Introduction to Machine Learning with Scikit-Learn

District Data Labs

These slides are based on:
https://www.slideshare.net/BenjaminBengfort/introduction-to-machine-learning-with-scikitlearn
by Benjamin Bengfort

and
https://www.slideshare.net/gabrielspmoreira/feature-engineering-getting-most-out-of-data-for-predictive-models-tdc-2017
by Gabriel Moreira

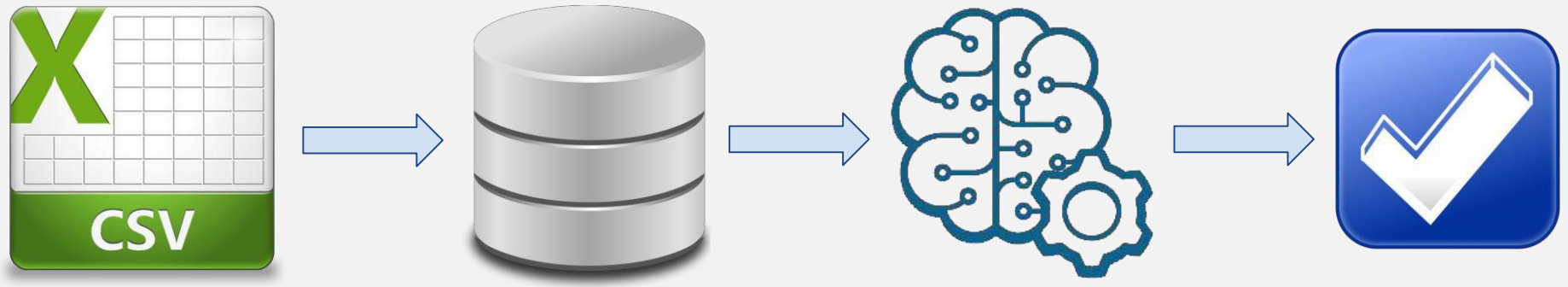
"Feature engineering is the process of transforming raw data into features that better represent the underlying problem to the predictive models, resulting in improved model accuracy on unseen data."

- Jason Brownlee

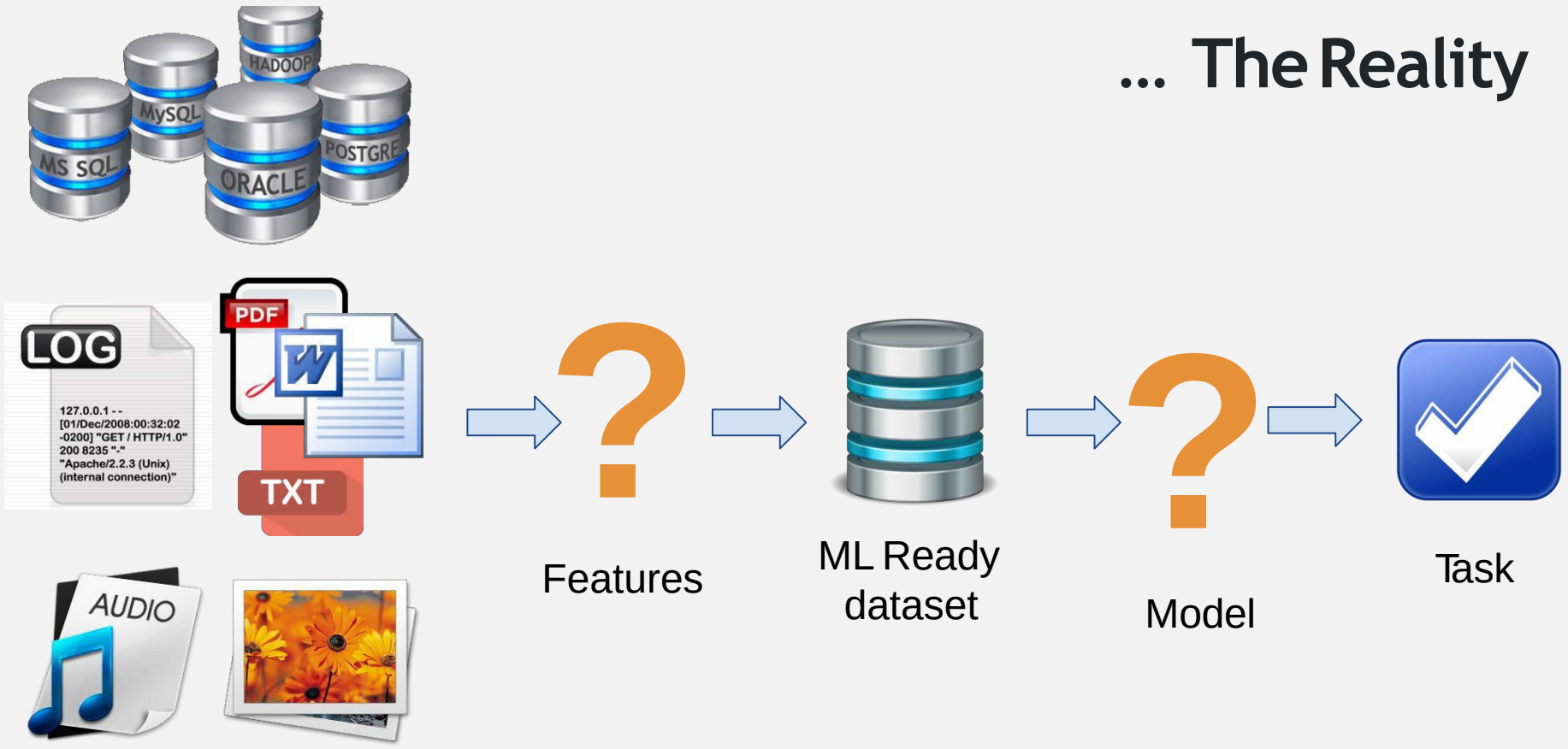
“Coming up with features is difficult,
time-consuming,
requires expert knowledge.
'Applied machine learning' is basically
feature engineering.”

