Applied Machine Learning for Business Analytics

Lecture 2: Machine Learning Practices

Lecturer: Zhao Rui

```
knn.fit(X, y)

# What kind of iris has 2cm x 5cm sepal and 1cm x 5cm petal?
# call the "predict" method:
result = knn.predict([[2, 5, 1, 5],])

print(iris.target_names[result])

# You can also do probabilistic predictions

knn.predict_proba([[2, 5, 1, 5],])
```

```
['setosa']
```

```
]: array([[1., 0., 0.]])
```

```
]: result
```

```
]: array([0])
```

Question: why the following code is not working?

```
]: result = knn.predict([2, 5, 1, 5])
```

Logistics

- 1-2 days response policy for course-related emails (Please address me Rui)
- Video presentation for group projects
- HW1 has been released (Simple EDA exercise) today, which due **Friday Jan 28, 11:59 pm**
- We miss 14 students in group projects. If you need any help, pls contact Sanjay
- The survey will be sent this weekend for your preference over remote learning and f2f learning.

Agenda

1. Feature Engineering
2. Model Selection: Cross-Validation
3. Hyper-parameter Selection
4. Data Leakage

1. Feature Engineering

Recall that computers only understand numbers

What is Feature Engineering

- Feature engineering:
  - Extract features to use in your model
  - How to represent examples by the feature vectors?

Feature Engineering

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

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**
- 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 Engineering

- 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

Discretization

ML models

Outputs

Can we use length directly?

Engineered Features

- For text data: BoW Models

Stopword removal	I have a dog. He's sleeping.
Lemmatization	I have dog. He's sleeping.
Contraction	I have dog. He's sleep.
Punctuation	I have dog. He is sleep.
Lowercase	I have dog He is sleep
N-gram	i have dog he is sleep

features

samples

0	3	0	0	...
1	0	0	0	...
0	0	1	0	..
...	...	...	...	...

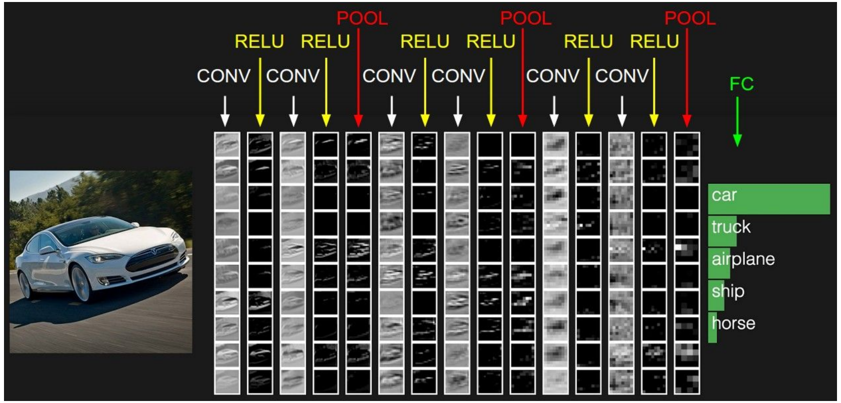
Classifier
(e.g. LogReg)

Features

I	you	have	dog	cat	he	she	is	they	sleep	I, have	have, dog	good, dog	...
1	0	1	1	0	1	0	1	0	1	1	1	0	...

Representation Learning

- Using Deep Learning Approach:
    - CNN, RNN, Attention Models
    - Learn representations from text, image, video, audio signals



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

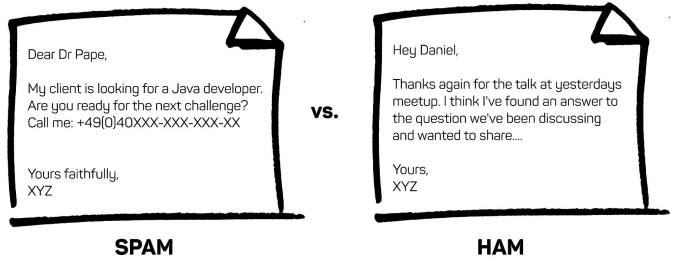
Feature Engineering

- In papers, deep learning papers promise no more feature engineering
  - We are still very far from that point
  - Deep learning are not the first choice in industry for many applications

Spam Classification

Except BoW Features:

- Post repetitiveness
- Language detection, typos, abnormal punctuations, ratio uppercase/lowercase
- IP, other users from the same IP
- Blacklisted links
- Targeted users
- ...



Feature engineering

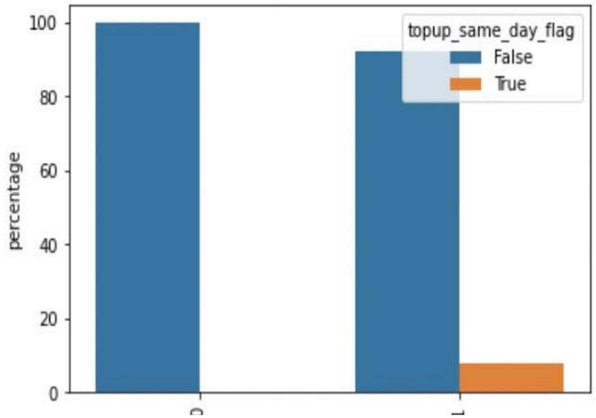
- For complex tasks, number of features can go up to millions or billions!
- Lots of ML production work involves coming up with new features
    - Fraudsters come up with new techniques very fast, so need to come up with new features very fast to counter
- Often require subject matter expertise
- Good 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

Several feature engineering tips

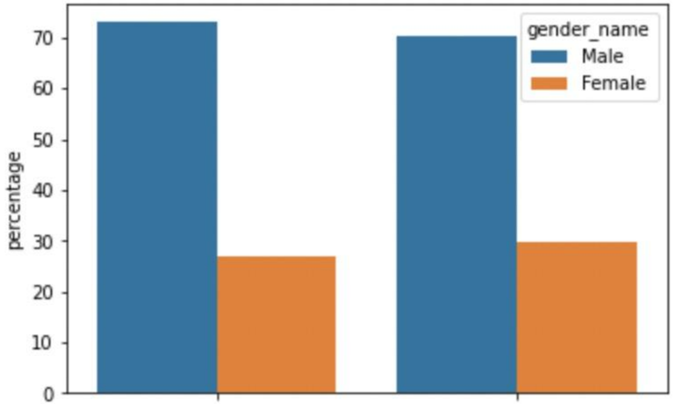
1. EDA
2. Handling missing values
3. Scaling
4. Discretization
5. Categorical features
6. Feature crossing

