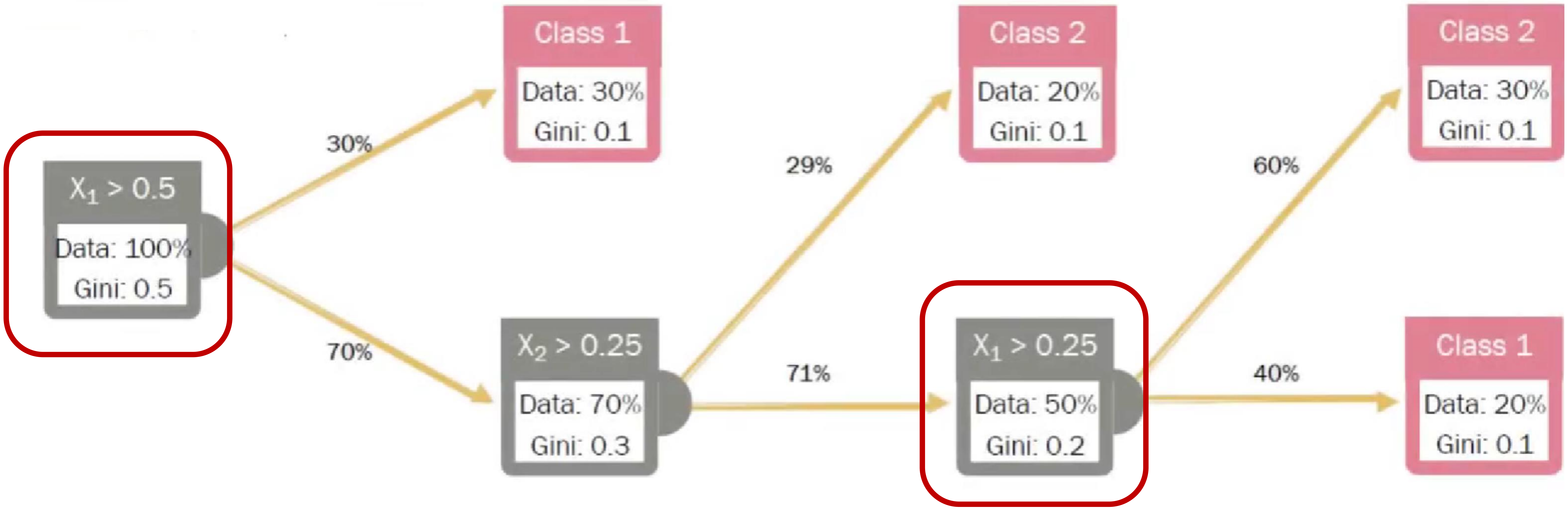
- 2 Features : X1 & X2
- 2 Classes : Class1 & Class2
- Impurity Metric : Gini

- Node Importance

$$ni_j = \frac{N_j}{N}\left(Gini_j - \mathbb{E}[Gini_{j-children}]\right)$$

- Feature Importance

$$fi_i = \frac{\sum_{j \in feature-inodes} ni_j}{\sum_{j \in allnodes} ni_j}$$



- Decrease in impurity for X1 at top:
  - Impurity in parent node – impurity in child node

$$0.5 - (0.7 \times .3 + 0.3 \times 0.1)$$

- Weighed by the ratio of data N_in/N

$$\frac{100}{100}[0.5 - (0.7 \times .3 + 0.3 \times 0.1)]$$

- How many times?

$$\frac{100}{100}[0.5 - (0.7 \times .3 + 0.3 \times 0.1)] + \frac{50}{100}[0.2 - (0.3 \times 0.1 + 0.2 \times 0.1)]$$

- Normalized Feature Importance = Sum of this feature importance divided by sum of all feature importance

Feature Importance in DT/RF summary

- Node Importance: Mean decrease in entropy/impurity from a parent node to child nodes after a feature split
  - Weighted by tree location (num examples at node)

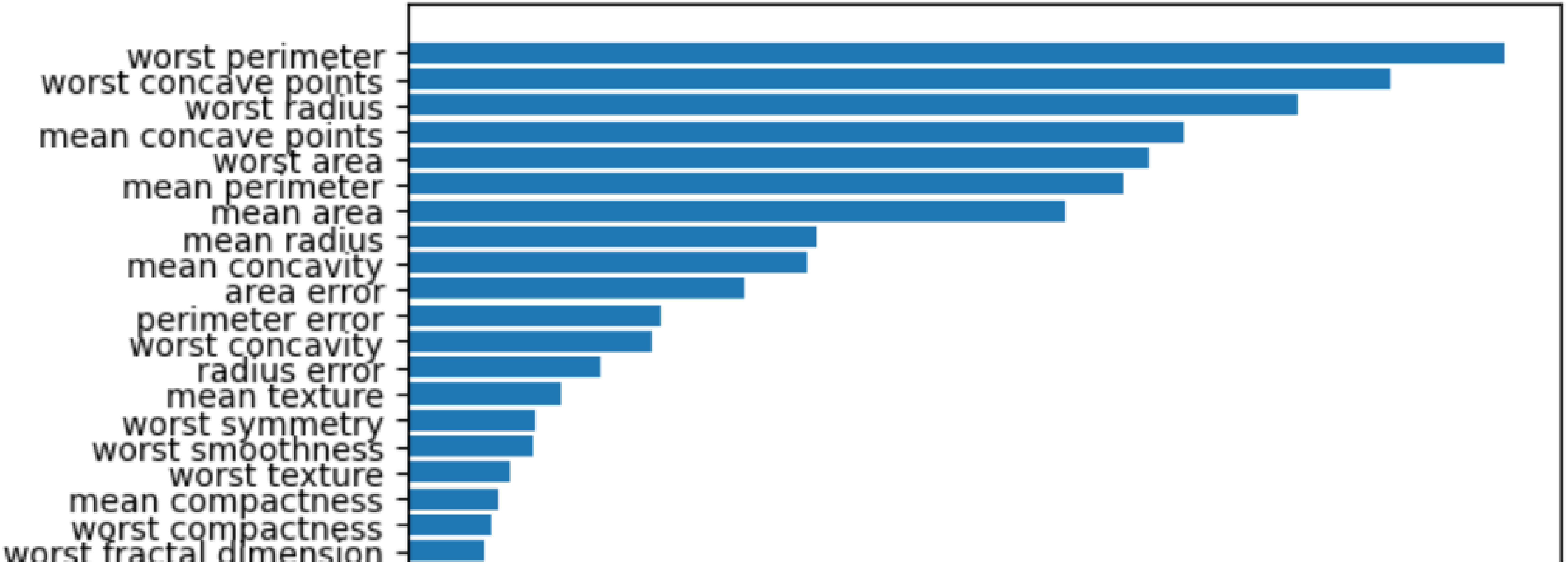
- for a given feature
  - for each tree
    - compute impurity decrease (Gini, Entropy)
    - weight by number of examples at that node
    - averaged over all trees
- normalize importances so that sum of feature importances sum to 1

Sklearn code

```
sorted_idx = model_best_rf.feature_importances_.argsort()
plt.barh(dataset.feature_names[sorted_idx], model_best_rf.feature_importances_[sorted_idx])
plt.xlabel("Random Forest Feature Importance")
```

✓ 0.3s

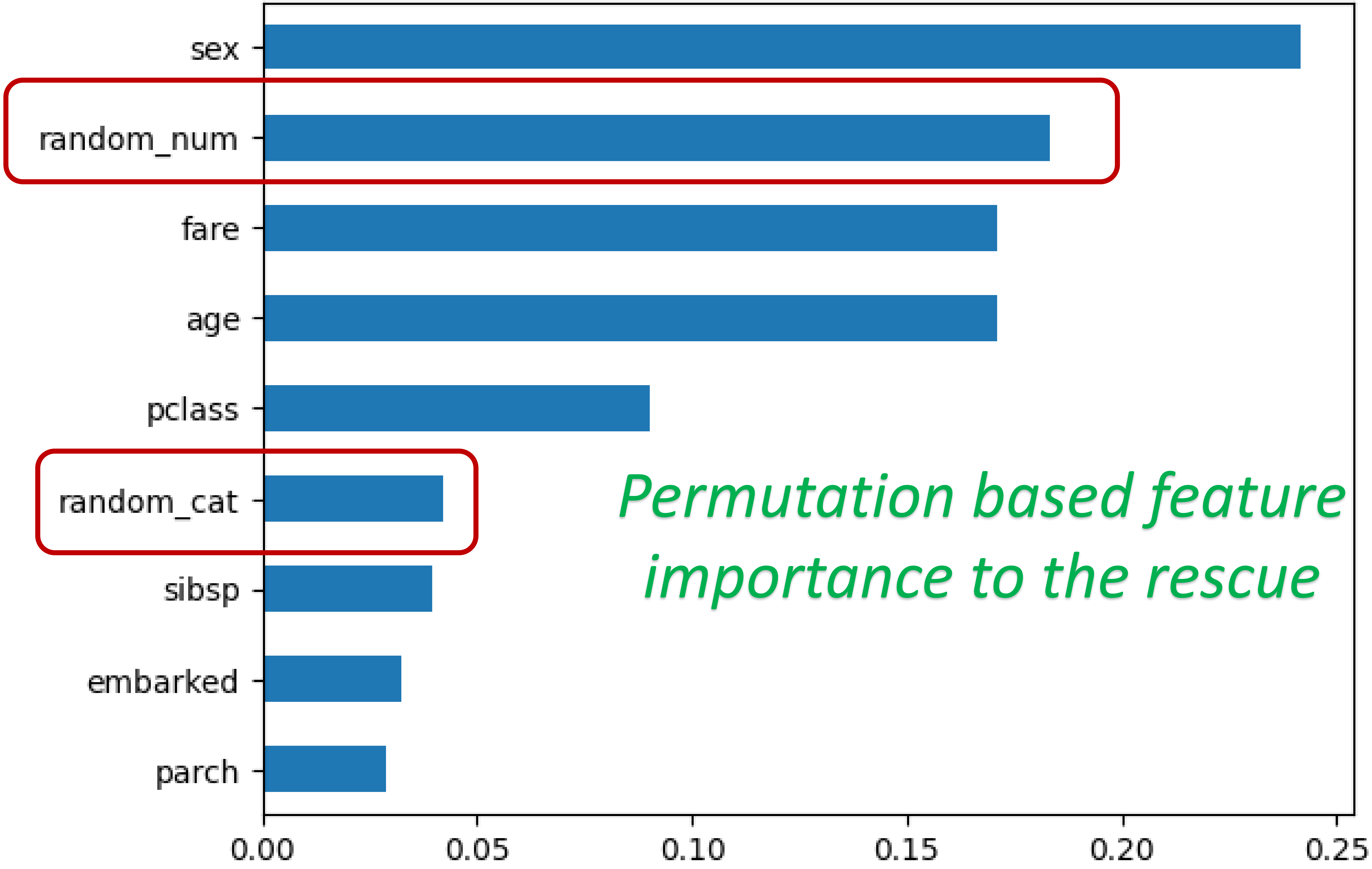
```
Text(0.5, 0, 'Random Forest Feature Importance')
```



Problems with Tree based Feature Importance

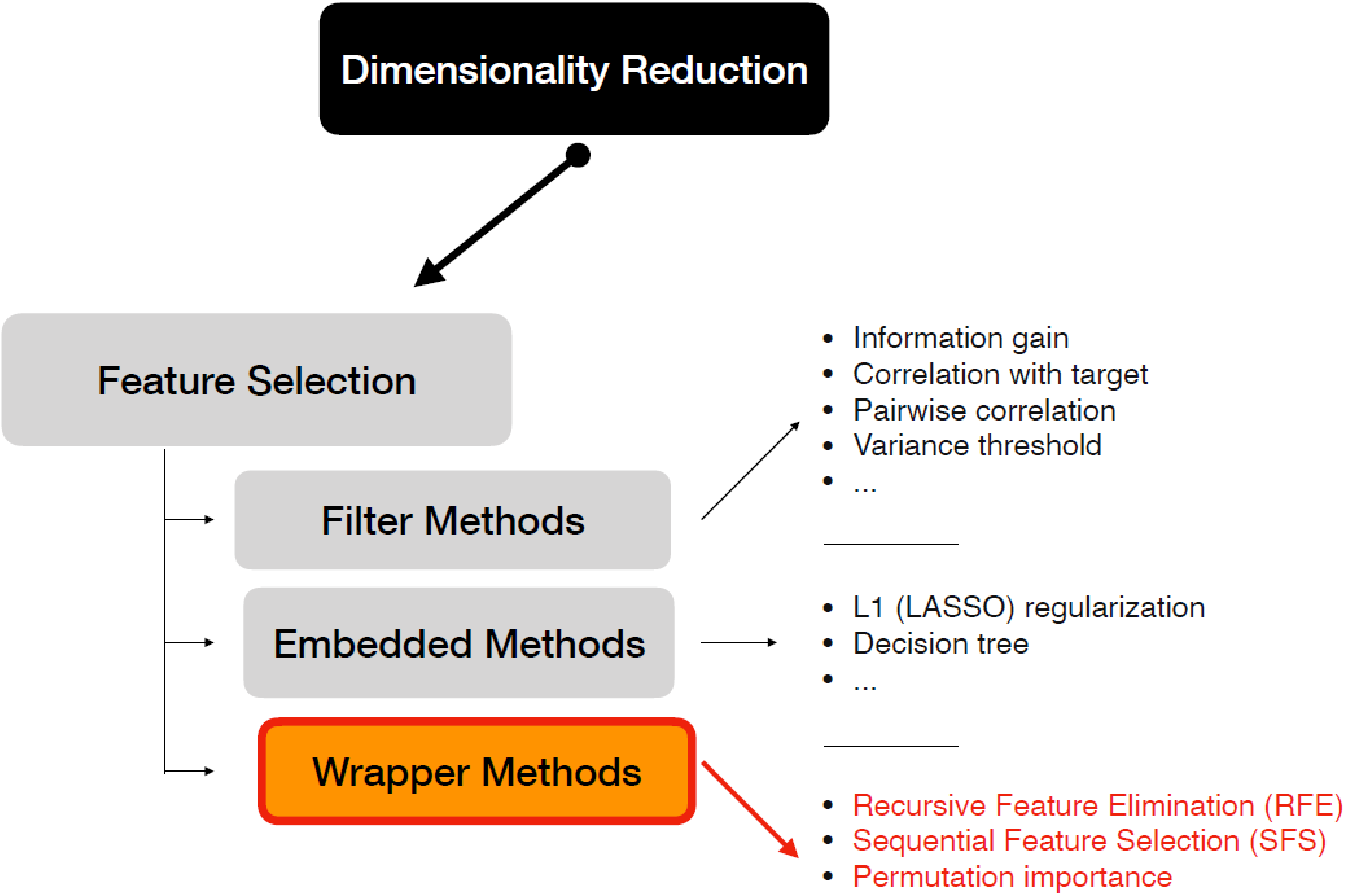
- Inflated feature importance for numerical feature
- Inflated feature importance for categorical feature with high cardinality

pclass	sex	age	sibsp	parch	fare	embarked	random_cat	random_num	survived
3.0	male	32.0	0.0	0.0	56.4958	S	0	-2.553921	1
2.0	male	27.0	0.0	0.0	26.0000	S	0	0.963879	0
3.0	male	35.0	0.0	0.0	7.8958	S	0	0.536653	0
3.0	female	26.0	1.0	1.0	22.0250	S	2	0.323079	1
3.0	male	33.0	0.0	0.0	8.6542	S	1	0.884045	0



