Introduction to Machine Learning with Scikit-Learn

District Data Labs

QCon SÃO PAULO 2017

Feature Engineering

Getting the most out of data for predictive models

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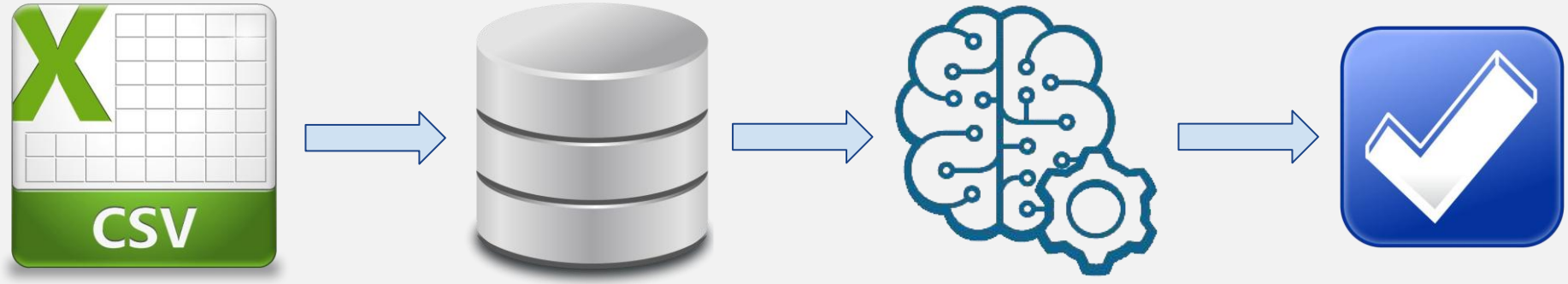
"Feature engineering is the process of transforming raw data into features