EDA for Discrete Features

- Predict Tranx. Probabilities for Onboarding Users



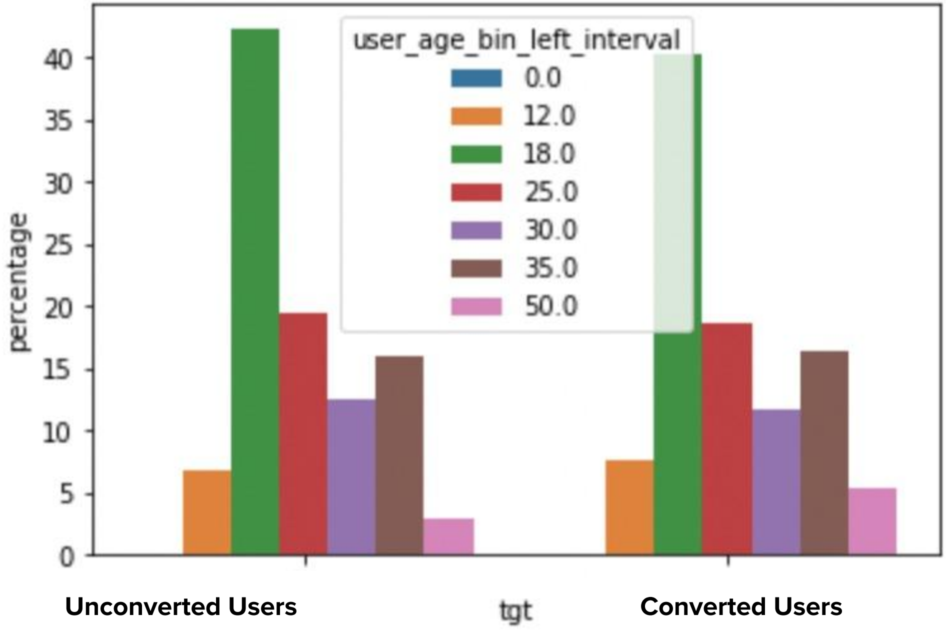
Unconverted Users Converted Users



Unconverted Users Converted Users

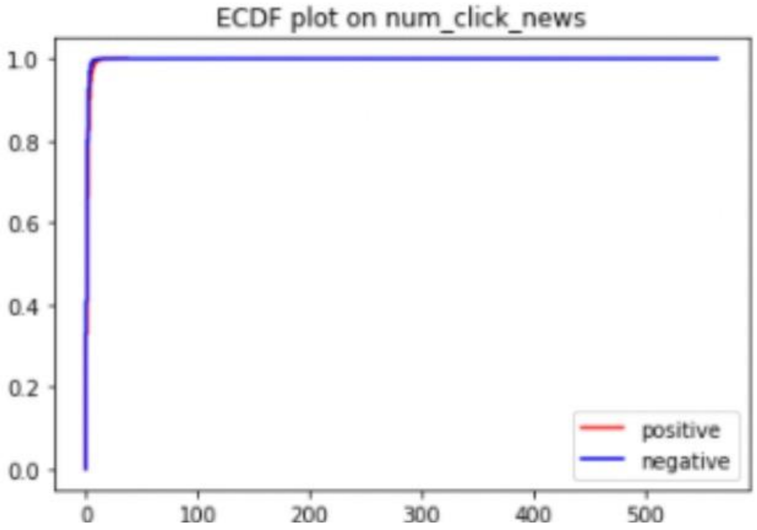
EDA for Continuous Features

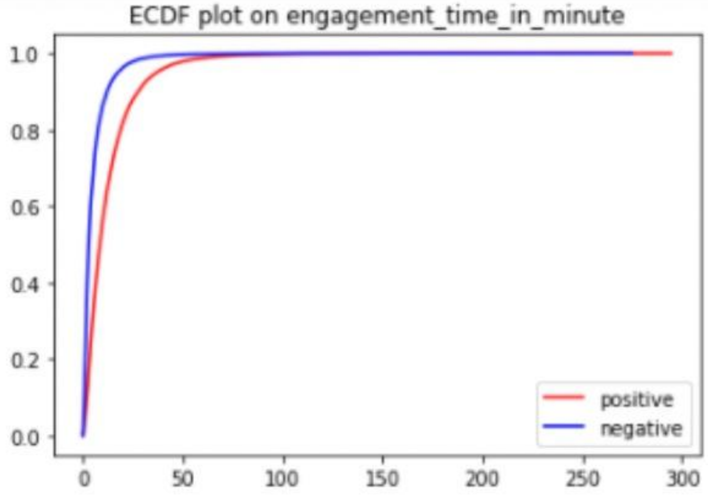
User Age Bin (legends = left interval limit, unit in years)



EDA for Continuous Features

- Empirical Cumulative Distribution Function: An estimator of the cumulative distribution function





Why Data Goes Missing

- Data missing has different reasons
  - Missing at random (MAR)
  - Missing not at random (MNAR)
  - Missing completely at random (MCAR)

Source: https://en.wikipedia.org/wiki/Missing_data

ID	Age	Gender	Annual income	Job	Buy?
1		A	150,000	Engineer	No
2	27	B	50,000	Teacher	No
3		A	100,000		Yes
4	40	B		Engineer	Yes
5	35	B		Doctor	Yes
6		A	50,000	Teacher	No

MAR

Missing at random – the missing data is related to another observed variable

ID	Age	Gender	Annual income	Job	Buy?
1		A	150,000	Engineer	No
2	27	B	50,000	Teacher	No
3		A	100,000		Yes
4	40	B		Engineer	Yes
5	35	B		Doctor	Yes
6		A	50,000	Teacher	No

MNAR

Missing not at random – the data missing is related to the value itself

ID	Age	Gender	Annual income	Job	Buy?
1		A	150,000	Engineer	No
2	27	B	50,000	Teacher	No
3		A	100,000		Yes
4	40	B	($350,0000?)	Engineer	Yes
5	35	B	($350,0000?)	Doctor	Yes
6		A	50,000	Teacher	No

MCAR

Missing completely at random – there is no pattern to which values are missing

ID	Age	Gender	Annual income	Job	Buy?
1		A	150,000	Engineer	No
2	27	B	50,000	Teacher	No
3		A	100,000		Yes
4	40	B		Engineer	Yes
5	35	B		Doctor	Yes
6		A	50,000	Teacher	No

Handling missing values

- Deletion – removing data with missing entries
- Imputation – filling missing fields with certain values

Handling missing values

- Deletion
  - Column deletion – remove columns with too many missing entries
    - drawbacks – even if half the values are missing, the remaining data still potentially useful information for predictions
    - e.g. even if over half the column for ‘Marital status’ is missing, marital status is still highly correlated with house purchasing
  - Row deletion

Marital status
Married
Single
Single

Handling missing values

- Row deletion
  - Good for: data missing completely at random (MCAR) and few values missing

ID	Age	Gender	Annual income	Job	Buy?
1	39	A	150,000	Engineer	No
2	27	B	50,000	Teacher	No
3		A	100,000		Yes
4	40	B	75,000	Engineer	Yes
5	35	B	35,000	Doctor	Yes
6	32	A	50,000	Teacher	No
7	33	B	60,000	Teacher	No
8	20	B	10,000	Student	No

Handling missing values

- Row deletion
    - Bad when many examples have missing fields

ID	Age	Gender	Annual income	Job	Buy?
1		A	150,000	Engineer	No
2	27	B	50,000	Teacher	No
3		A	100,000		Yes
4	40	B		Engineer	Yes
5	35	B		Doctor	Yes
6		A	50,000	Teacher	No
7	33	B	60,000	Teacher	No
8	20	B	10,000	Student	No

