# Lecture 10: Evaluating Machine Learning Models

Course: Biomedical Data Science

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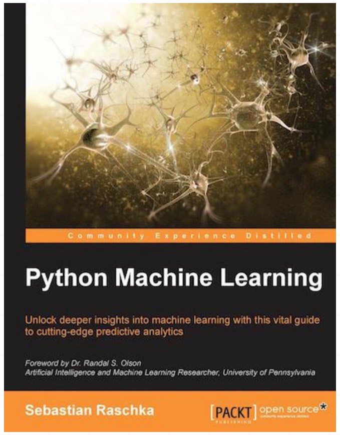
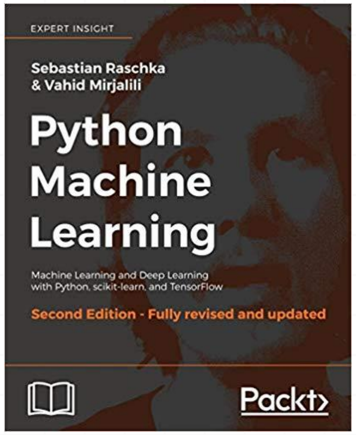
# Disclaimer

The following slides are partially based on:



# Important Steps

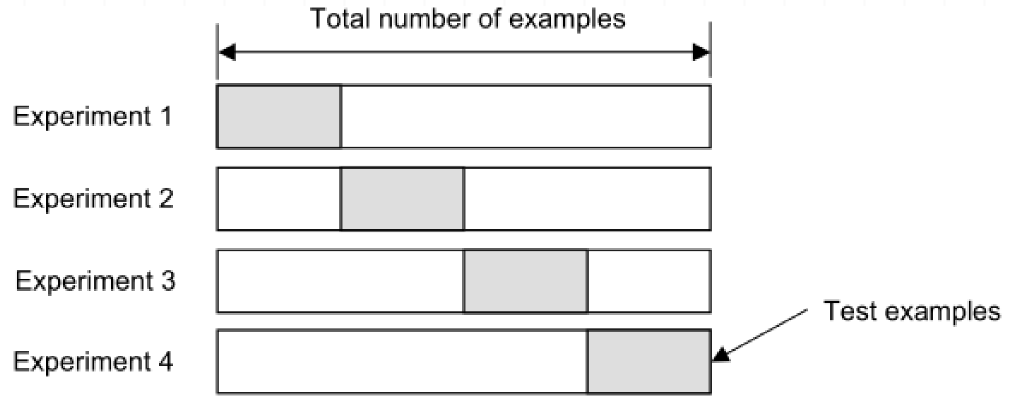
1. Determine relevant features (expert knowledge)
2. Collect data
3. **Split labeled data into training and test datasets**
4. Use training data to train machine learning algorithm.
5. Predict labels of examples in test data,
6. Evaluate algorithm.

# Test Data

- Remember: if we reuse the same test dataset over and over again during model selection,
  - Test data will become part of our training data and thus the model will be more likely to overfit.
  - The reported performance will not be correct
- Despite this issue, many people still use the test set for model selection, which is NOT a good machine learning practice.

# How to Split Data?

- Holdout
  - Training set
  - (validation set)
  - Test set
- K-fold Cross-validation
  - E.g. 10 fold cross validation



# Methods of Sampling

- Holdout
  - E.g. Reserve 2/3 for training and 1/3 for testing
- Random subsampling
- Cross validation
  - Partition data into k disjoint subsets
  - k-fold: train on k-1 partitions, test on the remaining one
  - Leave-one-out: $k=n$
- Stratified sampling
- Bootstrap
  - Sampling with replacement

# Cross-Validation


E= Average Error

$$E = \frac{1}{10}\sum_{i=1}^{10} E_i$$

$E_i$=Individual Error

# K-fold

- K =10 is typical
- If working with very small datasets, use leave-one-out (LOO)
  - If data from subjects, leave-one-subject-out
- cross_val_score() in scikit-learn
  - n_jobs can be set to distribute the evaluation across multiple CPUs
  - See Notebook

