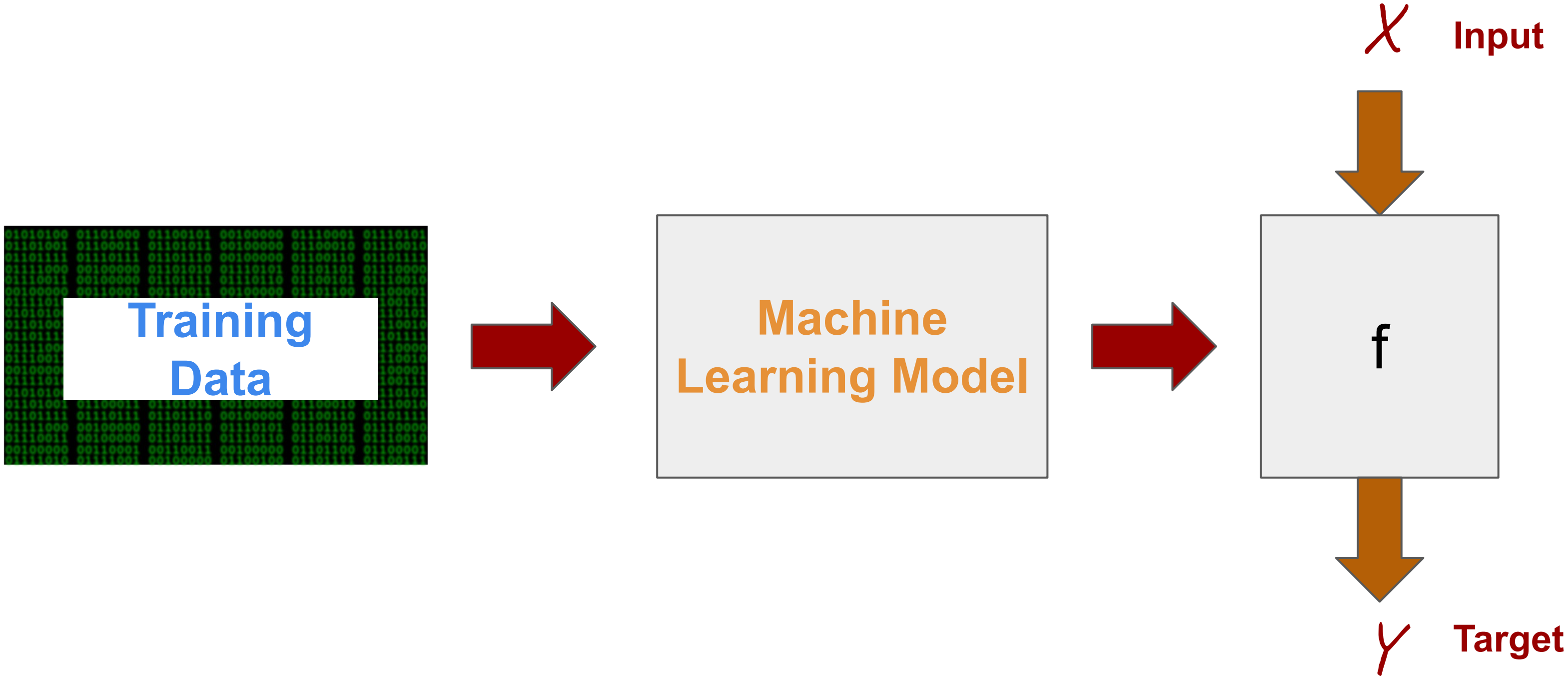
Machine Learning Practices

Framework (supervised)



Training Data

Machine Learning Model

f

X Input

Y Target

A “Real” Machine Learning Task

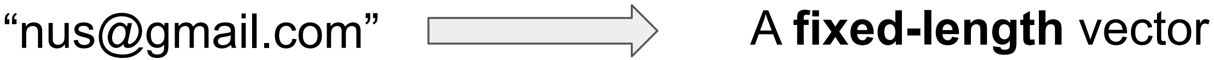
- Example task: predict y, whether a string x is an email address
  - x: “diszr@nus.edu.sg” **y:1**
  - x: “nusmsba” **y:0**
  - x: “@trump” **y:0**

- If we are going to using ML models?
  - What are T, P, E?

Feature Extraction

- **Question**: what properties of x **might be** relevant for predicting y?

- **Feature extractor**: Given input x, output a set of (**feature name**, **feature value**) pairs.



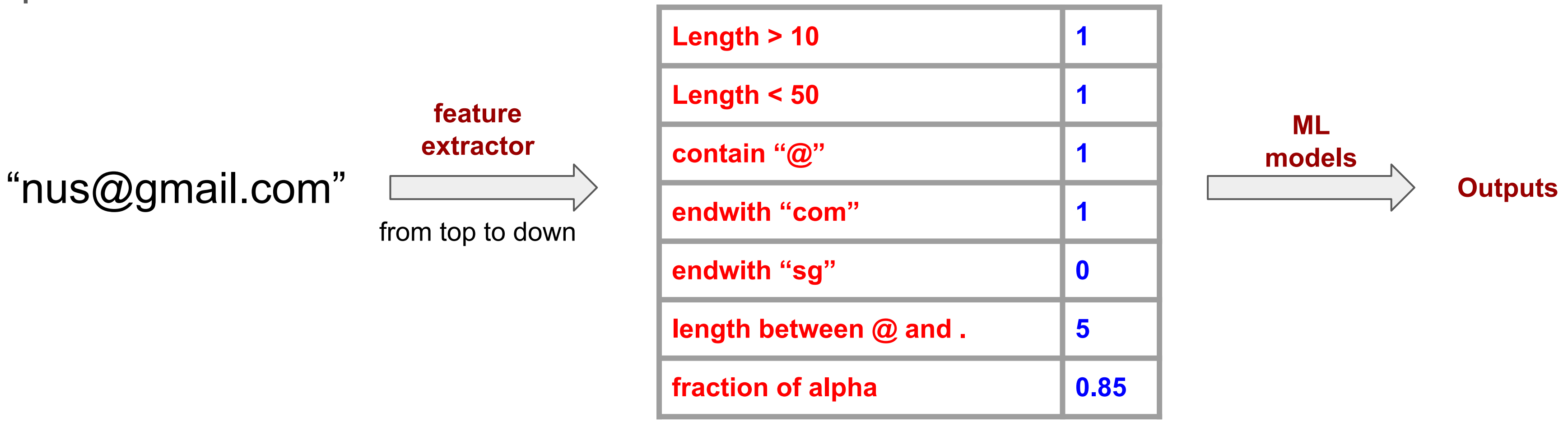
“nus@gmail.com”

A **fixed-length** vector

Feature Extraction

- **Question**: what properties of x **might be** relevant for predicting y?

- **Feature extractor**: Given input x, output a set of (**feature name**, **feature value**) pairs.