Permutation based feature importance to the rescue

Wrapper methods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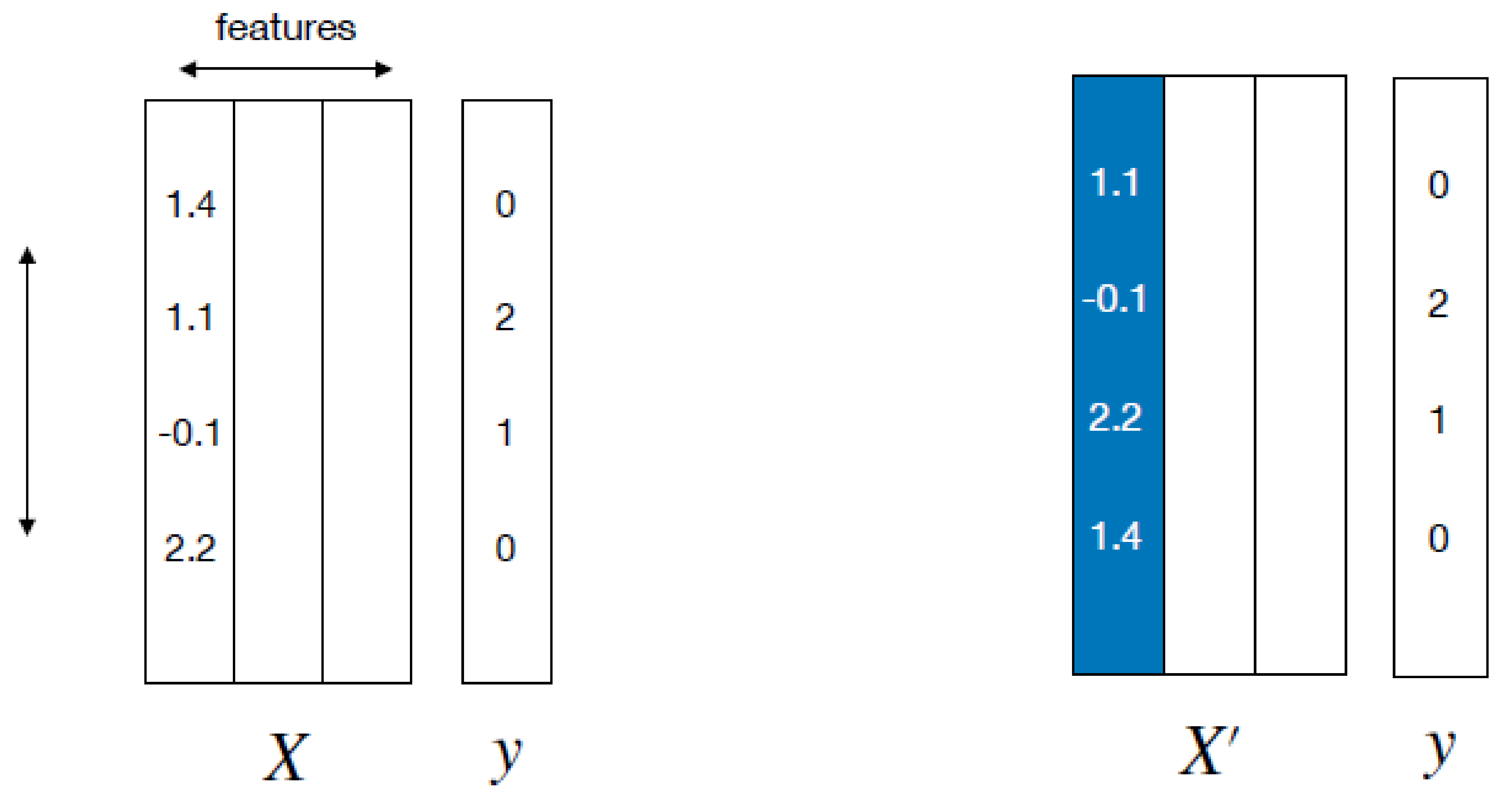
Wrapper methods

- General working
  - Wrap any algorithm to measure metrics
  - Make slight changes and run the algorithm again
  - The quantum of “slight changes” gives idea of feature importance
- E.g.:
  - RFE
  - Permutation Importance
  - Selective Feature Selection

Permutation based feature importance

Permutation importance

- model.fit(X_train, y_train),   model.score(X_test)



feature importance =

baseline performance – shuffled dataset performance

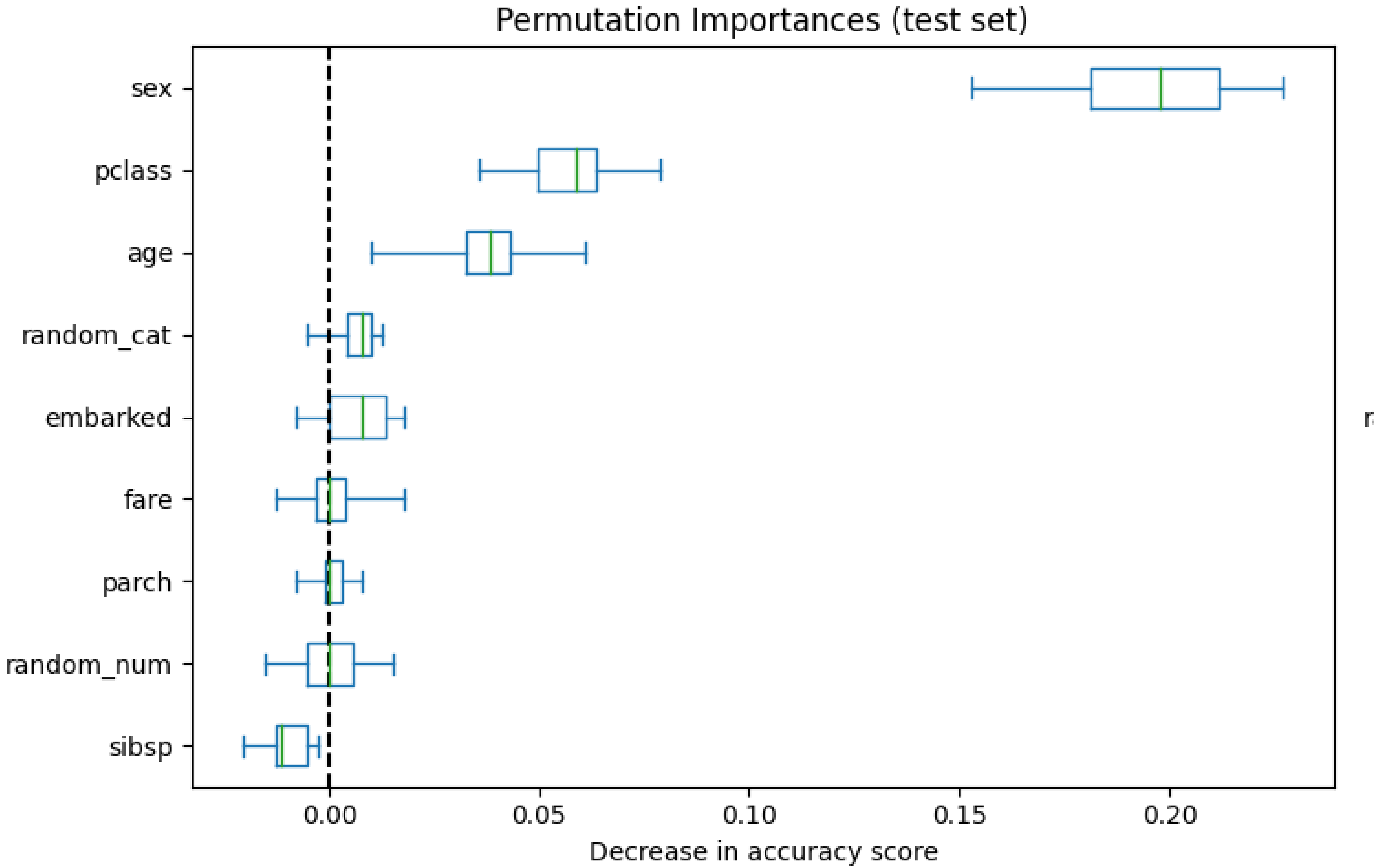
Permutation importance

- Train a baseline model
- Record model performance (any metric) on test dataset
- For each feature column in test dataset,
  - Shuffle that feature column alone, everything else unchanged
  - Observe performance and compare to original

  feature importance =

    baseline performance – shuffled dataset performance

- Do the shuffling for training dataset also & record feature importance


Permutation Importances (test set)
sex
pclass
age
random_cat
embarked
fare
parch
random_num
sibsp
0.00
0.05
0.10
0.15
0.20
Decrease in accuracy score

Column Drop Variant of permutation importance

- Train a baseline model
- Record model performance (any metric) on test dataset
- For each feature column in test dataset,
  - Drop column
  - Fit model
  - Compare test data set performance to original

- Accurate but very expensive

- Fixes the random_cat issue as well

Wrapper methods general features (except as noted)

- Permutation importance is model agnostic
  - No need for coeff_ or feature_importance implementation
    - (this is not applicable to other wrapper methods)
- Feature Importance is specific to model

- Permutation importance is flexible, can use any metric
- Feature importance is tied to impurity measure

- Permutation importance is easy to understand
- Feature importance is slightly tricky

Recursive Feature Elimination

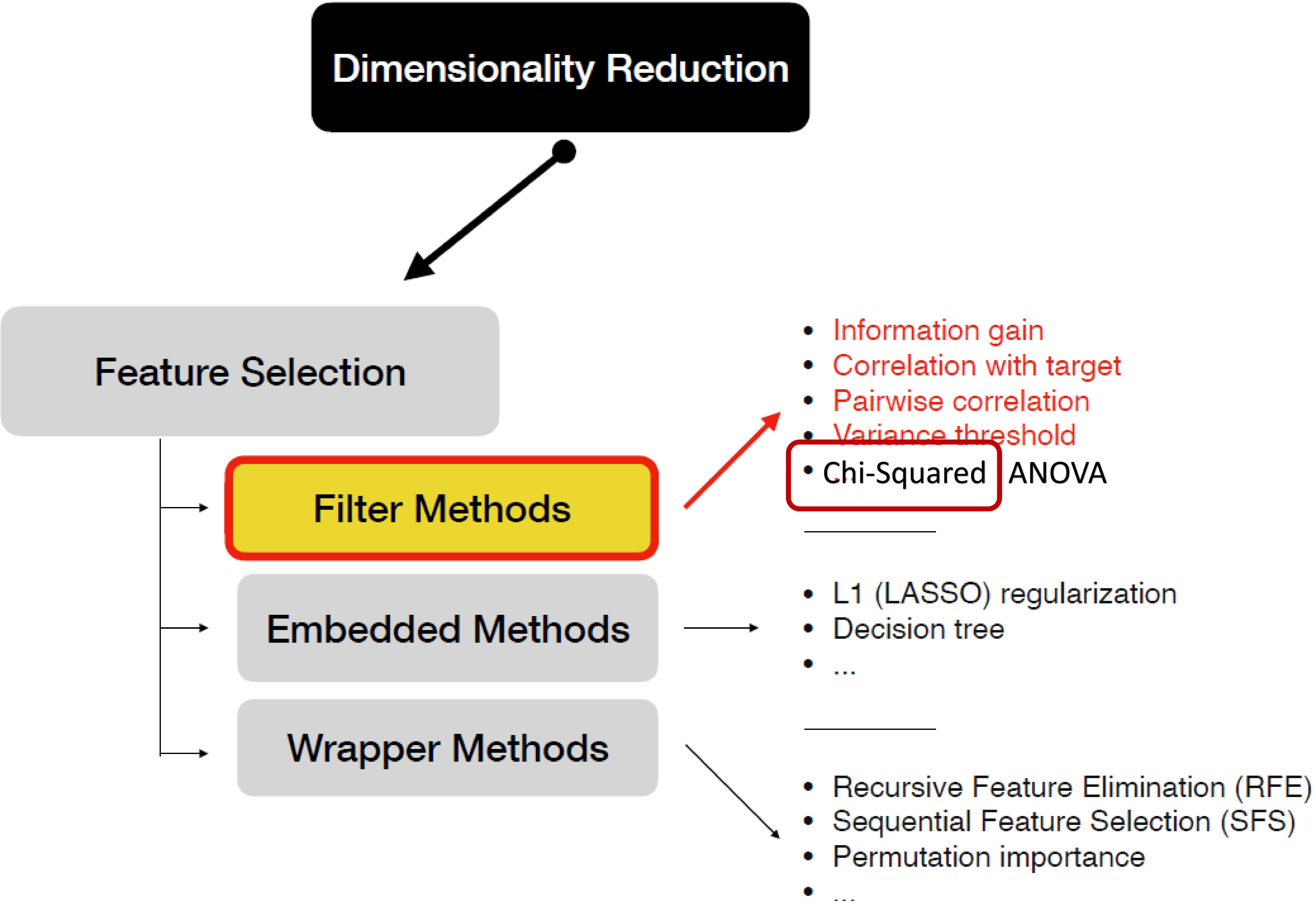
RFE

- Suppose you have number (or range) of features in mind
- Algorithm
  - Fit model to dataset
  - Eliminate feature with lowest coefficient (or lowest feature importance)
  - Repeat steps until desired features is reached

Why repeat steps? Why not delete all low coefficient features at the outset?

- Can be applied along with cross validation
- Comprehensive but expensive

Feature Selection with Chi Squared Test


Dimensionality Reduction
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Filter Methods
Embedded Methods
Wrapper Methods
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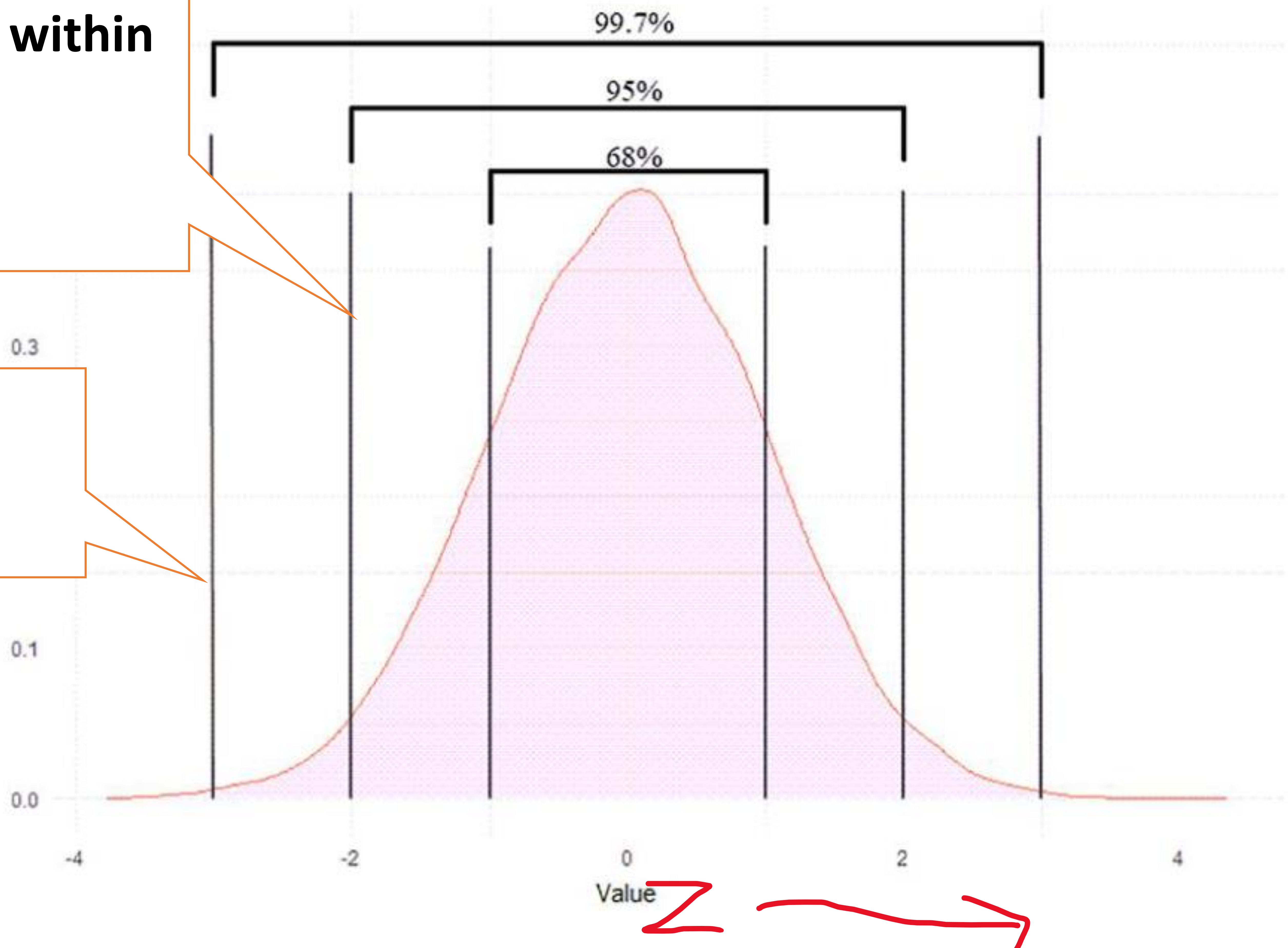
• Correlation with target
• Pairwise correlation
• Variance threshold
• Chi-Squared ANOVA
• L1 (LASSO) regularization
• Decision tree
• ...
• Recursive Feature Elimination (RFE)
• Sequential Feature Selection (SFS)
• Permutation importance
• ...