# Stratified k-fold

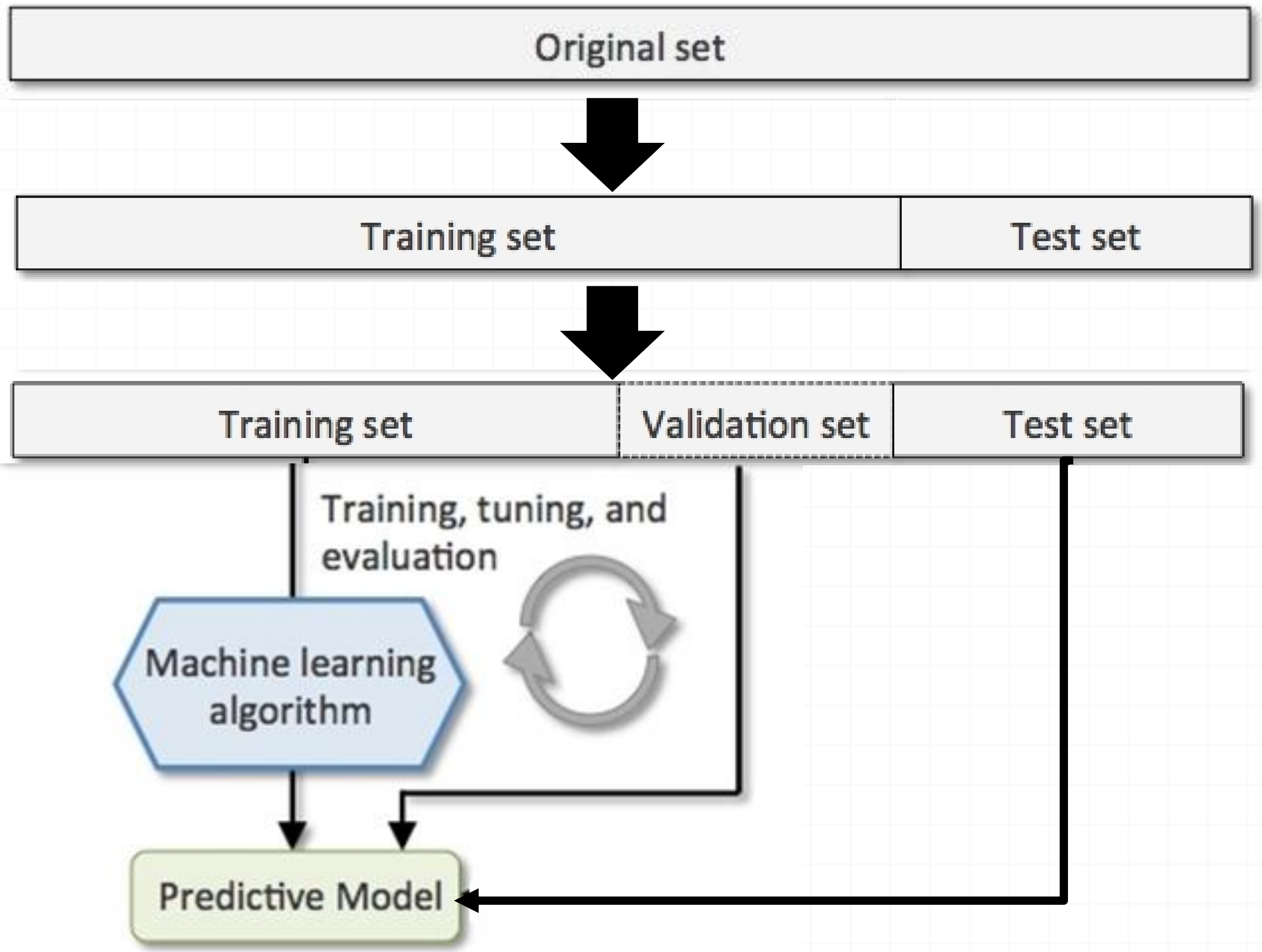
- The class proportions are preserved in each fold to ensure each fold is representative

# Recommended Approach

- Separate your data into three parts
  - training, validation, testing
- Use either
  - Holdout + k-folds cross-validation
  - Nested cross-validation

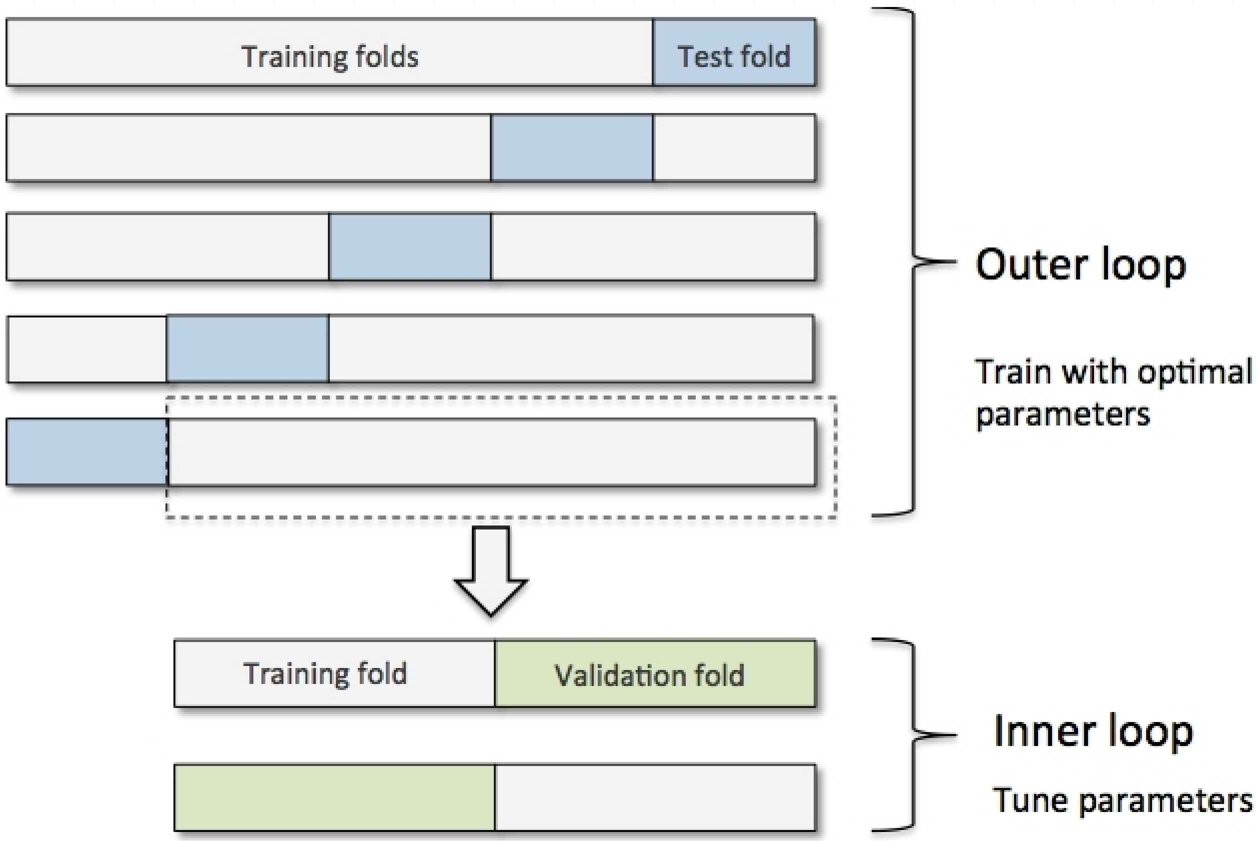
- Note: once you find satisfactory hyper-parameter values, you can retrain the model on the complete training set and obtain a final performance estimate using the independent test set.

