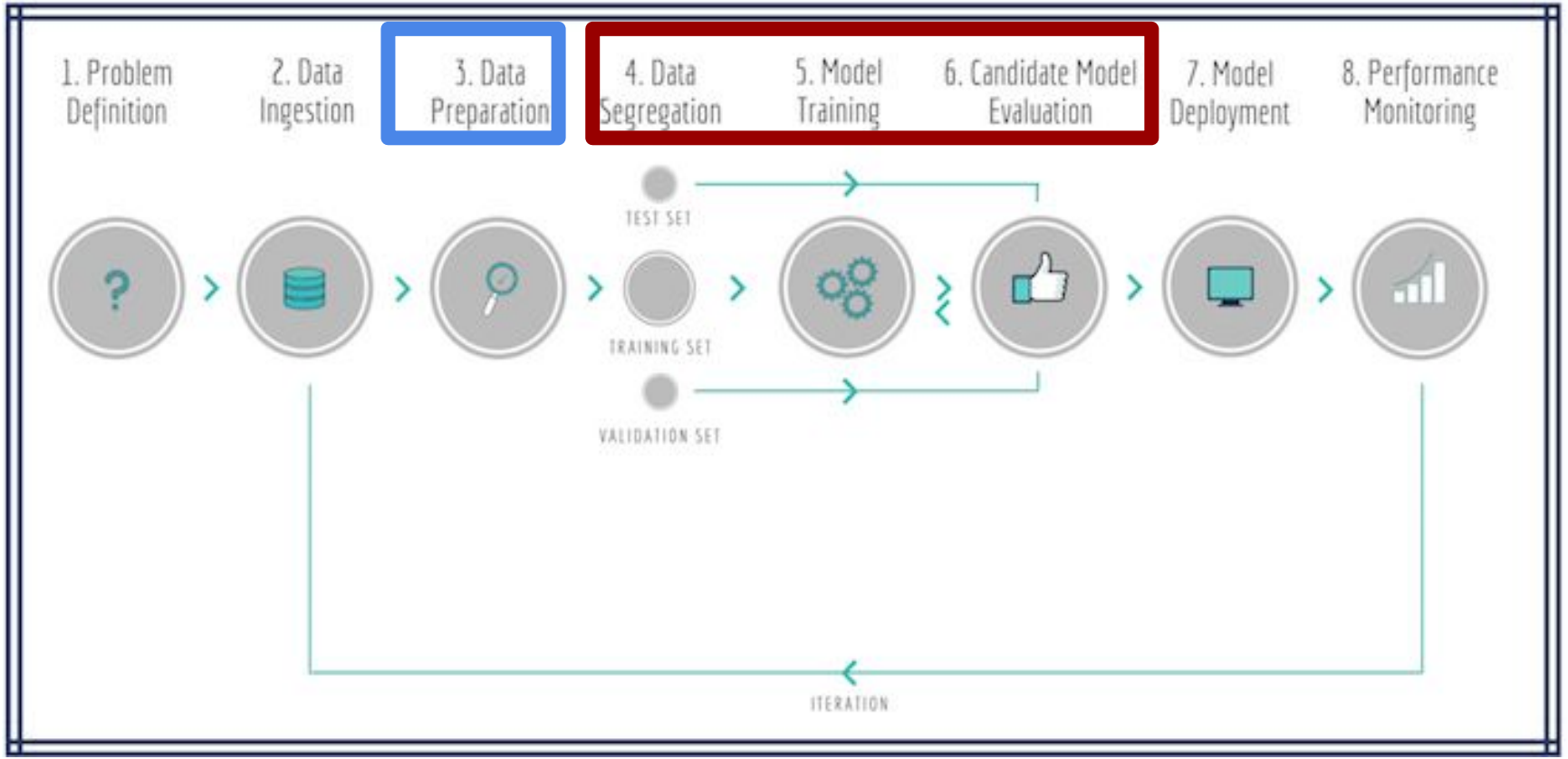
Machine Learning Practices

*Exploration
*Transformation
*Fea. Engineering

Modelling



Credit: Semi Koen

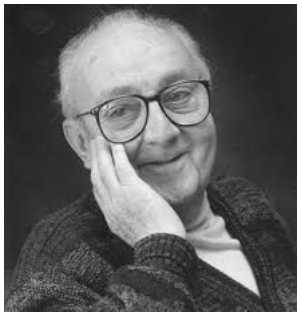
Agenda

1. Feature Engineering
2. Model Selection: Cross-validation
3. Hyperparameter Search
4. Hands-on Project: Cuisine Categorization

Feature Engineering

Recall that computers only understand numbers (binary)

What is Feature Engineering



George Box

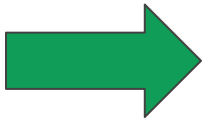
- Features never fully describe the situation
  - All models are wrong, but some are useful. The practical question is how wrong do they have to be to not be useful.

- Feature Engineering
  - How to represent examples by feature vectors
  - Suppose I would like to use examples from past to predict, at the current moment, which students will get an A in BT5153?
  - Some features may be useful: eg. GPA, prior programming experience
  - Other might cause me to overfit, e.g, birth month, weight.

Example: YouTube Impression

```
0 : {
  user_info : {
    age: 42
    ip_address: "192.168.0.1"
    watch_history: [ "abc123",
"def456" ]
  }
  impression {
    ui_position: 0
    video_id: "xyz789"
    was_clicked: true
    watch_time: 1.304
  }
}
```

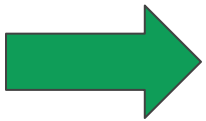
Real valued features can be copied over directly



```
age_feature = [ 42.0 ]
```

From Data to Features

```
0 : {
  user_info : {
    age: 42
    ip_address: "192.168.0.1"
    watch_history: [ "abc123",
"def456" ]
  }
  impression {
    ui_position: 0
    video_id: "xyz789"
    was_clicked: true
    watch_time: 1.304
  }
}
```



```
[
  42.0,
  1.0,
  0.0,
  0.0,
  0.0,
  9.321,
  -2.20,
  1.01,
  0.0,
  ...,
]
```