Standard Normal Distribution

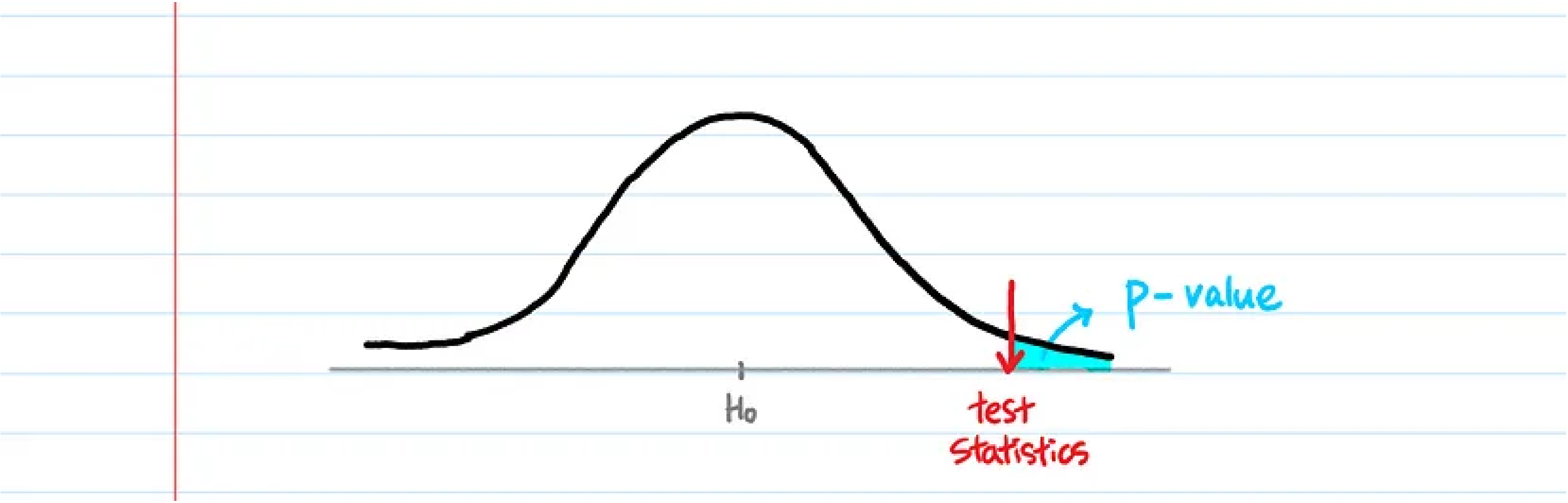
Probability of data within

1. z=1 is 0.68
2. z=2 is 0.95
3. z=3 is 0.997

Things are easy with normal distribution



Standard Normal distribution and p-values

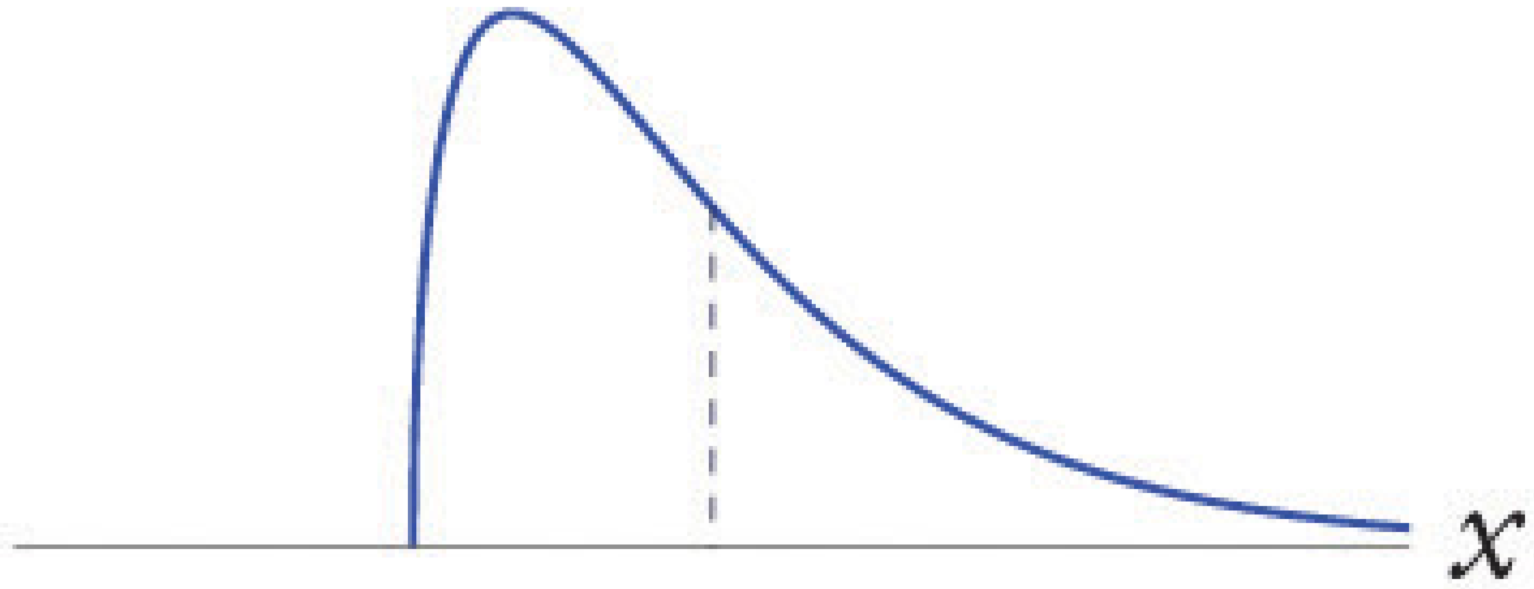


- P(X > k)

Why normal distribution?

- Not everything follows normal distribution

Some feature distribution



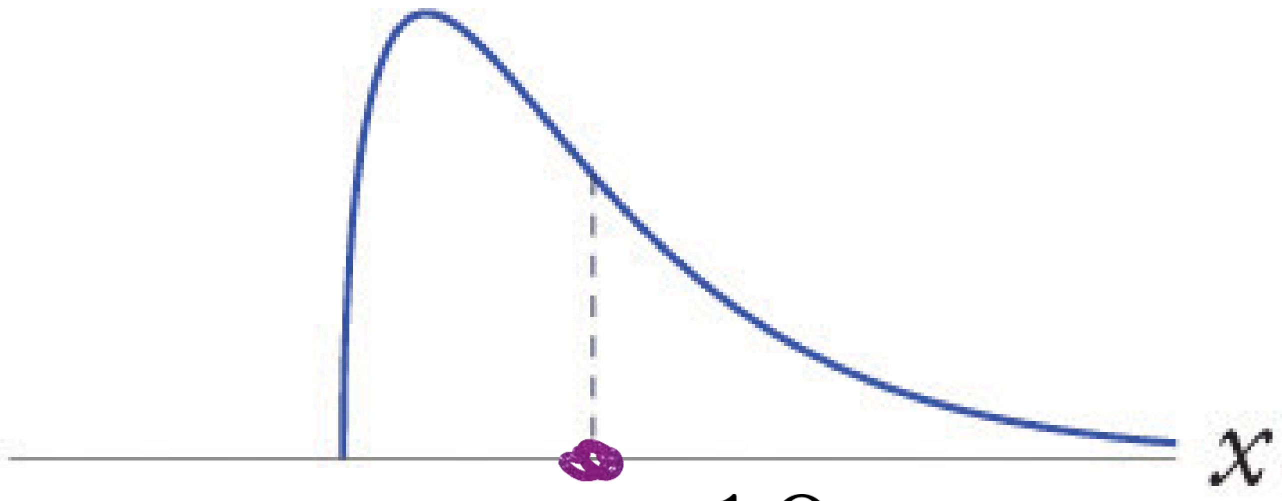
- Accidents on road follow Poisson distribution
- Volcanic eruption, asteroid strike: exponential distribution
- Why do we keep talking about normal distribution?
- The answer is in Central Limit theorem

Central Limit Theorem (CLT)

- Most fundamental to inferential statistics
- Aside: What is inferential statistics versus descriptive statistics?
- CLT provides mechanism to apply normal distribution to everything

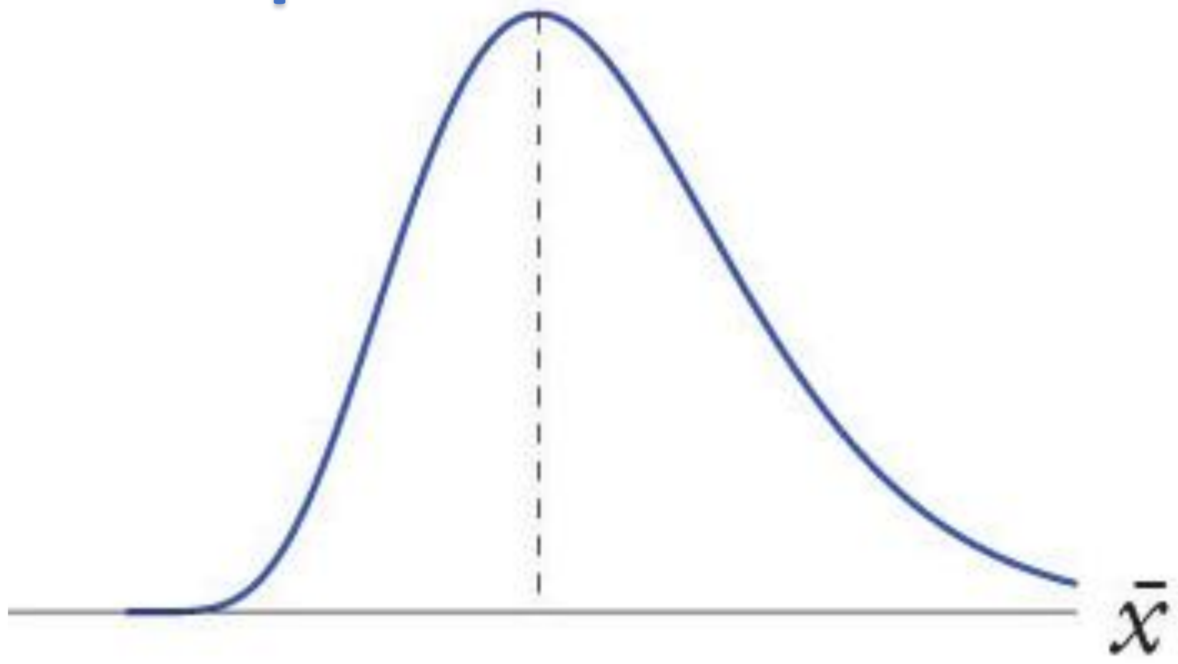
Central Limit Theorem – Sampling distribution of mean

Population distribution



$\mu = 10$

Sampling distribution of sample mean with n=5

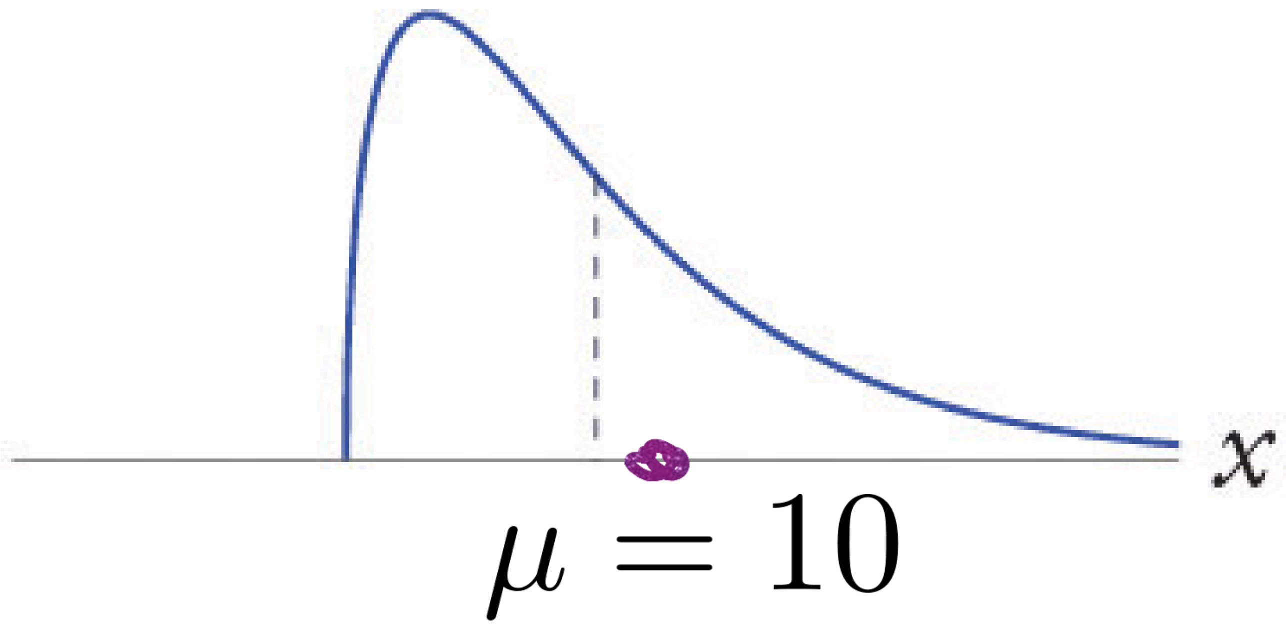


Sample size n = 5

Sampling	Mean
1	7.5
2	9.5
3	11
4	9
5	11.5
6	10.5
7	9.75
8	9
9	9.25
10	9.8

Central Limit Theorem – Sampling distribution of mean

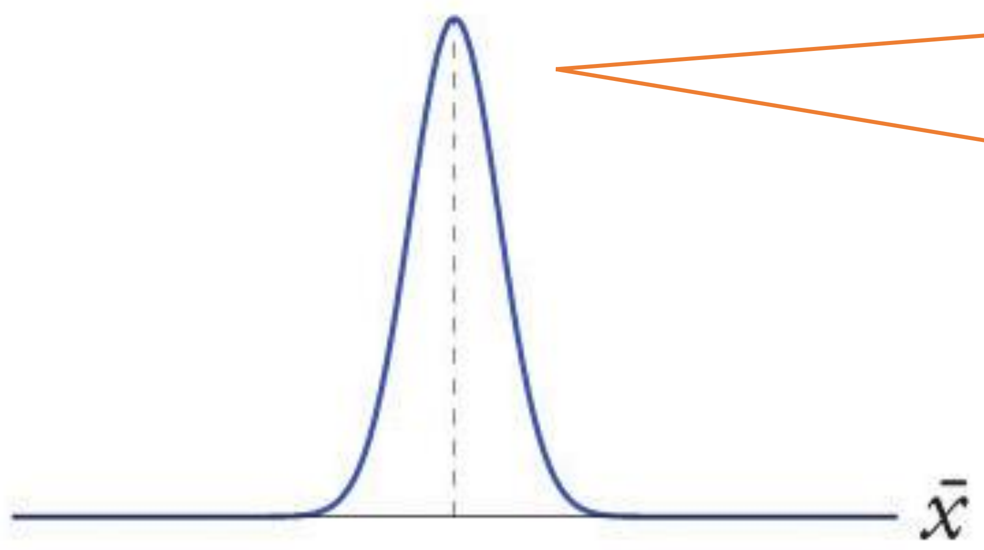
Population distribution



Sample size n = 30

Sampling	Mean
1	7.5
2	9.5
3	11
4	12
5	11.5
6	10.5
7	9.75
8	10
9	10.25
10	9.8

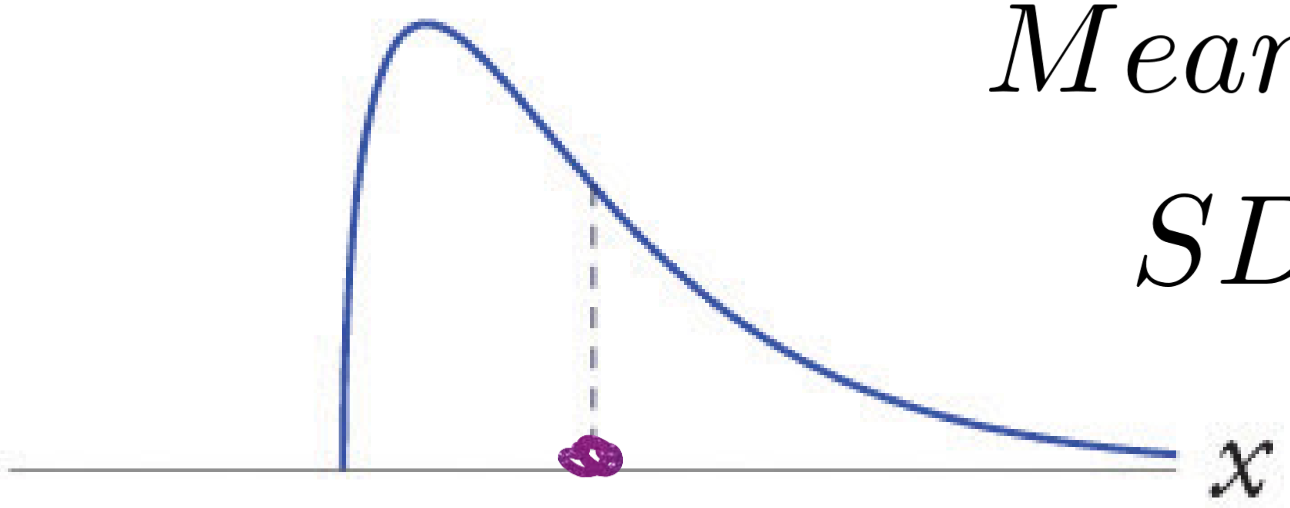
Sampling distribution of sample mean with n=30