# Hold-out + Cross-Validation



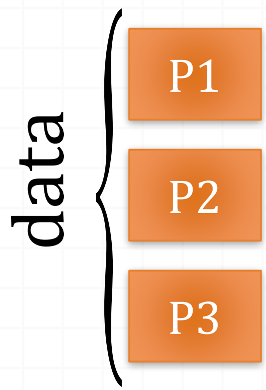
# 5×2 Cross-validation

- A form of nested variation



# Example of 3*2 nested cross-validation

Consider that we use 3-fold cross-validation and we want to optimize parameter C that takes values “1” and “2”.




***Outer Loop***

| Training set | Testing set | C | Accuracy | Average Accuracy |
|---|---|---|---|---|
| P1, P2 | P3 | 1 | 89% | 83% |
| P1,P3 | P2 | 2 | 84% | |
| P2, P3 | P1 | 1 | 76% | |

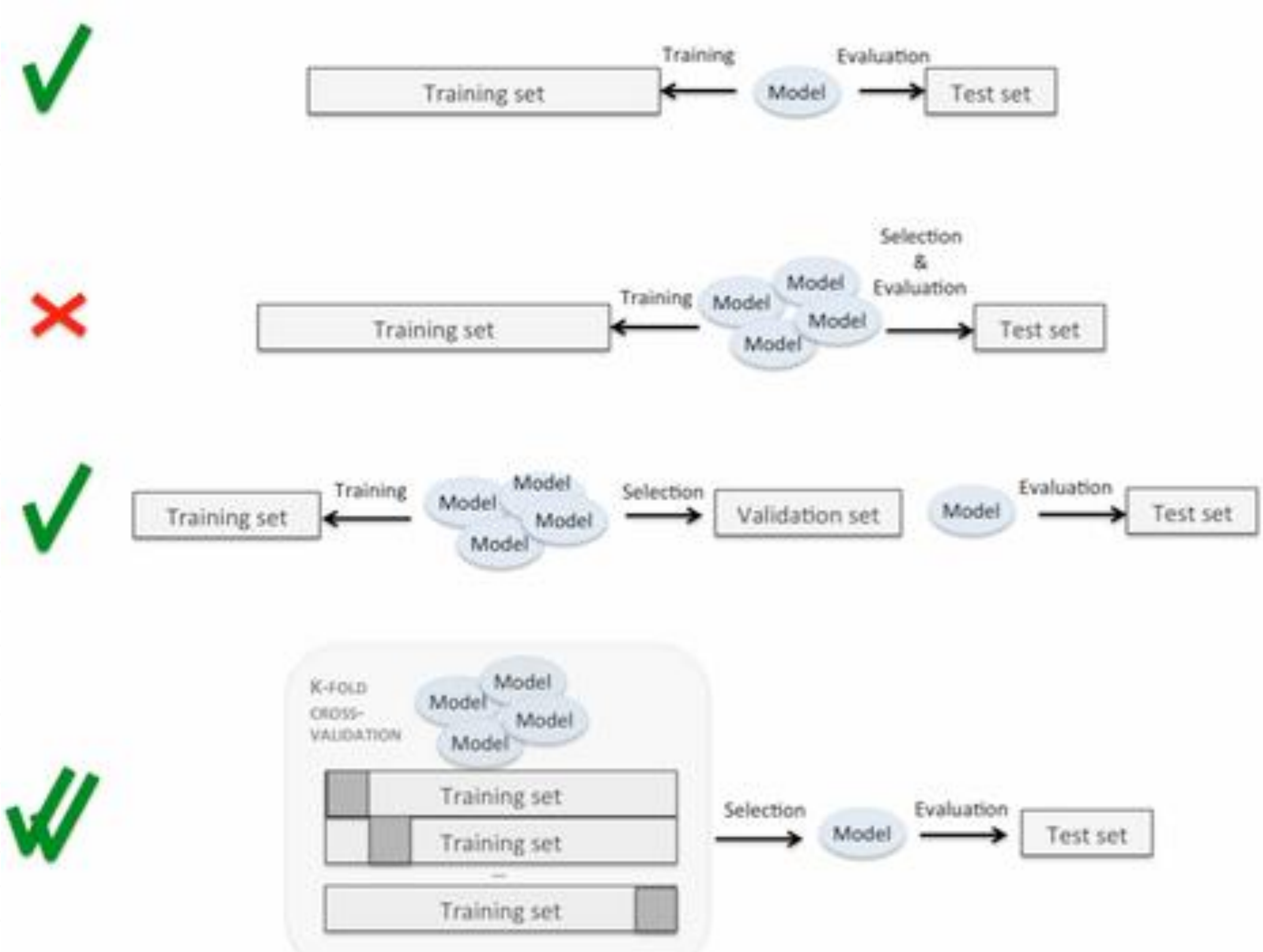
...

...