Handling missing values

- Row deletion
  - Bad for: missing data at random (MAR)
  - Can potentially bias data – we've accidentally removed all examples with gender 'A'

ID	Age	Gender	Annual income	Job	Buy?
1		A	150,000	Engineer	No
2	27	B	50,000	Teacher	No
3		A	100,000		Yes
4	40	B		Engineer	Yes
5	35	B		Doctor	Yes
6		A	50,000	Teacher	No
7	33	B	60,000	Teacher	No
8	20	B	10,000	Student	No

Handling missing values

- Row deletion
  - Bad for: missing values are not at random (MNAR)
  - Missing information is information itself

ID	Age	Gender	Annual income	Job	Buy?
1		A	150,000	Engineer	No
2	27	B	50,000	Teacher	No
3		A	100,000		Yes
4	40	B	($350,000?)	Engineer	Yes
5	35	B	($350,000?)	Doctor	Yes
6		A	50,000	Teacher	No
7	33	B	60,000	Teacher	No
8	20	B	10,000	Student	No

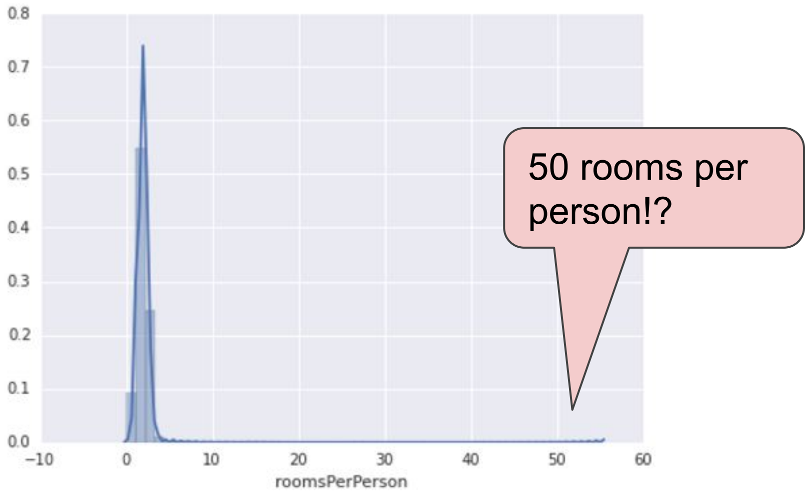
Imputation

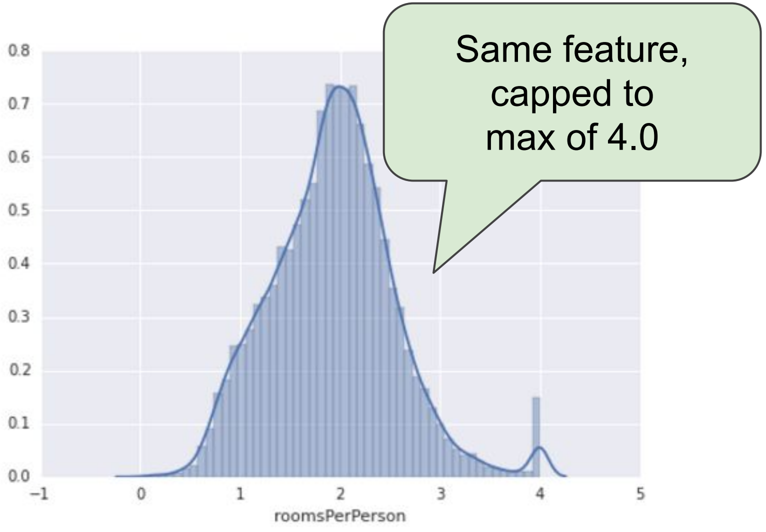
- Fill missing fields with certain values
  - Defaults
    - E.g. 0, or the empty string, etc.
  - Statistical measures – mean, median, mode
    - e.g. if a day in July is missing its temperature value, fill it with the median temperature in July

Scaling

Distribution should not have crazy outliers

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





Types of scaling

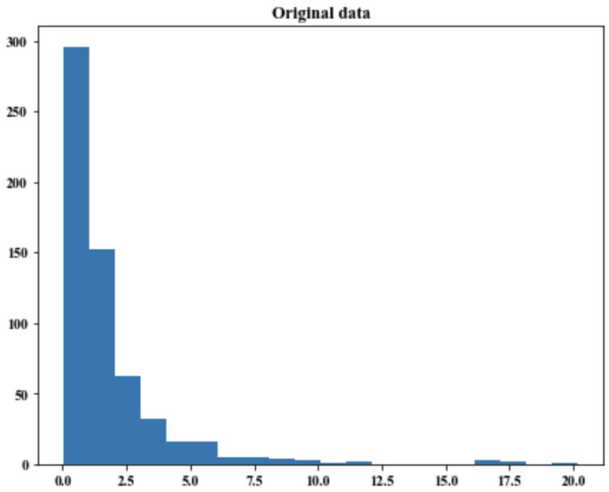
scaling type	use case
min/max normalization	Any -- no assumptions about variables
z-score normalization	When variables follow a normal distribution
log scaling	When variables follow an exponential distribution

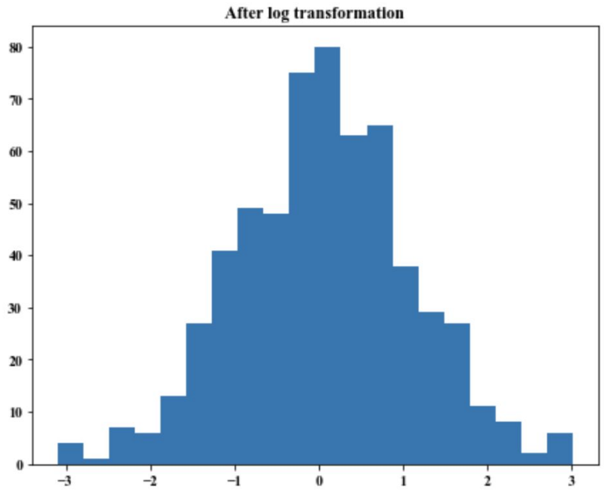
Feature Scaling

- Common Scaling Methods:
  - Min-max Scaler: $\hat{x} = \frac{x - x_{min}}{x_{max} - x_{min}}$
  - Z-score transformation: $\hat{x} = \frac{x - x_{mean}}{\sigma}$
- Which machine learning models require feature scaling?