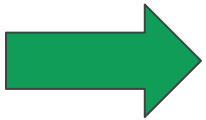
Process of creating features from data is Feature Engineering

Logs Data don't come to us a feature vectors

Example: YouTube Impression

```
0 : {
  user_info : {
    age: 42
    ip_address: "192.168.0.1"
    watch_history: [ "abc123",
"def456" ]
  }
  impression {
    ui_position: 0
    video_id: "xyz789"
    was_clicked: true
    watch_time: 1.304
  }
}
```

Real valued features can be copied over directly

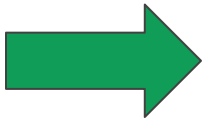


```
age_feature = [ 42.0 ]
```

From String to Features

```
0 : {
  user_info : {
    age: 42
    ip_address:
    watch_history
"def456" ]
  }
  impression {
    ui_position: 0
    video_id: "xyz789"
    was_clicked: true
    watch_time: 1.304
  }
}
```

String Features can be handled with one-hot encoding



```
impression_video_id_feature =
[  0,
 ...,
  0,
  1,
  0,
 ...,
  0 ]
```

K: number of unique videos

One-hot encoding. This has a 1 for “xyz789”, 0 for all others

Properties of a Good Feature

Feature values should appear with non-zero value more than a small handful of times in the dataset

my_device_id:8SK982ZZ1242Z

device_model:galaxy_s6

Properties of a Good Feature

Feature names should clearly describe the value's meaning, as well as indicate unit of measurement (where appropriate)

price_usd:29.99

feature_7:-10

Properties of a Good Feature

Features shouldn’t take on “magic” values

(Use an additional boolean feature like is_watch_time_defined instead!)

```
watch_time: -1.0
```

```
watch_time: 1.023
```

```
watch_time_is_defined: 1.0
```

Properties of a Good Feature

The definition of a feature shouldn’t change over time.

(Beware of depending on other ML systems!)

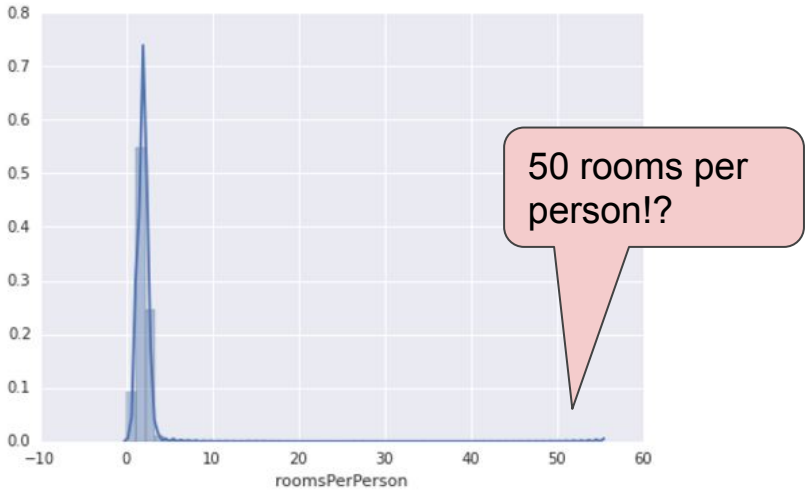
city_id:“br/sao_paulo”

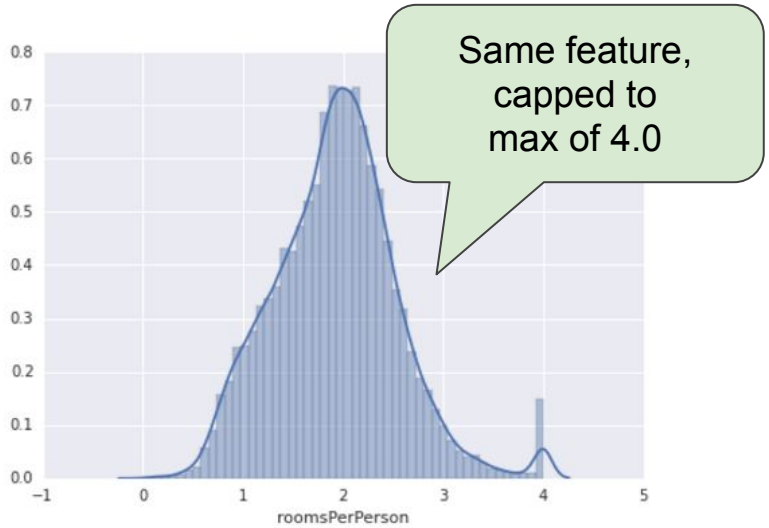
inferred_city_cluster_id:219

Properties of a Good Feature

Distribution should not have crazy outliers

Ideally all features transformed to a similar range, like (-1, 1) or (0, 5).





Why Scaling?

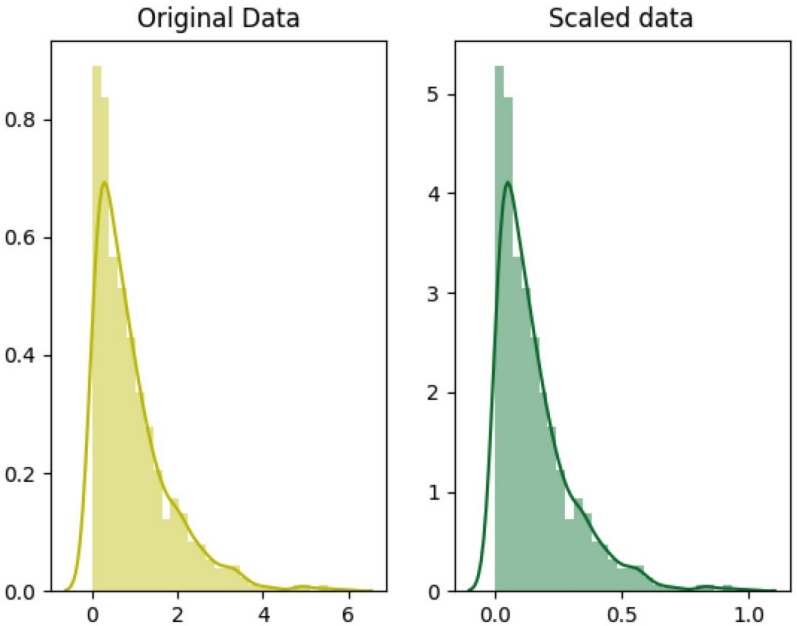
- Range of values of data may vary widely