***Inner Loop***

| Training set | Validation set | C | Accuracy | Average Accuracy |
|---|---|---|---|---|
| P1 | P2 | 1 | 86% | **85%** |
| P2 | P1 | | 84% | |
| P1 | P2 | 2 | 70% | 80% |
| P2 | P1 | | 90% | |

choose **C=1**




http://sebastianraschka.com/faq/docs/evaluate-a-model.html

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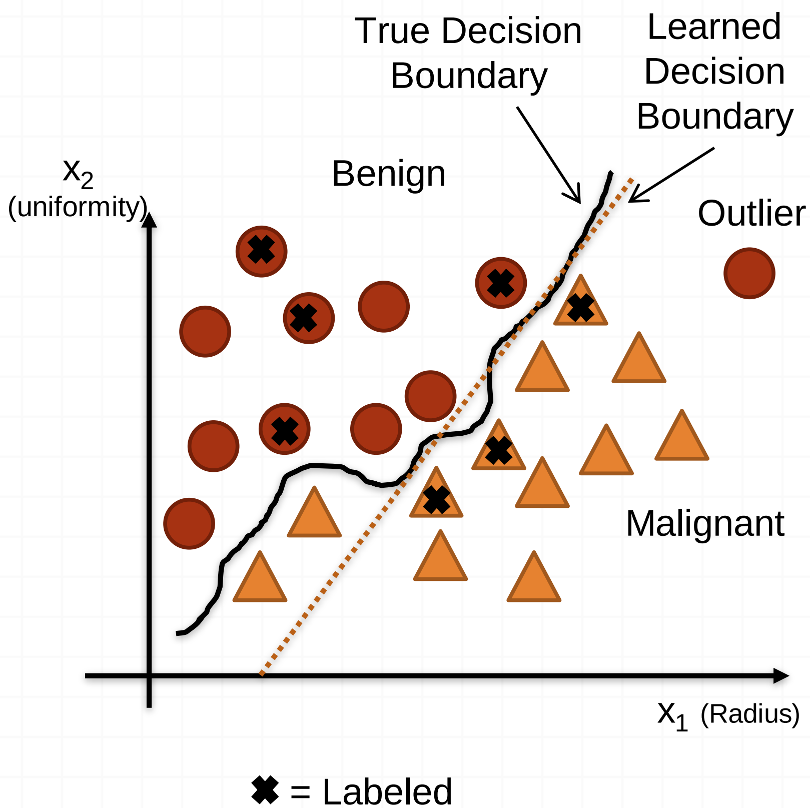
# Decision Boundary

- We seek to find this boundary

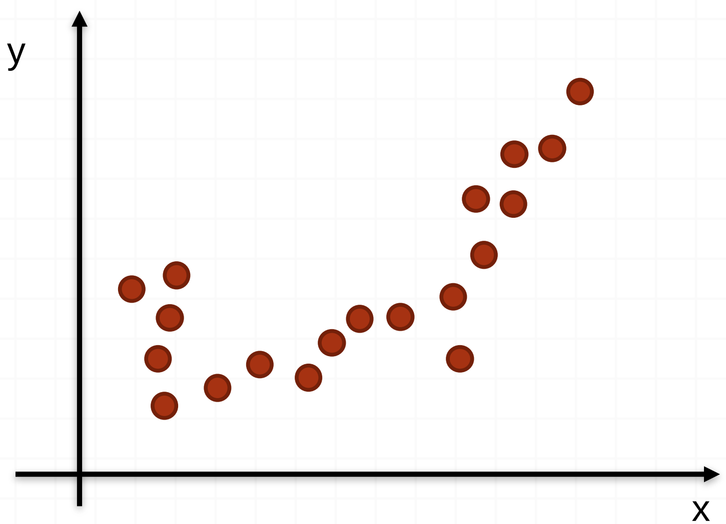


# Why Noise?

- Noise might be due to different reasons
  - Imprecision in recording the input data
  - Errors in labeling data
  - We might not have considered additional features (*latent*, or *hidden* features)
- When there is noise, the decision boundary becomes more complex

# Overfitting

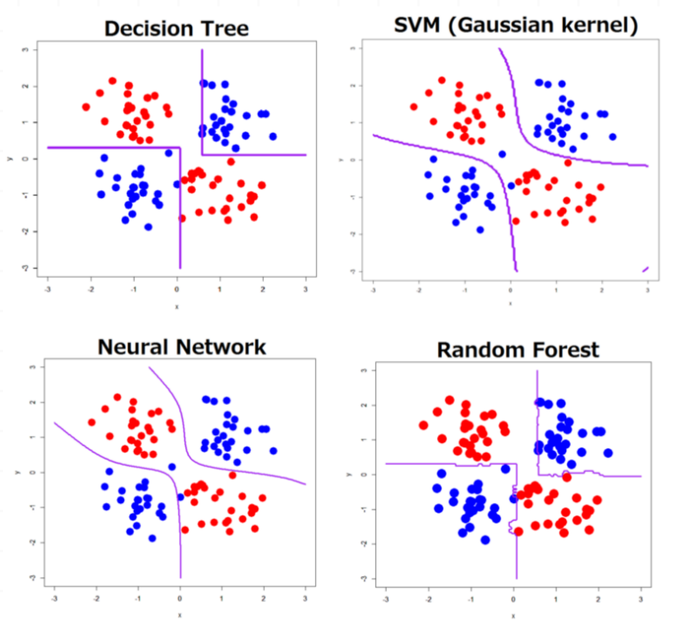
- Data are well described by our model, but the predictions do not generalize to new data.
  - A very rich hypothesis space
  - Training set too small