Sampling distribution approximates normal distribution when n>=30

Central Limit Theorem – Sampling distribution of mean

Population distribution

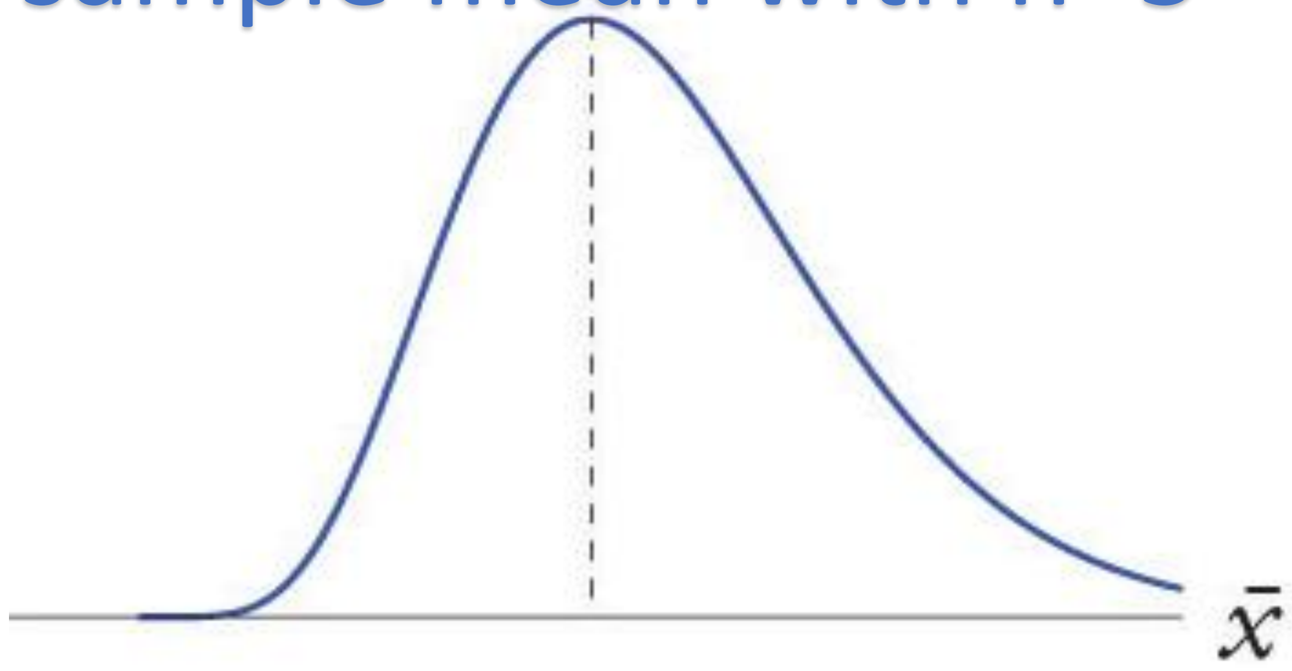


$$Mean = \mu$$

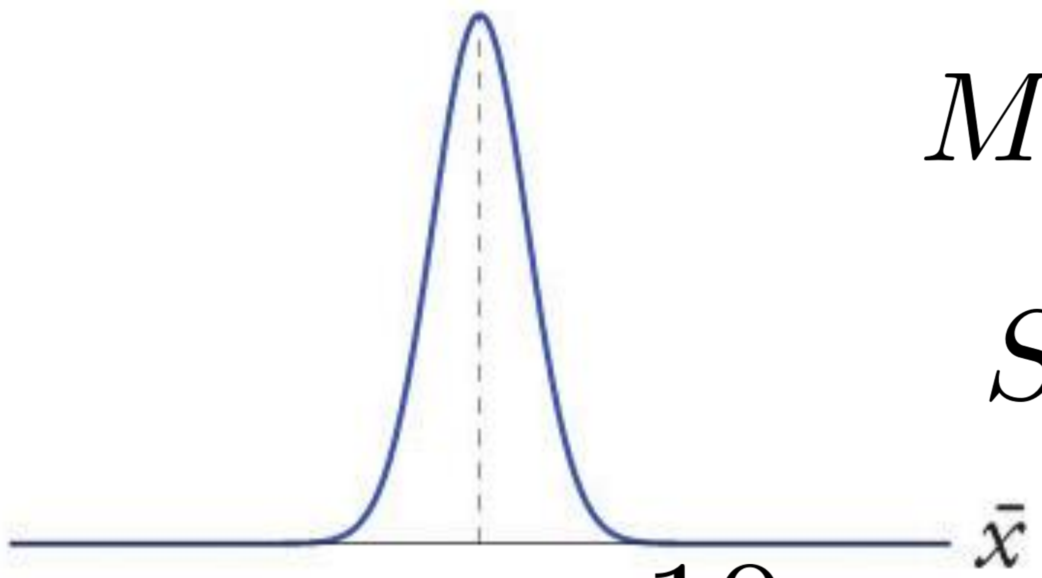
$$SD = \sigma$$

$$\mu = 10$$

Sampling distribution of sample mean with n=5



Sampling distribution of sample mean with n=30



$$Mean = \mu_s$$

$$SD = \frac{\sigma}{\sqrt{n}}$$

$$\mu_s = 10$$

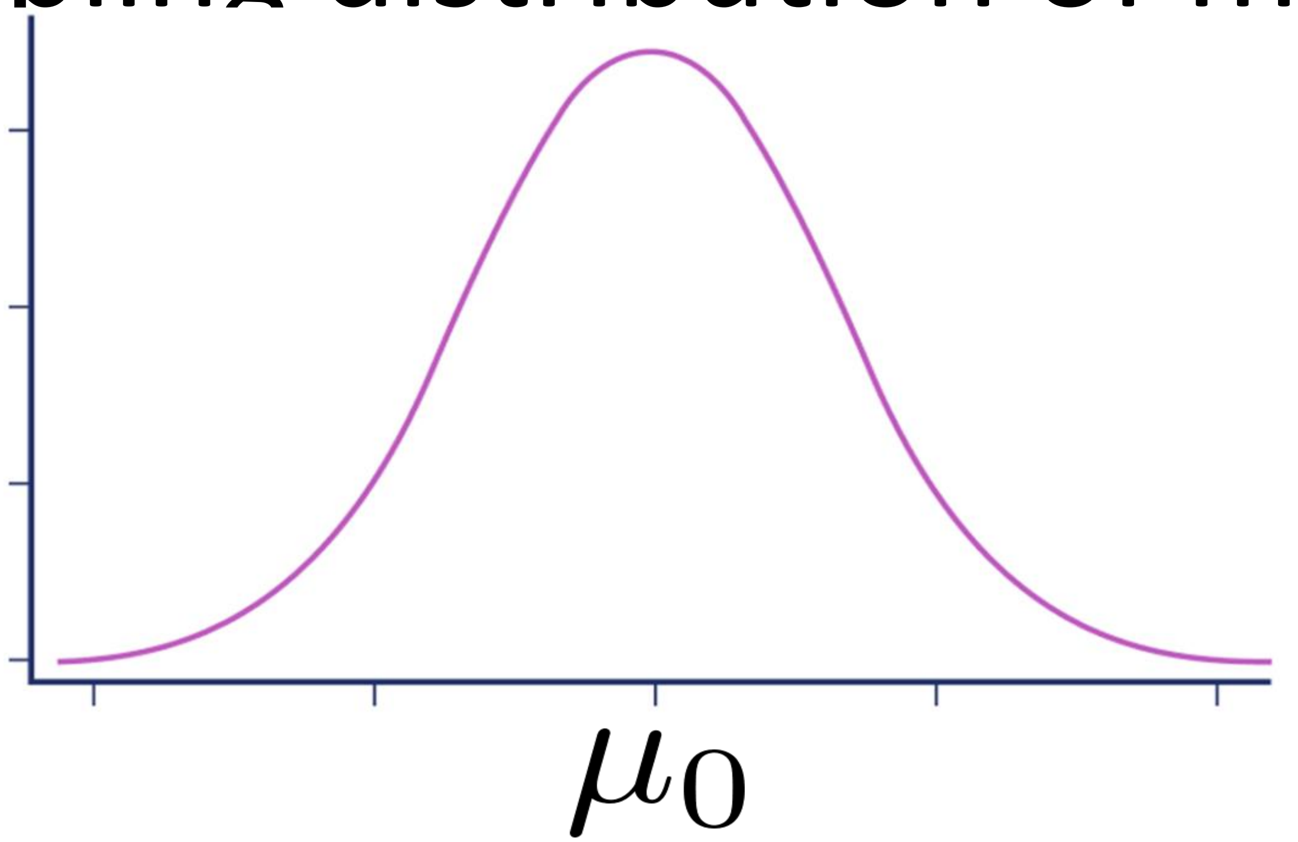
$$z \sim \mathcal{N}(\mu, \frac{\sigma}{\sqrt{n}})$$

Made in India iPhone 15 battery life

- iPhone 15 has mean battery life μ_0 & variance σ_0
- Population has some unknown distribution

$$X \sim Unknown(\mu_0, \sigma_0)$$

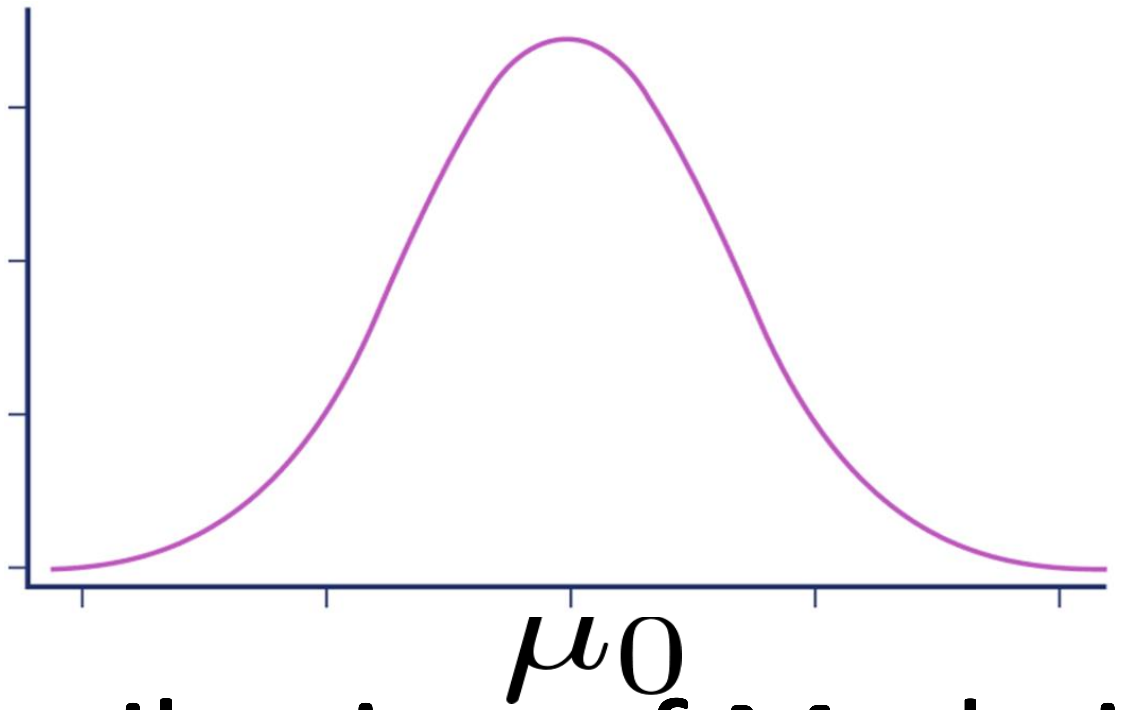
- How was population mean & variance found?
  - Draw samples (each of size >= 30) 10 times in population
  - Sampling distribution of mean battery life is gaussian

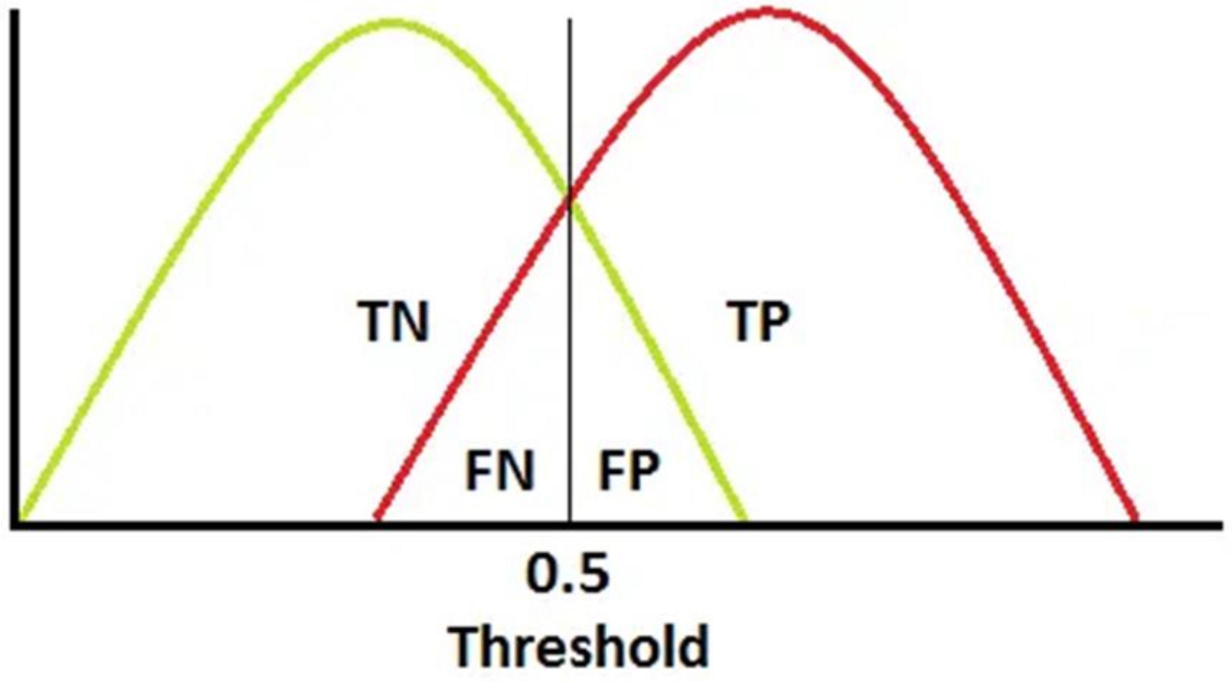


$$Y \sim \mathcal{N}(\mu_0, \frac{\sigma_0}{\sqrt{n}})$$

Made in China v/s India iPhone battery life

- Historical sampling distribution from China $Y \sim \mathcal{N}(\mu_0, \frac{\sigma_0}{\sqrt{n}})$





- v/s distribution of Made in India
- Where is the mean of new distribution?
- Should new distribution exactly align with historical distribution? What is confidence interval (CI)? $(\mu_0 \pm \frac{\sigma_0}{\sqrt{n}})$
- CI relation to TP/TN Type 1 Type2

