3011979 Practical Python for Data Sciences and Machine Learning

L6: Machine learning pipeline

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We seek understanding of mechanisms

Trajectory of the ball

Newton's laws of motion

Initial force and angle

Gravity

$$y = f(x)$$

Drug response in patient

Drug chemistry

Human biology

Clinical data

Genomics data

And a lot more…

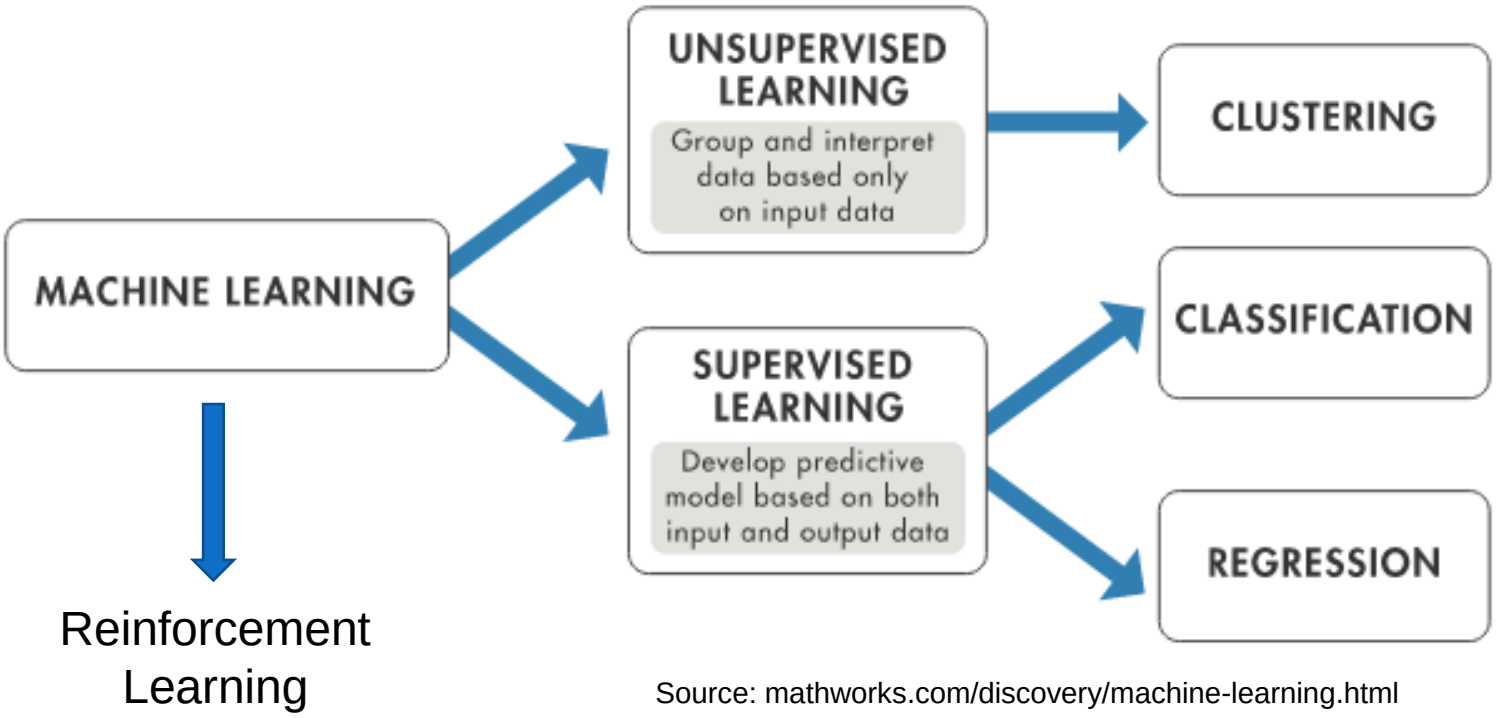
Statistics vs machine learning

$$y = f(x)$$

- **Statistics (and math modeling)** uses the whole (x, y) to learn about f
  - Constrained by our knowledge of the mechanisms
  - First order approximation = linear model

- **Machine learning** uses some of (x, y) to optimize the best f and then test it on the unseen data
  - Model can be more complex than the actual mechanisms
  - Even noises can be fitted almost perfectly
  - Multiple solutions exist!