– Andrew Ng

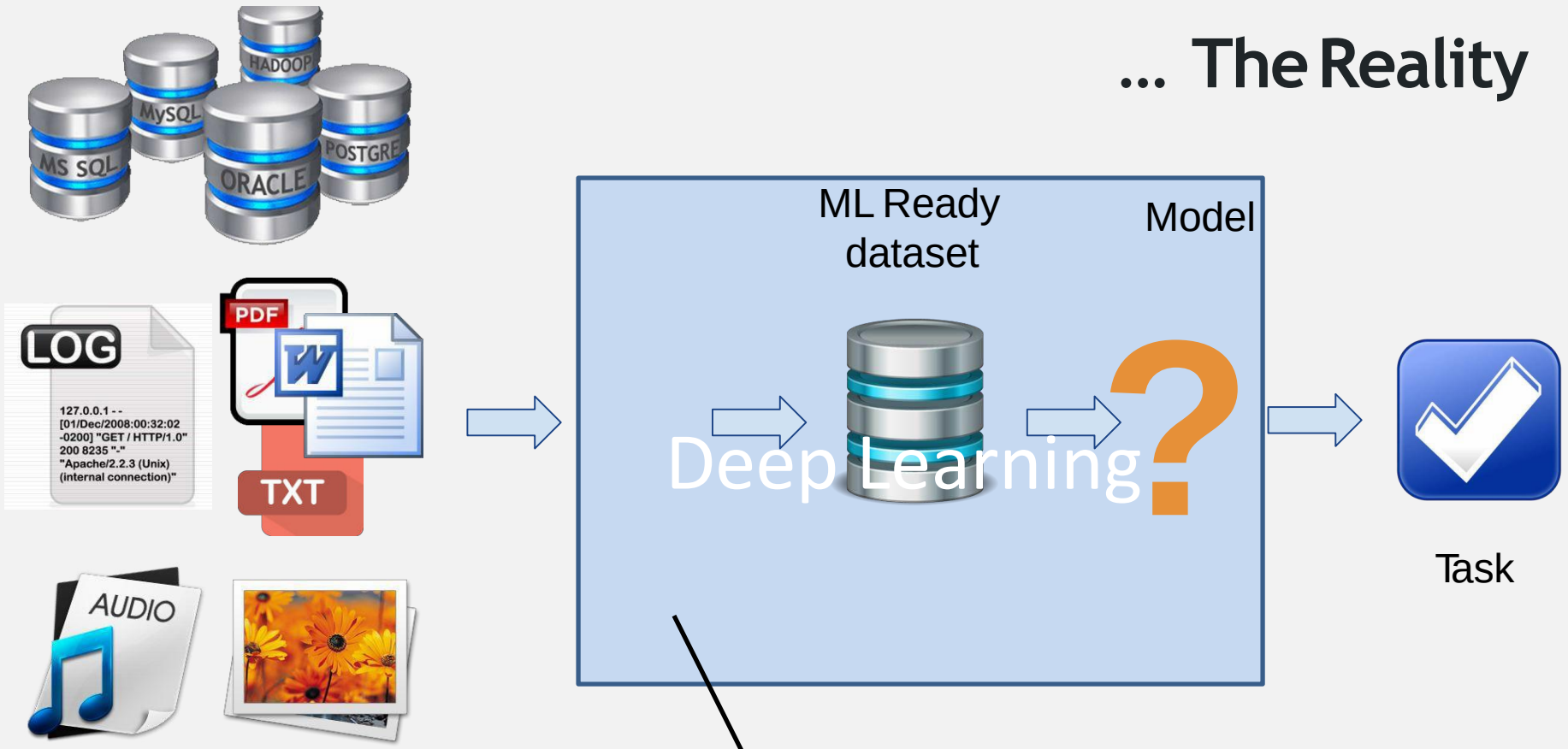
The Dream…



… The Reality


HADOOP
MySQL
MS SQL
ORACLE
POSTGRE
LOG
127.0.0.1 - -
[01/Dec/2008:00:32:02
-0200] "GET / HTTP/1.0"
200 8235 "-"
"Apache/2.2.3 (Unix)
(internal connection)"
PDF
TXT
AUDIO
?
?
Features
ML Ready
dataset
Model
Task
Raw data

… The Reality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TXT
AUDIO
ML Ready
dataset
Model
Deep Learning
?
Task
Raw data
But what architecture?
Scikit-learn can help a lot around here

What is Scikit-Learn?

Extensions to SciPy (Scientific Python) are called SciKits. SciKit-Learn provides machine learning algorithms and much more.

- Algorithms for supervised & unsupervised learning
- Built on SciPy and Numpy
- Standard Python API interface
- Sits on top of c libraries, LAPACK, LibSVM, and Cython
- Open Source: BSD License (part of Linux)

Probably the best general ML framework out there.

More on scikit-learn

- Data loading and pre-processing
- Feature engineering
- Hyperparameter tuning and Model evaluation
- Pipelines

Data Loading and pre-processing

- **Data Preparation / pre-processing** (this is where the magic comes☺) [scikit-learn (numpy, Pandas)]
  Data cleaning, inputs for missing values, features normalization, outliers detection
  Features augumentation / selection / construction / reduction
  - Transformers (fit -> transform)
  - https://scikit-learn.org/stable/modules/impute.html (deal with missing values)
  - https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.Normalizer.html (features/objects => axis=1/0)
  - https://scikit-learn.org/stable/modules/generated/sklearn.decomposition.PCA.html (too many correlated features)
  - https://scikit-learn.org/stable/modules/feature_extraction.html (transform feature space, e.g., numeric -> Binary)
  - https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.PolynomialFeatures.html (feature combinations)
  - https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.quantile_transform.html (transform to cum. distribution)
- **Exploration (iterates with pre-processing)** [scikit-learn / matplotlib / Seaborn…]
  Get some insights on the data, understand its structure, create initial hypothesis
  Clustering algorithms, histograms, plots, correlation…
  https://scikit-learn.org/stable/modules/clustering.html -> Agglomerative clustering
  https://seaborn.pydata.org/generated/seaborn.heatmap.html
  https://seaborn.pydata.org/generated/seaborn.pairplot.html
  https://seaborn.pydata.org/generated/seaborn.FacetGrid.html
  ...

Visualization (matplotlib, seaborn,...)

Data pre-processing and transformation

- Inputing for NaNs
- Normalization / standardization
- Transform nominals
- Transform numeric
- Data Aggregation
- Feature extraction / combination

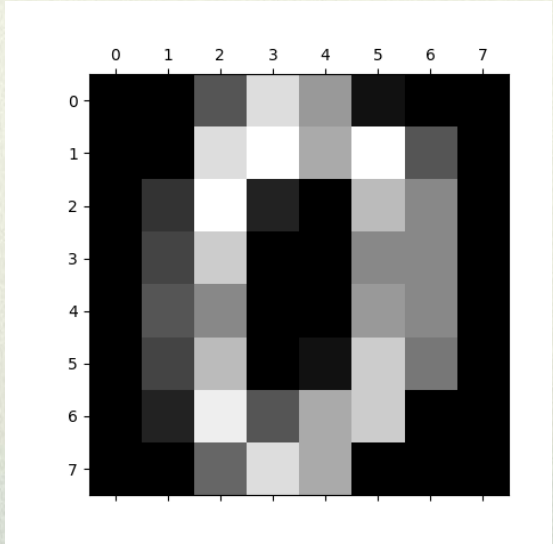
Mostly Transformer design patterns

- Fit on train data
- Transform both train and test data

Load dataset

- sklearn.datasets
  - Some „toy examples“ ready to use
    - datasets.load_iris()
    - datasets.load_wine()
  - Generate artificial data

```
>>> from sklearn.datasets import load_digits
>>> digits = load_digits()
>>> digits.data.shape
(1797, 64)
>>> digits.target_names
[0 1 2 3 4 5 6 7 8 9]
>>> import matplotlib.pyplot as plt
>>> plt.gray()
>>> plt.matshow(digits.images[0])
>>> plt.show()
```



Imputation for missing values

- Datasets contain missing values, often encoded as blanks, NaNs or other placeholders
- Ignoring rows and/or columns with missing values is possible, but at the price of loosing data which might be valuable
- Better strategy is to infer them from the known part of data
- Strategies
  - **Mean**: Basic approach
  - **Median**: More robust to outliers
  - **Mode**: Most frequent value
  - **Using a model**: Can expose algorithmic bias

Imputation for missing values

```
>>> import numpy as np
>>> from sklearn.preprocessing import Imputer
>>> imp = Imputer(missing_values='NaN', strategy='mean', axis=0)
>>> imp.fit([[1, 2], [np.nan, 3], [7, 6]])
Imputer(axis=0, copy=True, missing_values='NaN', strategy='mean',
verbose=0)
>>> X = [[np.nan, 2], [6, np.nan], [7, 6]]
>>> print(imp.transform(X))
[[ 4.          2.        ]
 [ 6.          3.666...]
 [ 7.          6.        ]]
```