Log scaling

- Help with skewed data
- Often gives performance gain





Potential Data Leakage

- scaling might lead to **data leakage**
- scaling variables requires “global” statistics

Discretization

- Turning a continuous feature into a discrete feature (quantization)
- Create buckets for different ranges
  - Incorporate knowledge/expertise about each variable by constructing specific buckets
- Examples
  - Income
    - Lower income: x < $35,000
    - Middle income: $35,000 <= x < $100,000
    - High income: x >= $100,000
  - Age
    - Minors: x < 18
    - College: 18 <= x < 22
    - Young adult: 22 <= x < 30
    - 30 <= x < 40
    - 40 <= x < 65
    - Seniors: x >= 65

Encoding Categorical Features

- Example: you want to build a recommendation system for Amazon
  - There are over 2 million brands that we need to recommend
  - It could be used as part of items features
  - Let us try one-hot encoding

Encoding Categorical Features

- one-hot encoding
- How to address unseen brands when the model is deployed

Encoding Categorical Features

- one-hot encoding!
- encode unseen brands with “UNKNOWN”

Did we solve the unseen problem?

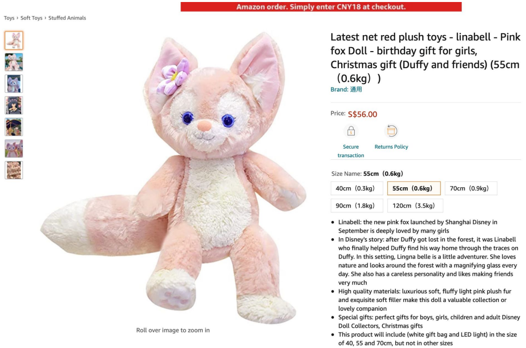
Encoding Categorical Features

- one-hot encoding!
- encode unseen brands with “UNKNOWN”
- Group low frequent 1% of brands and newcomers into “UNKNOWN” category

Did we solve the unseen problem?

Encoding Categorical Features

- one-hot encoding!
- encode unseen brands with “UNKNOWN”
- Group low frequent 1% of brands and newcomers into “UNKNOWN” category
- Problem – this treats all new brands the same as unpopular brands on the platform



What if Disney Linabell come to Amazon as a new brand

Encoding New Categories

1. The question is: how to implement a robust method of handling the potential new brands? (Out of Vocabulary Problems)
2. Two popular methods:
   a. Represent each category with its attribute
      i. For example, to represent a brand, use features: category, yearly revenue, company size, etc..
      ii. The similar trick could be found in BERT to address OOV words.
   b. Hashing Encoder
      i. Using a hash function to hash categories to different indexes
      ii. Suitable for highly cardinality features
      iii. Potential collision issues

More solutions: https://www.kaggle.com/waydeherman/tutorial-categorical-encoding

Feature Crossing

- Combine two or more features to create a new feature

Marriage	Single	Married	Single	Single	Married
Children	0	2	1	0	1
Marriage & children	Single, 0	Married, 2	Single, 1	Single, 0	Married, 1

Feature Crossing

- Helps models learn non-linear relationships between variables
- Warning – feature crossing can blow up your feature space
  - e.g. Feature A and B both have 100 categories → Feature A x B will have 10,000 categories
  - Need even more data to learn this new feature space
  - Blowing up feature space can increase risk of overfitting

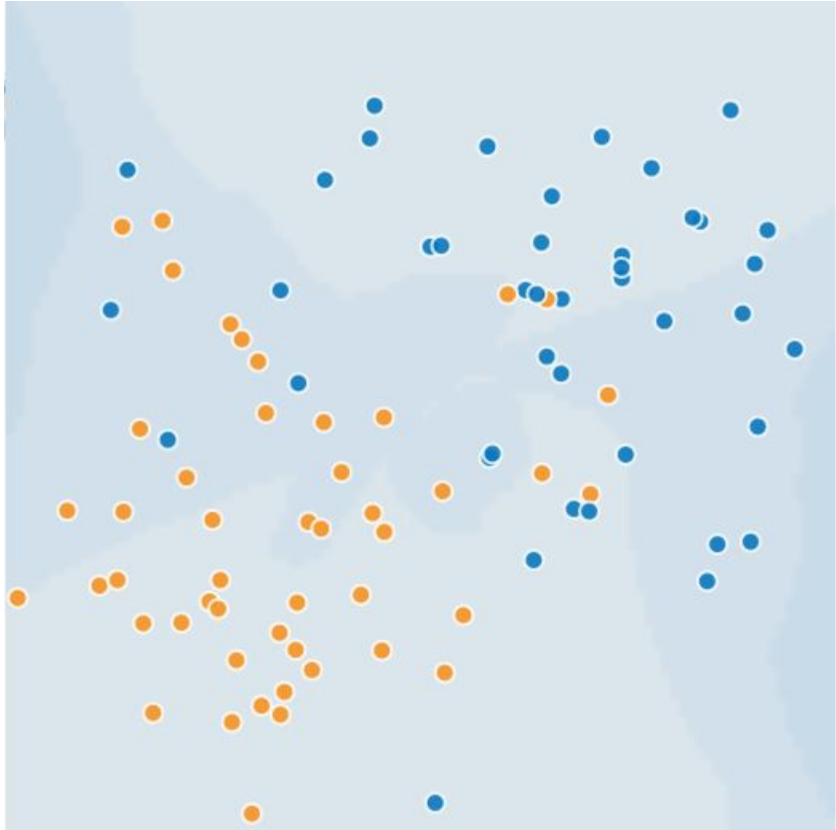
Feature crossing is widely used in recommendation system (CTR prediction)

1. https://ai.googleblog.com/2016/06/wide-deep-learning-better-together-with.html
2. https://www.ijcai.org/proceedings/2017/0239.pdf

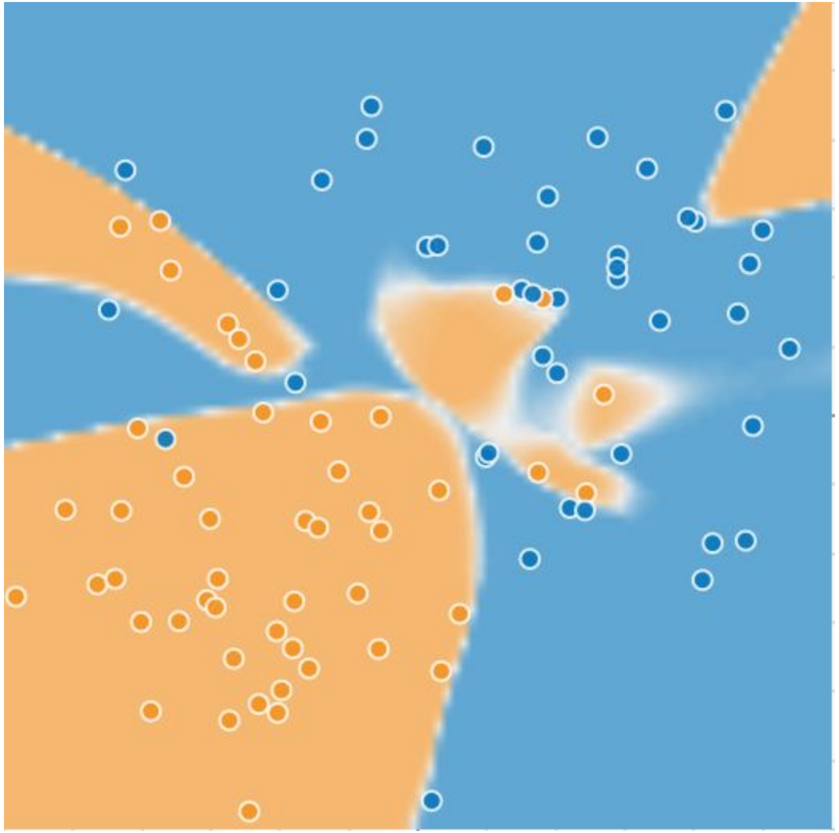
2. Cross-Validation

Which measure should we look for model evaluation?