that better represent the underlying problem to the predictive models, resulting in improved model accuracy on unseen data."

- Jason Brownlee

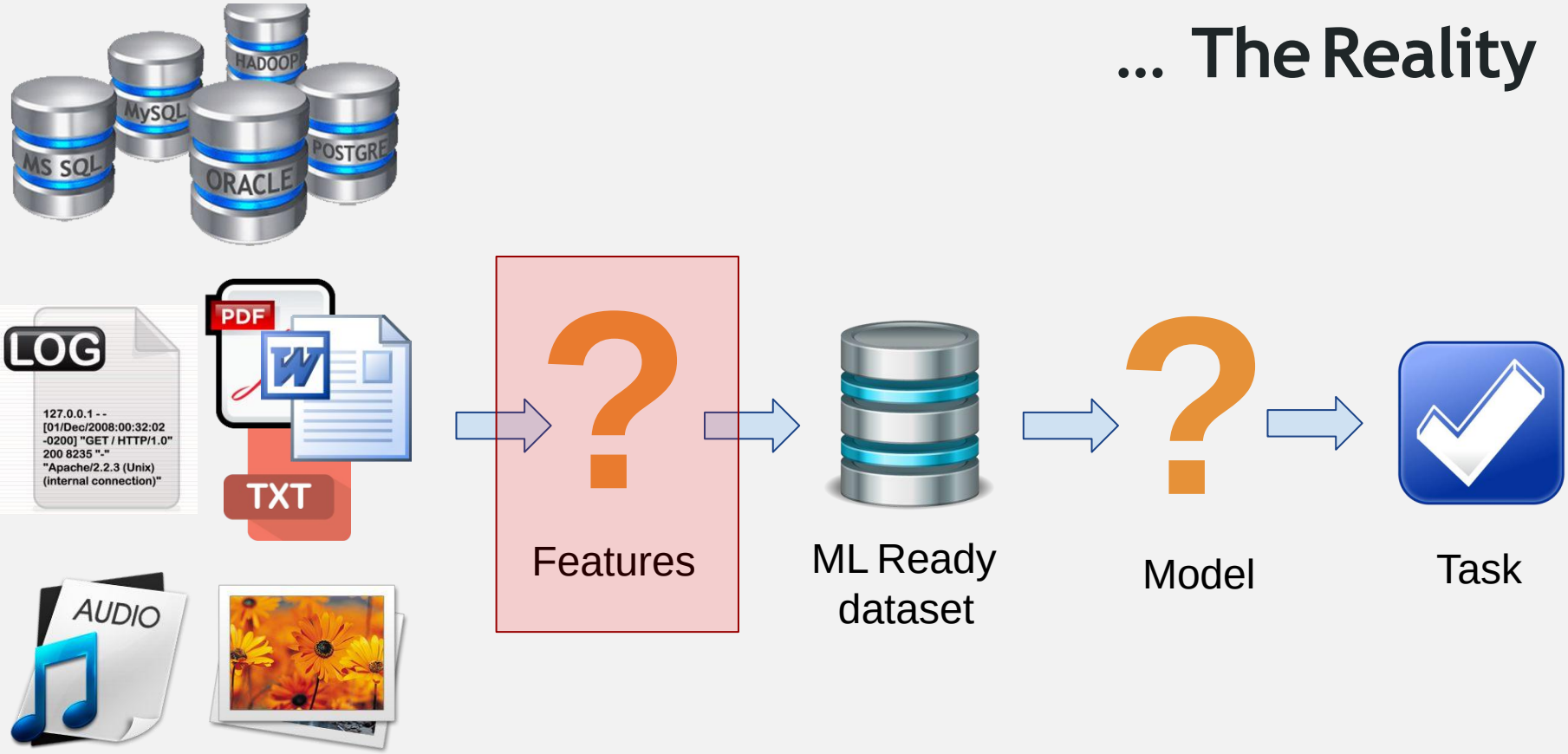
“Coming up with features is difficult,
time-consuming,
requires expert knowledge.
'Applied machine learning' is basically
feature engineering.”