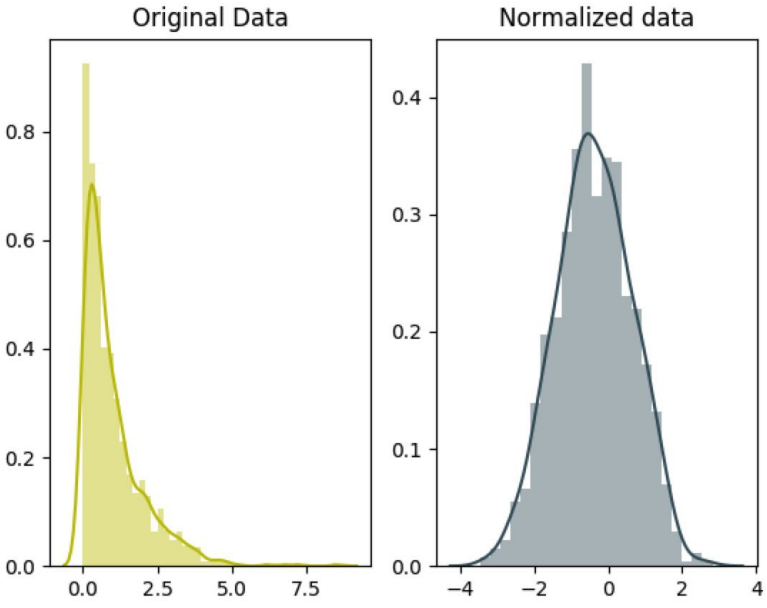
- Lots of machine learning algorithms are very senstiviative to scales of features
  - K-nearest Neighbors
  - K-means
  - Logistic Regression
  - SVMs
  - Gradient Descent
  - PCA
  - Etc

When distances of feature vector matter

Scaling Vs Normalization

Two ways to change the features of input data





Scaling Vs Normalization

- Feature Scaling: change the range of your data

$$\hat{x} = \frac{x - x_{min}}{x_{max} - x_{min}}$$

When distances measures are used in ML algorithms under the assumption that all features contribute equally

- Feature Normalization: change the shape of distribution of your data

$$\hat{x} = \frac{x - x_{mean}}{\sigma}$$

When machine learning models that assume that data is normally distributed e.g.linear regression, PCA, Gaussian Naive Bayes

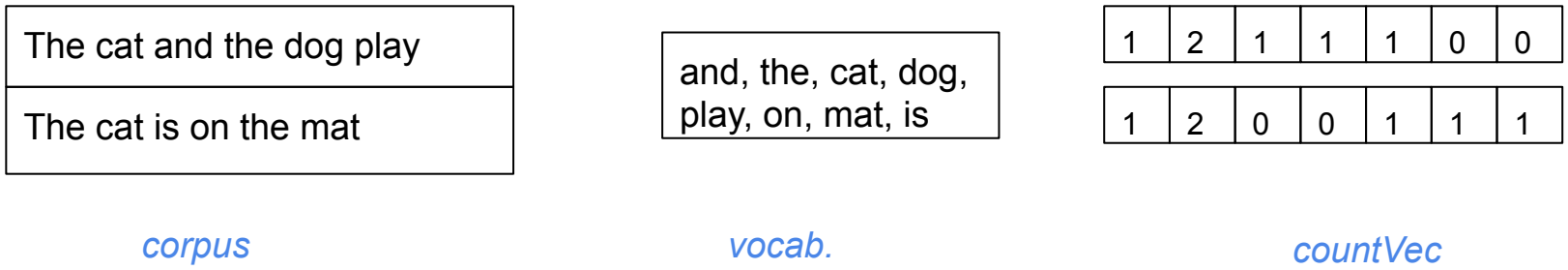
Good Habits: Know your data!!

- **Visualize:** Plot histograms, rank most to least common.
- **Debug**: Duplicate examples? Missing values? Outliers? Data agrees with dashboards? Training and Validation data similar?
- **Monitor**: Feature quantiles, number of examples over time?

How about Unstructured Data？

Bag-of-Words

- Steps
  - Build vocab i.e., set of all the words in the corpus
  - Count the occurrence of words in each document



N-gram model

- Steps
  - Build vocab, which set of all n-gram in the corpus
  - Count the occurrence of n-gram in each document

The cat and the dog play
The cat is on the mat

corpus

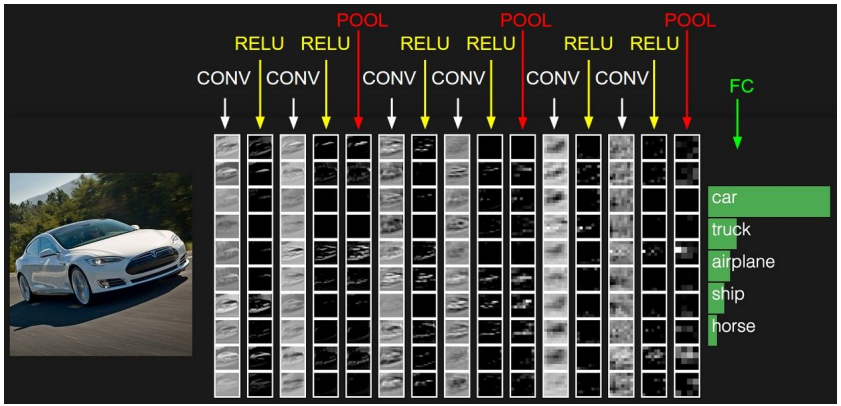
The cat, cat and, and the, the dog, dog play, cat is, is on, on the, the mat

vocab.