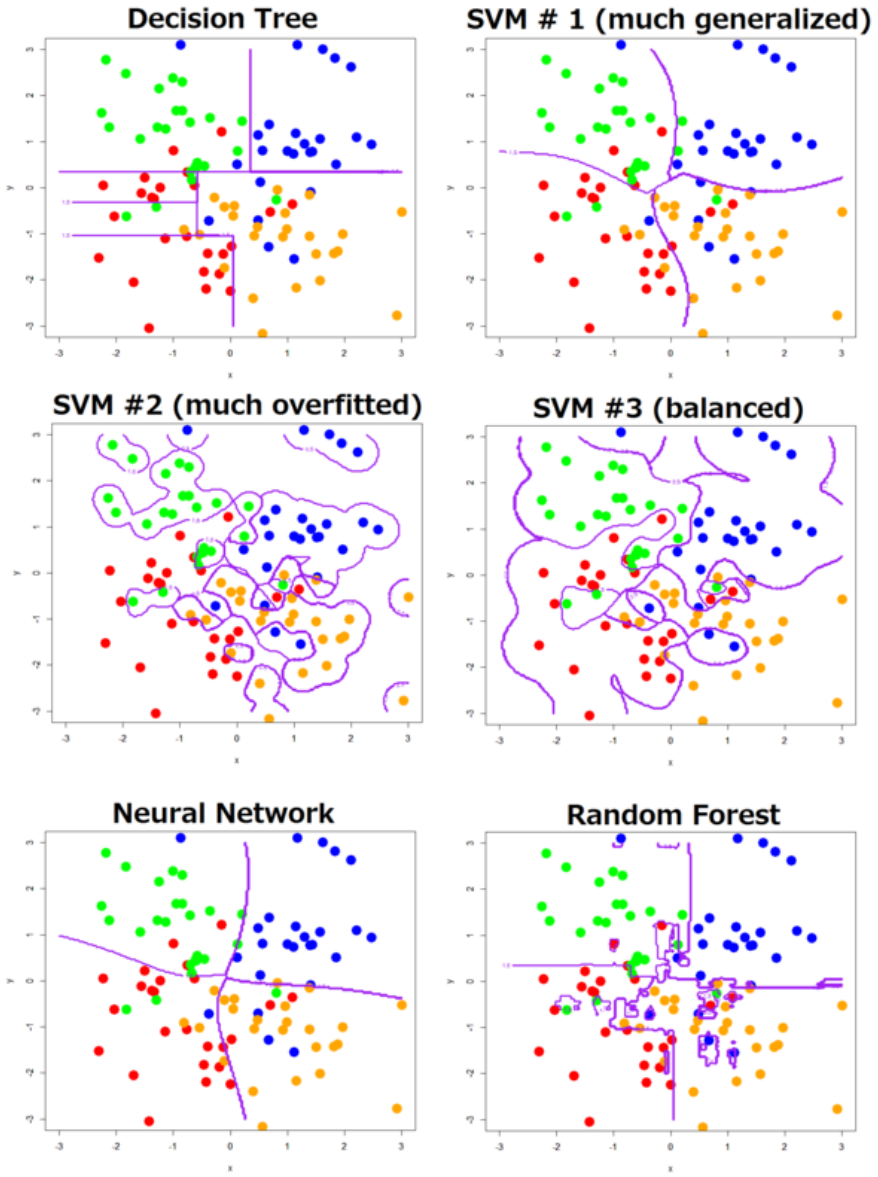
Supervised learning



Source: mathworks.com/discovery/machine-learning.html

- Classification = predict class (e.g., yes/no, subtype A/B/C)
- Regression = predict real number (e.g., p(sick), drug effect)