– Andrew Ng

The Dream…



… The Reality



Raw data

… The Reality

Raw data

Deep Learning

But what architecture?

Task

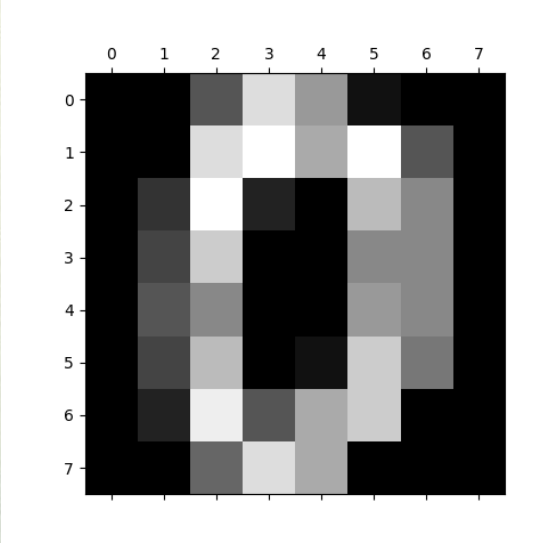
More on scikit-learn

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

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()
```



Data pre-processing and transformation

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

sklearn.preprocessing
sklearn.feature_extraction
sklearn.feature_selection

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

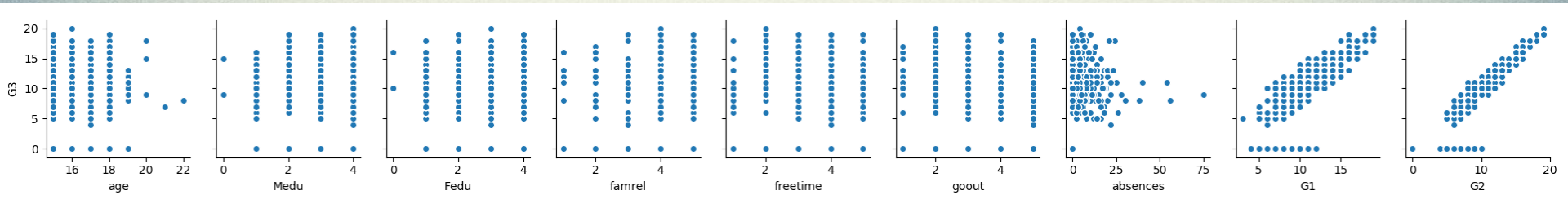
- correlation, covariation, linear dependence, dimensionality reduction…

Visualization

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

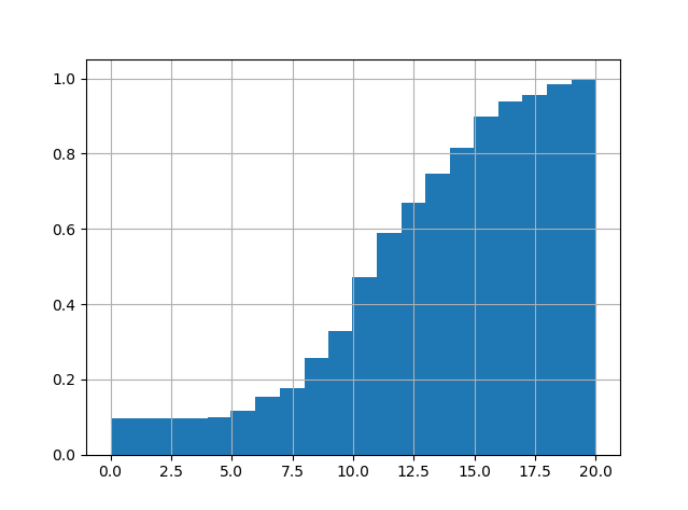
Exploratory Data Analysis (EDA) - pairplot

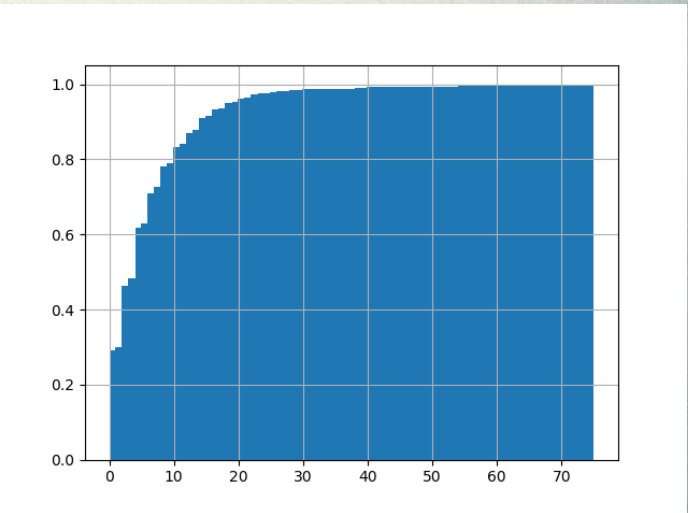
```
import pandas as pd
import seaborn as sns #statistical data visualization, based on matplotlib
import matplotlib.pyplot as plt