1	1	1	1	1	0	0	0	0
1	0	0	0	0	1	1	1	1

More Advanced Approach

- Using Deep learning
  - CNN, RNN, Attention Model
  - Learn representations from text, image, video, audio signal



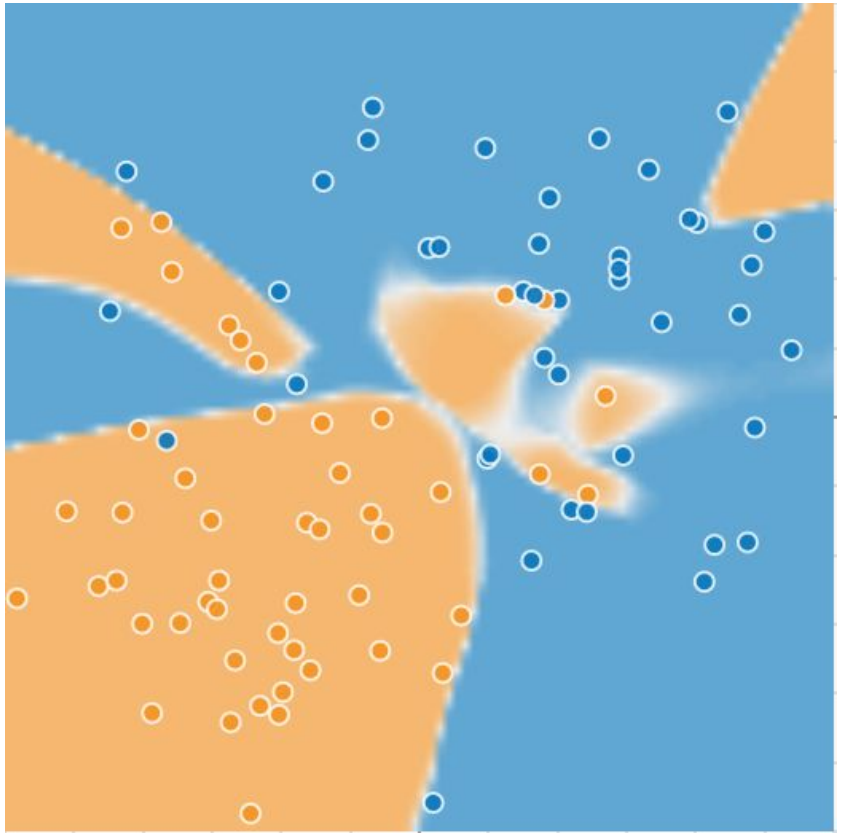
http://cs231n.github.io/convolutional-networks/

Cross-Validation

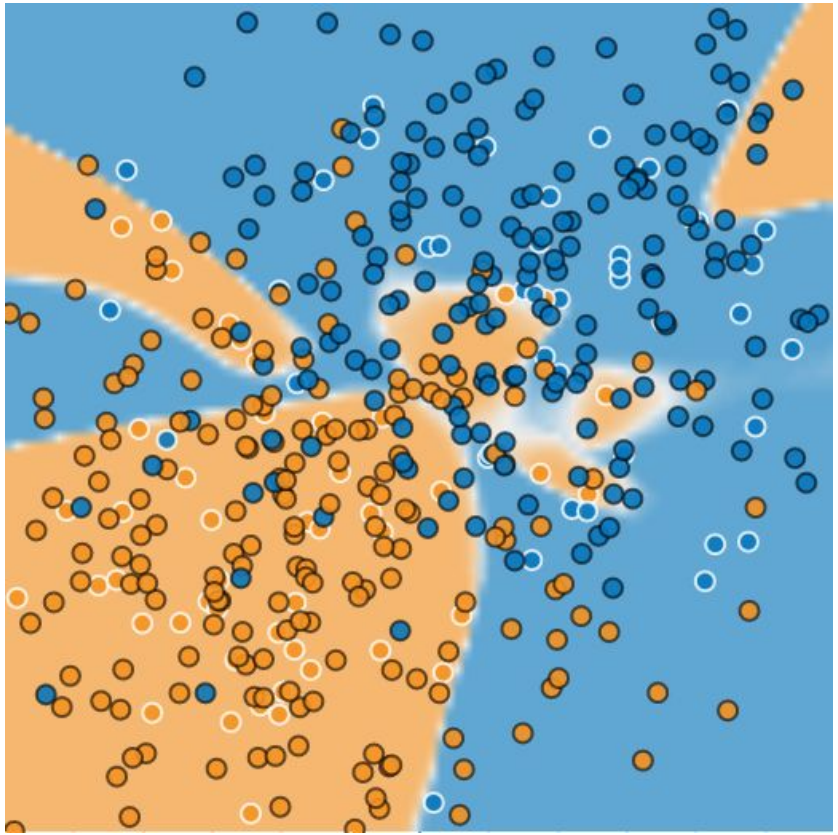
Which measure should we look for model evaluation?

Let’s try to train a model for this problem

How about this model?



Overfitting



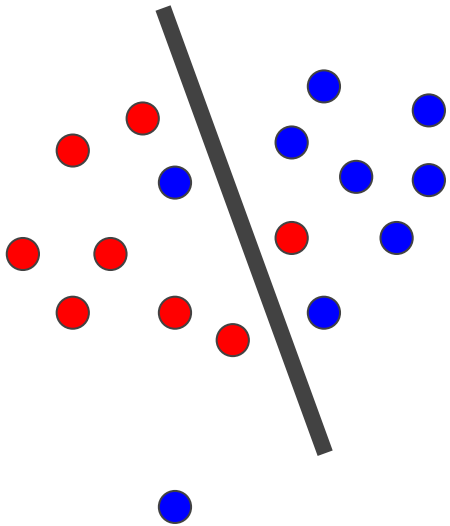
Which measure should we look for model evaluation?