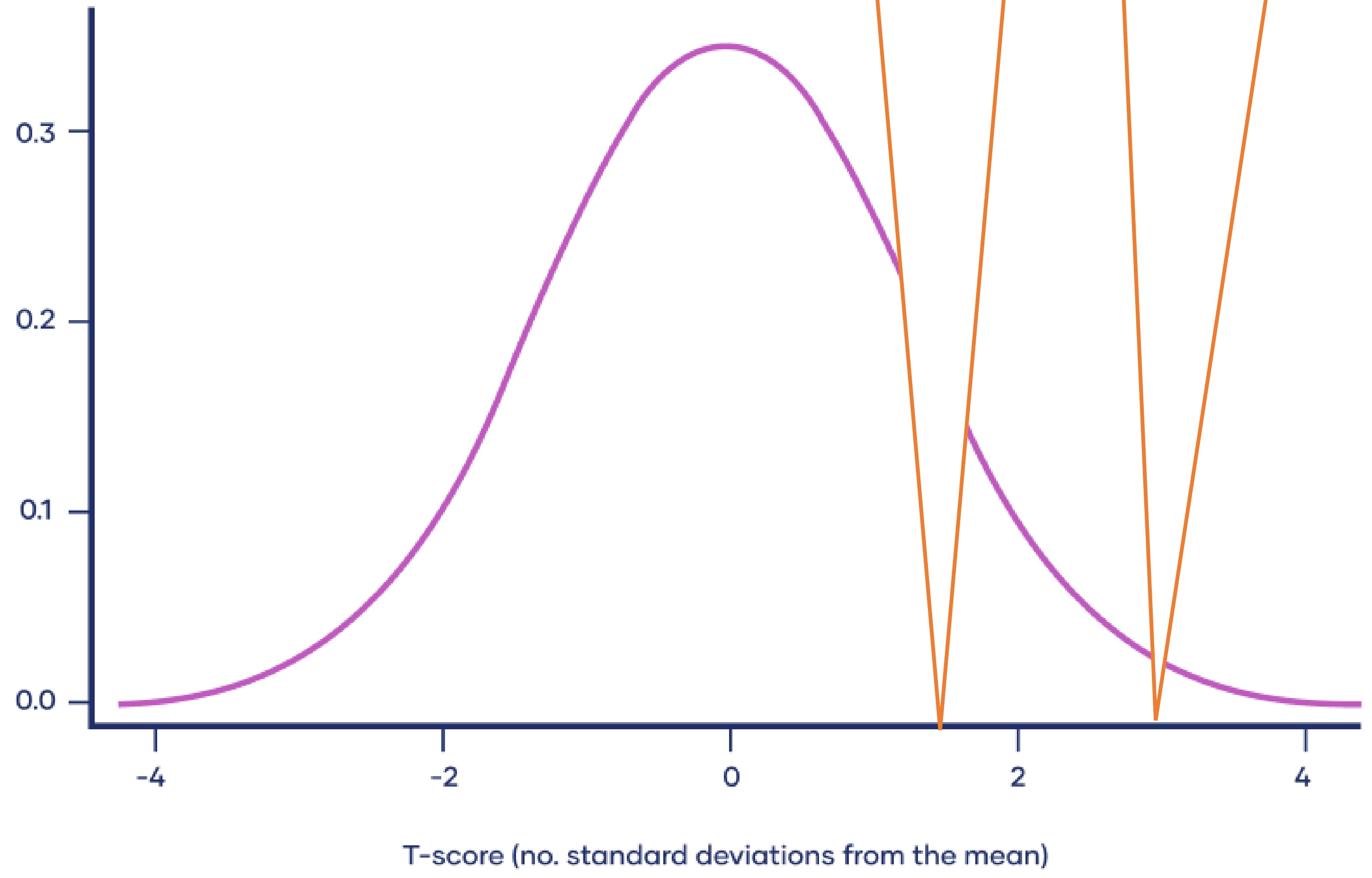
Clinical Trial of a new cancer medicine

- Current medicine has some efficacy
- Efficacy of current medicine decided by equation/past data
- Central Limit Theorem "sort of" gives bell curve (t distribution)
  - New medicine efficacy based on n samples
    - (n-1 degrees of freedom)

$$z \sim \mathcal{N}(\mu, \frac{\sigma}{\sqrt{n}})$$

$$t_{n-1} \sim \mathcal{T}(\mu, \frac{\sigma}{\sqrt{n}})$$

New medicine Mean efficacy is here



T Distribution

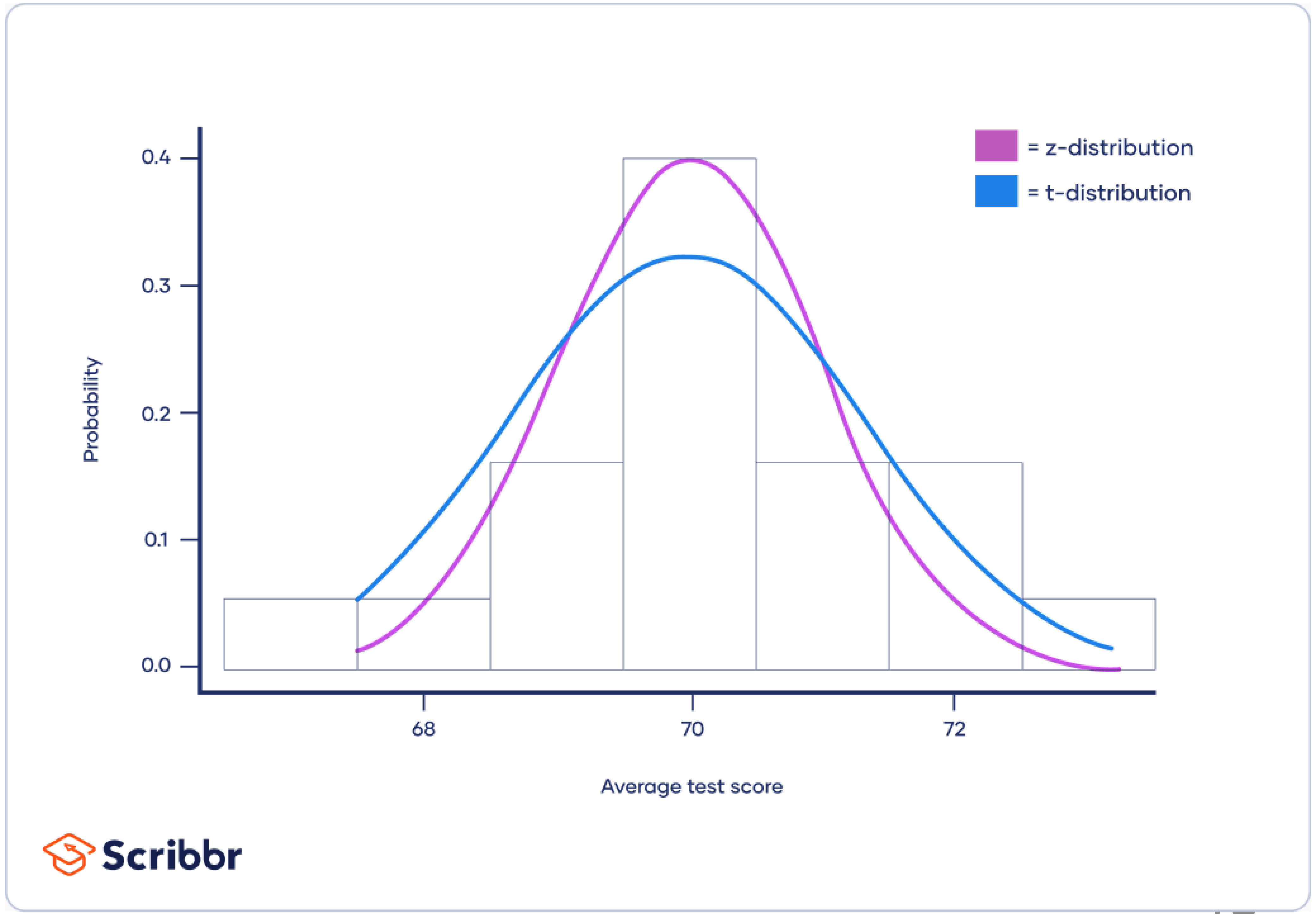
- Adjusted normal distribution for small sample sizes
- Number of samples = Degrees of freedom

$$z \sim \mathcal{N}(\mu, \frac{\sigma}{\sqrt{n}})$$

z statistic follows from this

t statistic follows from this

$$t_{n-1} \sim \mathcal{T}(\mu, \frac{\sigma}{\sqrt{n}})$$

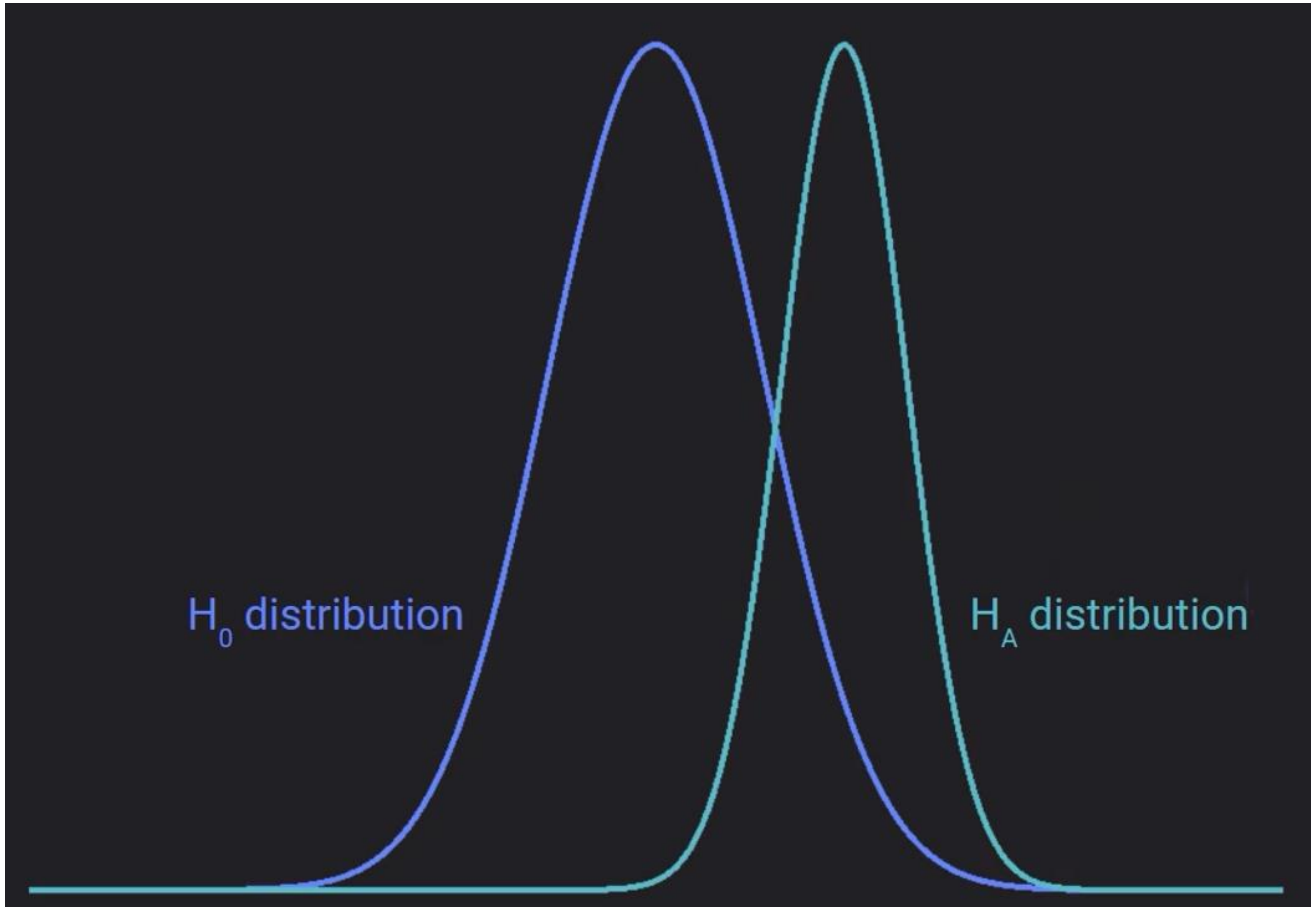


Intro to Hypothesis Test

- Null hypothesis – Ho,
- Alternate hypothesis – Ha

$$z \sim \mathcal{N}(\mu_0, \frac{\sigma_0}{\sqrt{n}})$$

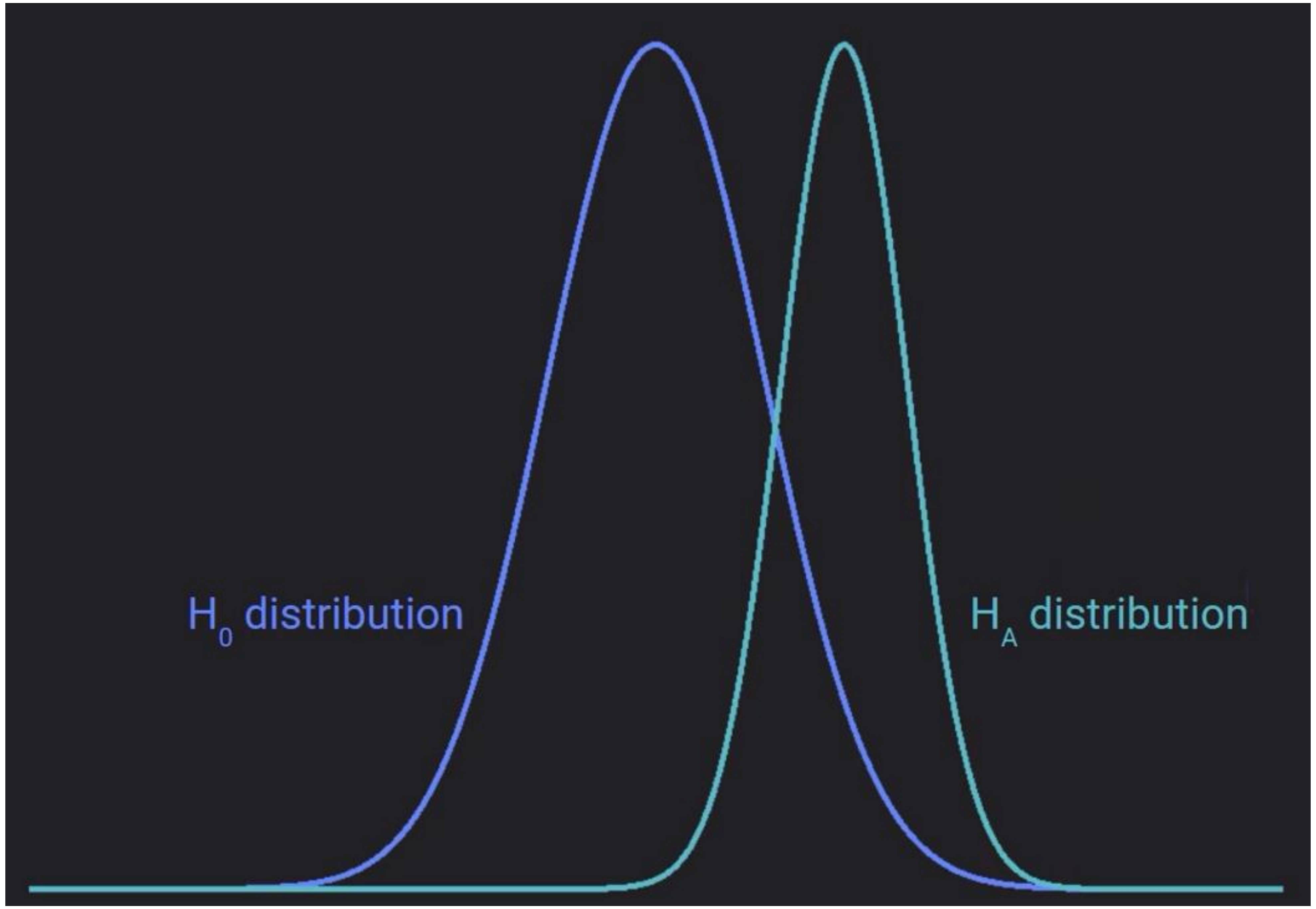
$$t_{n-1} \sim \mathcal{T}(\mu_0, \frac{\sigma_0}{\sqrt{n}})$$