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()
```





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

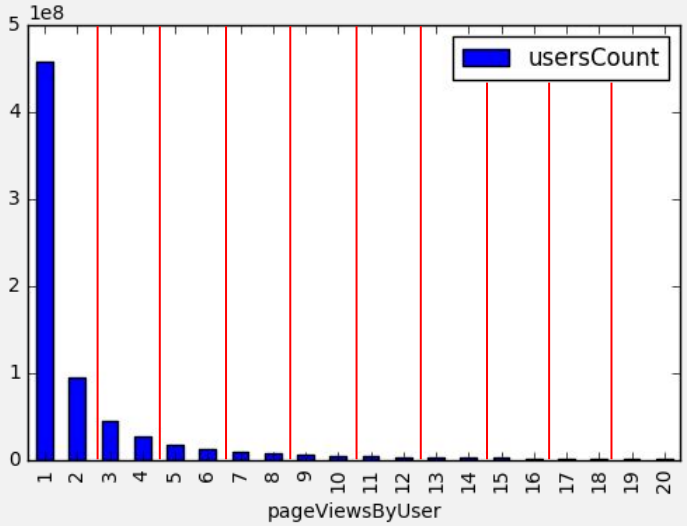
```
>>> from sklearn import preprocessing
>>> X = [[ 1., -1.,  2.],
...      [ 2.,  0.,  0.],
...      [ 0.,  1., -1.]]

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

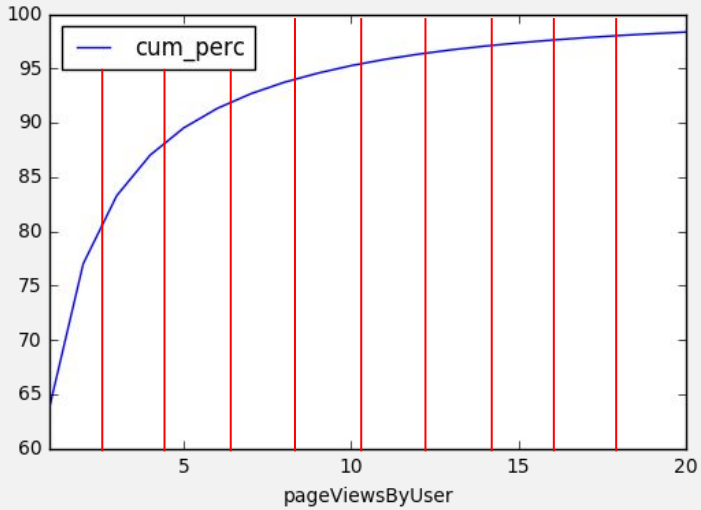
Binarization with scikit-learn

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?





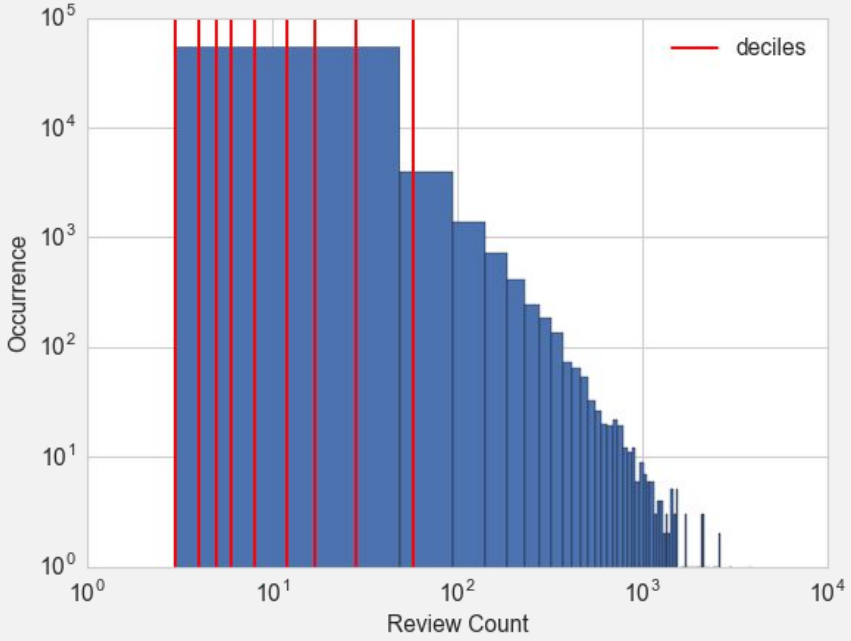
Most users (458,234,809 ~ 5*10^8) had only 1 pageview during the period.