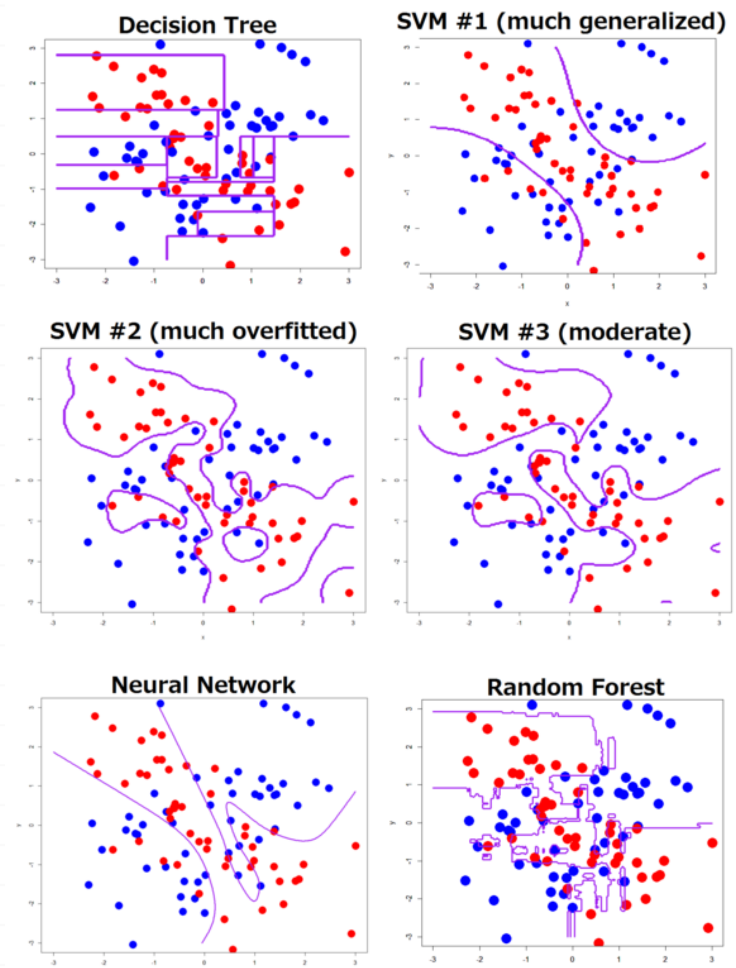


# Overfitting and Underfitting

- Underfitting
  - If your hypothesis is less complex than the actual function
    - Using a linear equation to model data generated by a third order polynomial
- Overfitting
  - If your hypothesis is more complex than the actual function
    - Using a fifth order polynomial to model data generated by a second order polynomial

# Over-fitted Decision Boundaries




http://www.kdnuggets.com/2015/06/decision-boundaries-deep-learning-machine-learning-classifiers.html

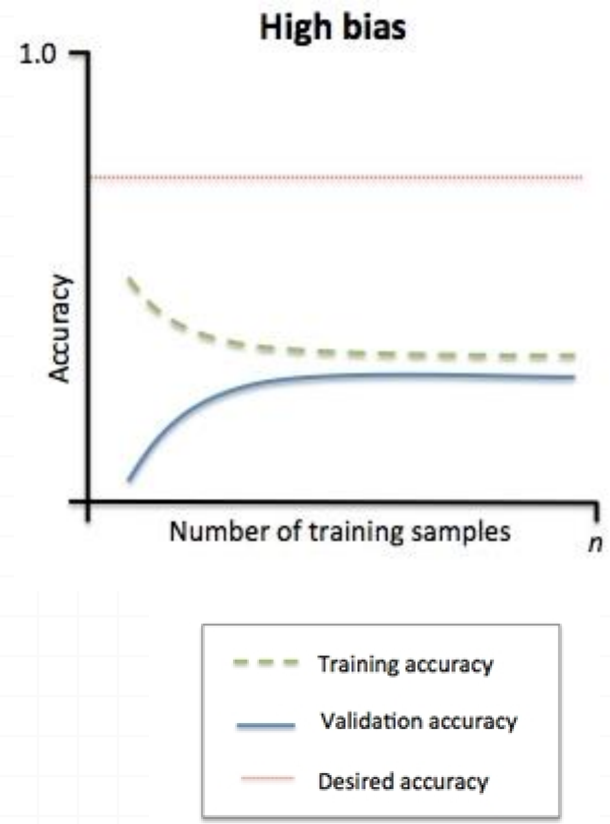
# Bias-Variance

- Variance = consistency of the model for a particular sample if we retrain the model multiple times, e.g. on different subsets of data
  - i.e. we can say the model is sensitive to the randomness in data
- Bias = how far off are the predictions from the correct values (systematic error not due to randomness in data)

- Simple linear model => high bias
- Complex model => high variance

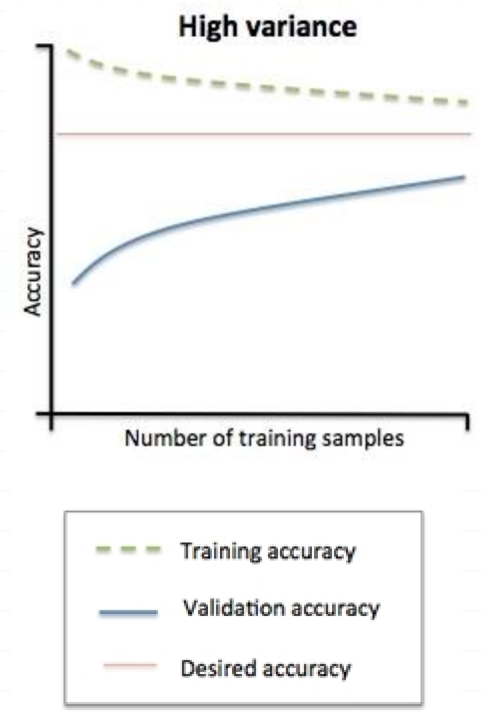
# Model Diagnosis Using Learning Curves

- This model has both low training and cross-validation accuracy, which indicates that it underfits the training data.
- We can
  - Increase the number of parameters of the model
    - More features
    - Decreasing regularization