“nus@gmail.com”

feature extractor

from top to down

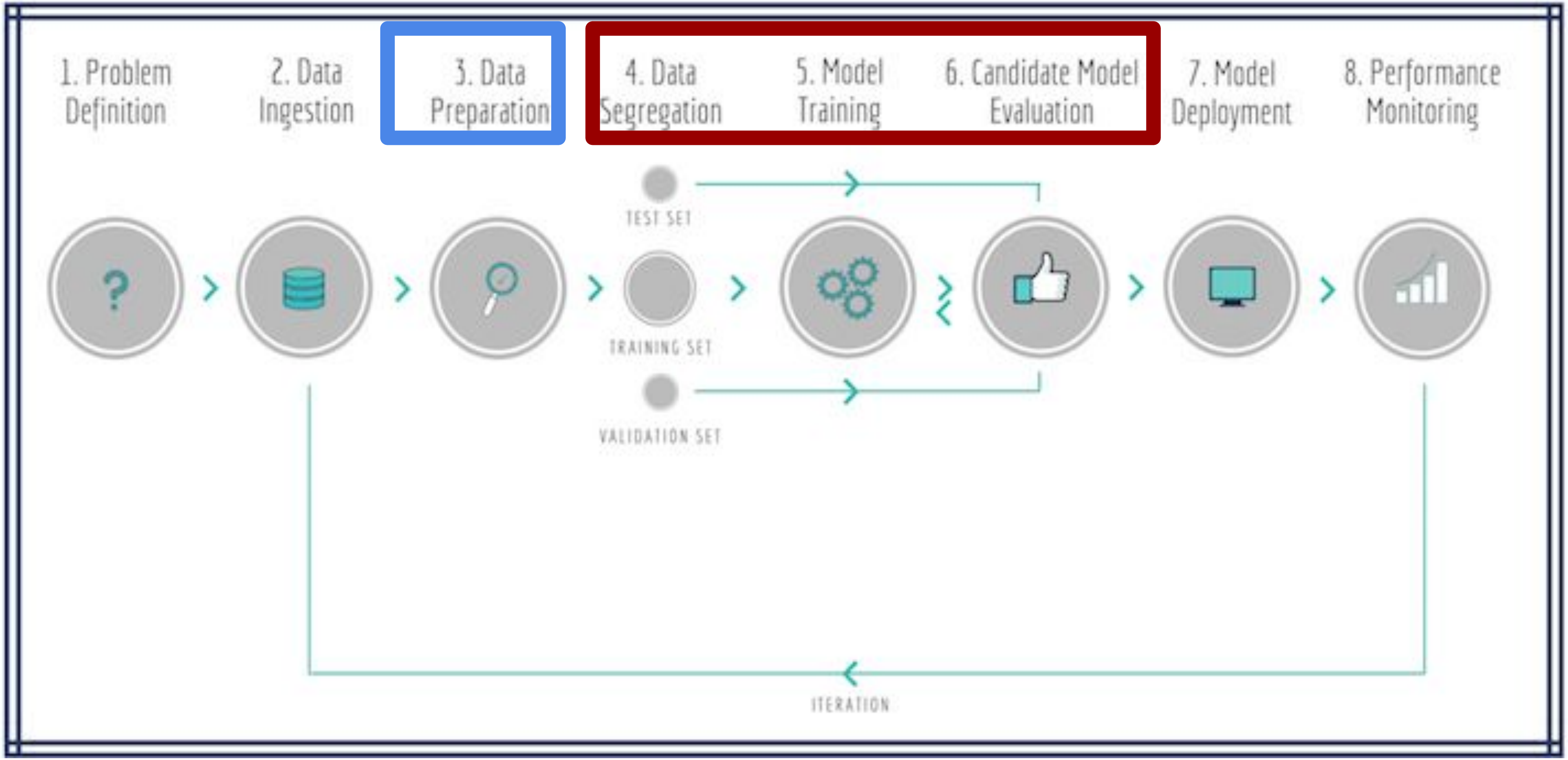
Length > 10	**1**
Length < 50	**1**
contain “@”	**1**
endwith “com”	**1**
endwith “sg”	**0**
length between @ and .	**5**
fraction of alpha	**0.85**

ML models

Outputs

*Exploration
*Transformation
*Fea. Engineering

Modelling



Credit: Semi Koen

Agenda

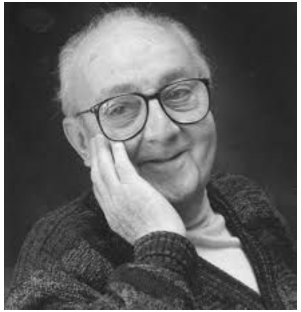
1. Feature Engineering
2. Model Selection: Cross-validation
3. Hyperparameter Search
4. Hands-on Project: Cuisine Categorization

Feature Engineering

Recall that computers only understand numbers (binary)

What is Feature Engineering

- 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.



George Box

- 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.

Feature Engineering

- Question u ask:

What properties of x **might be** relevant for predicting y?

This step is really important for linear models.

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

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!)

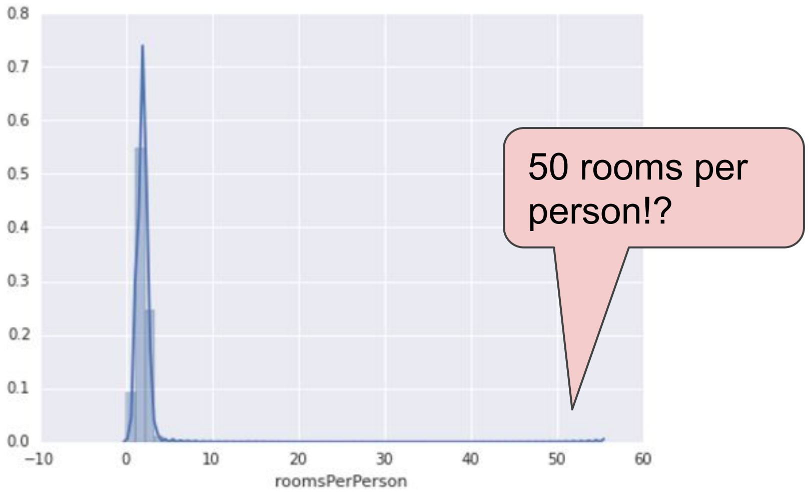
✓ `city_id:“br/sao_paulo”`

✗ `inferred_city_cluster_id:219`

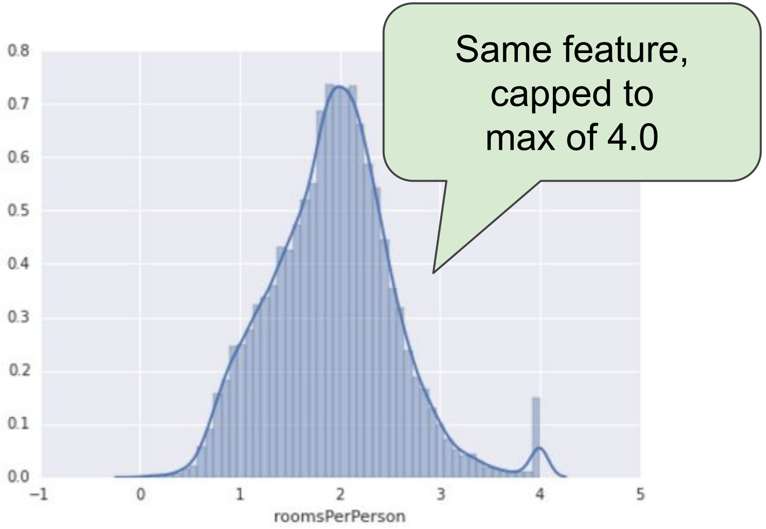
Properties of a Good Feature

Distribution should not have crazy outliers

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



50 rooms per person!?



Same feature, capped to max of 4.0

Why Scaling?