Missing values imputation with scikit-learn

Binarization

- Transform discrete or continuous numeric features in binary features

  Example: Number of user views of the same document

document_id	uuid	views_count
25792	6d82e412aa0f0d	8
25792	571016386ffee7	6
25792	6a91157d820e37	6
25792	ad45fc764587b0	6
25792	a743b03f2b8ddc	3

document_id	uuid	viewed
25792	6d82e412aa0f0d	1
25792	571016386ffee7	1
25792	6a91157d820e37	1
25792	ad45fc764587b0	1
25792	8d87becfb35857	1
25792	abcdefg1234567	0

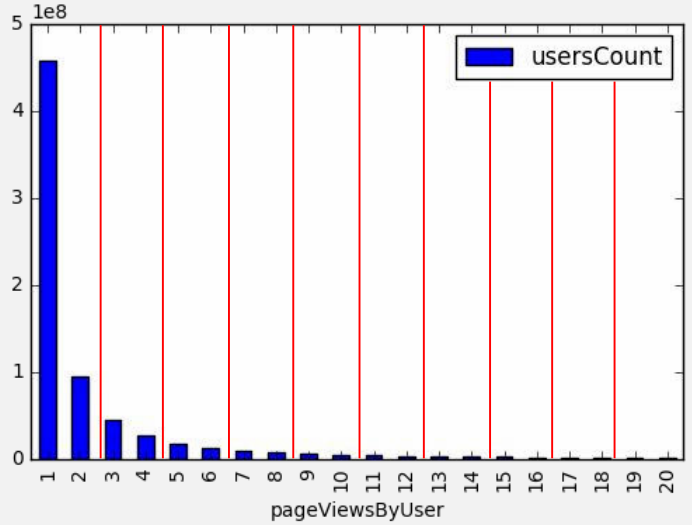
```
>>> from sklearn import preprocessing
>>> X = [[ 1., -1.,  2.],
...      [ 2.,  0.,  0.],
...      [ 0.,  1., -1.]]

>>> binarizer =
preprocessing.Binarizer(threshold=1.0)
>>> binarizer.transform(X)
array([[ 1., 0.,  1.],
       [ 1., 0.,  0.],
       [ 0., 1.,  0.]])
```

Binarization with scikit-learn

Binning

- Split numerical values into bins and encode with a bin ID
- Can be set arbitrarily or based on distribution
- **Fixed-width binning**

Does fixed-width binning make sense for this long-tailed distribution?




```
>>> x = np.array([0.2, 6.4, 3.0, 1.6])
>>> bins = np.array([0.0, 1.0, 2.5, 4.0, 10.0])
>>> inds = np.digitize(x, bins)
>>> inds
array([1, 4, 3, 2])
```

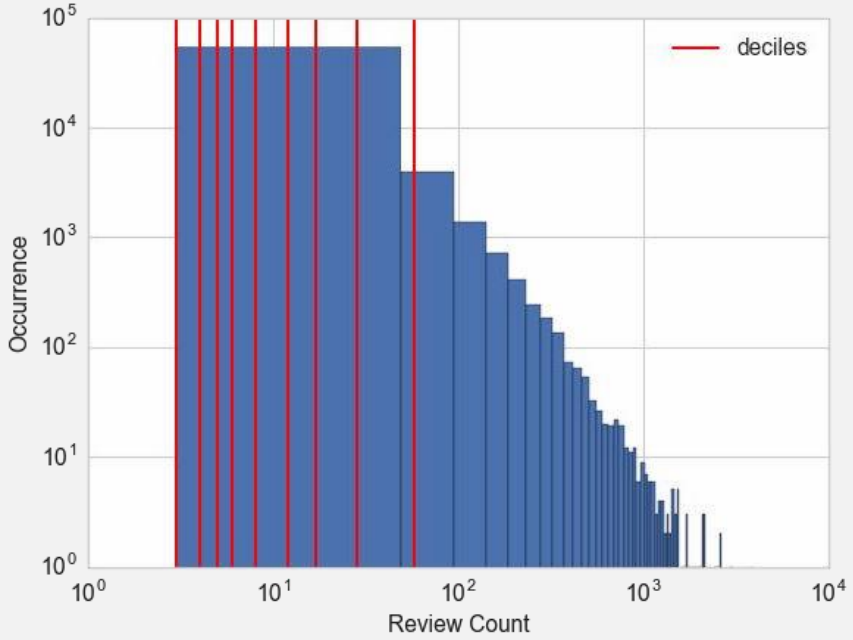
Most users (458,234,809 ~ 5*10^8) had only 1 pageview during the period.

numpy.digitize

Binning

- **Adaptative or Quantile binning**

  Divides data into equal portions (eg. by median, quartiles, deciles)




```
>>> deciles = dataframe['review_count'].quantile([.1, .2, .3, .4, .5, .6, .7,
.8, .9])
>>> deciles
0.1     3.0
0.2     4.0
0.3     5.0
0.4     6.0
0.5     8.0
0.6    12.0
0.7    17.0
0.8    28.0
0.9    58.0
```

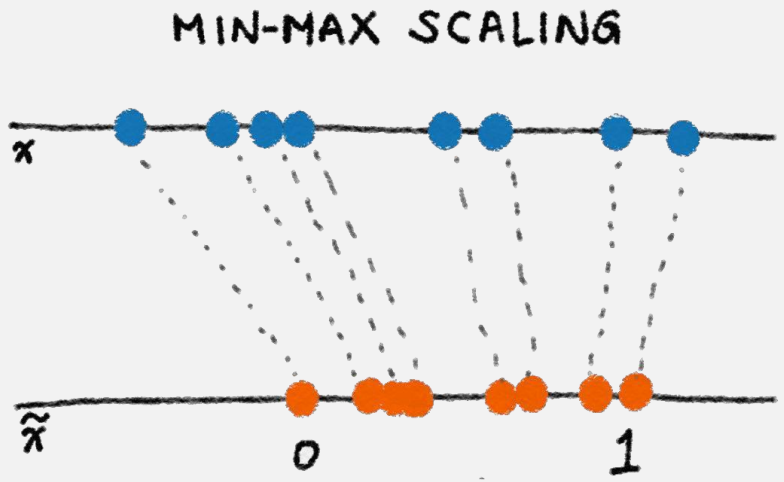
Quantile binning with Pandas

Scaling

- Models that are smooth functions of input features (or utilize similarity) are sensitive to the scale of the input (eg. Linear Regression, KNN)
- Scale numerical variables into a certain range, dividing values by a normalization constant (no changes in single-feature distribution)
- Popular techniques
  - MinMax Scaling
  - Standard (Z) Scaling
  - L2 normalization

Min-max scaling

- Squeezes (or stretches) all values within the range of [0, 1] to add robustness to very small standard deviations and preserving zeros for sparse data.