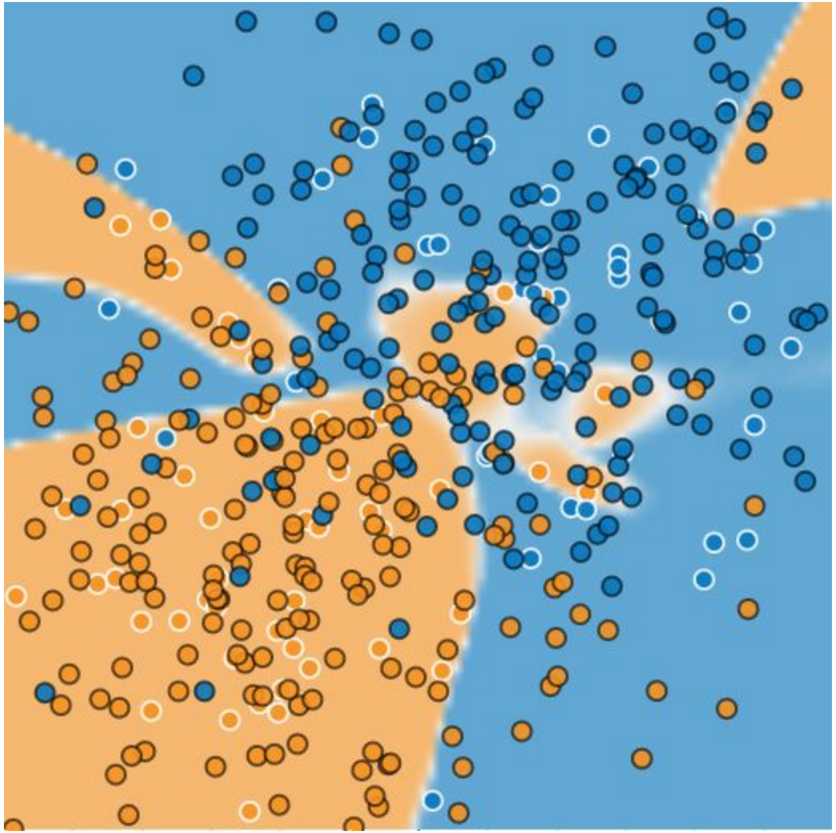
Let’s try to train a model for this problem



How about this model?



More data



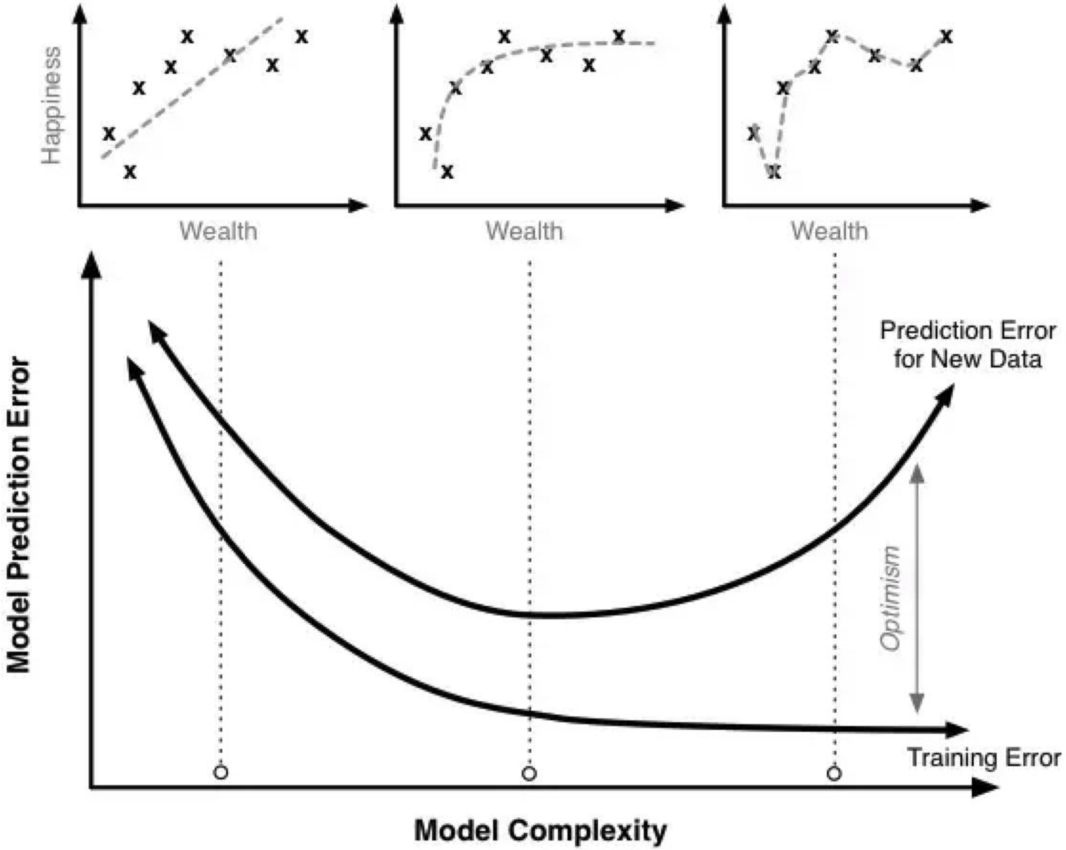
Which measure should we look for model evaluation?

Training performance is not suitable

Generalization

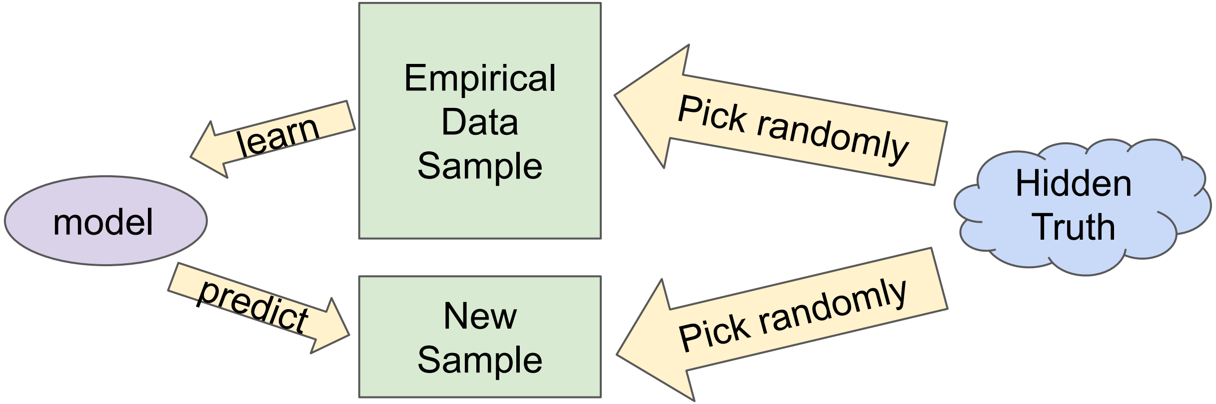
- In ML, a model is used to fit the data
- Once trained, the model is applied upon new data
- Generalization is the prediction capability of the model on live/new data