- Range of values of data may vary widely
- Lots of machine learning algorithms are very sensitive to scales of features
  - K-nearest Neighbors
  - K-means
  - Logistic Regression
  - SVMs
  - Gradient Descent
  - PCA
  - Etc

When distances of feature vector matter

How to scale data

- 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

- Z-score Transformation: **Force the mean to be zero and std to be one**

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

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

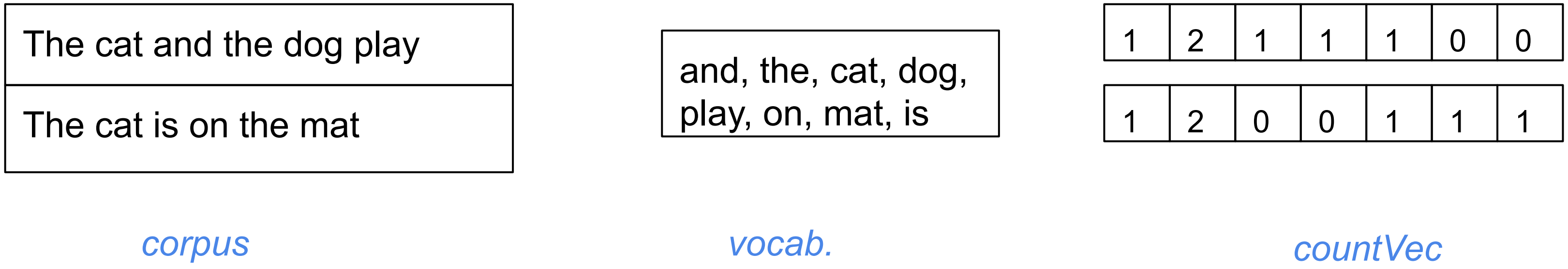
Good Habits: Know your data!!

- **Visualize:** Plot histograms, rank most to least common value.
- **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



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

corpus

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

vocab.

1	2	1	1	1	0	0
1	2	0	0	1	1	1

countVec

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

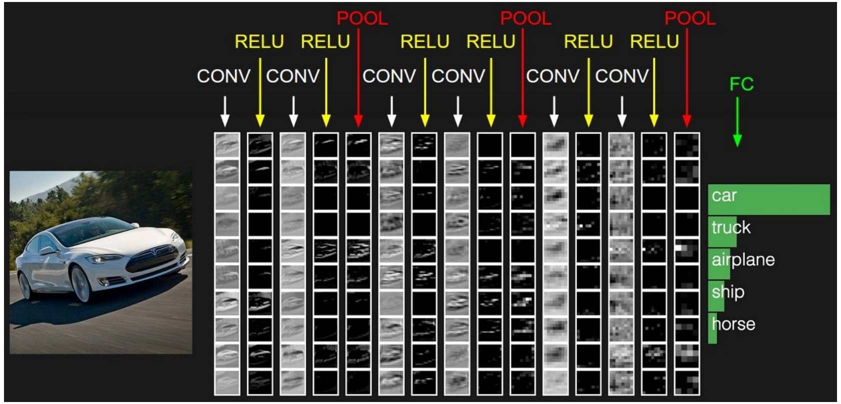
vocab.

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

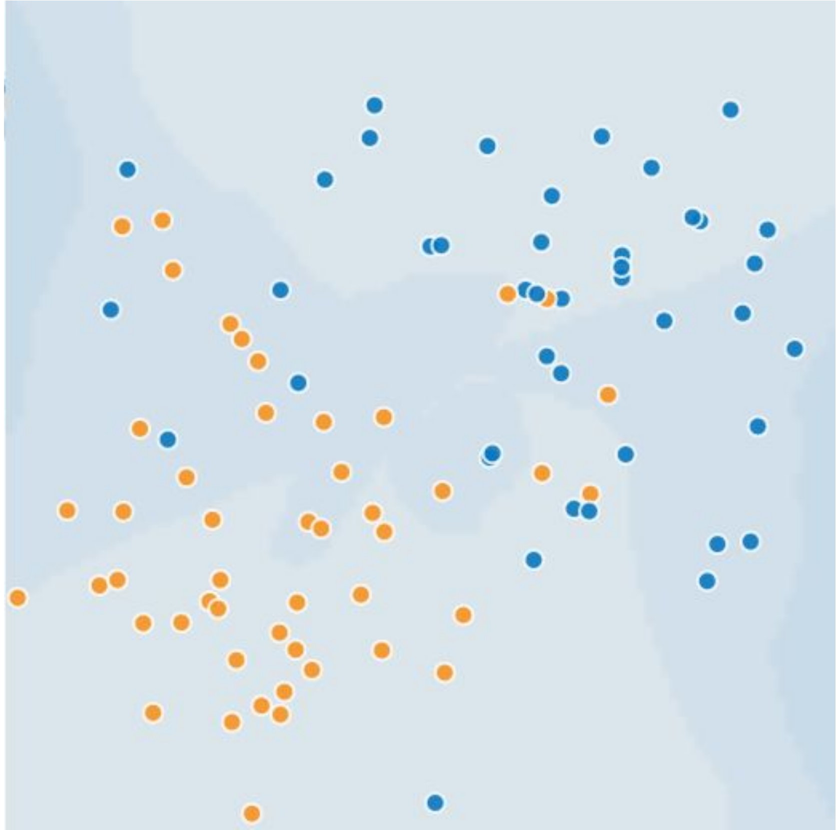


http://cs231n.github.io/convolutional-networks/

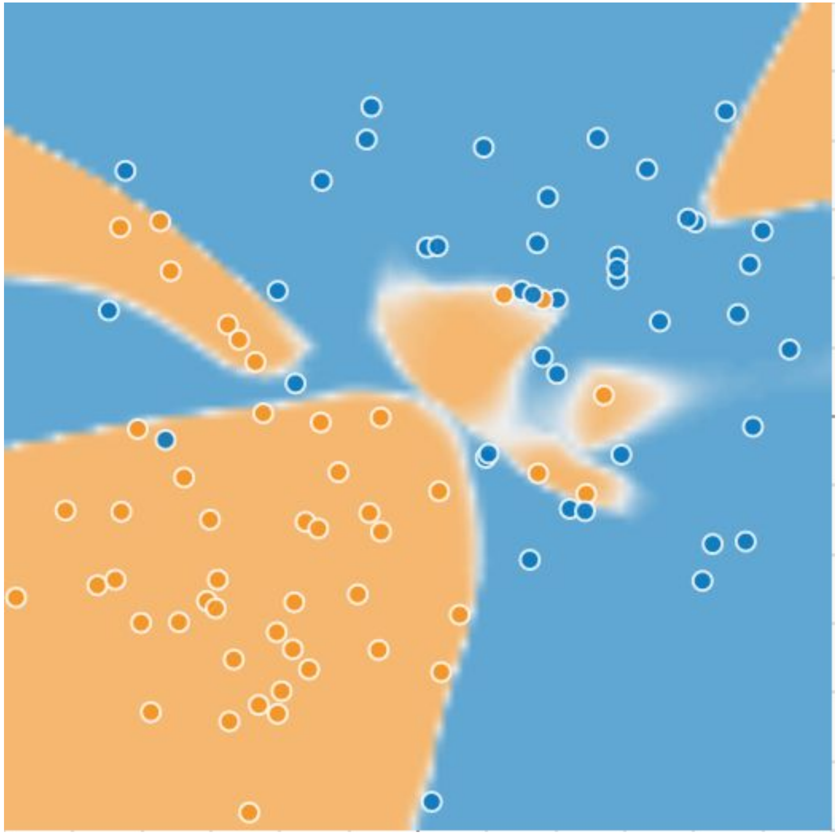
Cross-Validation

Which measure should we look for model evaluation?