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
```

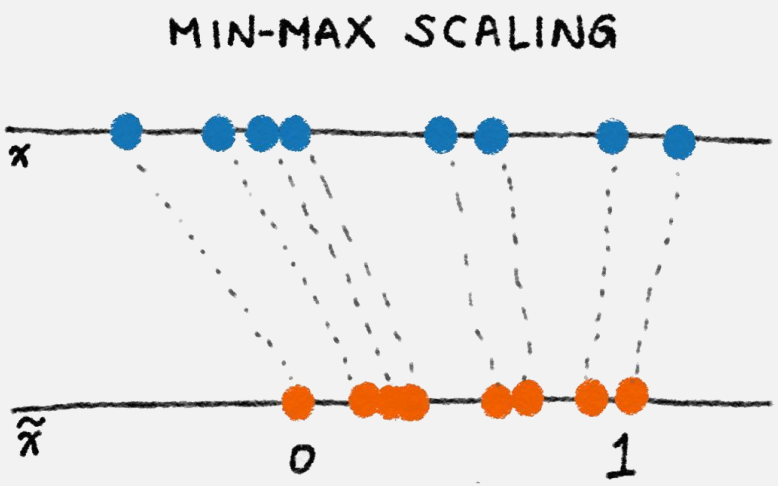
Quantile binning with Pandas

Scaling

- Models that are smooth functions of input features are sensitive to the scale of the input (eg. Linear Regression)
- 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

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.



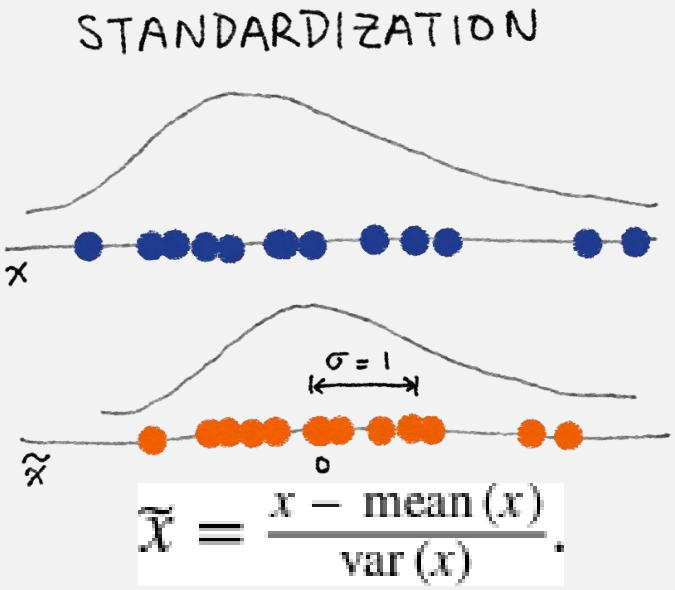
$$\tilde{x} = \frac{x - \min(x)}{\max(x) - \min(x)}$$

```
>>> 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)



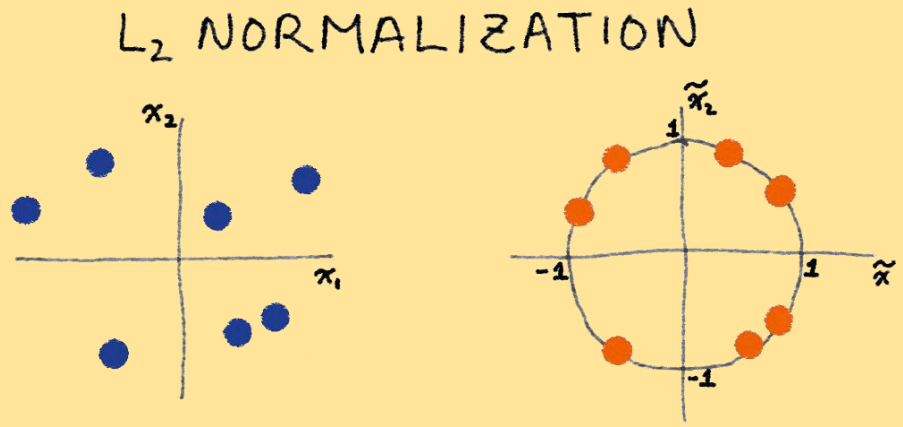
$$\tilde{x} = \frac{x - \text{mean}(x)}{\text{var}(x)}.$$

```
>>> 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...]])
```