Model Complexity



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

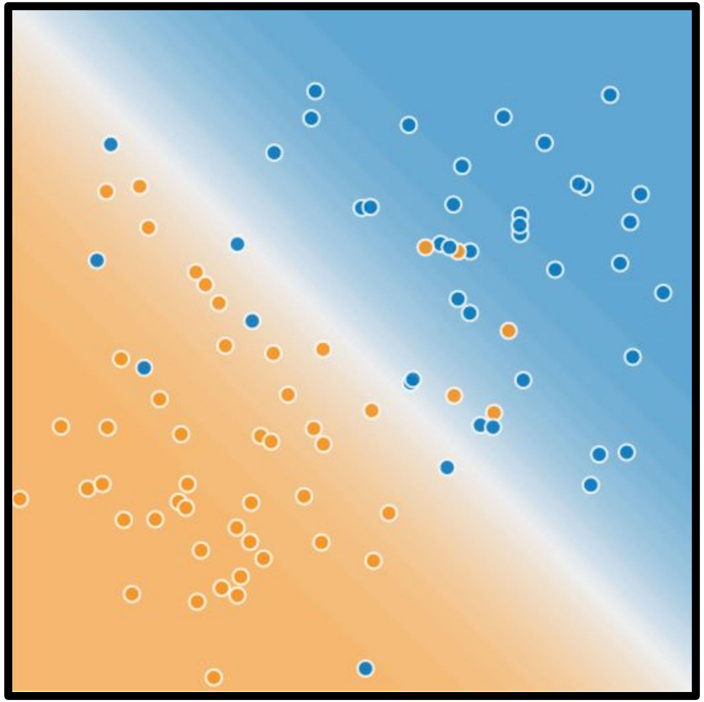
Is the model overfitting?

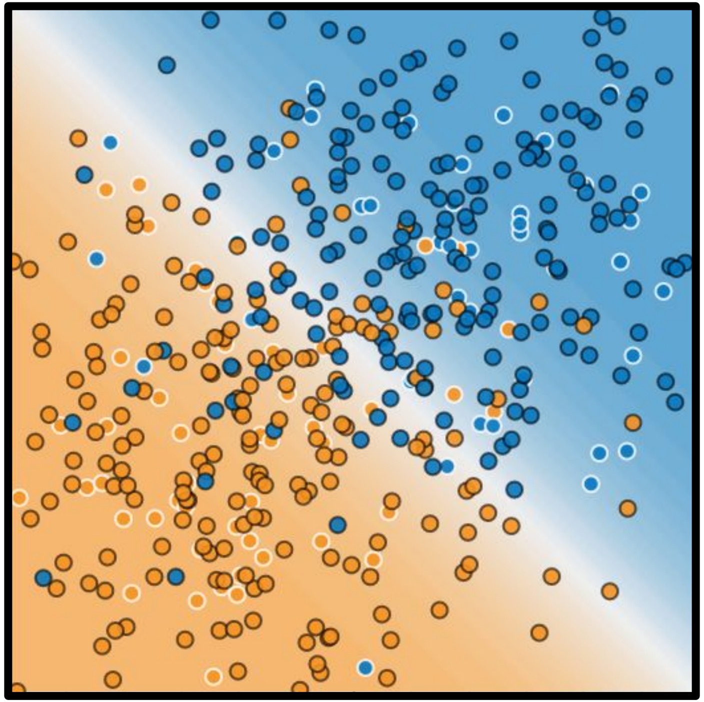
- Empirically:
  - Key point: will our model be good on new samples?
  - Evaluate: get new samples of data (test set)
  - If test set is large enough and we do not cheat by using test set over and over, the good performance on test set can be a useful indicator of model's generalization capability

Training/Test Splitting

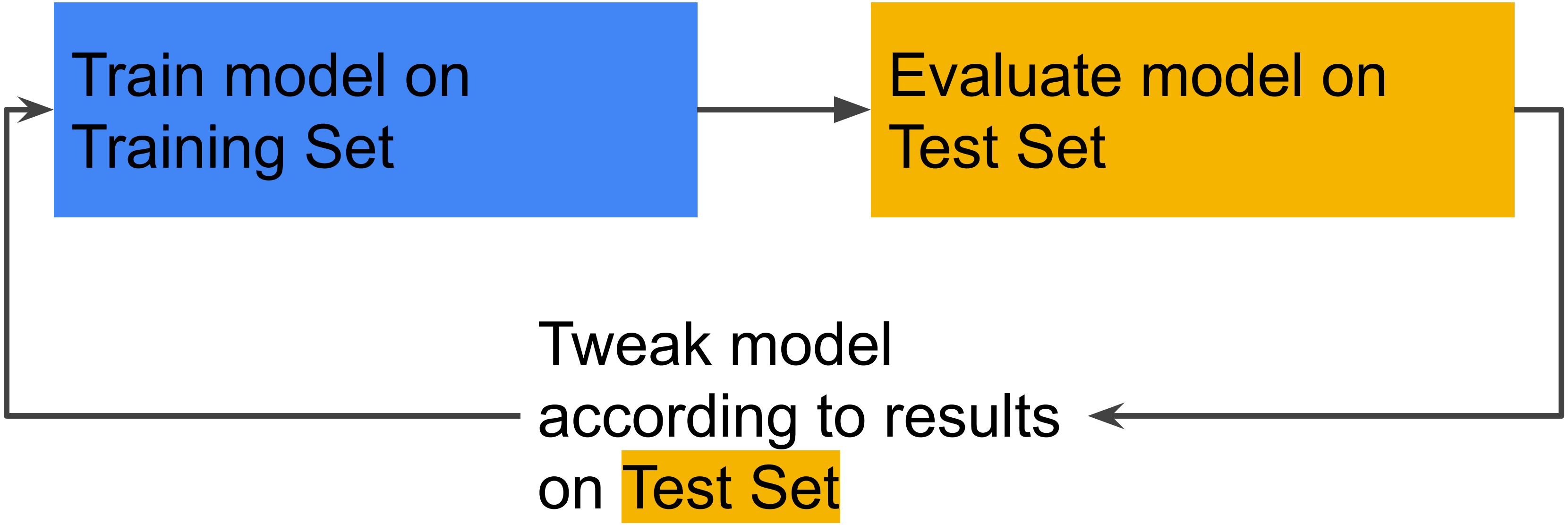
- If models do much better on the training set than the testing set, then models are likely overfitting.
- How do we divide?
  - Randomization for splitting
  - Larger training data size -> better model
  - Larger testing data size -> more confident in model’s evaluation
  - One practical rule: 10-15%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

Training vs Test





How about this workflow?