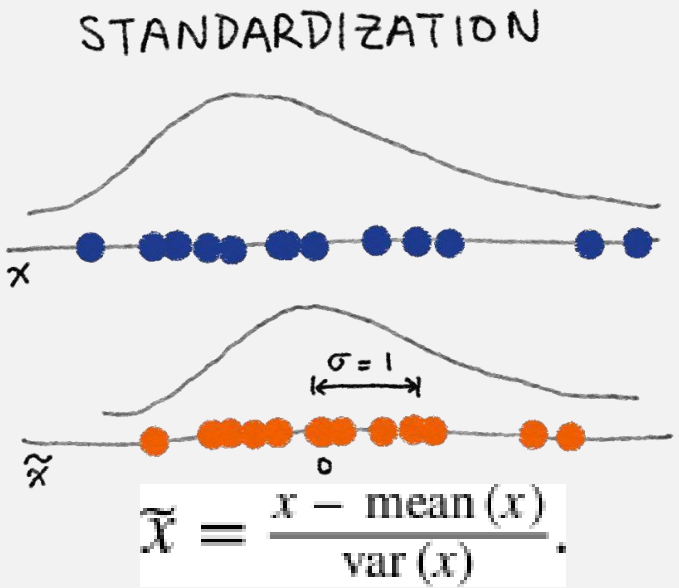
$$\tilde{x} = \frac{x - \min(x)}{\max(x) - \min(x)}$$

```
>>> from sklearn import preprocessing
>>> X_train = np.array([[ 1., -1.,  2.],
...                     [ 2.,  0.,  0.],
...                     [ 0., 1., -1.]])
...
>>> min_max_scaler =
preprocessing.MinMaxScaler()
>>> X_train_minmax =
min_max_scaler.fit_transform(X_train)
>>> X_train_minmax
array([[ 0.5       ,  0.        ,  1.        ],
       [ 1.        ,  0.5       ,  0.33333333],
       [ 0.        ,  1.        ,  0.        ]])
```

Min-max scaling with scikit-learn

Standard (Z) Scaling

After Standardization, a feature has mean of 0 and variance of 1 (assumption of many learning algorithms)



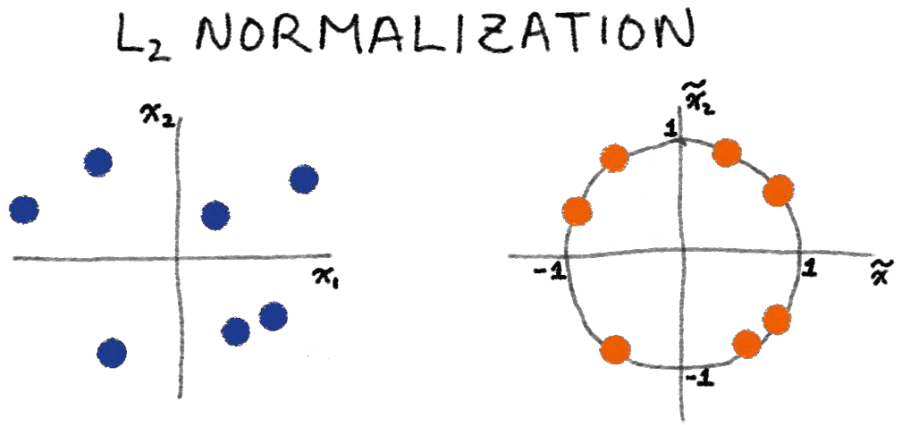
$$\tilde{x} = \frac{x - \text{mean}(x)}{\text{var}(x)}.$$

```
>>> from sklearn import preprocessing
>>> import numpy as np
>>> X = np.array([[ 1., -1.,  2.],
...               [ 2.,  0.,  0.],
...               [ 0., 1., -1.]])
>>> X_scaled = preprocessing.scale(X)
>>> X_scaled
array([[ 0.  ..., -1.22...,  1.33...],
       [ 1.22...,  0.  ..., -0.26...],
       [-1.22..., 1.22..., -1.06...]])
>> X_scaled.mean(axis=0)
array([ 0., 0.,  0.])
>>> X_scaled.std(axis=0)
array([ 1., 1.,  1.])
```

Standardization with scikit-learn

Normalization

- Scales individual samples (rows) to have unit vector, dividing values by vector's L^2 norm, a.k.a. the Euclidean norm
- Useful for quadratic form (like dot-product) or any other kernel to quantify similarity of pairs of samples. This assumption is the base of the **Vector Space Model** often used in **text classification and clustering** contexts



$$\tilde{x} = \frac{x}{\| x \|_2}.$$

Normalized vector

$$\| x \|_2 = \sqrt{x_1^2 + x_2^2 + \ldots + x_m^2}$$

Euclidean (L^2) norm

Normalization

```
>>> from sklearn import preprocessing
>>> X = [[ 1., -1.,  2.],
...      [ 2.,  0.,  0.],
...      [ 0.,  1., -1.]]
>>> X_normalized = preprocessing.normalize(X, norm='l2')
>>> X_normalized
array([[ 0.40..., -0.40...,  0.81...],
       [ 1.  ...,  0.  ...,  0.  ...],
       [ 0.  ...,  0.70..., -0.70...]])
```

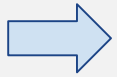
Normalization with scikit-learn

Log transformation

Compresses the range of large numbers and expand the range of small numbers.

Eg. The larger x is, the slower log(x) increments.

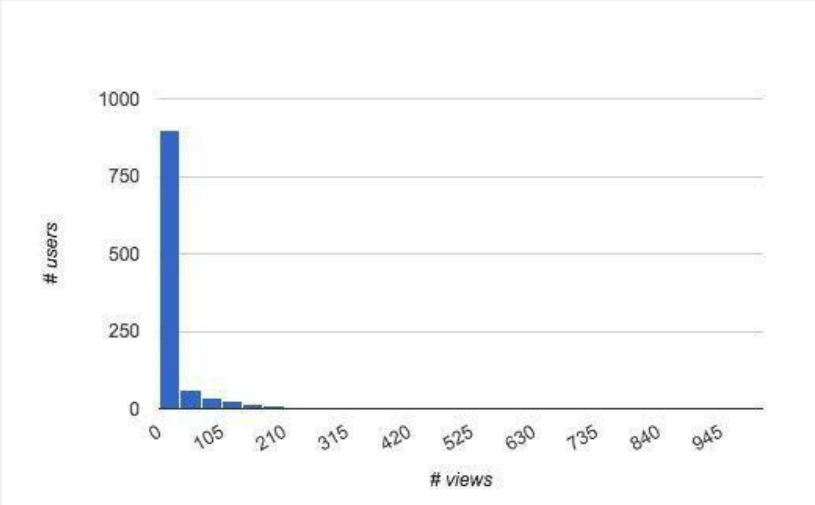
user_id	views_count
a	1000
b	500
c	300
d	200
e	150
f	100
g	70
h	50
i	30
j	20
k	10
l	5
m	1

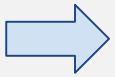


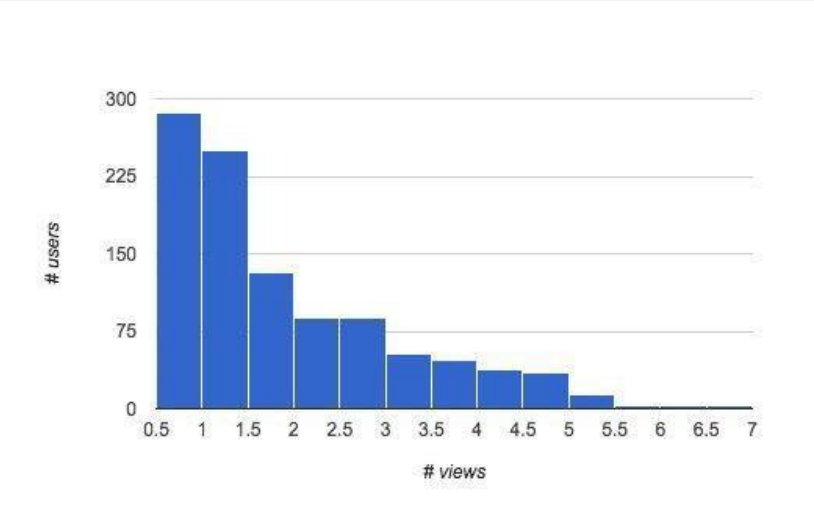
log(1+views_count)
6.91
6.22
5.71
5.30
5.02
4.62
4.26
3.93
3.43
3.04
2.40
1.79
0.69

Log transformation

Smoothing long-tailed data with log







Histogram of # views by user

Histogram of # views by user smoothed by log(1+x)