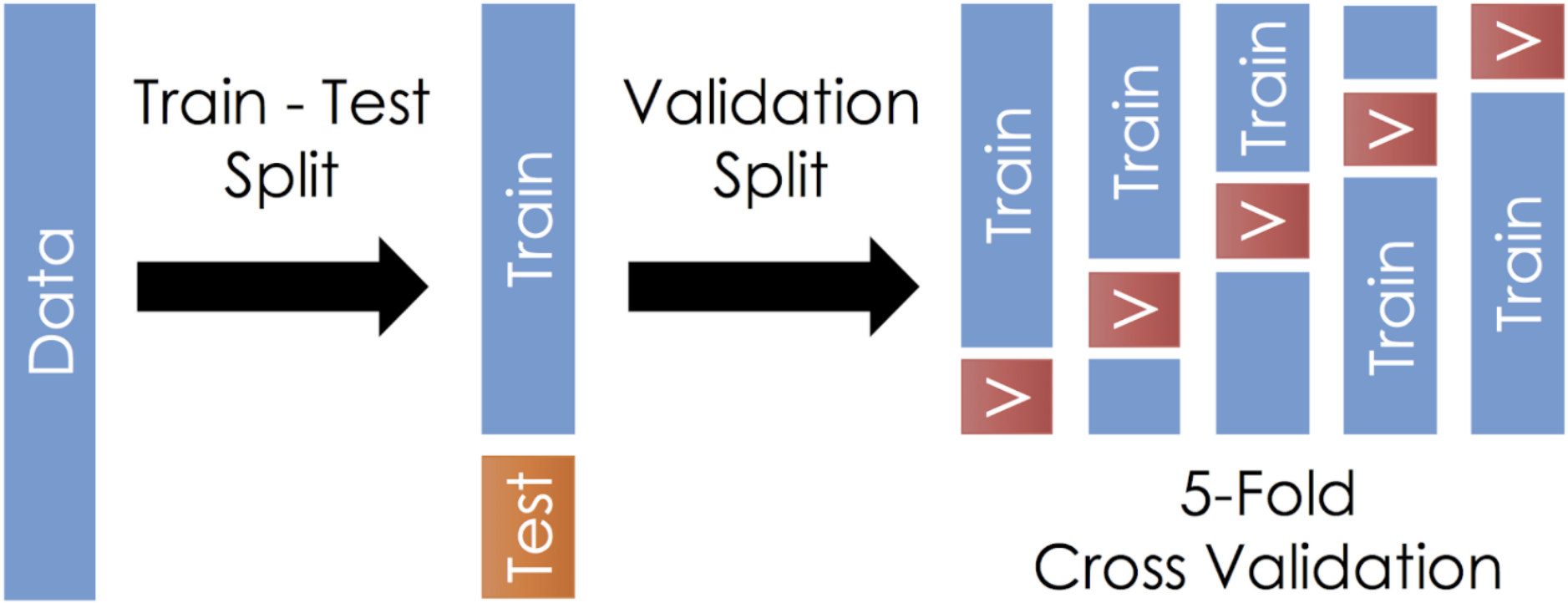
Complex model **tends to** overfits



- Most of what we do in machine learning is to <u>prevent overfitting</u>
- Use of validation set
- Remove noisy features
- Regularize model complexity

Validation

Validation



Source: medium.com

- **Training set** is used to optimize model f
  - Select the model that performs best on the **validation set(s)**
  - Cross-validation lessens the chance that the model overfit
- Then check the model's performance on the **test set**

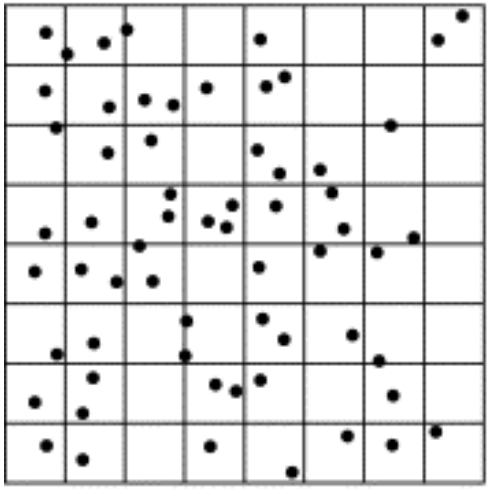
Expected model behavior

- Performance on **training set** is near perfect
- Performance on **validation set** is lower
  - But this is still an over-estimation of the model's performance
- Performance on **test set** is most representative

- **Key assumption**: all sets are representative of the distribution of input data

- In practice, you may find that performance on the validation set is lower than on the test set
  - It's about how the data were split