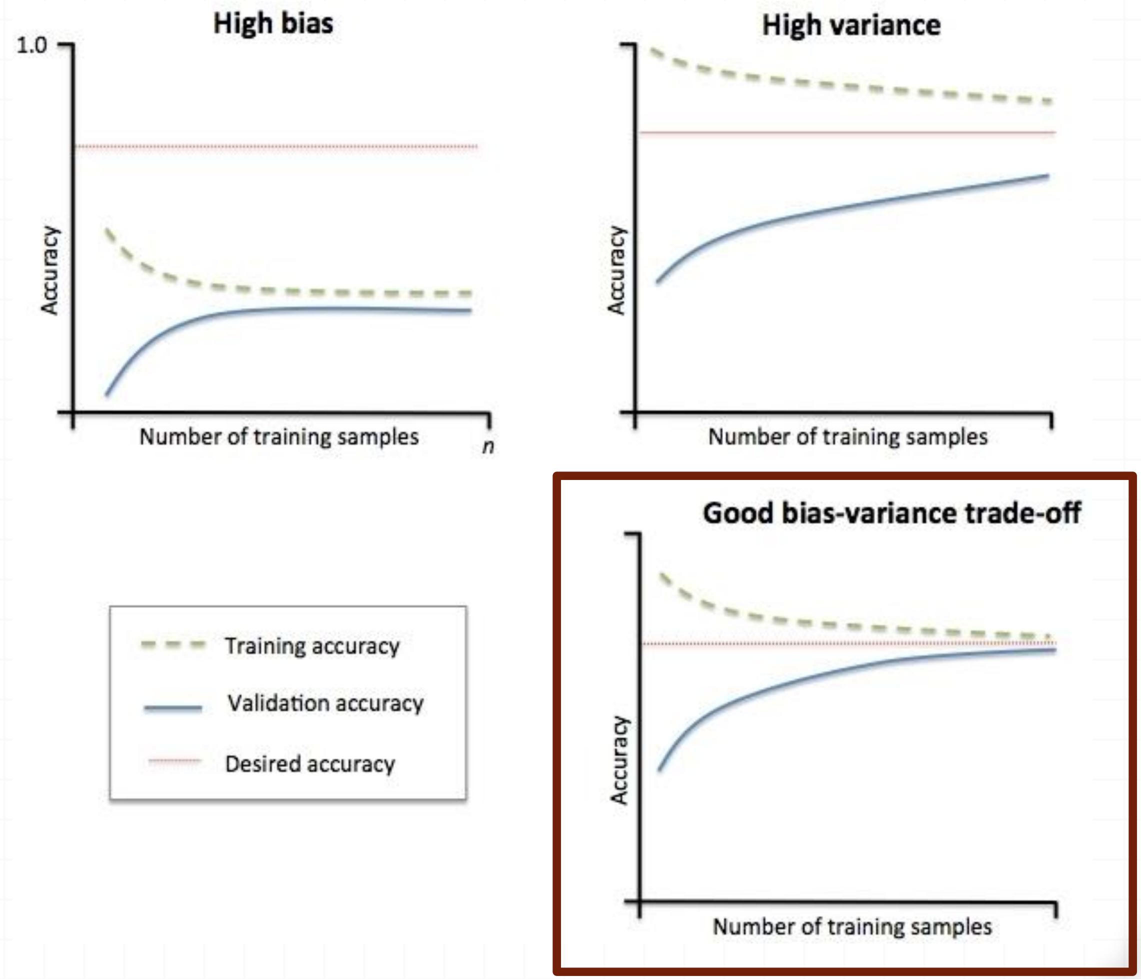
# Model Diagnosis Using Learning Curves

- A model that suffers from high variance, which is indicated by the large gap between the training and cross-validation accuracy.
- To address this problem
  - we can collect more training data
  - or reduce the complexity of the model, e.g. more regularization parameter
  - or decrease the number of features via feature selection