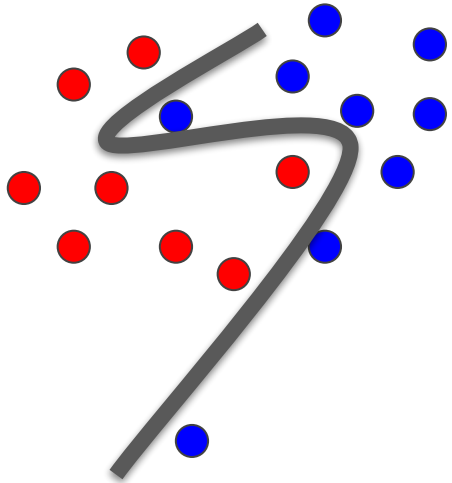
Training performance is not suitable

Generalization

- In ML, a model is used to fit the data
- Once trained, the model is applied upon new data
- Generalization is the prediction capability of the model on live/new data

Which model is better?



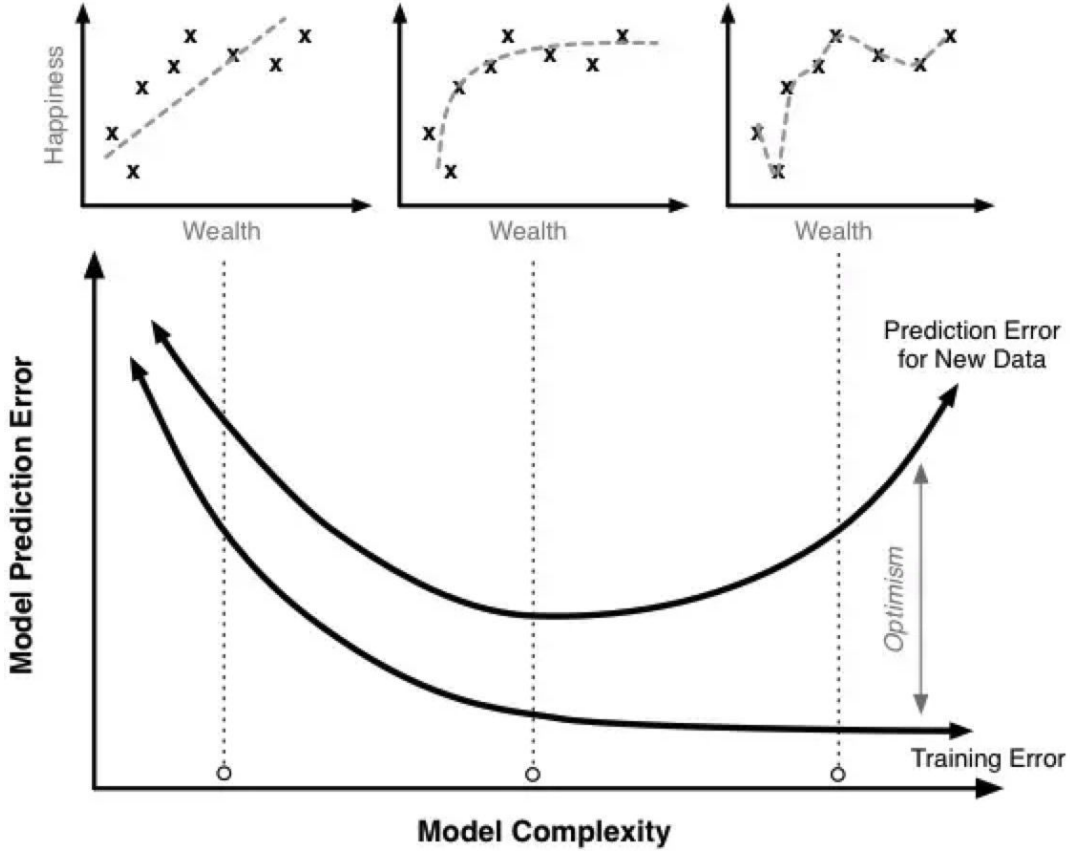


SPAM VS **Not SPAM**

Model Complexity

- Complex model easily overfits the training data
- Then, the trained model is unable to generalize on testing data
- overfitting vs underitting
  - overfitting: small training error but large testing error
  - underfitting: large training and testing errors

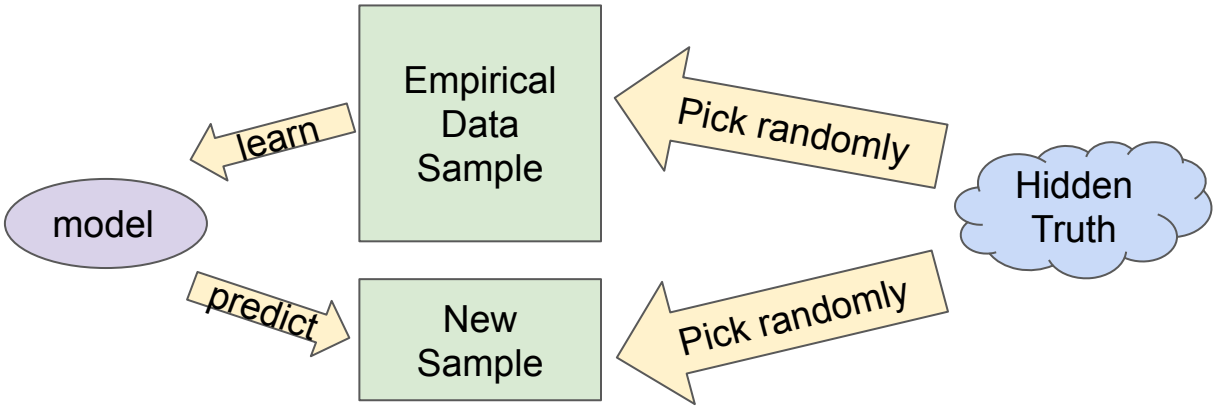
Model Complexity



source: stackoverflow

The Big Picture

- Goal: predict well on new data drawn from (hidden) true distribution.
- Problem: we don’t see the truth.
  - We only get to sample from it.
- If model *h* fits our current sample well, how can we trust it will predict well on other new samples?



Is the model overfitting?

- Intuition: Occam's Razor principle
  - The less complex a model is, the more likely that a good empirical result is not just due to the peculiarities of our samples.