Feature extraction

Interaction Features

$$(X_1, X_2) \Longrightarrow (1, X_1, X_2, X_1^2, X_1X_2, X_2^2)$$

```
>>> import numpy as np
>>> from sklearn.preprocessing import PolynomialFeatures
>>> X = np.arange(6).reshape(3, 2)
>>> X
array([[0, 1],
       [2, 3],
       [4, 5]])
>>> poly = poly = PolynomialFeatures(degree=2, interaction_only=False,
include_bias=True)
>>> poly.fit_transform(X)
array([[  1.,   0.,   1.,   0.,   0.,   1.],
       [  1.,   2.,   3.,   4.,   6.,   9.],
       [  1.,   4.,   5.,  16.,  20.,  25.]])
```

Polynomial features with scikit-learn

One-Hot Encoding (OHE)

- Transform a categorical feature with *m* possible values into *m* binary features.
- If the variable cannot be multiple categories at once, then only one bit in the group can be on.

platform
desktop
mobile
tablet

platform=desktop	platform=mobile	platform=tablet
1	0	0
0	1	0
0	0	1

- Sparse format is memory-friendly
- sklearn.feature_extraction.DictVectorizer

Large Categorical Variables

- Common in applications like targeted advertising and fraud detection
- Example:

categorical_feature	unique_values
landing_page_document_id	636482
ad_id	418295
ad_document_id	143856
content_entities	52439
advertiser	2052
publisher	830
country_state	1892

Some large categorical features from Outbrain Click Prediction competition

Feature hashing

- Hashes categorical values into vectors with fixed-length.
- Lower sparsity and higher compression compared to OHE
- Deals with new and rare categorical values (eg: new user-agents)
- May introduce collisions

country
brazil
chile
venezuela
colombia
... 222 countries

100 hashed columns

country_hashed_1	country_hashed_2	country_hashed_3	country_hashed_4	...
1	0	0	0	...
0	0	0	1	...
0	0	1	0	...
0	0	1	0	...
...	...	...	...	...

https://scikit-learn.org/stable/modules/generated/sklearn.feature_extraction.FeatureHasher.html

Bin-counting

- Instead of using the actual categorical value, use a global statistic of this category on historical data.
- Useful for both linear and non-linear algorithms
- May give collisions (same encoding for different categories)
- Be careful about leakage
- Strategies
  - Count
  - Average CTR

Bin-counting

ad_id
423654
123646
68655
54345

ad_views		ad_clicks		ad_CTR
18339	or	1355	or	0.074
335		12		0.036
1244		132		0.106
35387		1244		0.035

Counts

Click-Through Rate

P(click | ad) = ad_clicks / ad_views

Textual features

- sklearn.feature_extraction.text
- Count, Tf-IDF,

Image features

- sklearn.feature_extraction.image
- Patches, img to graph,…

Feature selection

Feature selection

- Decrease complexity of model
- Remove redundant and irrelevant features

https://scikit-learn.org/stable/modules/feature_selection.html

- sklearn.feature_selection.SelectKBest
  - Scoring function
  - K features
  - Threshold
  - …

Data exploration (Exploratory data analysis, EDA)

- Get the knowledge about your data
  - What does the data model look like?
  - What is the features distribution?
  - What are the features with missing or inconsistent values?
  - What are the most predictive features?

Exploratory Data Analysis (EDA)

- Get the knowledge about your data

  - get a basic description of the data
  - visualize it
  - identify patterns in it
  - identify challenges of using the data
  - form hypothesis about the data
  - …

Exploratory Data Analysis (EDA)

Basic knowledge

-Describe data (quantiles, med, mean, max, min…)

- *head(), tail()*
- *Pd.Query(), sorting,*

Challenges

-NaNs, outliers, numeric -> nominal and vice versa

Patterns

- correlation, covariation, linear dependence, clusters, dimensionality reduction…

Visualization

- boxpolots, histograms, cummulative distribution, pairplots, scatter plots, corr matrices, …

Patterns

https://pandas.pydata.org/pandas-docs/stable/reference/api/pandas.DataFrame.corr.html
- Pairwise correlation for dataframe columns

https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LinearRegression.html
- Linear regression (Estimator class, fit and predict methods)

https://scikit-learn.org/stable/modules/clustering.html
- Several variants of clustering, perhaps hierarchical one would be most appropriate

https://scikit-learn.org/stable/modules/generated/sklearn.decomposition.PCA.html
- Linear dimensionality reduction (are my features correlated?)

Visualization

Matplotlib
- Basics

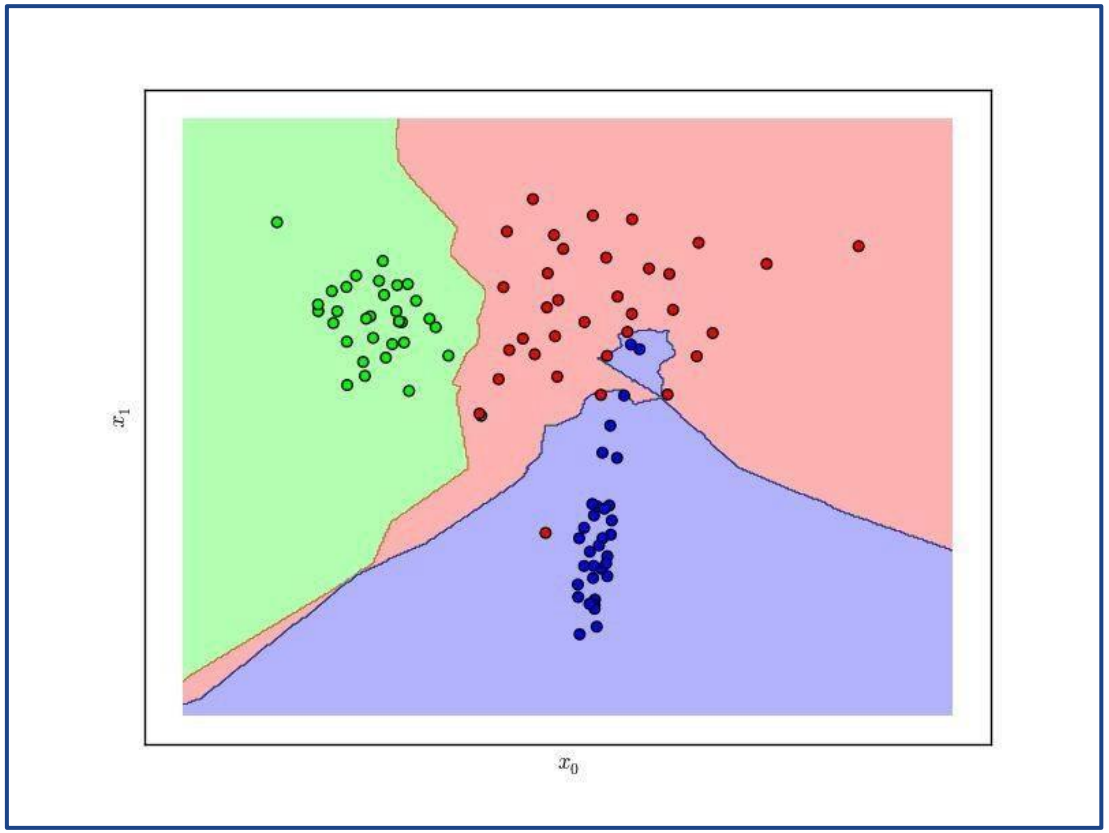
Seaborn
- Extends over matplotlib (compatible calls)
- Easier processing
- Nicer graphs by default
- Several additional graph types (pairplot, facetedGrid) especially useful
- https://www.slideshare.net/nishantupadhyaysbi/python-seaborn-cheatsheet