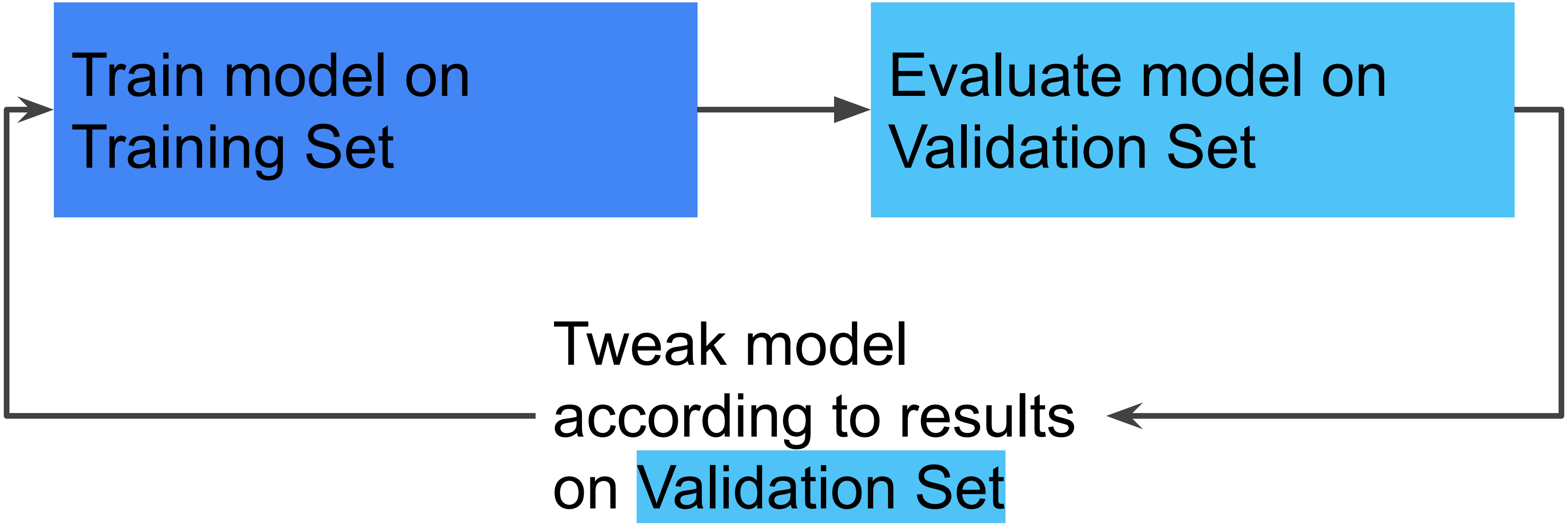


Pick model that does best on Test Set.

Partition Data Sets

Training Set Validation Set Test Set

Better Workflow: Use a validation set



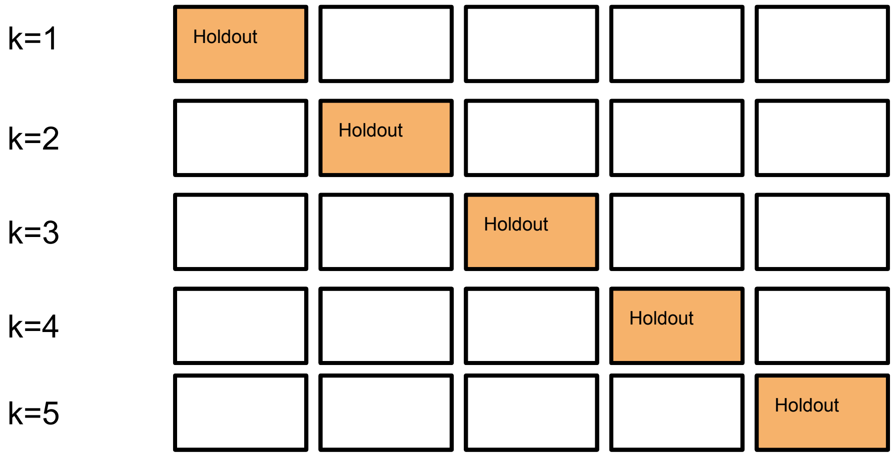
Pick model that does best on Validation Set
Confirm results on Test Set

Cross-Validation

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



CV

- 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.

`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.

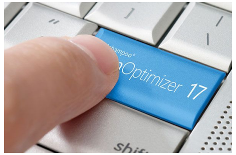
Alpha is the controlling parameter, which is also hyperparameter