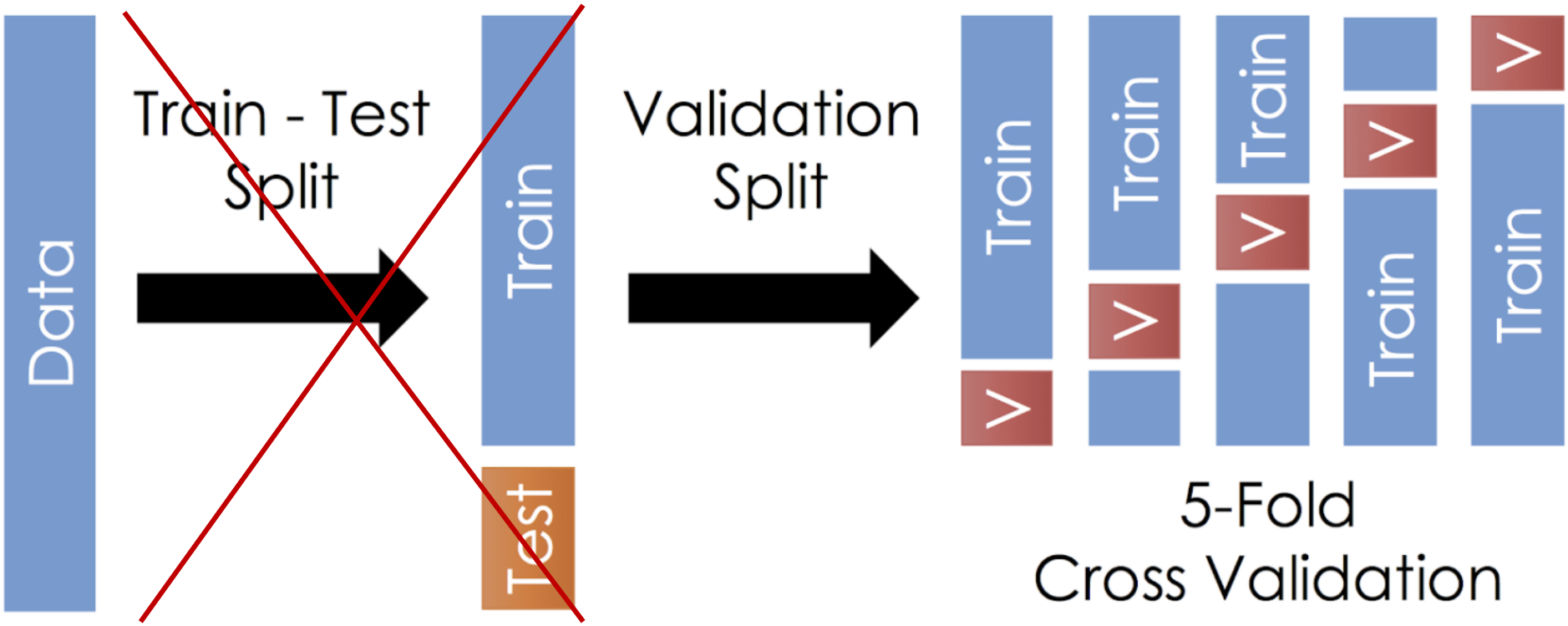
Dealing with small dataset



Some parts of data distribution are unobserved

- Small dataset may not reflect the whole data distribution
  - Further amplified by data splitting
- Which set would you assign less samples to?
  - Small test set = cannot trust the estimated performance
  - Small validation set = cannot reliably identify the best model
  - Small training set = the model does not fit some part of the distribution

It is ok to not have the (external) test set



- With small dataset, train-test split is appropriate
  - Splitting reduces the amount of data for training and tuning
  - Small test set cannot represent the true data distribution anyway
- Can only propose the method, not the trained model

Validation schemes

- ***k*-fold** cross-validation
  - Split data into ***k*** equal-sized partitions
  - In each round, train models on ***k* – 1** partitions and evaluate the performance on the last partition
  - ***k*** models are trained and evaluated

- **Leave-one-out** (LOO) cross-validation
  - ***k*-fold** cross-validation with ***k*** = number of samples – 1
  - **number of samples – 1** models are trained and evaluated
  - The performance is either 0 or 1 (for classification)

- **Bootstrapping**
  - **Randomly split x%** of the data as training set
  - Repeat the process multiple times

Feature selection

Uninformative features can be detrimental

- Uninformative features can correlate with the outcome by chance and fool the model
  - Often the case for small dataset
  - Complex model can always discover a combination of noisy features that fit the data well
- Some models have built-in ability to avoid uninformative features, but many do not
  - Linear models are forced to consider all features
    - Alleviated by L1-regularization (LASSO)
  - Random forest can handle this well
  - Neural network suffers the most from this problem

Univariate feature selection

- A preliminary filter using univariate technique can be helpful
  - Correlation between an input feature and an output (regression)
  - Test of mean or ANOVA between input feature means across different output classes (classification)

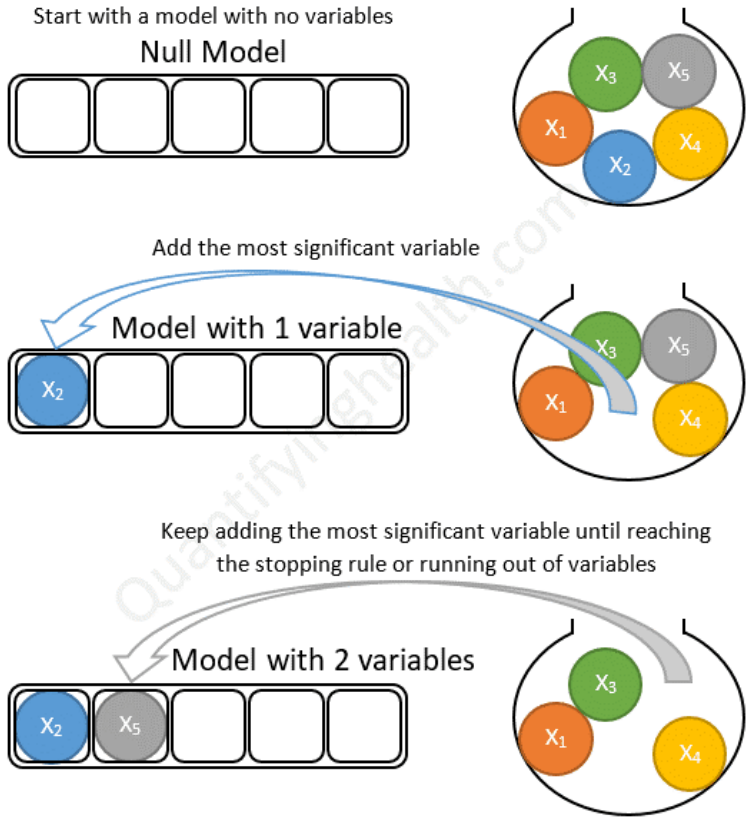
- Some features might be predictive only on a subpopulation and do not exhibit high correlation on the whole dataset
  - Do not be too aggressive on the univariate step