Matplotlib slides follows
More reading:
https://elitedatascience.com/python-seaborn-tutorial
https://seaborn.pydata.org/examples/index.html

Supervised ML algorithms

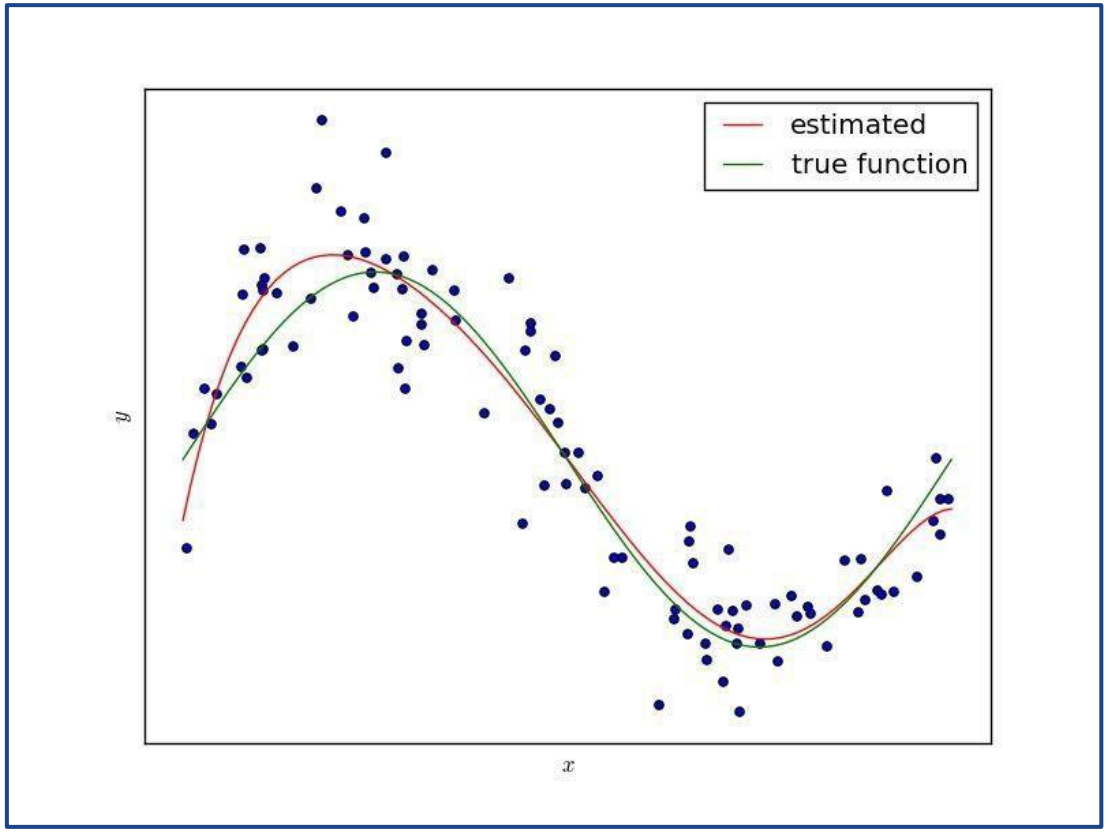
(just the very basics now, more later)

Classification



Given labeled input data (with two or more labels), fit a function that can determine for any input, what the label is.

Regression



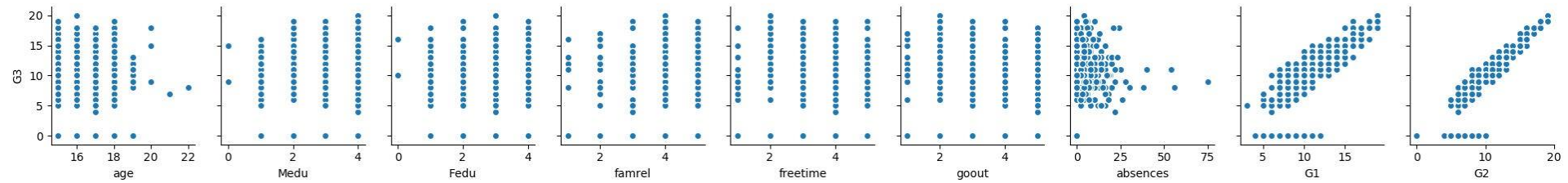
Given continuous input data fit a function that is able to predict the continuous value of input given other data.

K-nearest neighbors

Linear regression

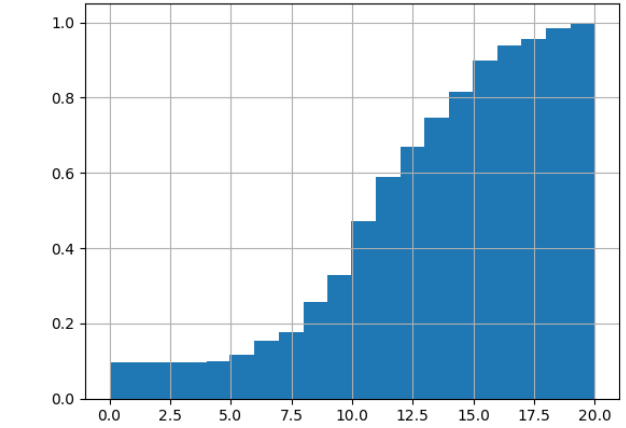
Exploratory Data Analysis (EDA) - pairplot

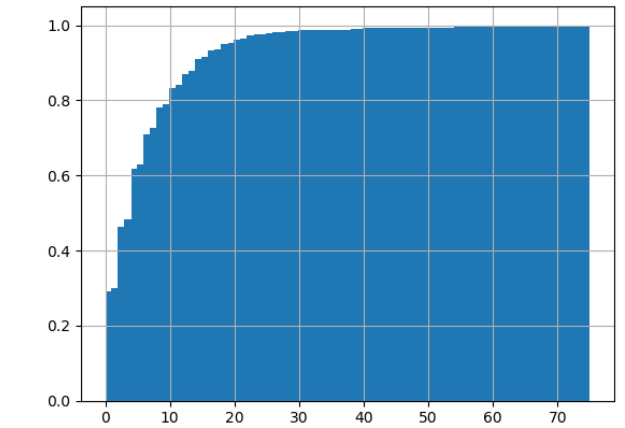
```
import pandas as pd
import seaborn as sns #statistical data visualization, based on matplotlib
import matplotlib.pyplot as plt

df = pd.read_csv("C:/Users/peska/Documents/uceni/2017_2018/NPRG065/cviceni/student-mat.csv", delimiter=";")

sns.pairplot(data=df,
                x_vars= ["age","Medu","Fedu","famrel","freetime","goout","absences","G1","G2"],
                y_vars= ['G3'])
plt.show()
```



Exploratory Data Analysis (EDA) - CDF

```
import pandas as pd
import matplotlib.pyplot as plt

df = pd.read_csv("C:/Users/peska/Documents/uceni/2017_2018/NPRG065/cviceni/student-mat.csv", delimiter=";")


df.G3.hist(cumulative=True, normed=1, bins=len(df.G3))
#df.absences.hist(cumulative=True, normed=1, bins=len(df.absences))
plt.show()
```