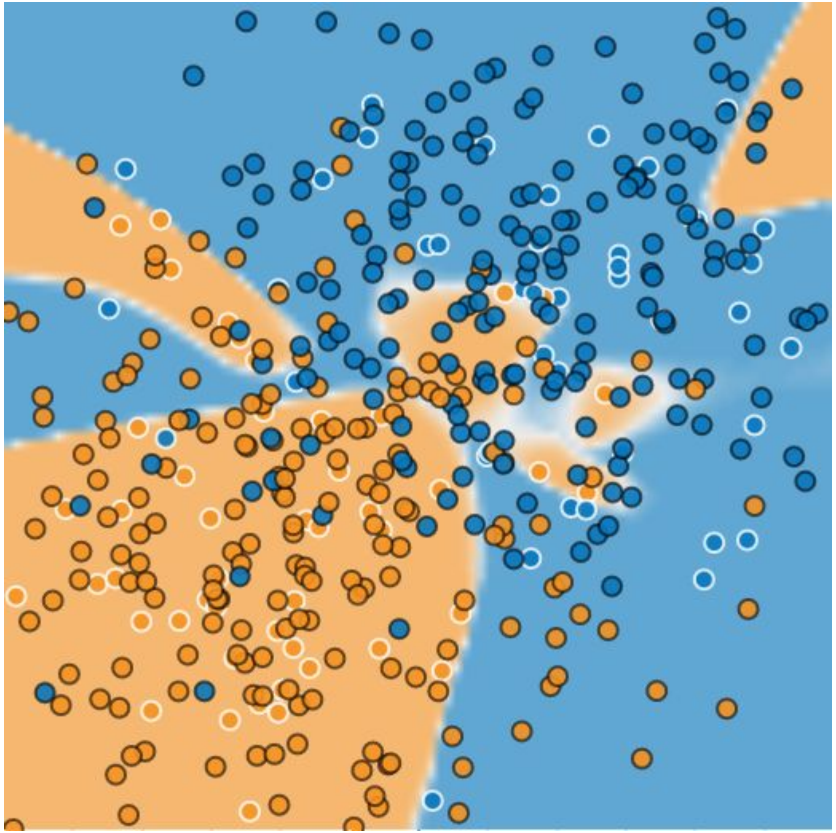
Let’s try to train a model for this problem



How about this model?



More data



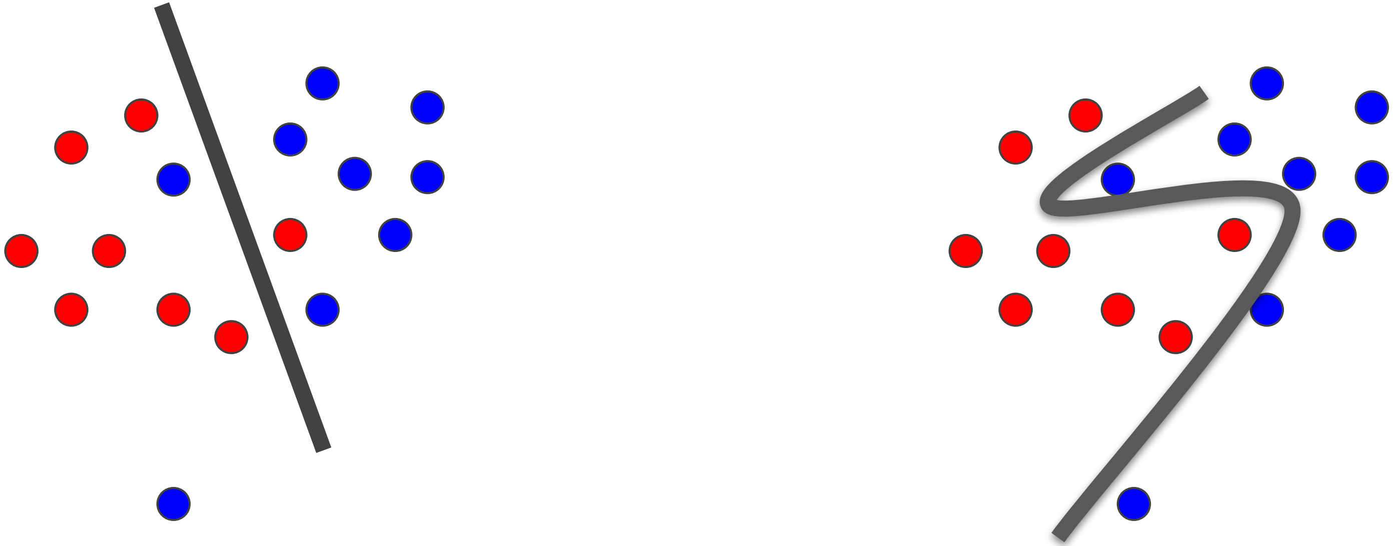
Which measure should we look for model evaluation?

Training performance is not suitable

Generalization

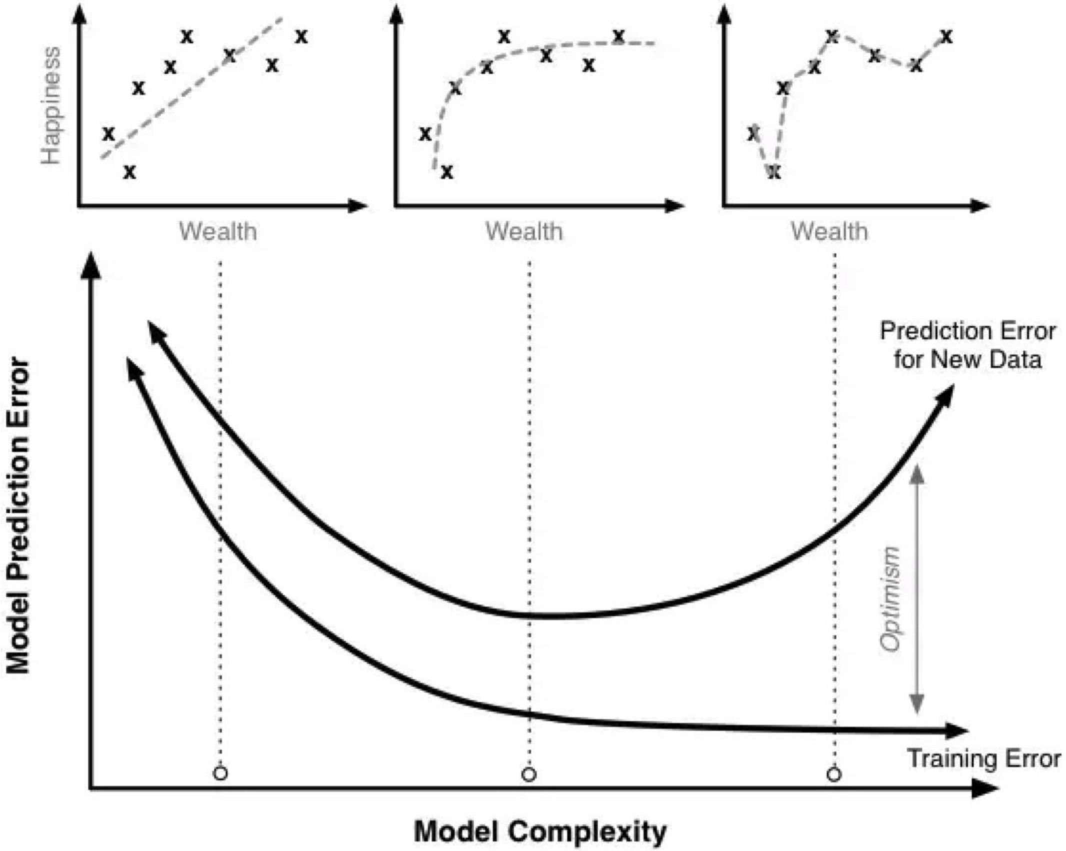
- In ML, a model is used to fit the data
- Once trained, the model is applied upon new data
- Generalization is the prediction capability of the model on live/new data

Which model is better?