Sequential feature selection schemes

Forward Selection

Add one good feature at a time

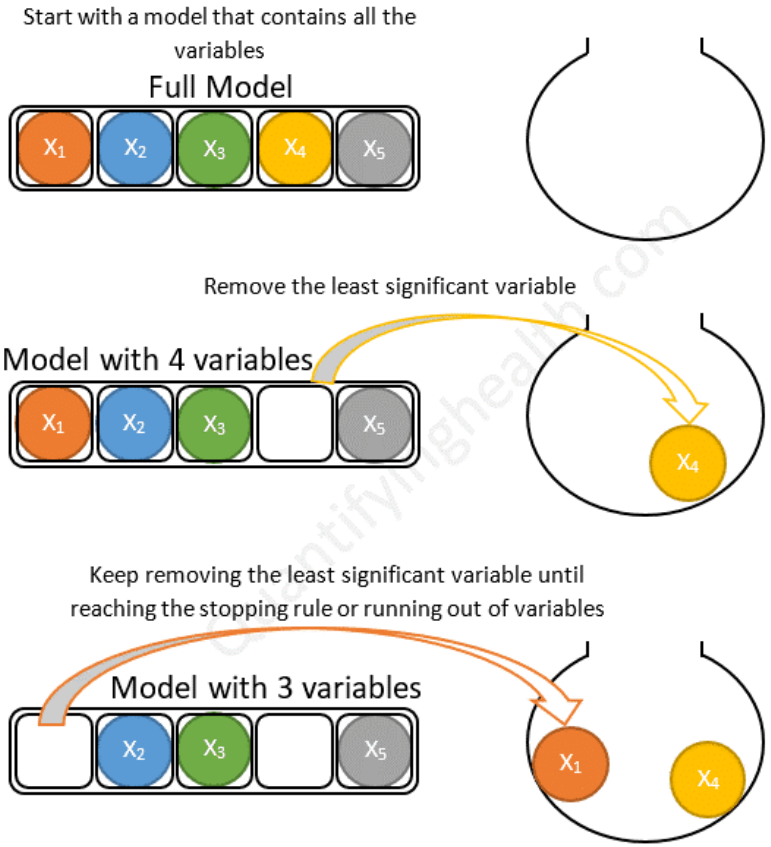
Forward stepwise selection example with 5 variables:



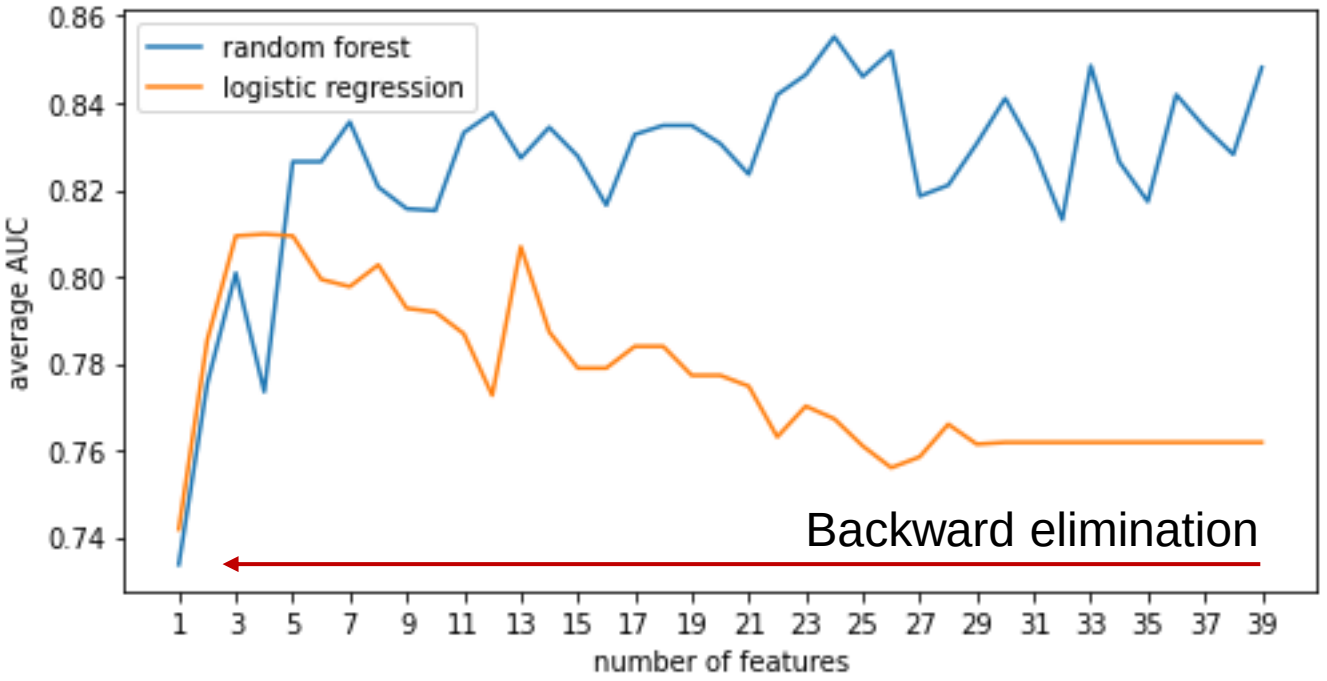
Backward Elimination

Remove one poor feature at a time

Backward stepwise selection example with 5 variables:

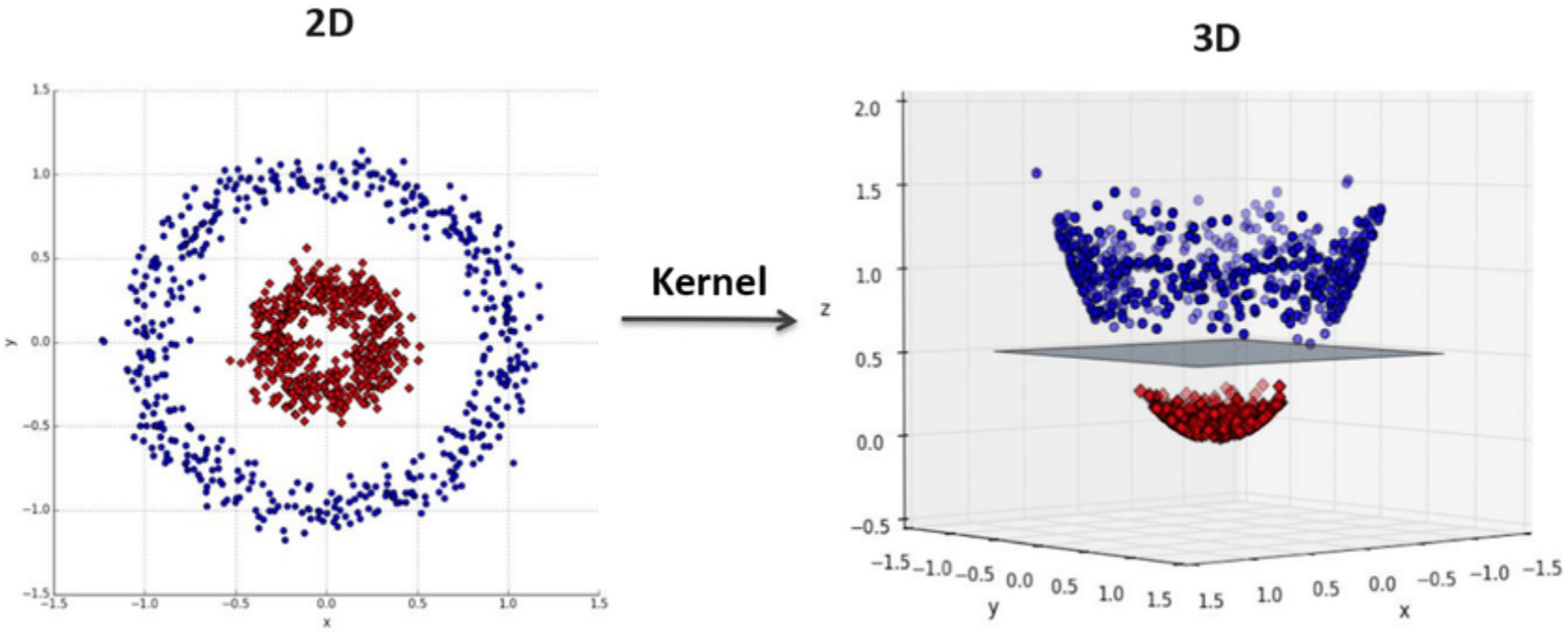


Impact of feature selection



- Random forest does not need help select feature
  - But doing so can reduce the burden of future data collection
- Logistic regression benefits a lot from feature selection
- There are ~5-7 essential features that cannot be removed