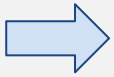
Normalization with scikit-learn

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.

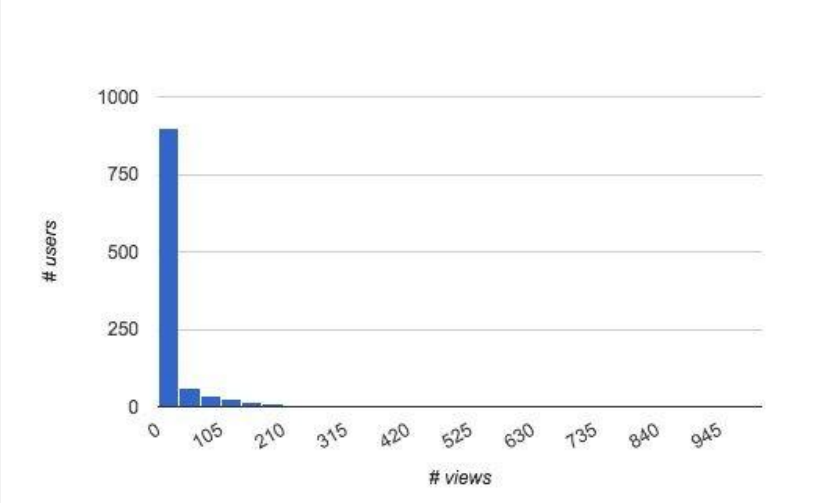
user_id	views_count
a	1000
b	500
c	300
d	200
e	150
f	100
g	70
h	50
i	30
j	20
k	10
l	5
m	1



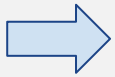
log(1+views_count)
6.91
6.22
5.71
5.30
5.02
4.62
4.26
3.93
3.43
3.04
2.40
1.79
0.69

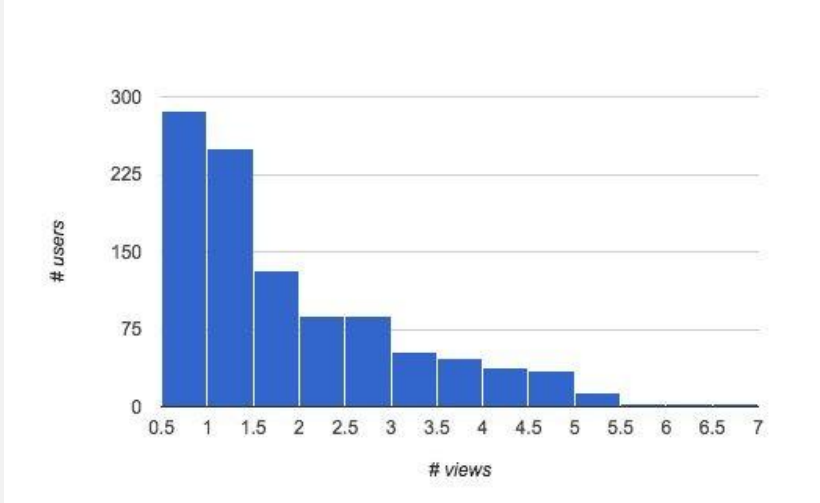
Log transformation

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

100 hashed columns

country
brazil
chile
venezuela
colombia
... 222 countries

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	...
...	...	...	...	...