3. 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

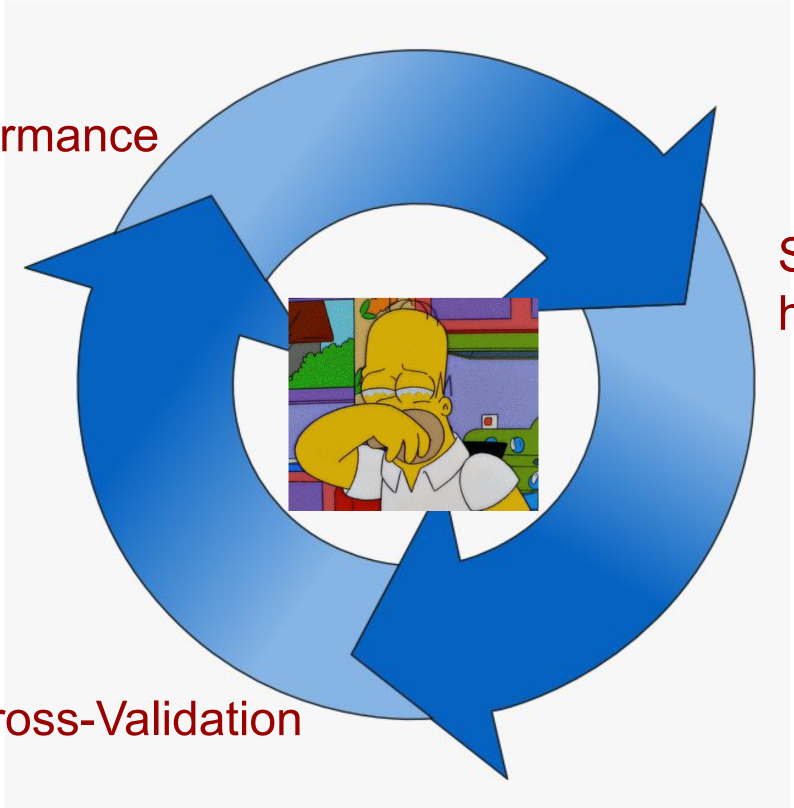
Scores

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()
```

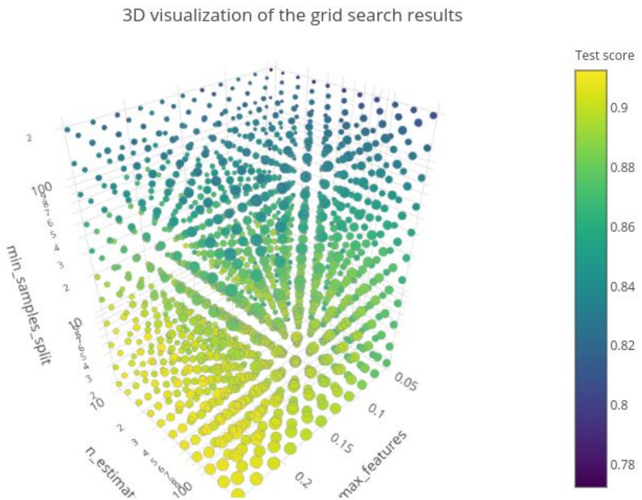
Hyperparameters should be passed when you initialize the machine learning model **before training**

Searching is Iterative, then Expensive



Grid Search

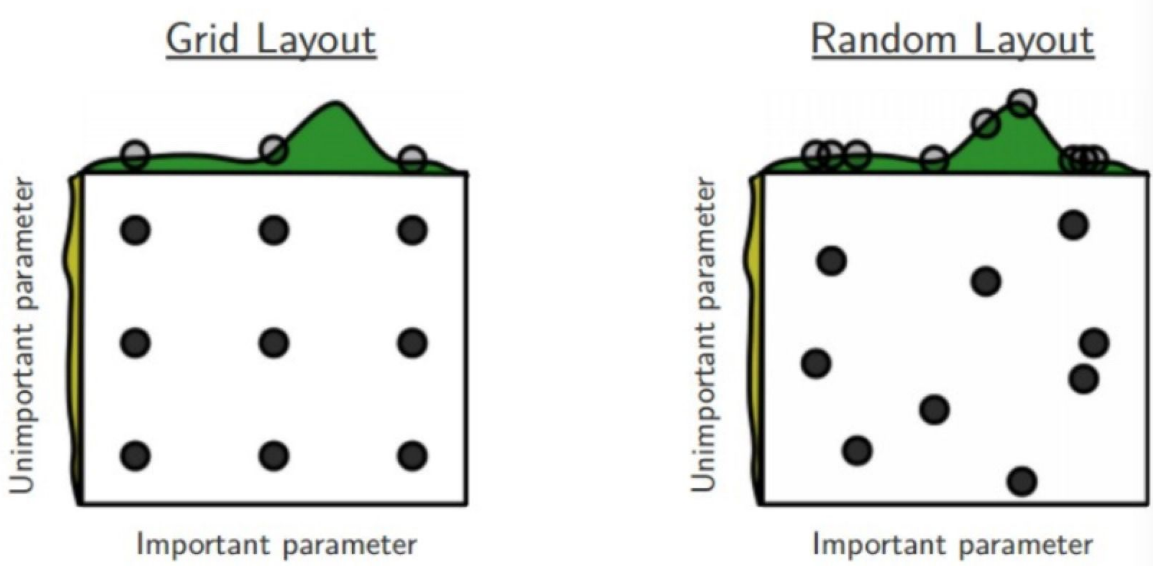
- Define a grid on n-dimensions, where each of these maps for an hyperparameter
- For each dimension, define the range of possible values
- Search for all combinations and select the best one



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

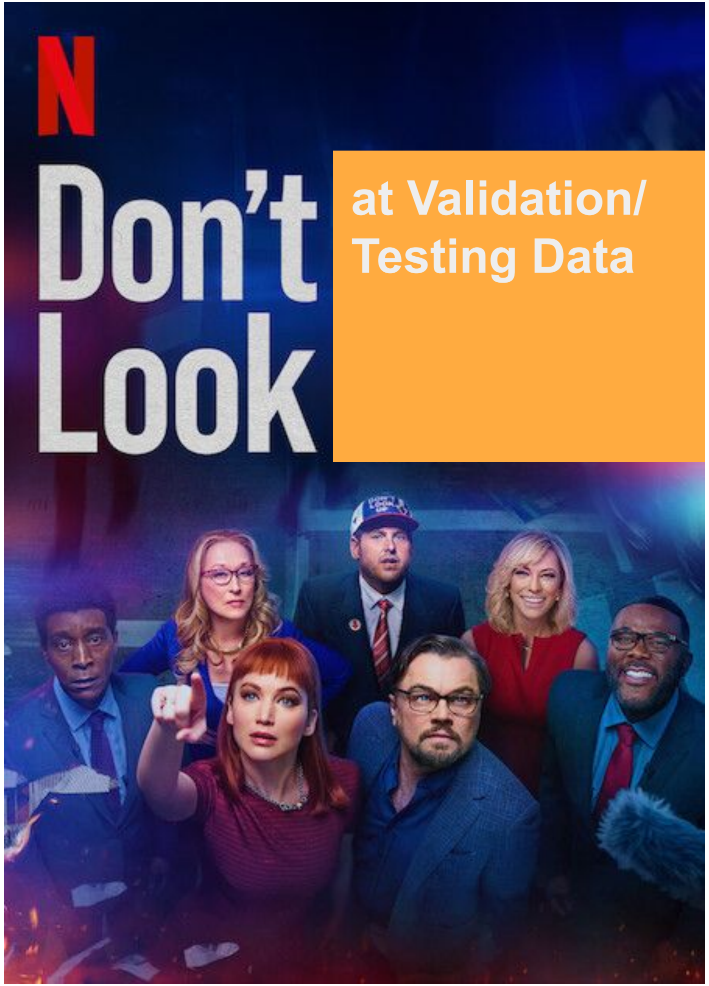
Advanced Search Algorithms

- 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

GCP Implementation:
https://cloud.google.com/blog/products/ai-machine-learning/hyperparameter-tuning-cloud-machine-learning-engine-using-bayesian-optimization

4. Data Leakage



at Validation/
Testing Data

Data Leakage

- Training data leakage
  - Oversampling before splits
    - Training data may overlap with testing data
  - Prepare features on the entire data instead of just training data
    - Create vocab/preprocessing scaler from train+test data
  - Group leakage
    - A patient has 2 CT scans, 1 in train, 1 in test.
- **Feature leakage**
  - Some form of the label “slip” into the features
  - **This same information is not available during inference**

Feature Leakage Example I

- Detect Lung Cancer from CT Scans
- Collected from Hospital I
- Performs well on unseen data from I
- Performs poorly on new data from Hospital II

Date
Doctor note
Medical record
Scanner type
CT scan Image

Feature Leakage Example I

- Detect Lung Cancer from CT Scans
- Collected from Hospital I
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Date
Doctor note
Medical record
Scanner type
CT scan Image

At hospital I, when doctors suspect that a patient has lung cancer, they send that patient to a higher-quality scanner

How to avoid leakage

- Check for duplication between train and valid/test splits
- Use only train splits for feature engineering (model training for sure)
- Train model on subset of features
    - If performance very high on subset, either high quality features or leakage!
- Monitor model performance as more features are added
    - If sudden increase, either high quality features or leakage!
- Check the correlation between feature and label
- Keep asking yourself during model development: can we use this information when the model is deployed for inference?