- Convert x to z or t

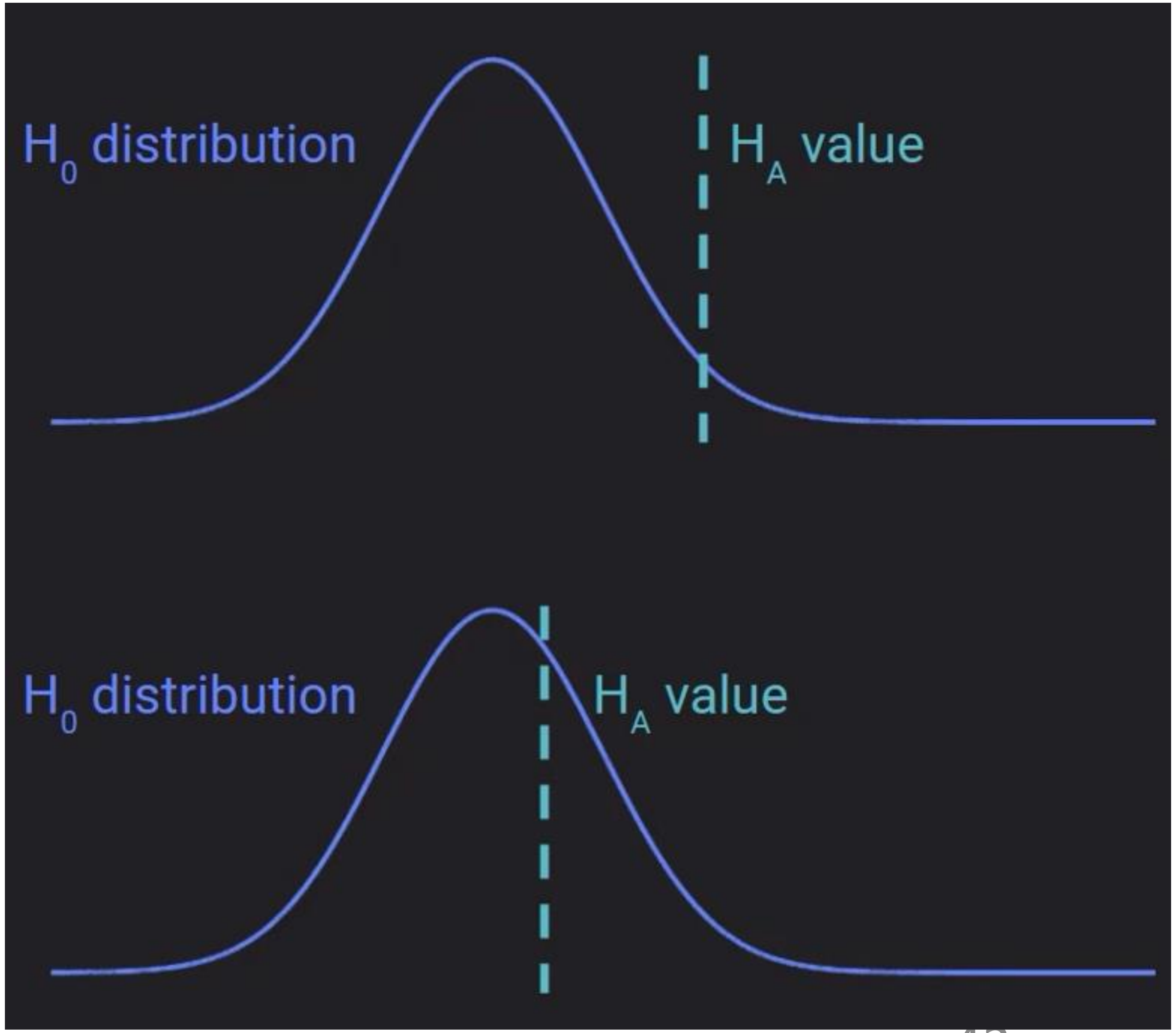
$$t_{n-1} = \frac{x - \mu_0}{\sigma/\sqrt{n}}$$

Intro to p-values in Hypothesis Test



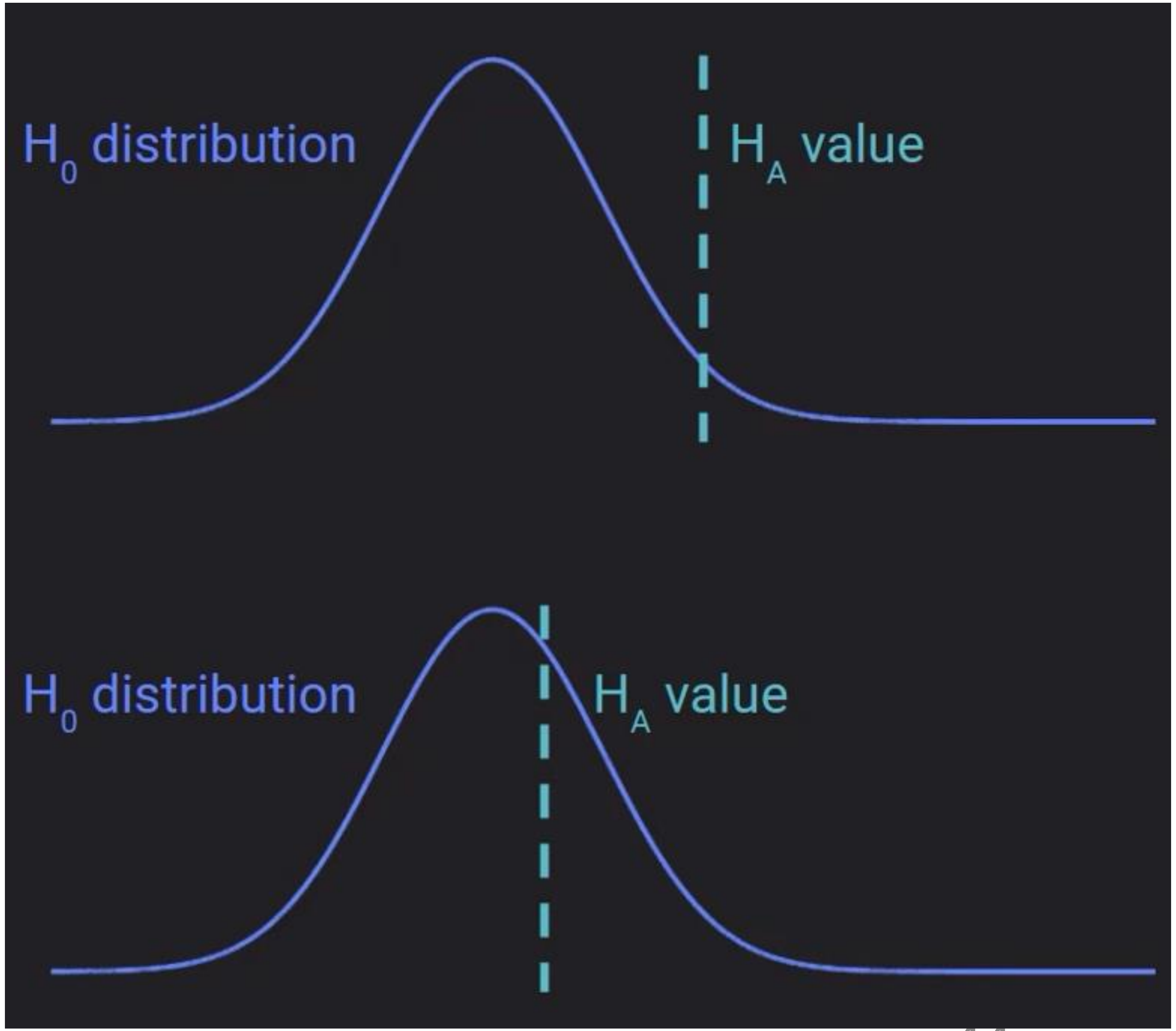
Indicates what is the probability value >= t-statistic

$$t_{n-1} = \frac{x - \mu}{\sigma / \sqrt{n}}$$



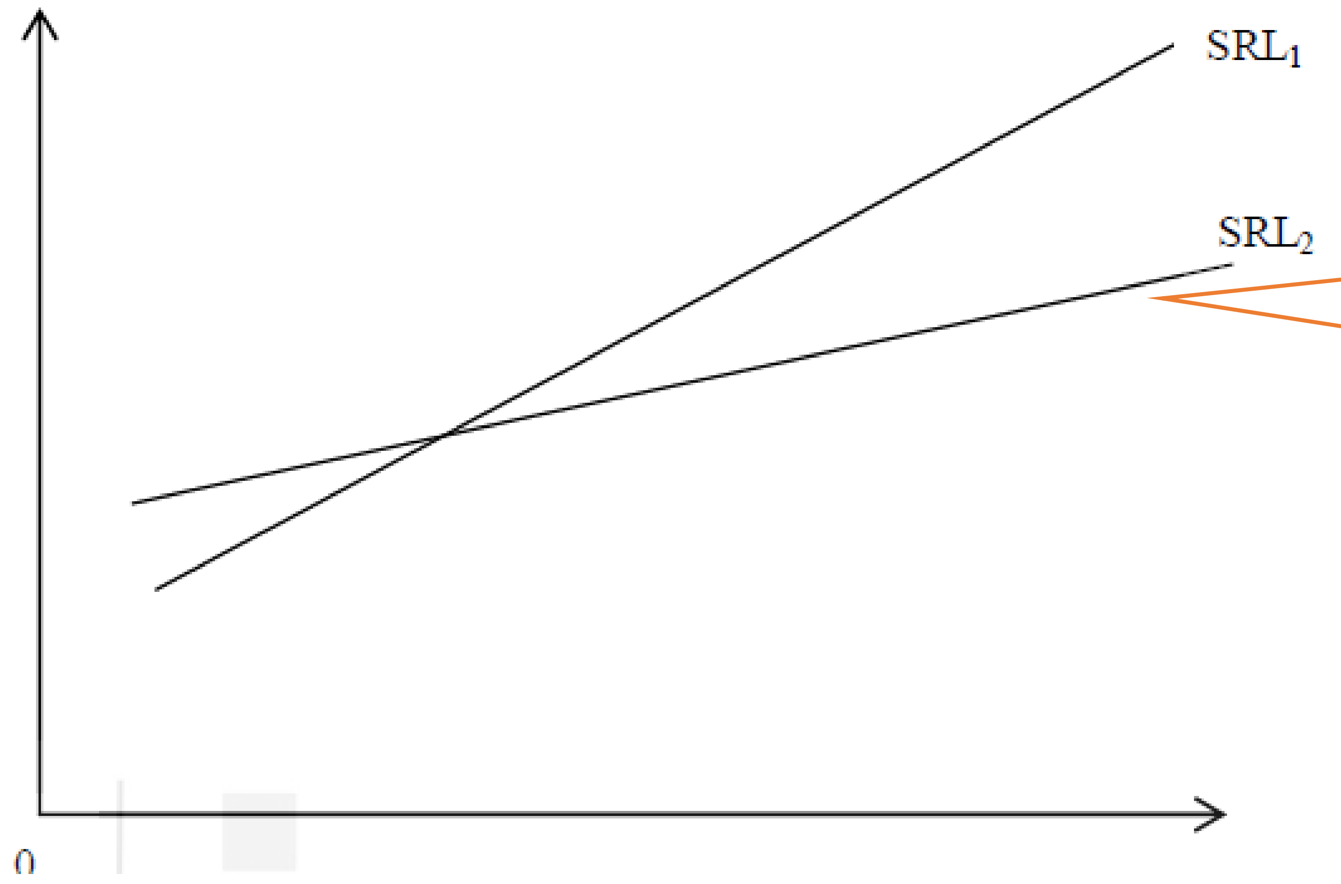
p-values in Hypothesis Test

- How likely for the Ha value to occur if Ho is true?
- What is the probability of observing a value of Ha larger than current value if there was no true effect?
- P(Ha | Ho)
- Definite Integral
  - Lookup table or coding



Regression - Population versus Sample View

- Sample Regression Functions
  - Different Regression Line/Plane/Hyperplane



Hypothesis function(s) corresponding to different null hypothesis (of what?)

- Difference between lines – values of coefficients
- Distribution of coefficients

$$\hat{y} = h(x) = w_1 TV + w_2 radio + w_3 newspaper$$

P value tells us total probability of given value under null hypothesis

Null Hypothesis is coefficient = 0

Alternate Hypothesis is coefficient not 0

OLS Regression Results

Dep. Variable:	sales	**R-squared (uncentered):**	0.982
Model:	OLS	**Adj. R-squared (uncentered):**	0.982
Method:	Least Squares	**F-statistic:**	3566.
Date:	Sun, 28 Mar 2021	**Prob (F-statistic):**	2.43e-171
Time:	13:42:33	**Log-Likelihood:**	-423.54
No. Observations:	200	**AIC:**	853.1
Df Residuals:	197	**BIC:**	863.0
Df Model:	3		
Covariance Type:	nonrobust		

	coef	**std err**	**t**	**P>|t|**	**[0.025**	**0.975]**
TV	0.0538	0.001	40.507	0.000	0.051	0.056
radio	0.2222	0.009	23.595	0.000	0.204	0.241
newspaper	0.0168	0.007	2.517	0.013	0.004	0.030

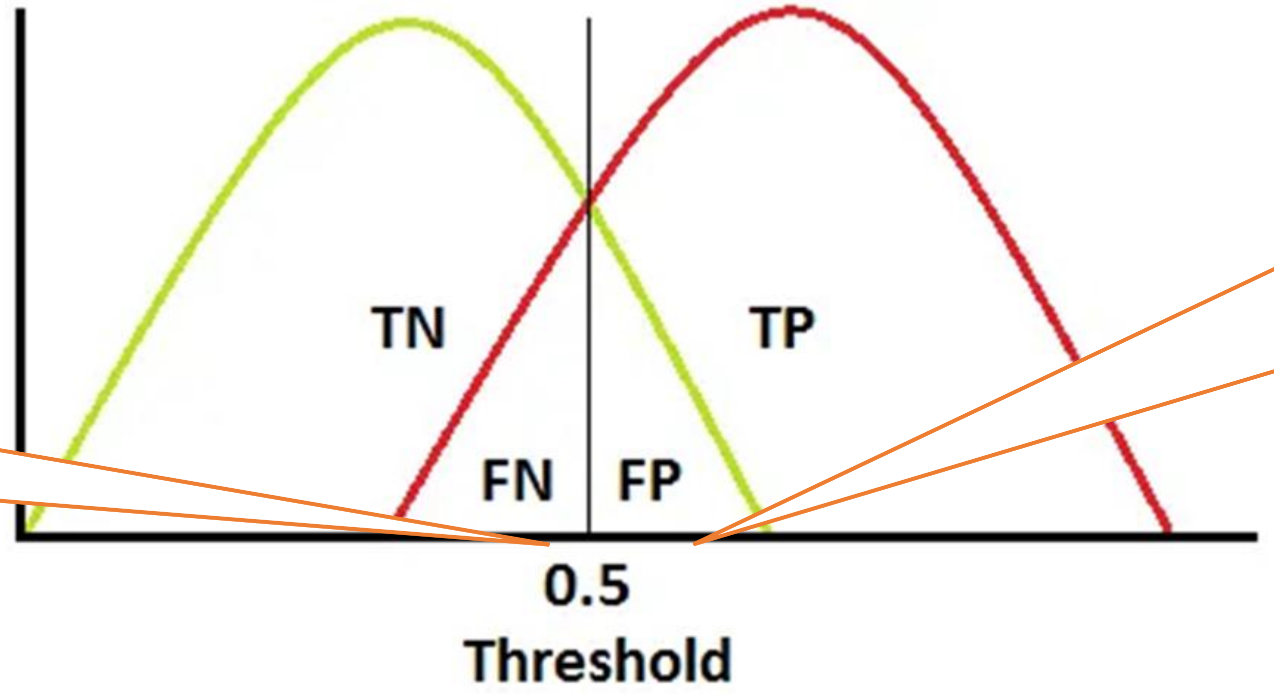
Omnibus:	5.982	**Durbin-Watson:**	2.038
Prob(Omnibus):	0.050	**Jarque-Bera (JB):**	7.039
Skew:	-0.232	**Prob(JB):**	0.0296
Kurtosis:	3.794	**Cond. No.**	12.6

Viewing hypothesis test from generative ML perspective

- p values & statistical significance
- Machine Learning
  - Training is not a strict Ho, but a foundation
  - Each X_test record is sample from different dist (RV)
  - Each X_test record is the mean of the RV
  - Prediction on each X_test is different Ha