- Theoretically:
  - Interesting field: generalization theory
  - Based on ideas of measuring model simplicity / complexity

William of Occam

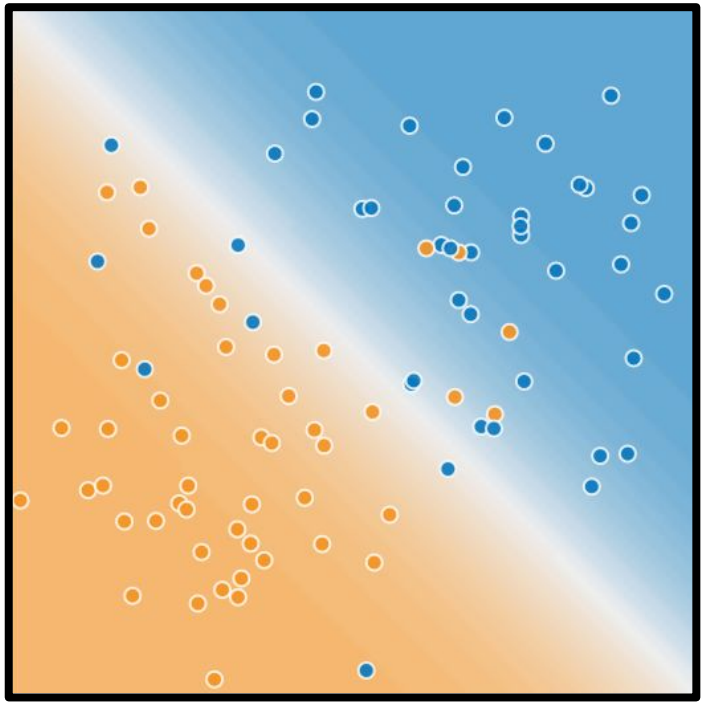
Is the model overfitting?

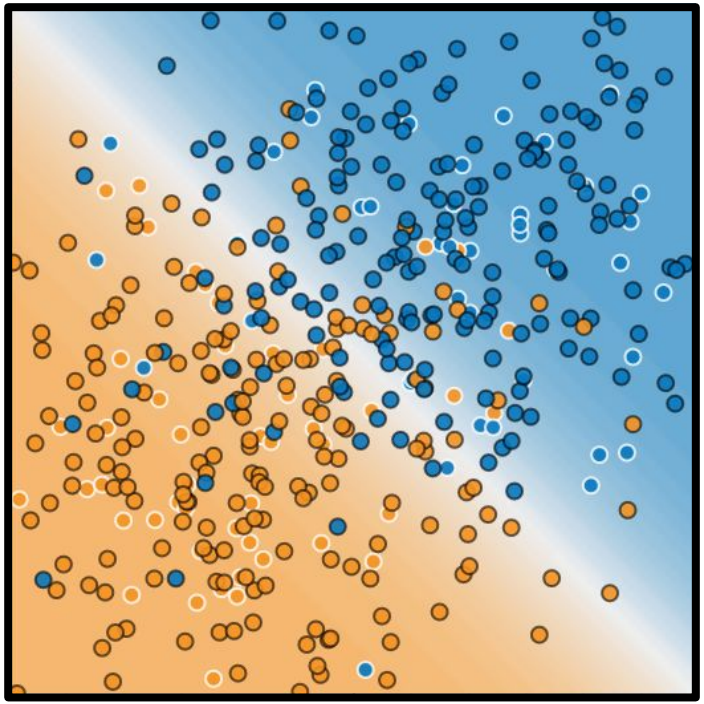
- Empirically:
  - Key point: will our model be good on new samples?
  - Evaluate: get new samples of data (test set)
  - If test set is large enough and we do not cheat by using test set over and over, the good performance on test set can be a useful indicator of model's generalization capability

Training/Test Splitting

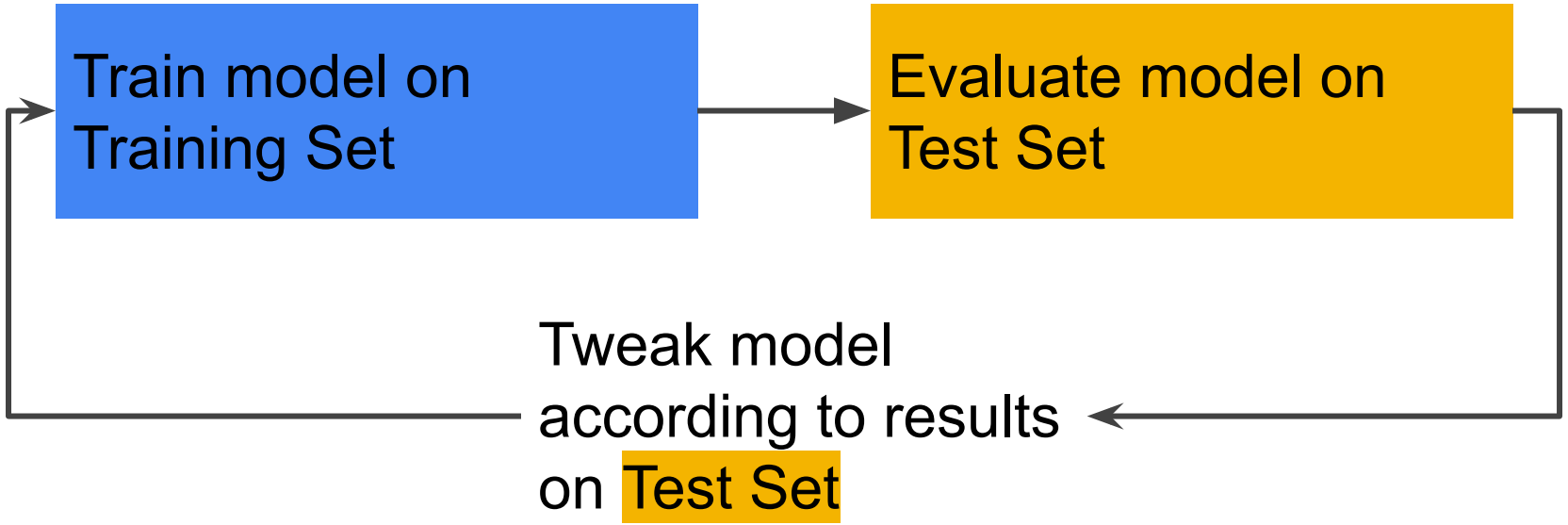
- If models do much better on the training set than the testing set, then models are likely overfitting.
- How do we divide?
  - Randomization for splitting
  - Larger training data size -> better model
  - Larger testing data size -> more confident in model's evaluation
  - One practical rule: 10-15% left for testing, the rest for training

Training Evaluation v.s. Test Evaluation





How about this workflow?