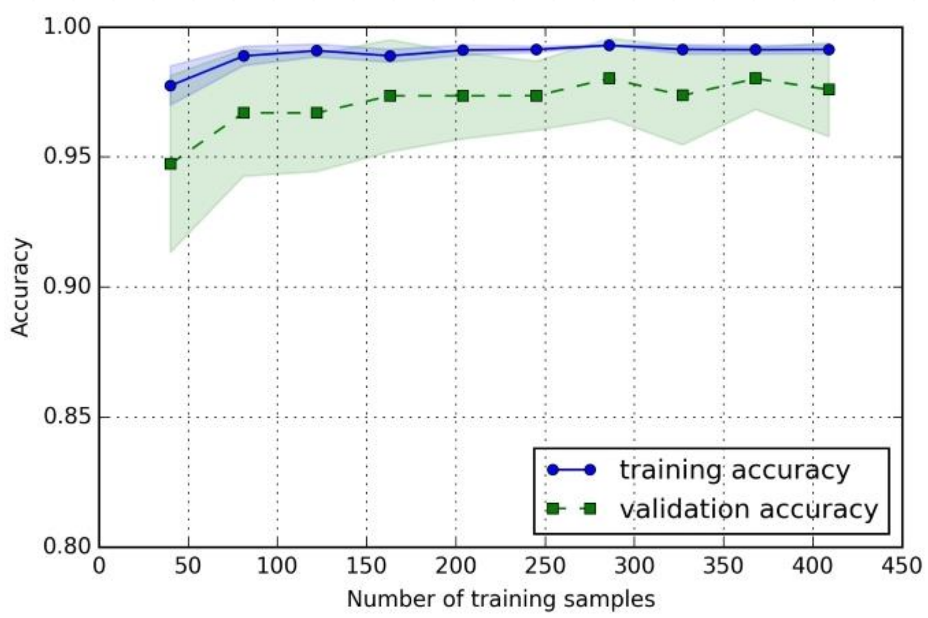
# Model Diagnosis Using Learning Curves

- A good balance



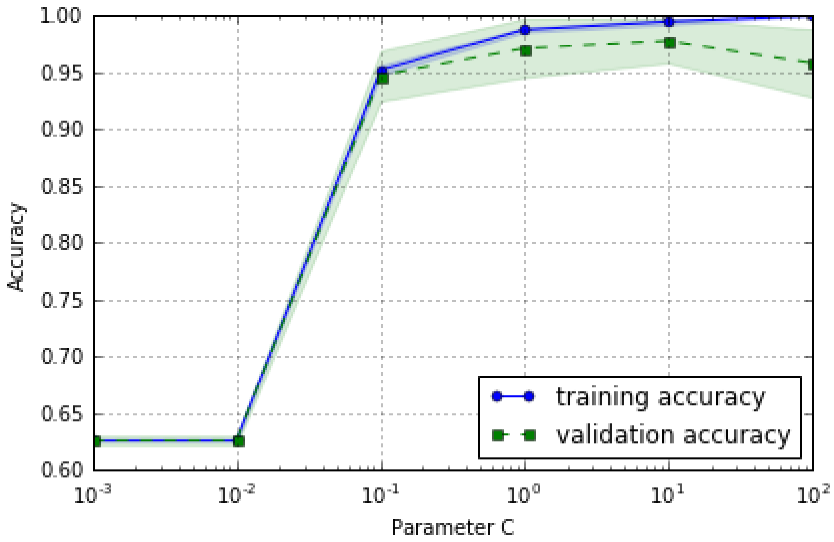
# Learning Curve in scikit-learn

- Use the learning_curve() function in sklearn
- See notebook



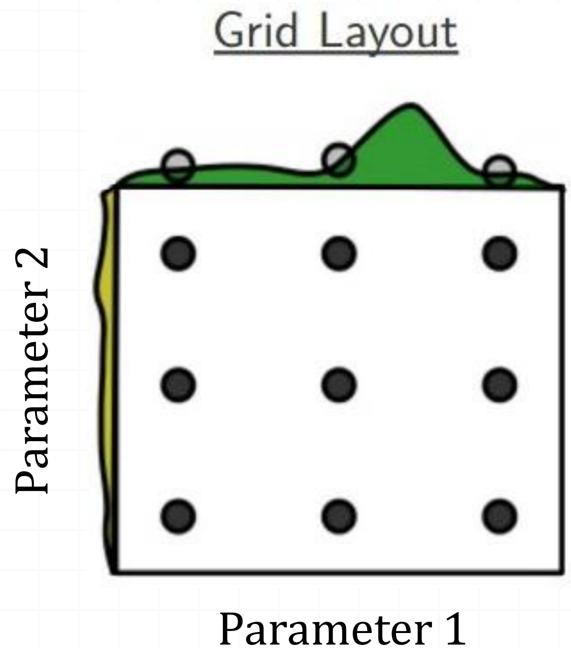
# Validation Curve

- Similar to learning curves
  - Instead of plotting against the sample size, we vary the values of the model parameters, e.g. C in SVM
  - Use validation_curve()



# Fine-tune via Grid Search

- You can use Grid Search to automate the process of finding the best parameter values



# Important Steps

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# Model Evaluation

- Metrics for Performance Evaluation
  - How to evaluate the performance of a model?

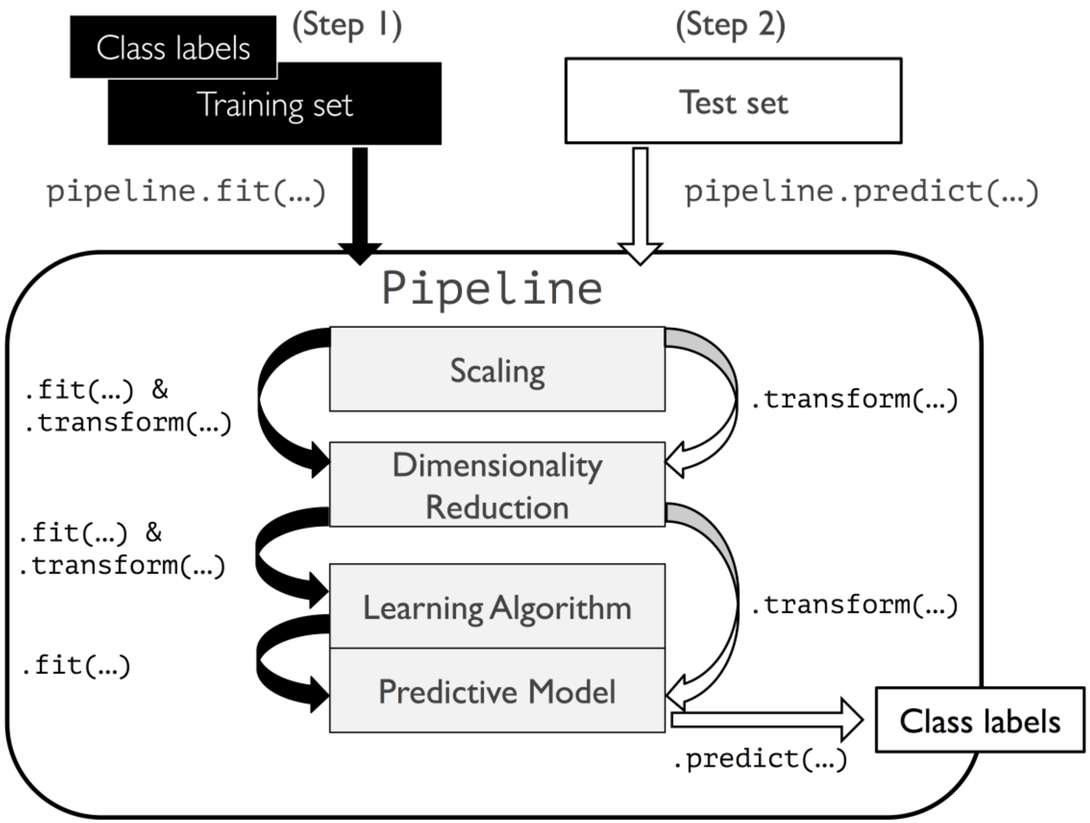
- Methods for Model Comparison
  - How to compare the relative performance among competing models?