SPAM VS Not SPAM

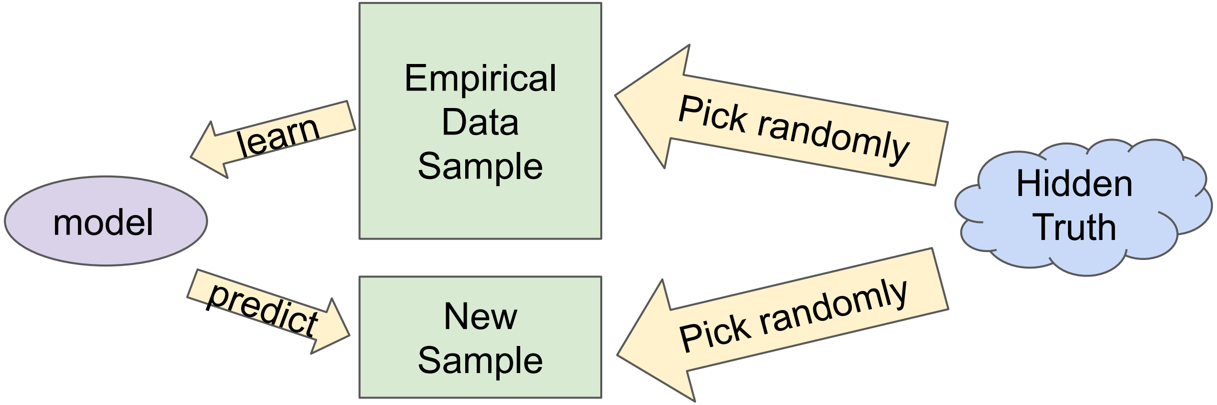
Model Complexity



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.

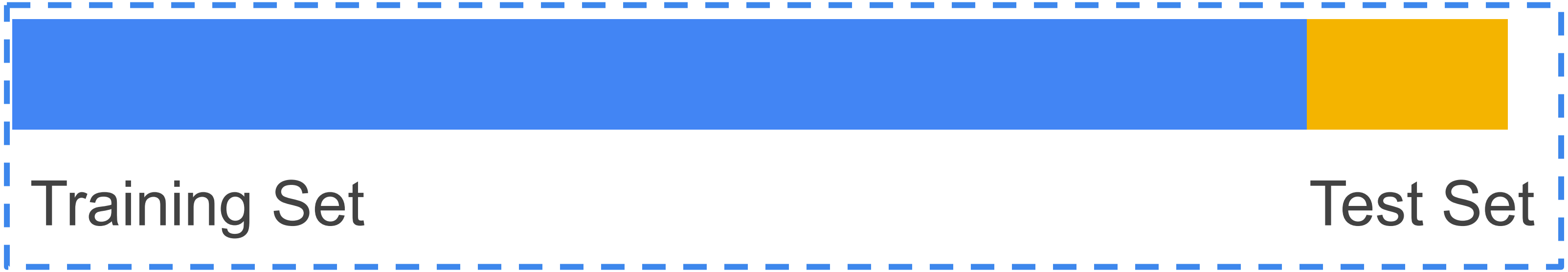
- Theoretically:
  - Interesting field: generalization theory
  - Based on ideas of measuring model simplicity / complexity

William of Occam

Is the model overfitting?

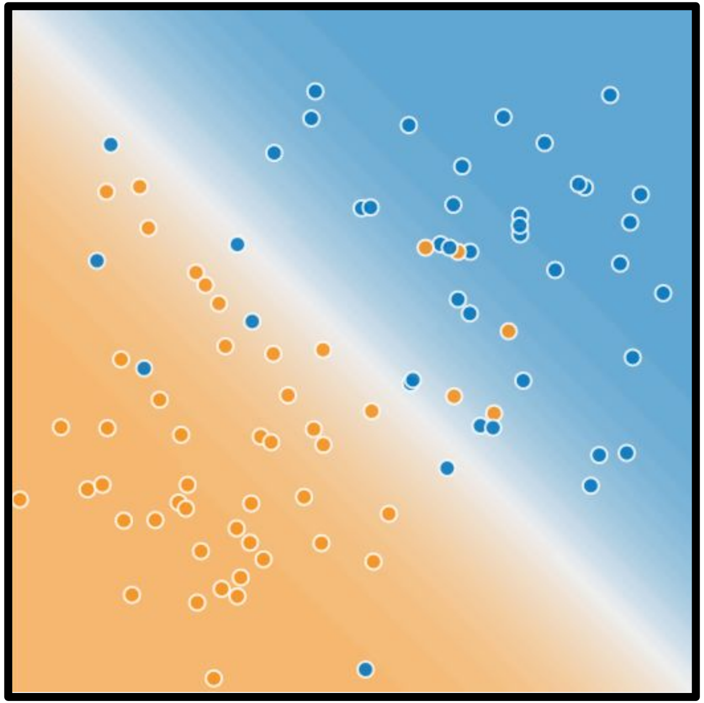
- Empirically:
  - Key point: will our model be good on new samples?
  - Evaluate: get new samples of data (test set)
  - If test set is large enough and we do not cheat by using test set over and over, the good performance on test set can be a useful indicator of model’s generalization capability