Hypothesis testing looks for conservative threshold for a given p-value

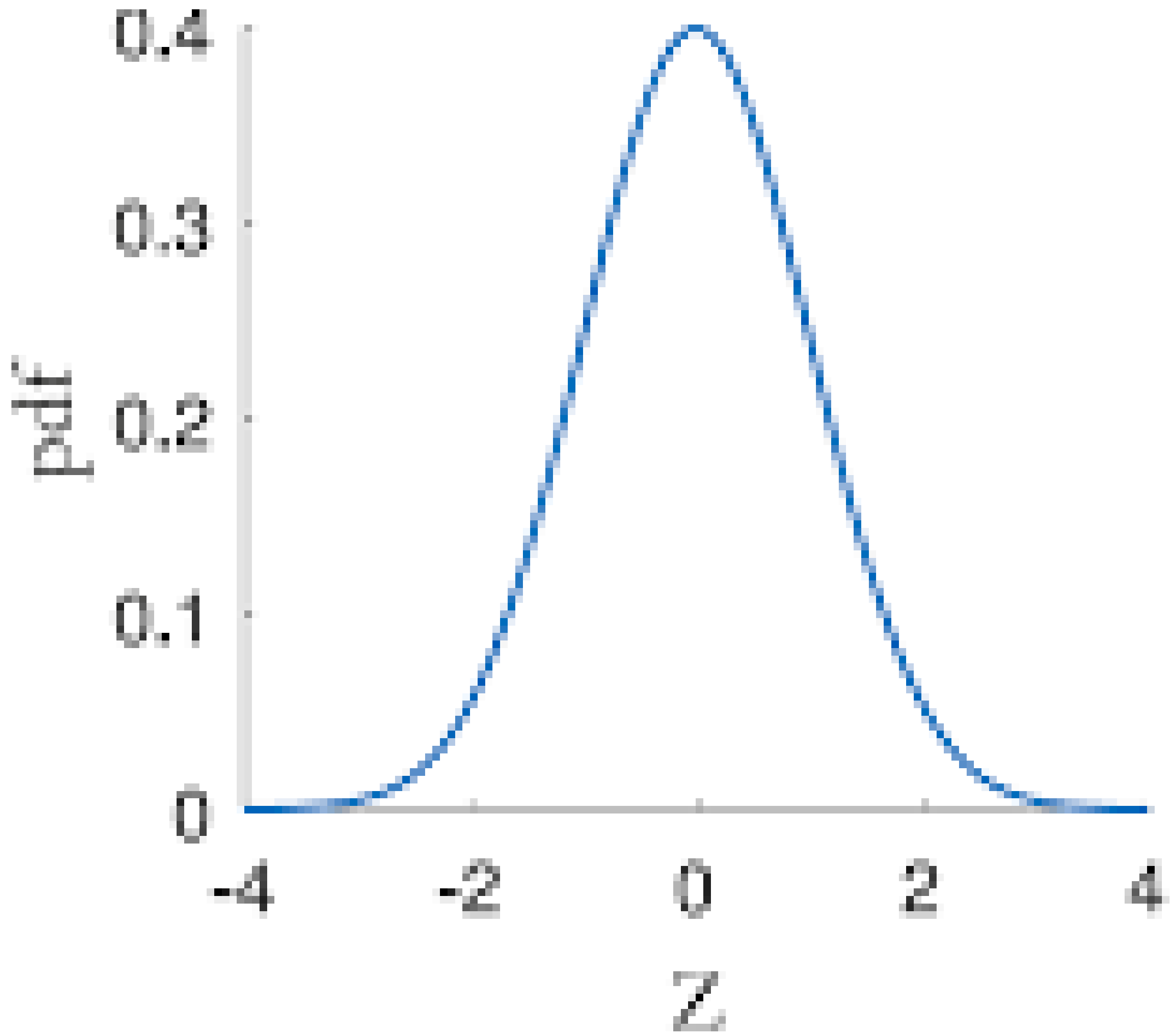
ML looks for optimal threshold



Chi-squared Distribution

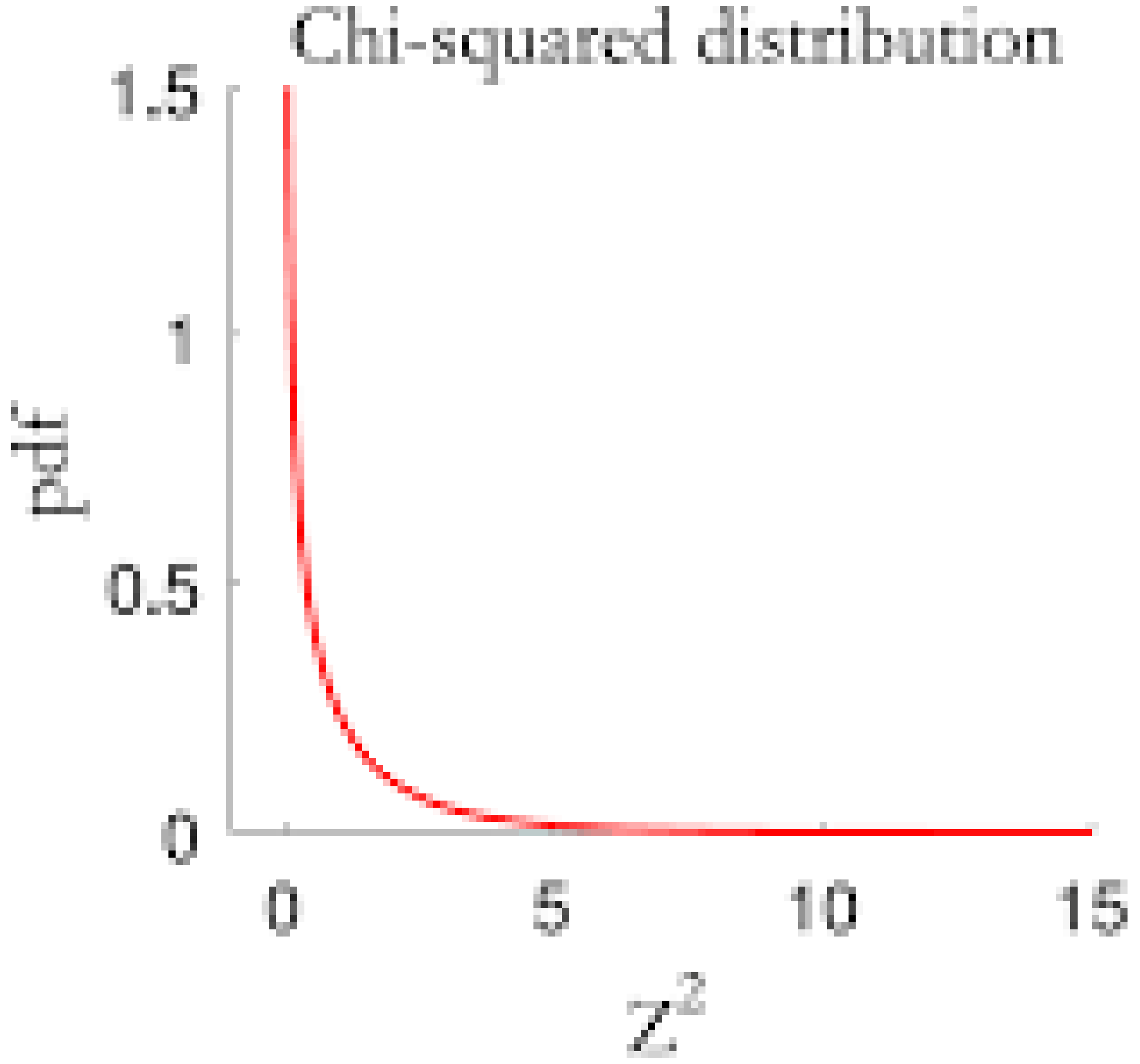
$$Z \sim N(0,1)$$

Standard Normal Distribution



$$Q = Z^2 \sim \chi^2$$

Chi-Squared Distribution

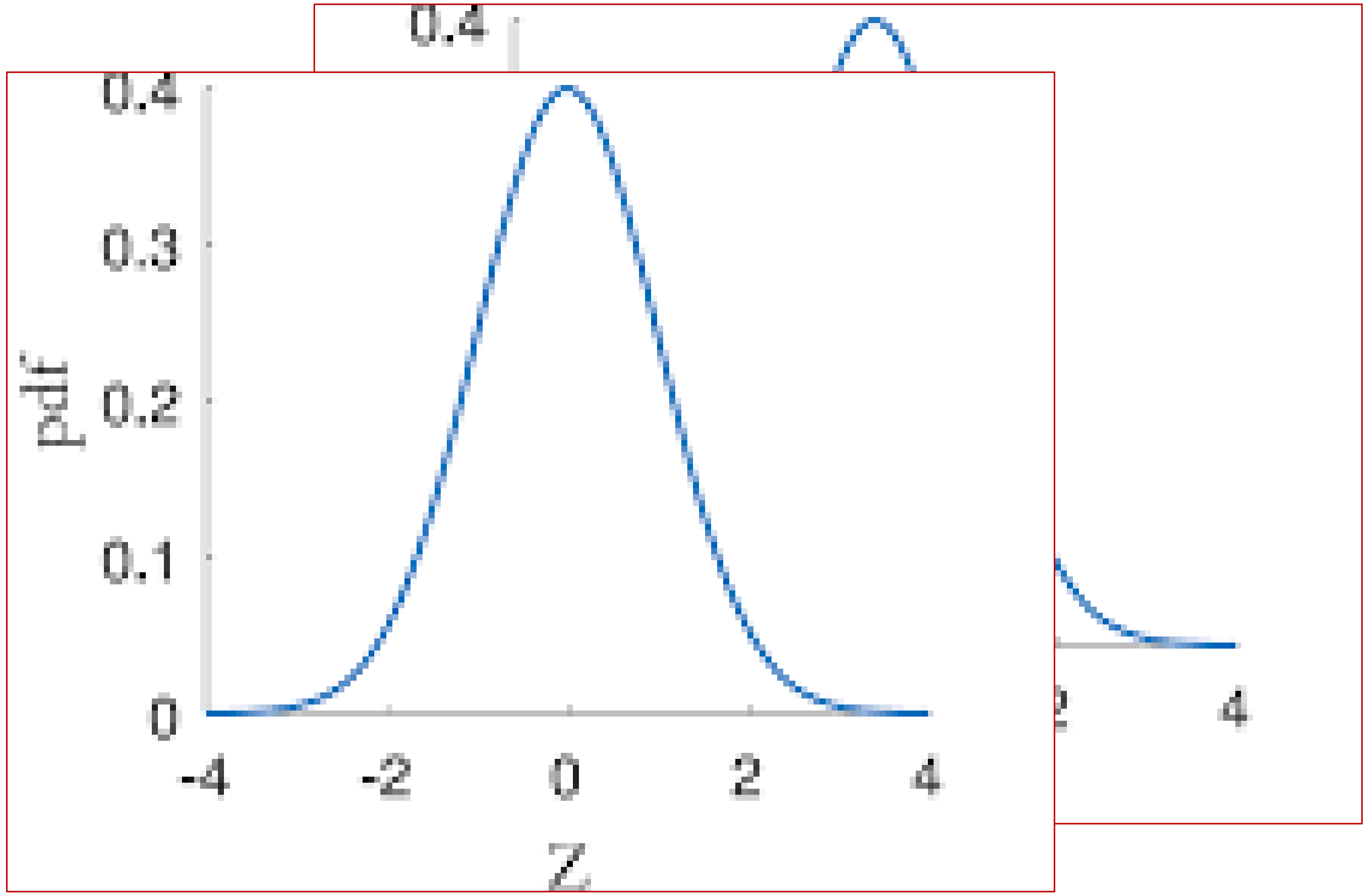


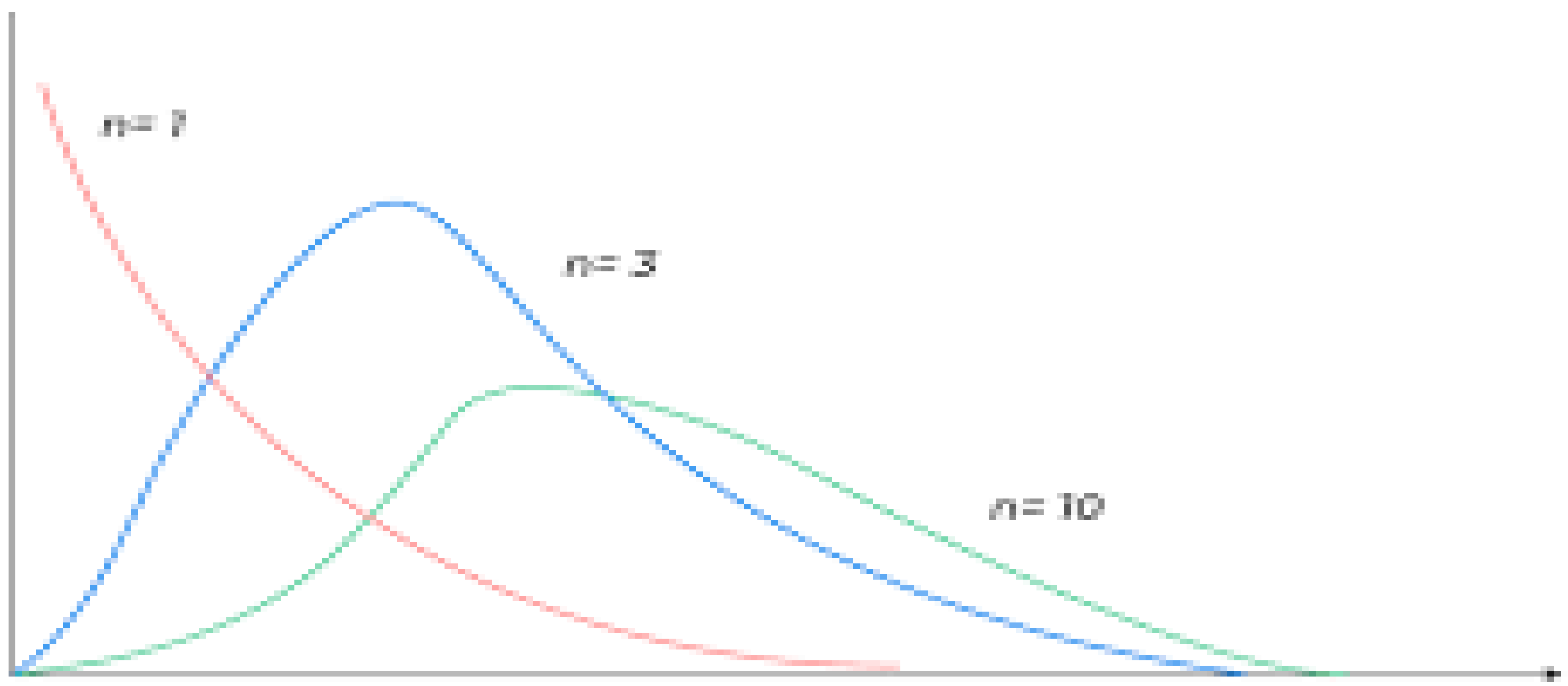
Chi-squared Distribution with two degrees of freedom