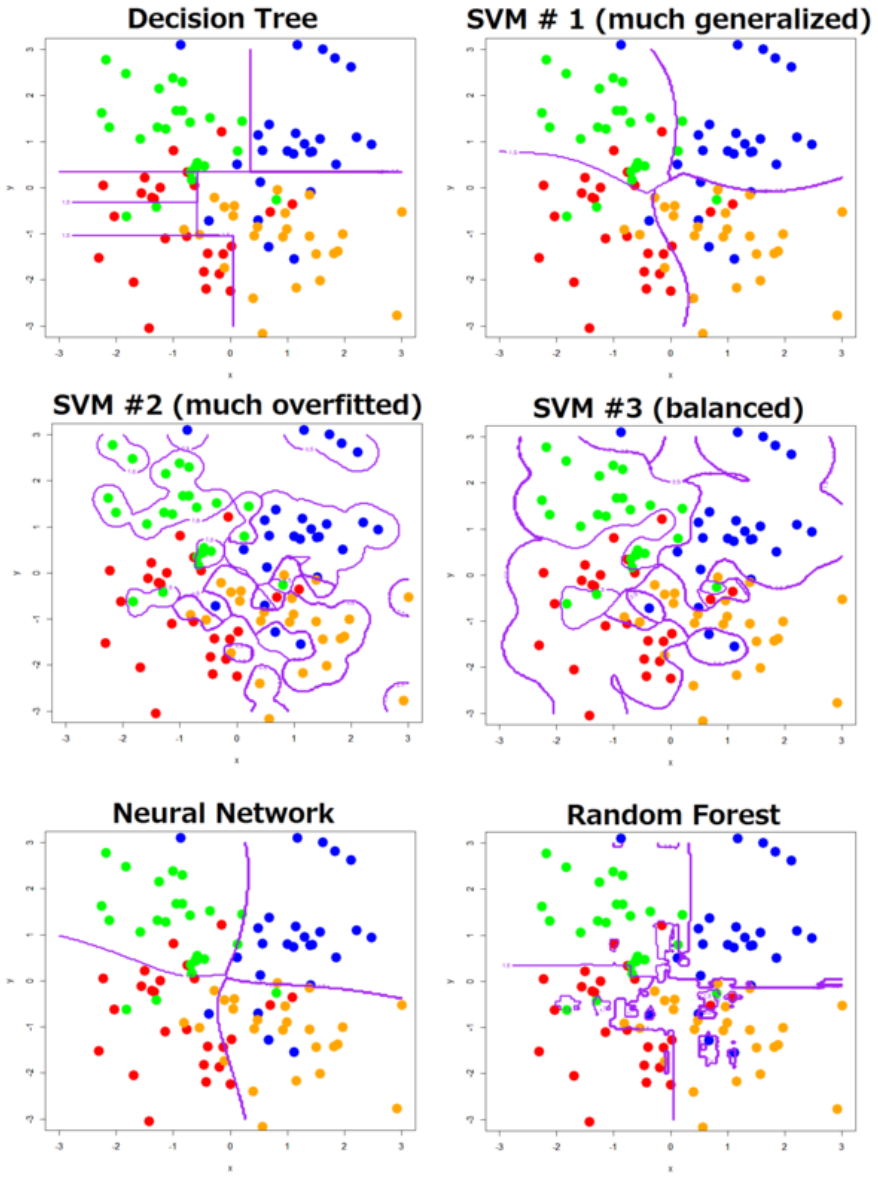
Feature engineering



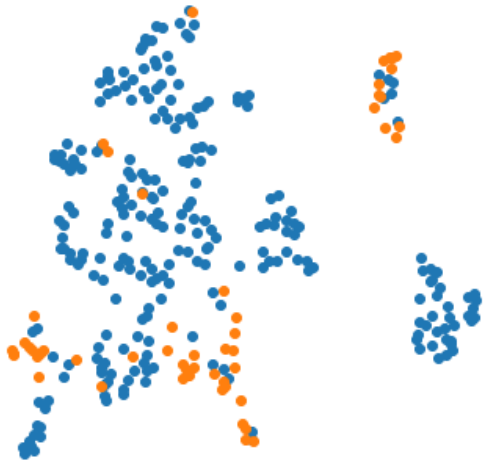
- Transform (x, y) to (x, y, $x^2 + y^2$)
  - Blue data points are further away from origin → larger $x^2 + y^2$
  - Separating hyperplane is a linear combination of x, y, and $x^2 + y^2$ which is nonlinear with respect to x and y

Model regularization

Simple model can perform better



- Similar to nested model testing in statistics
- Develop a simple model as **baseline**
  - Linear / logistic regression
- Visualize data distribution



Coefficient regularization

$$\text{Ridge Loss} = C \cdot \sum_i \left(y_i - [b_0 + b_1 x_1^{(i)} + \cdots + b_n x_n^{(i)}] \right)^2 + \sum_i {b_i}^2$$