Pick model that does best on Test Set.

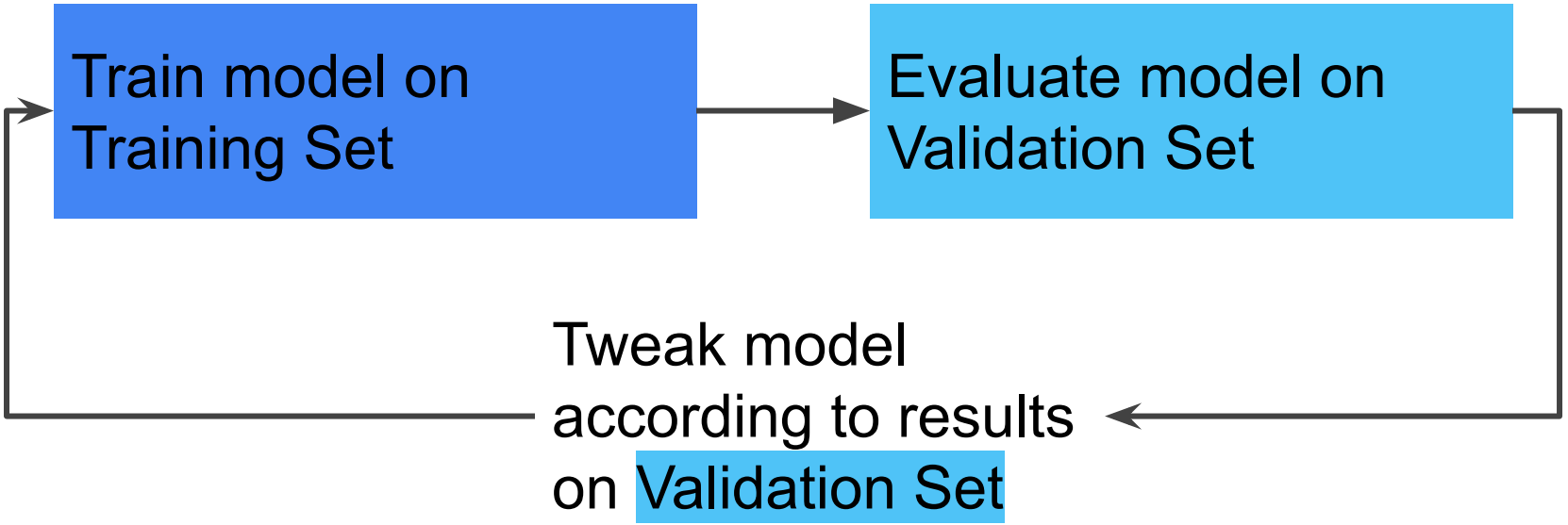
Partition Data Sets

Training Set

Validation Set

Test Set

Better Workflow: Use a validation set



Pick model that does best on Validation Set
Confirm results on Test Set

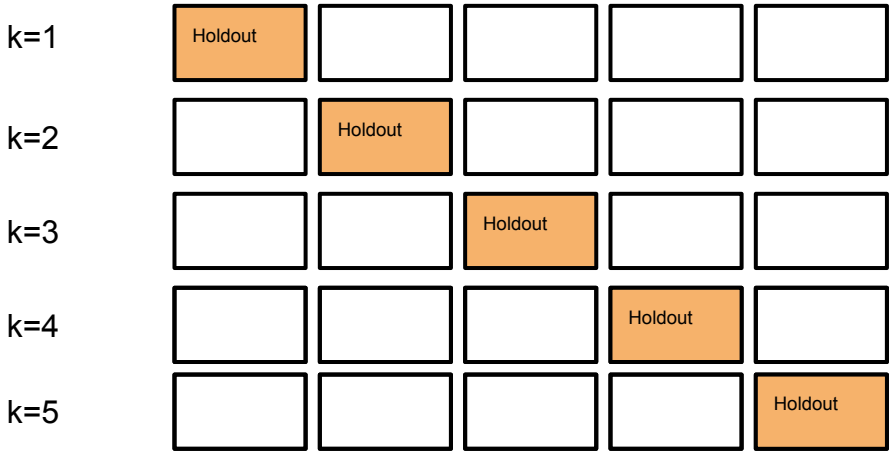
Cross-validation

- If we have a small dataset: CV can be conducted

- Idea is simple but smart:
  - Use your initial training data to generate multiple mini train-test splits. Use these splits to evaluate your model
  - K is a hyper-parameters. K is equal to the number of generated train-test splits.

Cross-validation

- Partition data into k subsets, i.e., folds
- Iteratively train the model on k-1 folds while using the remaining fold as the test set (hold-out set)
- Compute the average performances over the K folds



Summary

- Divide into three sets
  - training set
  - validation set
  - test set

- Classic gotcha: only train the model on training data
  - Getting surprisingly low loss?
  - Check the whole procedure

How to detect overfitting

- After training/testing splitting, training loss is much less than testing loss.

- Start with a simple model as the benchmark
  - When add model complexity, you will have a reference point to see whether the additional complexity is worthy.

How to prevent overfitting

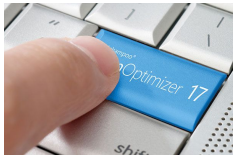
- Train with more data
  - Filter noisy data (outlier)
- Remove features
  - Remove irrelevant features
- Regularization
  - Control model complexity
  - Different machine learning models have their own regularization methods.