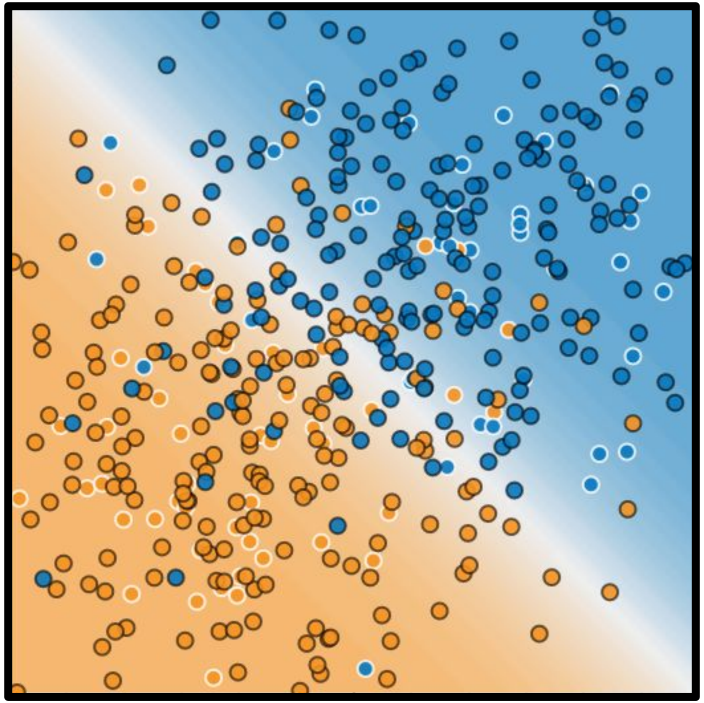
Training/Test Splitting



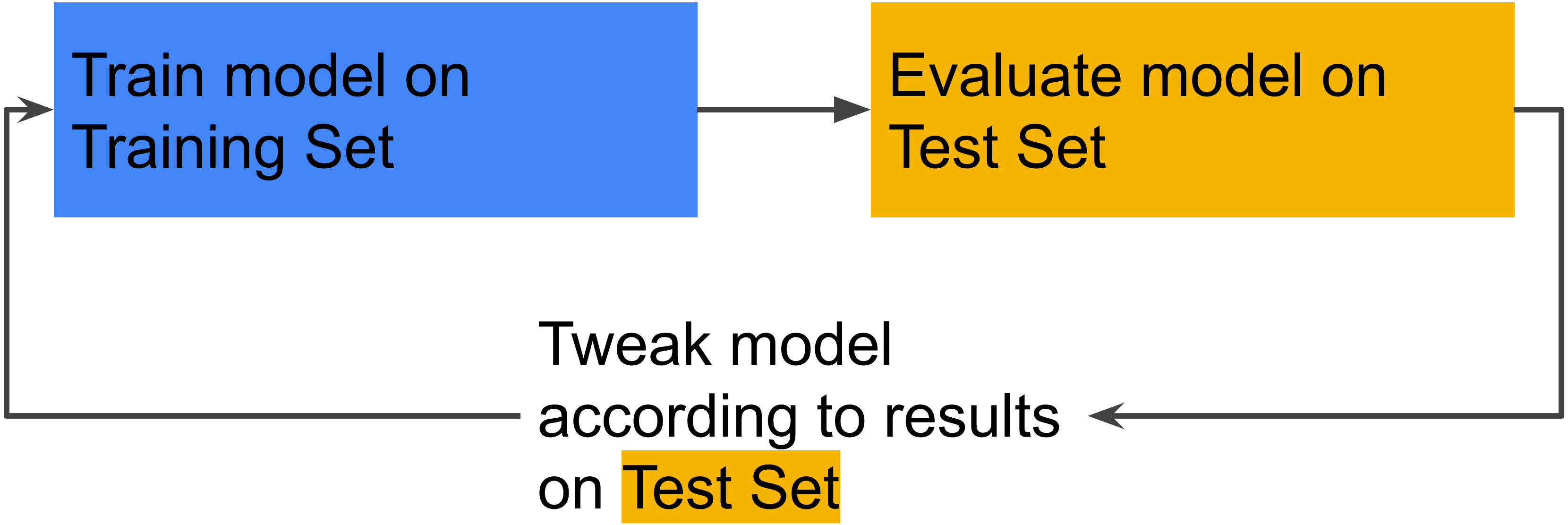
- If models do much better on the training set than the testing set, then models are likely overfitting.
- How do we divide?
  - Randomization for splitting
  - Larger training data size -> better model
  - Larger testing data size -> more confident in model's evaluation
  - One practical rule: 10-15%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

Training Evaluation v.s. Test Evaluation





How about this workflow?



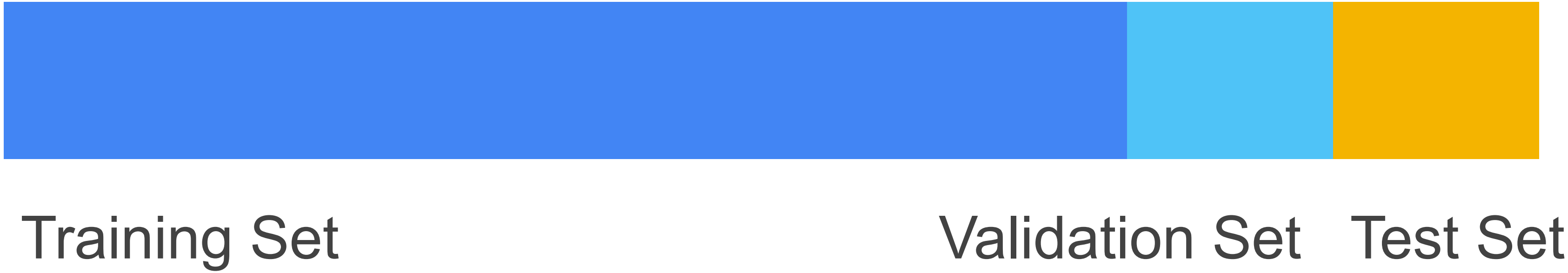
Train model on Training Set

Evaluate model on Test Set

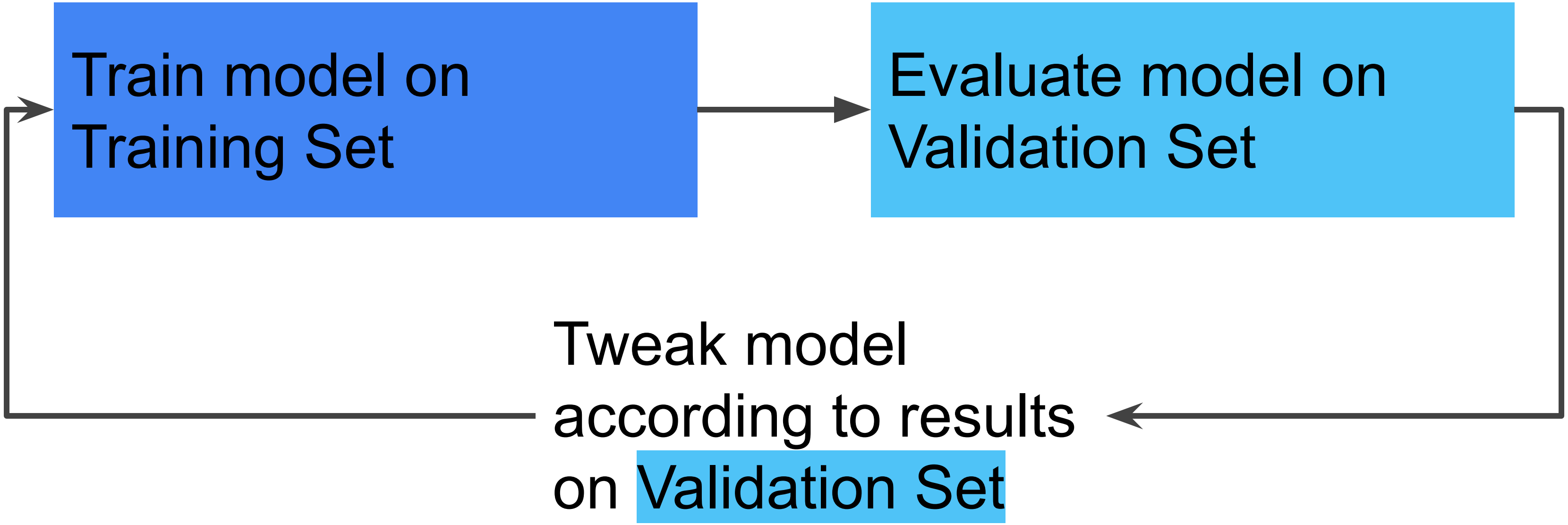
Tweak model according to results on Test Set

Pick model that does best on Test Set.