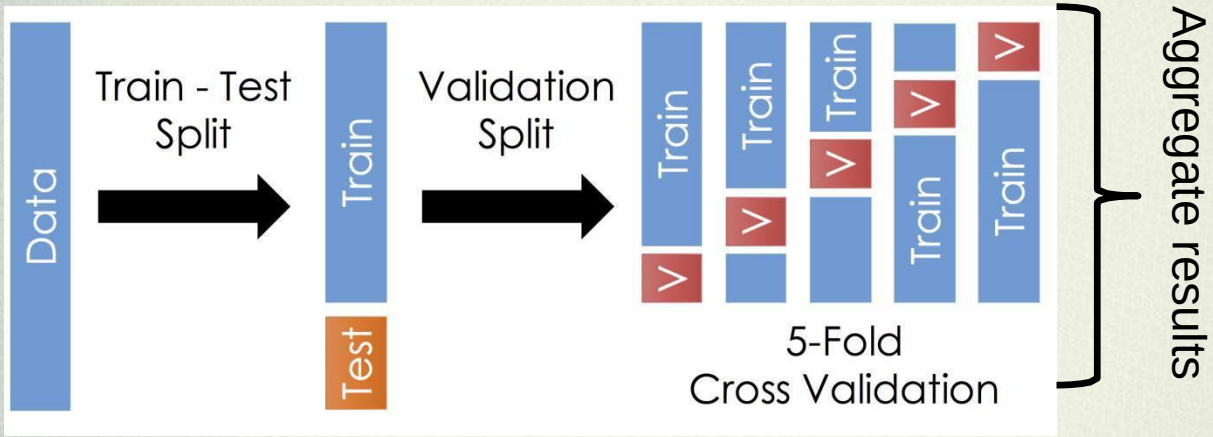




Model Fitting & Evaluation

Model Fitting Protocol

How to learn model's hyperparameters: grid search & cross-validation



Instead of Train – Test split, you may use additional „outer" cross-validation

Get results from all parts of the dataset

Never use any knowledge of the test set data

E.g. For mean ratings, object similarities etc

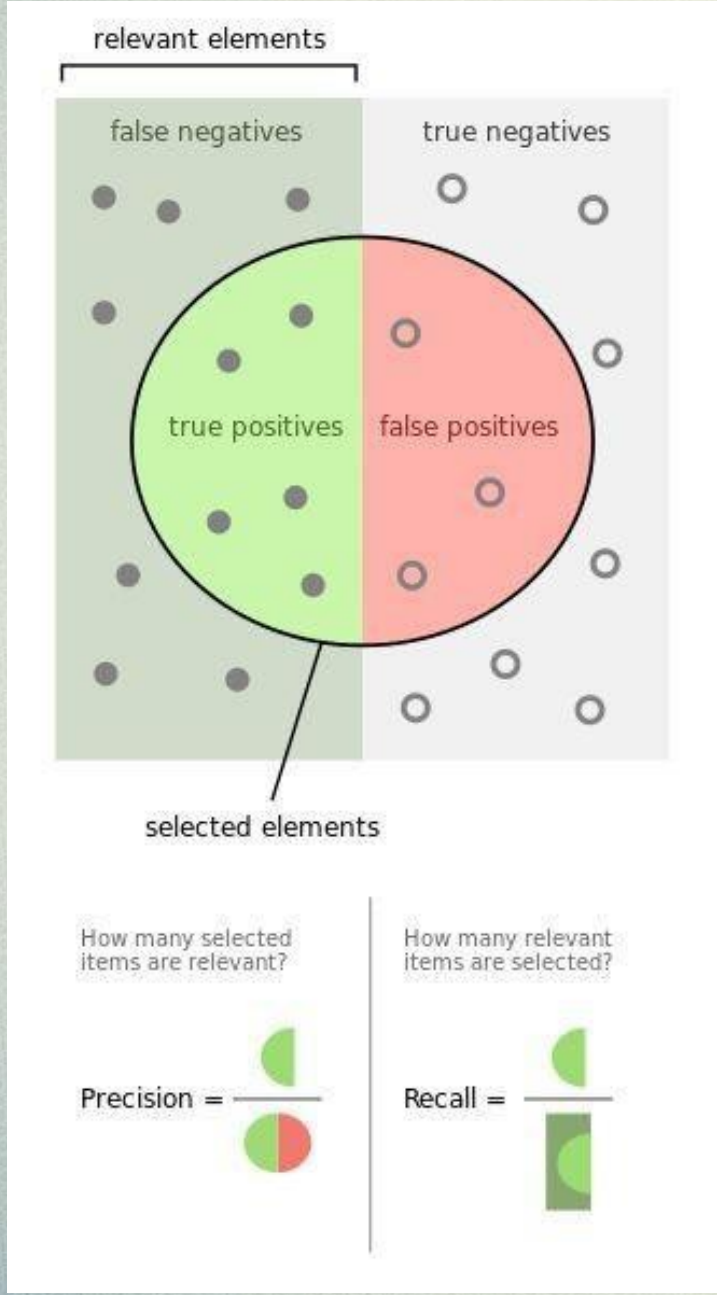
Model Fitting Protocol

Further variants:

- Monte-Carlo cross validation:
  - random splits, arbitrary size (cold start problems)

- Bootstrap validation:
  -only one split (if you have abundant data)

-Temporal splits:
  -if domain changes over time



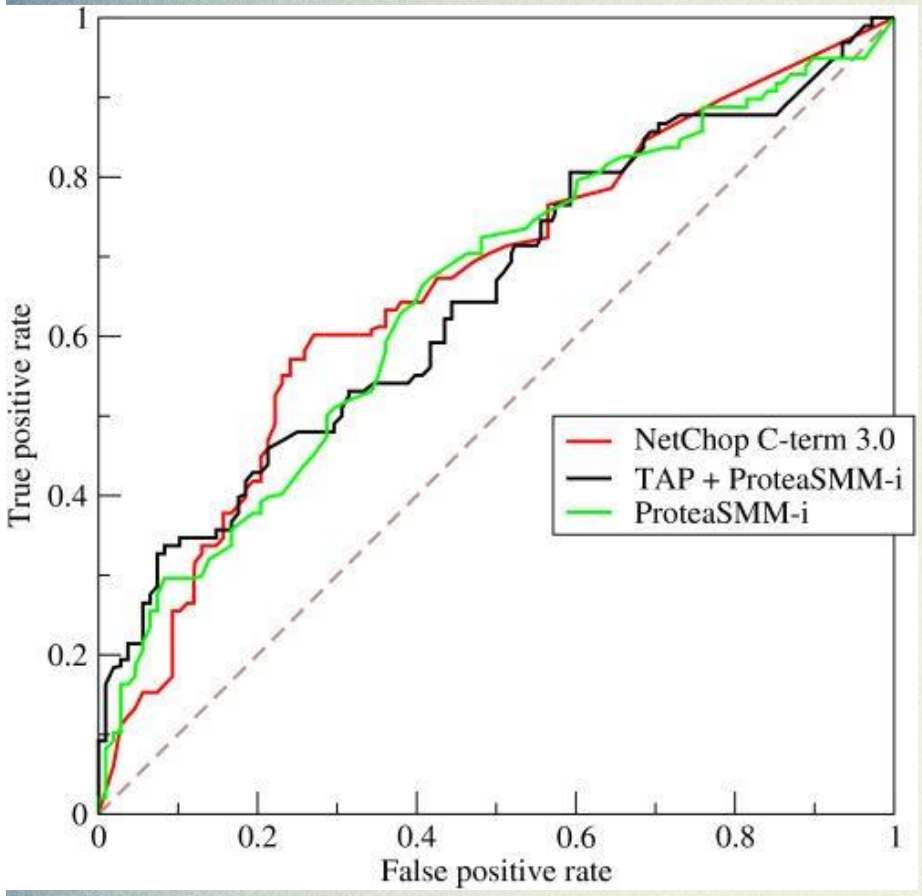
accuracy =
true positives + true negatives / total

precision =
true positives / (true positives + falsepositives)

recall =
true positives / (false negatives + true positives)