Hyperparameter Optimization

Hyperparameters

- Machine learning algorithms usually have two kinds of weights:
  - ***Parameters***: learned by data during training such as slope of linear regression, layer weights of neural networks
  - **Hyperparameters**: left to us to select beforehand such as K in KNN, number of layers in neural networks

Hyperparameters

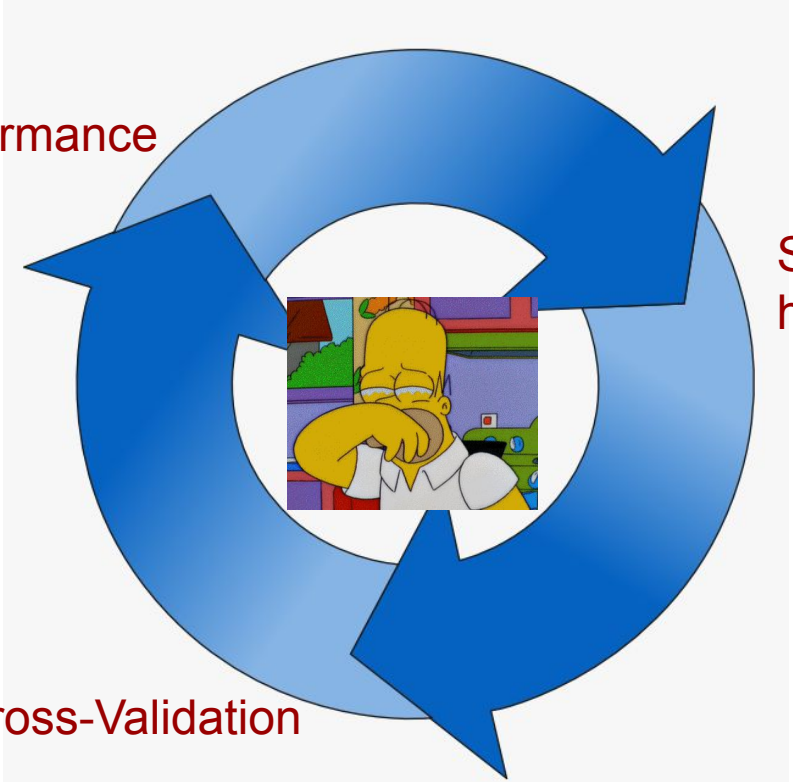


Parameters

Scores

Searching is Iterative, then Expensive

Track the performance

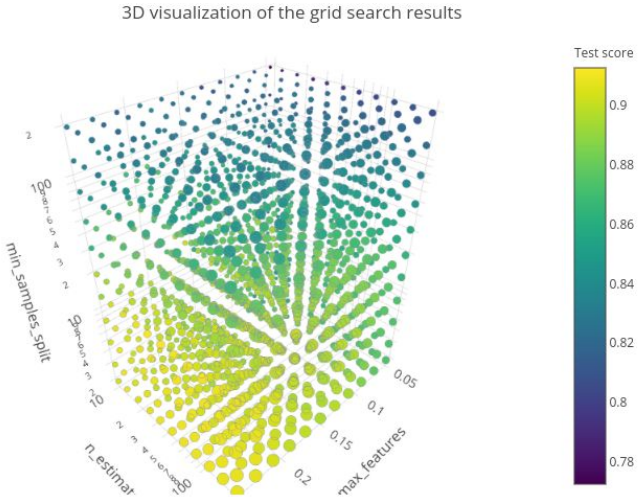


Select one potential hyperparameter set

Run Cross-Validation

Grid Search

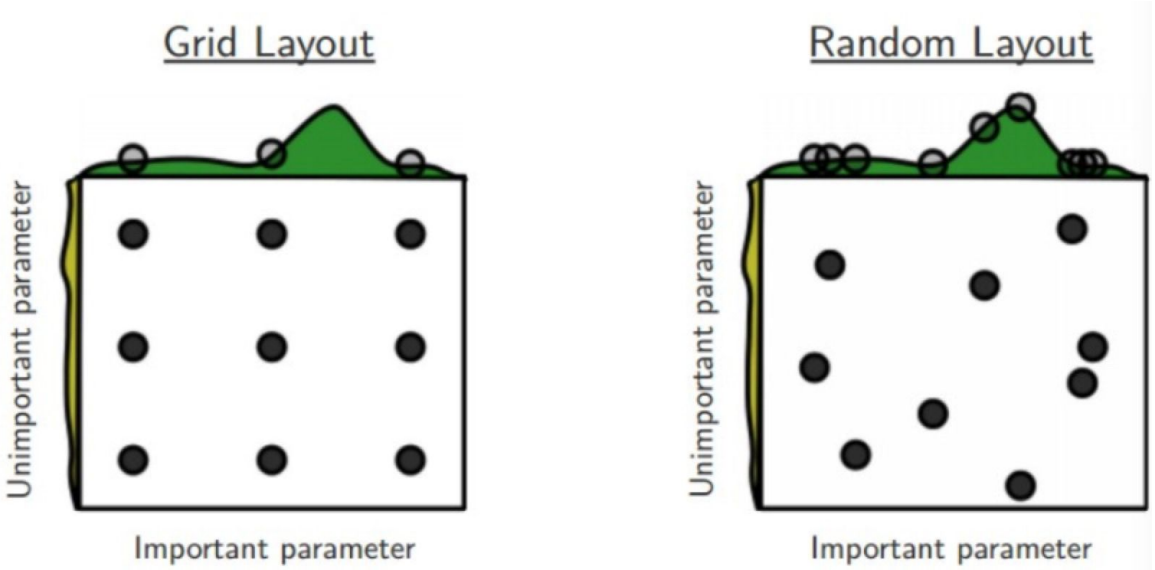
- Define a grid on n-dimensions, where each of these maps for an hyperparameter
- For each dimension, define the range of possible values
- Search for all combinations and select the best one



Inefficient !!!

Random Search

- Randomly pick the point from the configuration space
- The rest is the same as grid search



Good on high-dim spaces

From Bergstra and Bengio

Advanced Search Algorithms

- For grid and random search, the previous trials can not contribute to each new guess.

- Try to model the hyperparameter search as a machine learning task
  - Tree-structured Parzen Estimator
  - Gaussian Process
  - Other bayesian optimization methods

Main idea: based on the distribution of the previous results, decide which set of parameters should be explored firstly