- Two random var Z_1, Z_2 with std normal distribution

$$Z_1 \sim N(0,1) \quad Z_2 \sim N(0,1)$$

$$Q = Z_1^2 + Z_2^2 \sim \chi_2^2$$



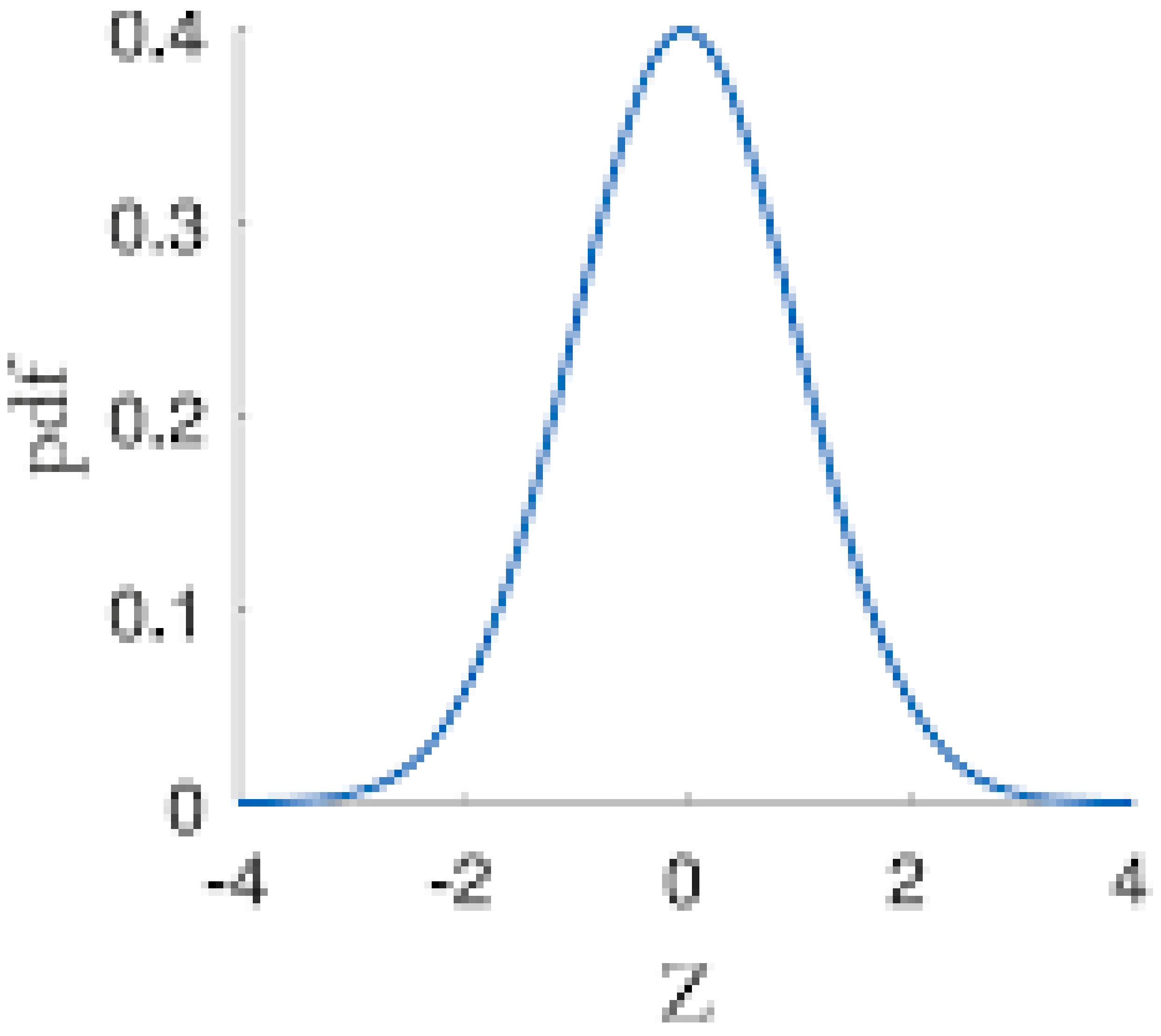


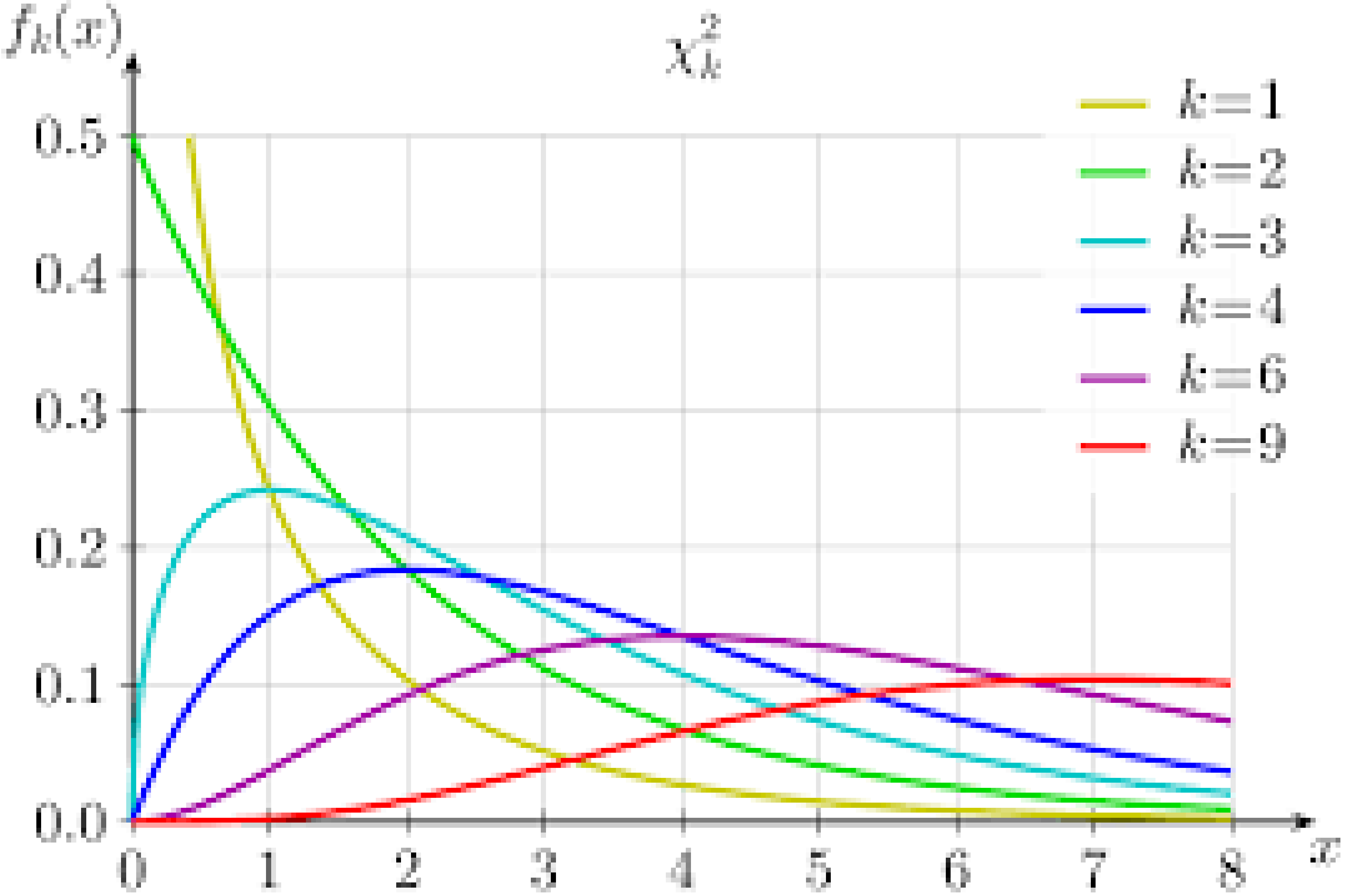
Chi-squared Distribution with n degrees of freedom

- n random var $Z_1, ..Z_n$ with std normal distribution

$Z_1 \sim N(0,1) \quad Z_n \sim N(0,1)$

$$Q = \sum_{i=1}^{n} Z_i^2 \sim \chi_n^2$$





Revisiting the contingency table for independence

- Titanic dataset
  - Sex & Survived (x & y)

sex	female	male	
survived			
0	91	479	570
1	235	109	344
Total	326	588	914

Observed

	Female	Male	Total
Survived	0.1	0.52	0.62
Not Survived	0.26	0.12	0.38
Total	0.36	0.64	1

Expected

	Female	Male	Total
Survived	.22	0.4	0.62
Not Survived	0.14	0.25	0.38
Total	0.36	0.64	1

Observed counts to expected counts

Observed

sex	female	male	
survived			
0	91	479	570
1	235	109	344
Total	326	588	914

	Female	Male	Total
Survived	0.1	0.52	0.62
Not Survived	0.26	0.12	0.38
Total	0.36	0.64	1

$P(X,Y) = P(X)P(Y)$

Expected

	Female	Male	Total
Survived	.22	0.4	0.62
Not Survived	0.14	0.25	0.38
Total	0.36	0.64	1

	Female	Male	Total
Survived	0.22 x 570	0.4 x 570	570
Not Survived	0.14 x 344	0.25 x 344	344
Total	0.36	0.64	1

Distribution of a single column in contingency table

sex	female
survived	
0	91
1	235
Total	326

Observed

	Female
Survived	0.1
Not Survived	0.26
Total	0.36

Binomial distribution with large n

- n = 326
- p=0.1
- X =91

$$Z = \frac{X - np}{\sqrt{np(1-p)}} \sim \mathbb{N}(0,1)$$

$$Z^2 = \frac{(X-np)^2}{np(1-p)}$$

$$Z^2 = \frac{(X-np)^2}{np} + \frac{(n-X-np(1-p))^2}{n(1-p)}$$

$$Z^2 = \sum_i \frac{(o_i - e_i)^2}{e_i}$$

Chi-Squared distribution

sex	female	male	
survived			
0	91	479	570
1	235	109	344
Total	326	588	914

$$\chi^2 = Z^2 = \sum_{all-cells} \frac{(o_i - e_i)^2}{e_i}$$

- How many degrees of freedom
- Ho Two features or feature-target are independent

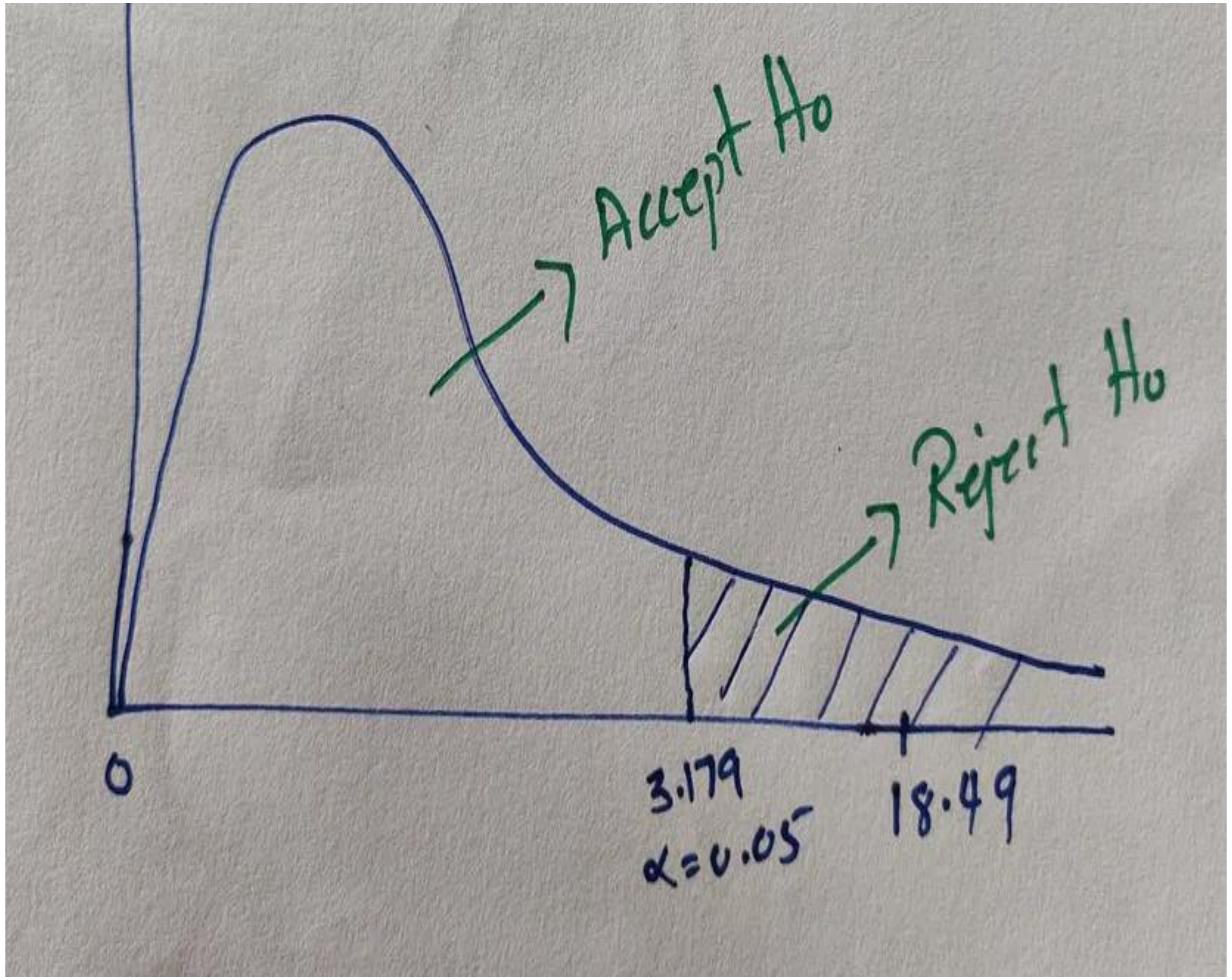
Ha Features not independent

	Female	Male	Total
Survived	0.22 x 570	0.4 x 570	570
Not Survived	0.14 x 344	0.25 x 344	344
Total	0.36	0.64	1

$$Z_1^2 = \sum_{i \in k} \frac{(o_i - e_i)^2}{e_i} \qquad Z_2^2 = \sum_{i \in k} \frac{(o_i - e_i)^2}{e_i}$$

$$\chi^2 = Z_1^2 + Z_2^2 = \sum_{all-cells} \frac{(o_i - e_i)^2}{e_i}$$

$$\chi^2 = Z_1^2 + Z_2^2 + ... = \sum_{all-cells} \frac{(o_i - e_i)^2}{e_i}$$



- Ho Two features (or feature-target) are independent
- Ha Features (or feature-target) not independent

- Observed diverges A LOT from expected
- Chi-Squared value increases


X²– 4X ≤ 0
n (B∩C) = 22
n (B) = 68
n (C) = 84
n (B∪C) = n (B) + n (C)-n (B∩C)
M = 0.046765 / 3 0L
He = 4.002602
Na = 22.989769
Ar = 39.948
x̄₁ = 1+3+3+6+8+9 / 6 = 5
x̄₂ = 2+4+4+8+12 = 30
x̄₃ = 4+7+1+6 = 18
log_b b^x = x
log_a x = log_b x / log_b a
20 →
6 →
(0,1)
f = R/2

ANOVA

ANOVA intuitively from ML perspective

- Categorical Feature: Crime rate = High, Medium, Low
- Numerical target: House price
- Does crime rate have impact on house price?

- Is the price difference between groups a mere chance (noise) or significant enough to be good predictor?
- Quantifying the difference as not significant/significant
- Think of it as lining up all combinations of Ho-Ha between categorical values

$$SSB = \sum_{i=1}^{m} n_i(\bar{x}_i - \bar{x})^2$$

$$SSW = \sum_{i=1}^{m}\sum_{j=1}^{n}(x_{i,j} - \bar{x}_i)^2$$

$$F = \frac{SSB/n_1}{SSW/n_2}$$

F-statistic from F distribution Has its own p-values

- n1, n2 degrees of freedom
- Ho Categorical feature has no variance between groups
- Ha Categorical feature has significant variance between groups

- Ho Categorical target cannot be predicted by a numerical feature
- Ha ??

Code example in sklearn

```python
from sklearn.feature_selection import f_classif

from sklearn.datasets import load_iris
data = load_iris()
X = data.data
y = data.target
```

```python
# Perform ANOVA
F_scores, p_values = f_classif(X, y)

for feature, F, p in zip(data.feature_names, F_scores, p_values):
    print(f"Feature: {feature}, F-score: {F}, p-value: {p}")
```

```
Feature: sepal length (cm), F-score: 119.26450218449871, p-value: 1.669669107731823e-31
Feature: sepal width (cm), F-score: 49.16004008961098, p-value: 4.492017133311986e-17
Feature: petal length (cm), F-score: 1180.161182529776, p-value: 2.856776610962102e-91
Feature: petal width (cm), F-score: 960.0071468018025, p-value: 4.169445839445031e-85
```

F-statistic in OLS

$$\hat{y} = h(x) = w_1 TV + w_2 radio + w_3 newspaper$$

P value tells us total probability of given value under null hypothesis

Null Hypothesis is coefficient = 0

Alternate Hypothesis is coefficient not 0

OLS Regression Results

Dep. Variable:	sales	**R-squared (uncentered):**	0.982
Model:	OLS	**Adj. R-squared (uncentered):**	0.982
Method:	Least Squares	**F-statistic:**	3566.
Date:	Sun, 28 Mar 2021	**Prob (F-statistic):**	2.43e-171
Time:	13:42:33	**Log-Likelihood:**	-423.54
No. Observations:	200	**AIC:**	853.1
Df Residuals:	197	**BIC:**	863.0
Df Model:	3		
Covariance Type:	nonrobust		

	coef	std err	t	P>|t|	[0.025	0.975]
TV	0.0553	0.001	40.507	0.000	0.051	0.056
radio	0.2222	0.009	23.595	0.000	0.204	0.241
newspaper	0.0168	0.007	2.517	0.013	0.004	0.030

Omnibus:	5.982	**Durbin-Watson:**	2.038
Prob(Omnibus):	0.050	**Jarque-Bera (JB):**	7.039
Skew:	-0.232	**Prob(JB):**	0.0296
Kurtosis:	3.794	**Cond. No.**	12.6

F-statistic in OLS

ANOVA intuitively from ML perspective

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QUESTIONS