Partition Data Sets



Better Workflow: Use a validation set



Train model on Training Set

Evaluate model on Validation Set

Tweak model according to results on Validation Set

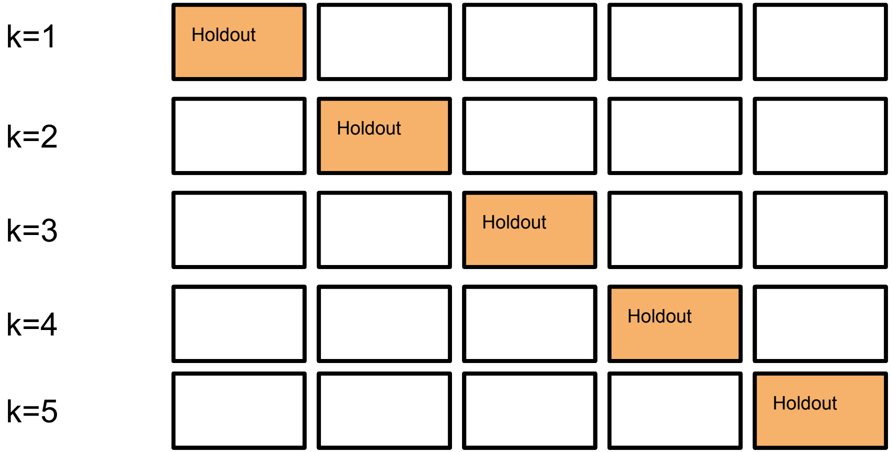
Pick model that does best on Validation Set
Confirm results on Test Set

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



k=1	Holdout				
k=2		Holdout			
k=3			Holdout		
k=4				Holdout	
k=5					Holdout

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.

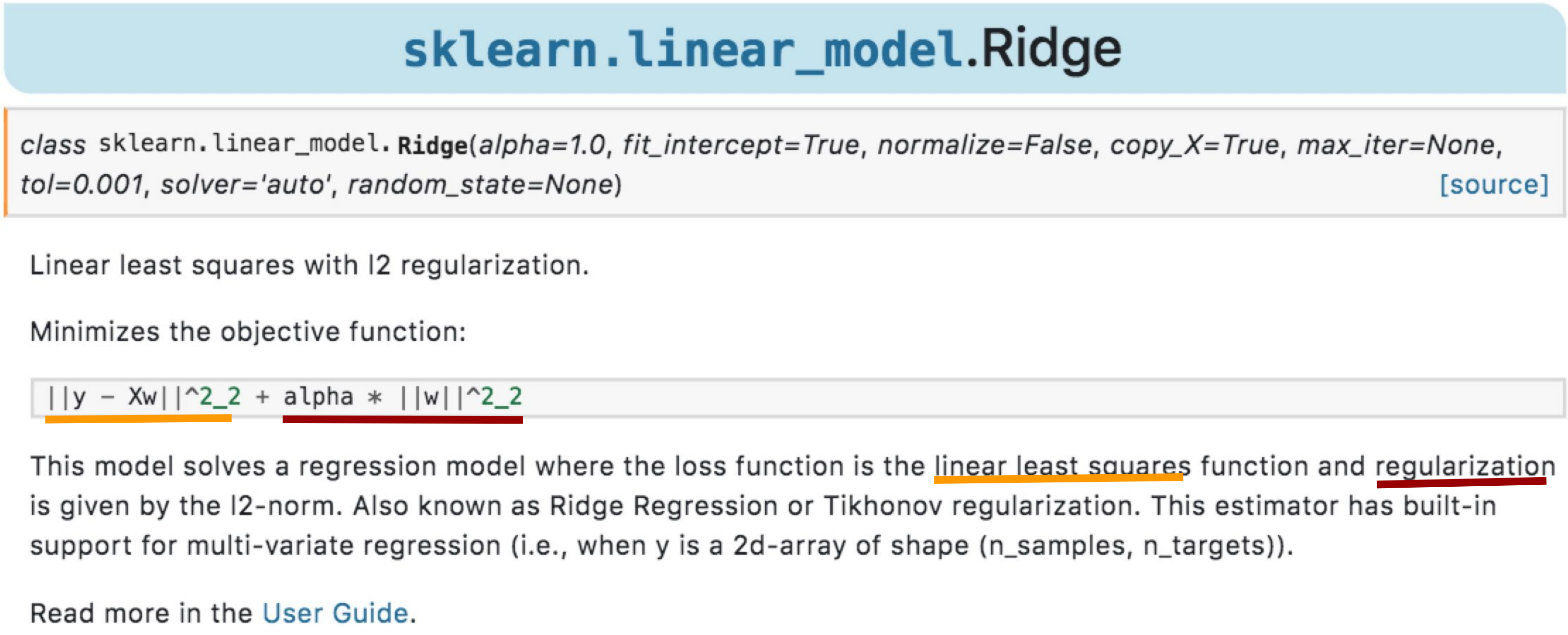
- Start with a simple model as the benchmark
  - When add model complexity, you will have a reference point to see whether the additional complexity is worthy.

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.

As a Summary

- What should be the targets set for Machine Learning
  - Minimize loss on the training set
  - Minimize loss on the validation set
  - Minimize loss on the test set
  - Minimize loss on unseen future examples



sklearn.linear_model.Ridge

class sklearn.linear_model.**Ridge**(*alpha=1.0, fit_intercept=True, normalize=False, copy_X=True, max_iter=None, tol=0.001, solver='auto', random_state=None*) [source]

Linear least squares with l2 regularization.

Minimizes the objective function:

```
||y - Xw||^2_2 + alpha * ||w||^2_2
```

This model solves a regression model where the loss function is the linear least squares function and regularization is given by the l2-norm. Also known as Ridge Regression or Tikhonov regularization. This estimator has built-in support for multi-variate regression (i.e., when y is a 2d-array of shape (n_samples, n_targets)).

Read more in the User Guide.

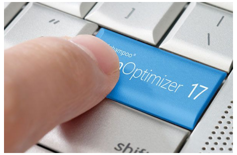
Alpha is the controlling parameter, which is also hyperparameter

Hyperparameter Optimization

Hyperparameters

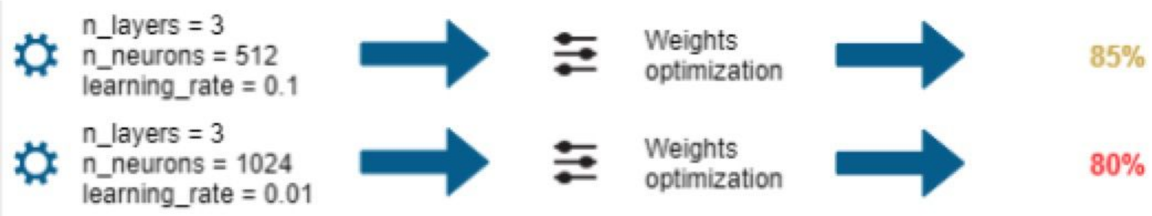
- Machine learning algorithms usually have two kinds of weights:
  - ***Parameters***: learned by data during training such as slope of linear regression, layer weights of neural networks
  - **Hyperparameters**: left to us to select beforehand such as K in KNN, number of layers in neural networks