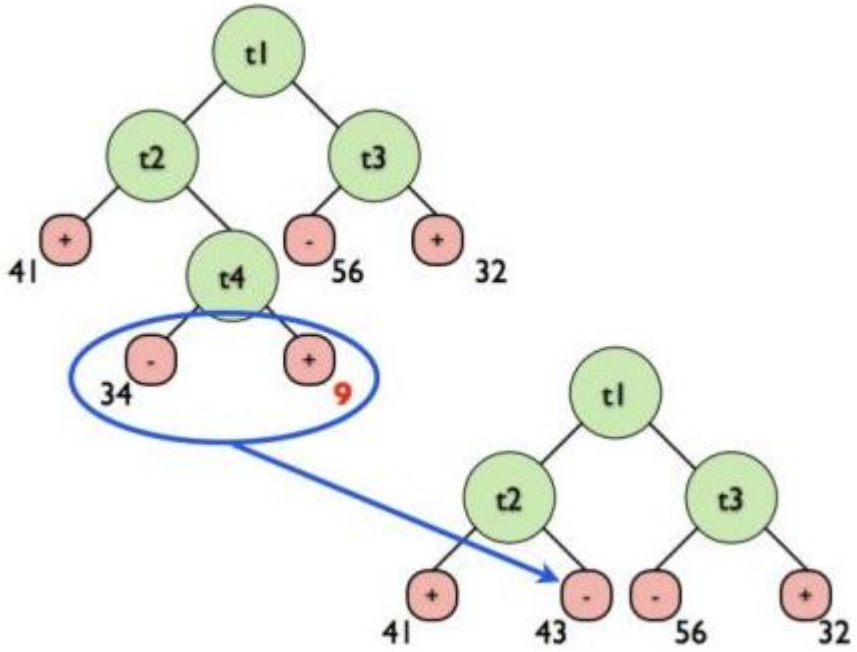
$$\text{LASSO Loss} = C \cdot \sum_i \left(y_i - [b_0 + b_1 x_1^{(i)} + \cdots + b_n x_n^{(i)}] \right)^2 + \sum_i |b_i|$$

- In addition to minimizing prediction error, we can force the model to consider other objectives
  - Make the magnitude of $b = (b_0, b_1, \ldots, b_n)$ small
  - Assign similar b_i's to clinical features from the same group

- **Small coefficient** means that a unit change in input feature will lead to **small change** in prediction output
  - Model becomes more robust to input noises

- Works with neural network as well

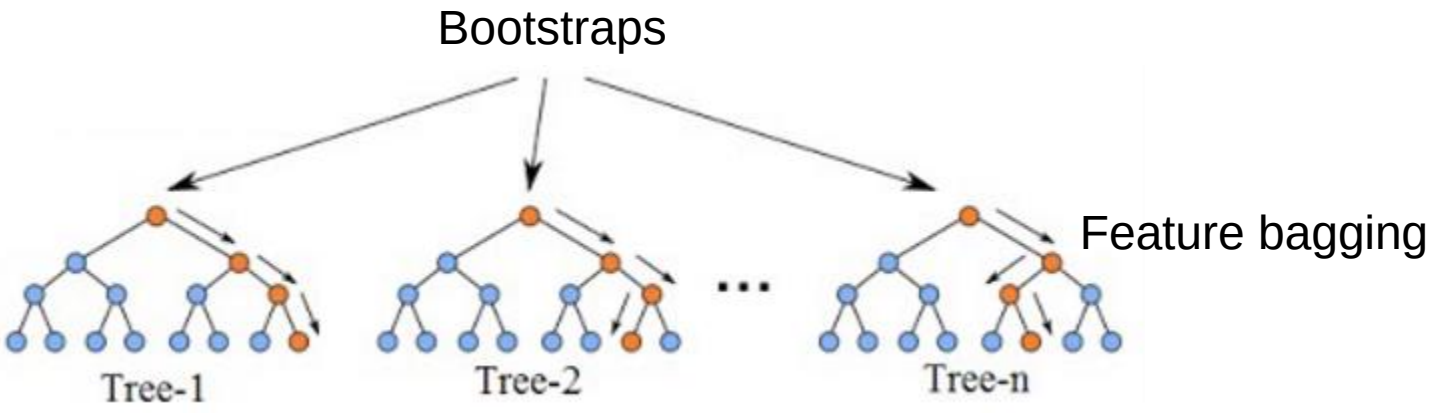
Tree pruning



Patel, N. and Upadhyay, S. “Study of Various Decision Tree Pruning Methods with their Empirical Comparison in WEKA” IJCA 2012

- Tree model’s complexity = number of decisions
  - $R_\alpha(\text{Tree}) = \text{Performance}(\text{Tree}) + \alpha \cdot \text{Number of leaves}$
  - α indicates the penalty on tree complexity

Ensemble approach



- Bootstrap bagging to generate multiple training sets
  - One model for each split
  - Aggregate prediction with a vote or average
- Ensemble can be formed between different model families
  - Logistic regression + decision tree

Any question?