# Triple Tradeoff

- Complexity of the hypothesis space: $C$
- Amount of training data: $N$
- Generalization error on new data: $E$

- $N\uparrow \rightarrow E\downarrow$
- $C\uparrow \rightarrow$ *first* $E\downarrow$, *then* $E\uparrow$

# Development Pipeline



# Scikit-Learn: Pipeline

- The Pipeline object takes a list of tuples as input
  - first value = an arbitrary identifier string
  - second value = a scikit-learn transformer or estimator.

**Combining transformers and estimators in a pipeline**

```
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA
from sklearn.svm import SVC
from sklearn.pipeline import Pipeline

pipe_svc = Pipeline([('scl', StandardScaler()),
                     ('pca', PCA(n_components=2)),
                     ('clf', SVC())])

pipe_svc.fit(X_train, y_train)
print('Test Accuracy: %.3f' % pipe_svc.score(X_test, y_test))
y_pred = pipe_svc.predict(X_test)
```

# Notes on Paper 5

# Study Guidelines & Checklists

- STROBE used in observational studies
- TRIPOD used in predictive model development and validation
- PRISMA-P used in systematic review protocols

# Error in Regression

- Mean Absolute Error (MAE)
- Root mean squared error (RMSE)

$$\mathrm{MAE} = \frac{1}{n}\sum_{j=1}^{n}|y_j - \hat{y}_j|$$

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{j=1}^{n}(y_j - \hat{y}_j)^2}$$

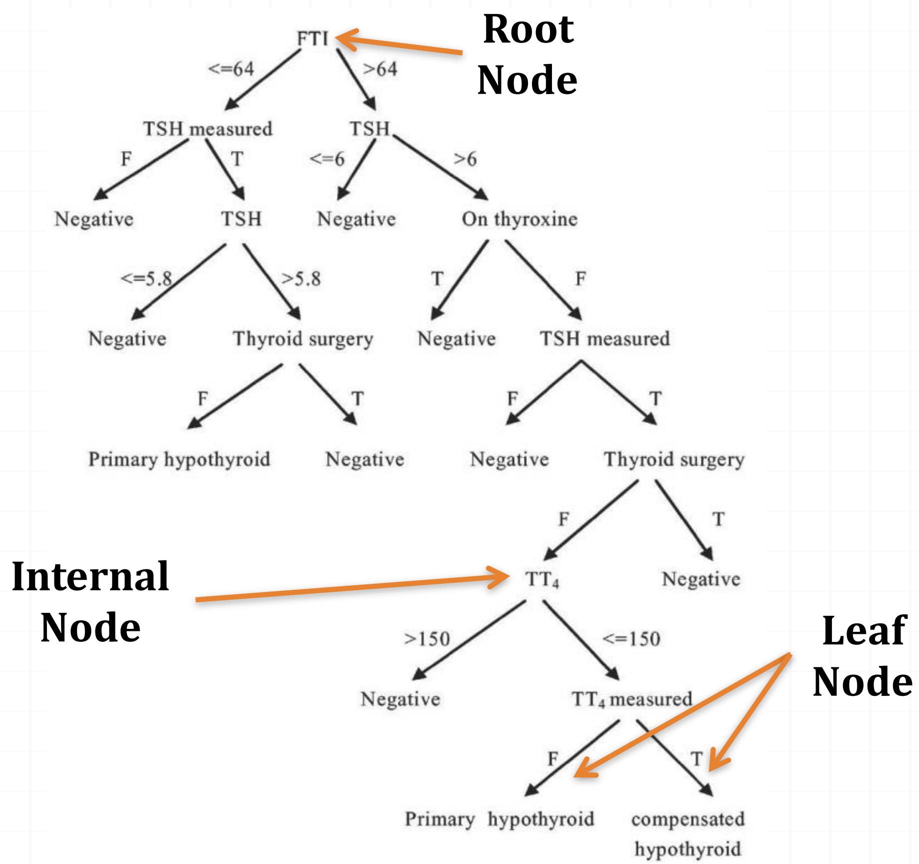
- Both are indifferent to the direction of errors
- RMSE gives relatively high weight to large errors

# Errors in Forecasting

- MAPE: Mean Absolute Percentage Error

$$\mathrm{MAPE} = \frac{1}{h}\sum_{j=1}^{h}\frac{|y_{t+j} - \hat{y}_{t+j}|}{y_{t+j}}$$

# Decision Tree




*Chou, Kuang-Yi, et al. "The Irrelevant Values Problem of Decision Tree in Medical Examination." Journal of Applied Science and Engineering 15.1 (2012): 89r96.

# Random Forest

- A random forest is a collection of decision trees
- it searches for the best feature among a random subset of features.

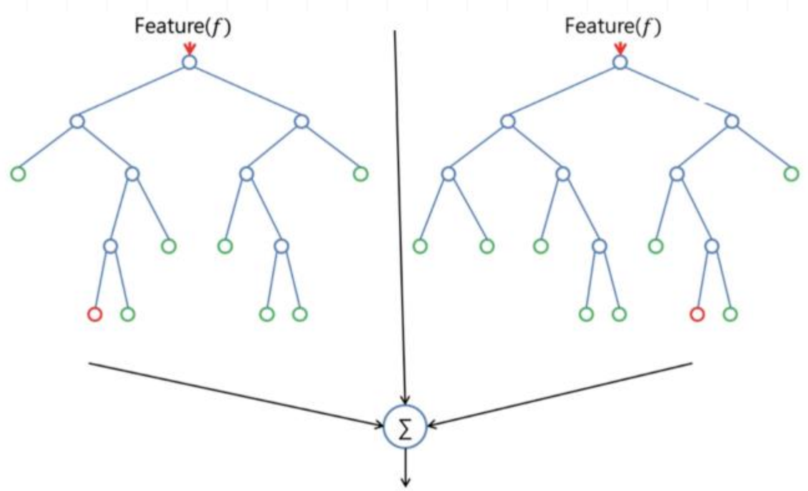



Image from https://towardsdatascience.com/the-random-forest-algorithm-d457d499ffcd