Hyperparameters



Parameters

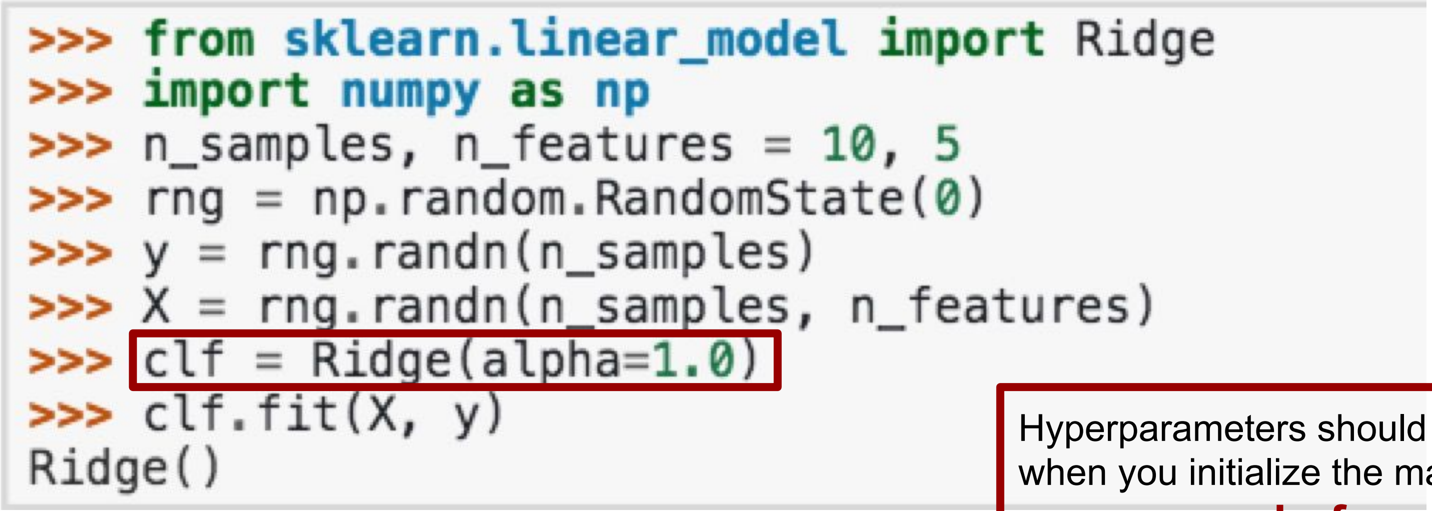
Scores



n_layers = 3
n_neurons = 512
learning_rate = 0.1
Weights optimization
85%

n_layers = 3
n_neurons = 1024
learning_rate = 0.01
Weights optimization
80%

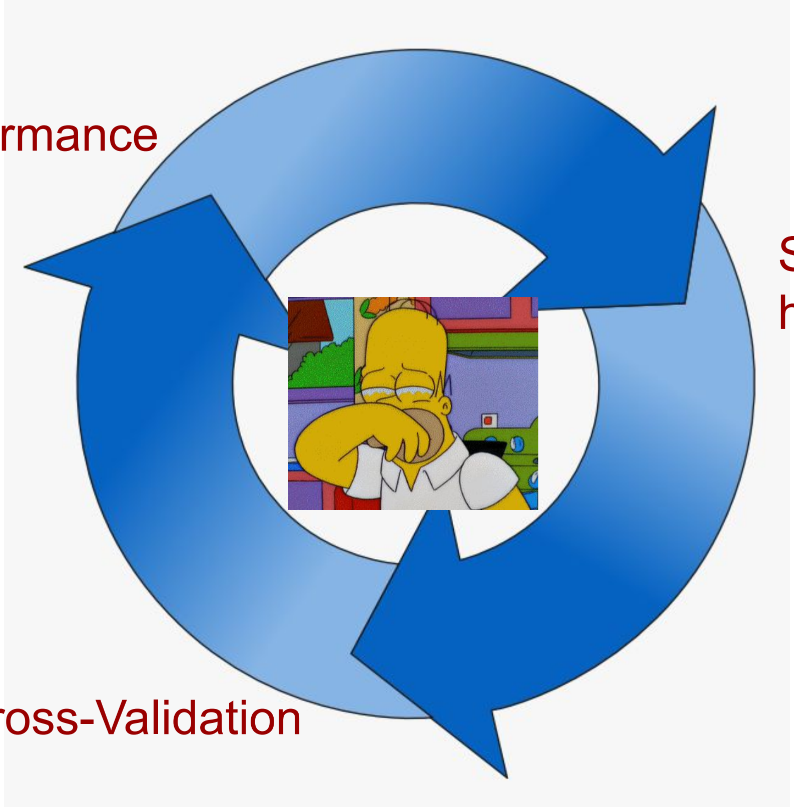
Hyperparameters



```
>>> from sklearn.linear_model import Ridge
>>> import numpy as np
>>> n_samples, n_features = 10, 5
>>> rng = np.random.RandomState(0)
>>> y = rng.randn(n_samples)
>>> X = rng.randn(n_samples, n_features)
>>> clf = Ridge(alpha=1.0)
>>> clf.fit(X, y)
Ridge()
```

Hyperparameters should be passed when you initialize the machine learning model **before training**

Searching is Iterative, then Expensive



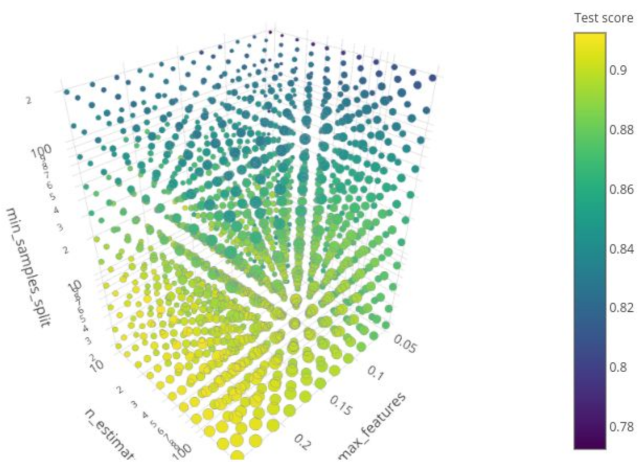
Track the performance

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

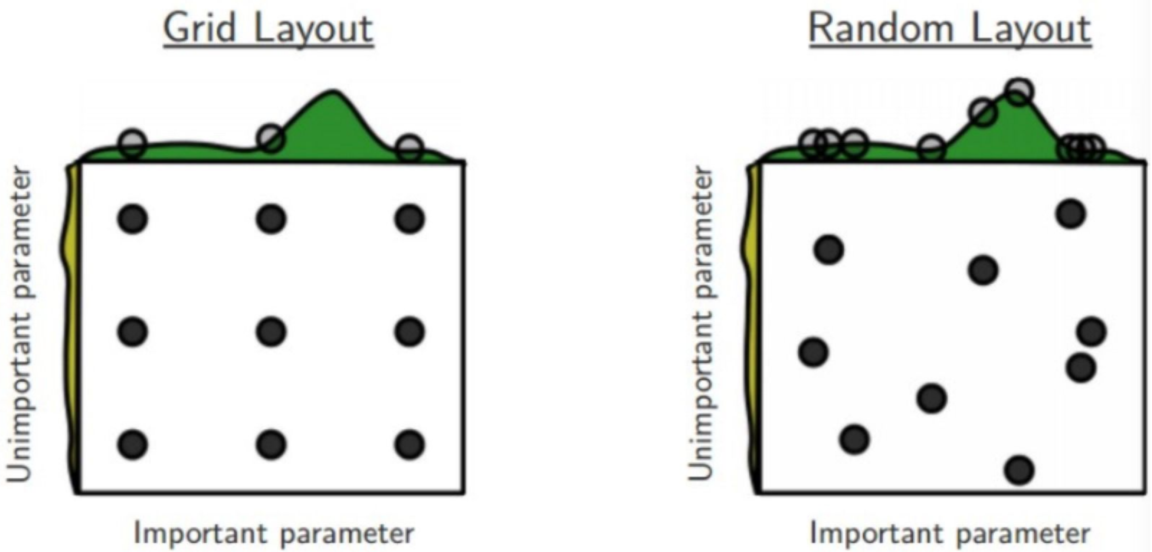


3D visualization of the grid search results

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