F1 score =
2 * ((**precision** * **recall**) / (**precision** + **recall**))

https://en.wikipedia.org/wiki/Precision_and_recall

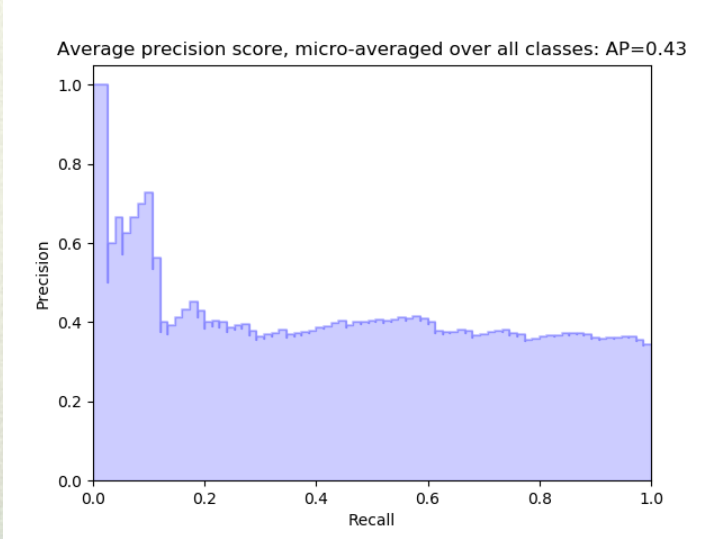


ROC (reciever-operator curve)

True Positive Rate /
False Positive Rate

AUC (AUROC) = area under ROC

- *probability that random positive example will be ranked higher than random negative*
- calculate empirically from test results



AUPR (area under precision-recall curve)

https://en.wikipedia.org/wiki/Receiver_operating_characteristic
http://scikit-learn.org/stable/modules/generated/sklearn.metrics.auc.html#sklearn.metrics.auc

MSE & Coefficient of Determination

MAE / MSE / RMSE

MSE = np.mean((predicted-expected)**2)

Coefficient of determination

R^2 is a predictor of "goodness of fit" and is a value ∈ [0,1] where 1 is perfectfit.

-the proportion of the variance in the dependent variable that is predictable from the independent variable(s)

-independent from the scale of the output feature

$$SS_{\text{tot}} = \sum_i (y_i - \bar{y})^2,$$

$$SS_{\text{res}} = \sum_i (y_i - f_i)^2 = \sum_i e_i^2$$

$$R^2 \equiv 1 - \frac{SS_{\text{res}}}{SS_{\text{tot}}}.$$

Evaluation - sklearn

sklearn.model_selection
-GridSearchCV
-train_test_split()
-LeaveOneOut (predict for each example separately)

- Split data / Learn hyperparameters / Validate metrics

Evaluation - sklearn

sklearn.metrics: metric(true, predicted/rank,…)
Classification
-classification_report()
-precision, recall, auc, f1_score, jaccard,…
-confusion matrix

Regression
-r2_score(), MAE, MSE

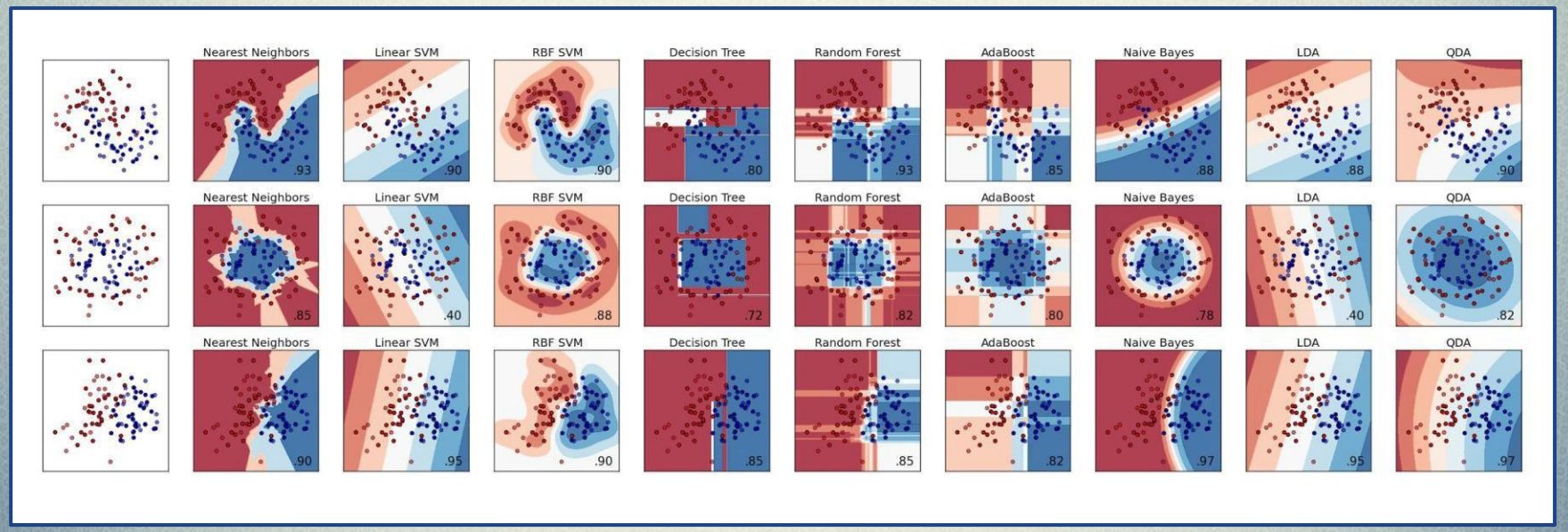
Clustering
Pairwise
- cosine / euklidean distance, …
…
-http://scikit-learn.org/stable/modules/classes.html#module-sklearn.metrics

```
from sklearn import svm, datasets
from sklearn.model_selection import GridSearchCV, train_test_split
from sklearn.metrics import classification_report

iris = datasets.load_iris()
parameters = {'kernel':('linear', 'rbf'), 'C':[1, 10]}
svc = svm.SVC()
X = iris.data
y = iris.target
X_train, X_test, y_train, y_test = train_test_split(X, y,
test_size=0.3, random_state=0)

clf = GridSearchCV(svc, parameters)
clf.fit(X,y)
print(clf.cv_results_['mean_test_score'])
print(clf.cv_results_['params'])
print(clf.best_params_)

y_pred = clf.predict(X_test)
print(classification_report(y_test, y_pred))
```

Other Evaluation

How to evaluate clusters?

Visualization (but only in 2D)



Unpredictable Future

Machine learning models attempt to predict the future as new inputs come in - but human systems and processes are subject to change.

Solution: Precision/Recall tracking over time

Pipelines

Pipelines

`sklearn.pipeline.Pipeline(steps)`

- Sequentially apply *repeatable* transformations to final estimator that can be validated at every step.
- Each step (except for the last) must implement Transformer, e.g. `fit` and `transform` methods.
- Pipeline itself implements both methods of `Transformer` and `Estimator` interfaces.

```
>>> from sklearn.preprocessing import  PolynomialFeatures
>>> from sklearn.pipeline import  make_pipeline
>>> model = make_pipeline(PolynomialFeatures(2), linear_model.
Ridge())
>>> model.fit(X_train, y_train)


>>> mean_squared_error(y_test, model.predict(X_test))
3.1498887586451594


>>> model.score(X_test, y_test)
0.9709057634510810 4
```

Pipelined Model