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
18339
335
1244
35387

or

ad_clicks
1355
12
132
1244

or

ad_CTR
0.074
0.036
0.106
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

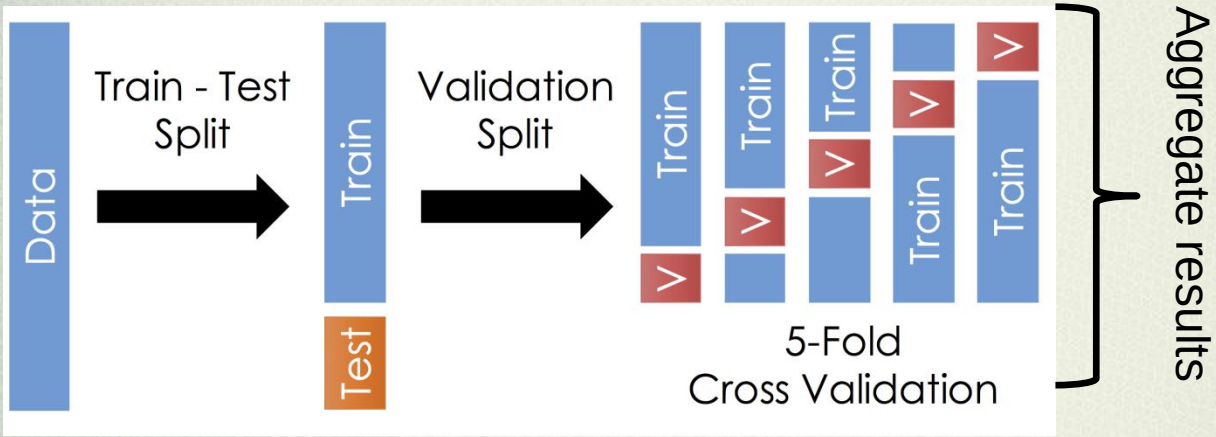
- Decrease complexity of model
- Remove redundant and irrelevant features

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

Model Fitting & Evaluation

Model Fitting Protocol

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



Istead 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

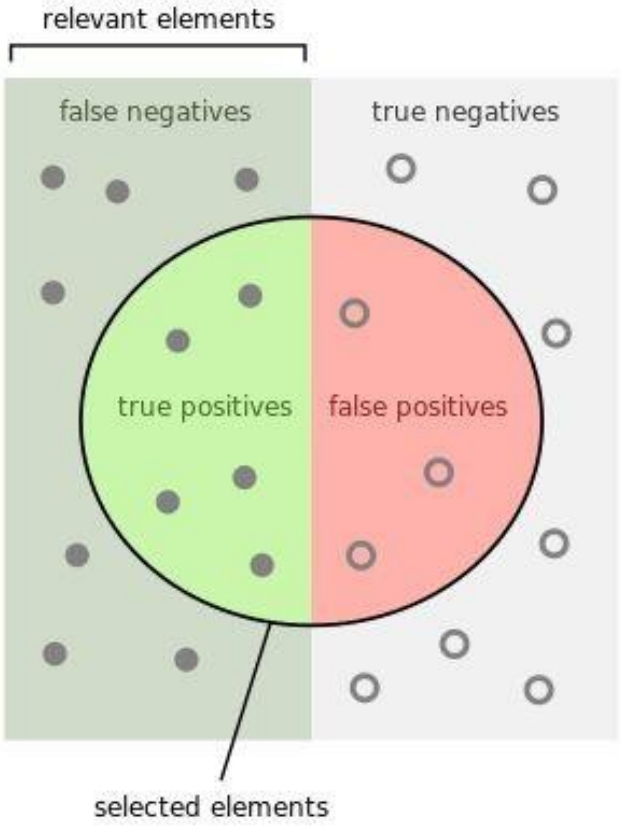
Model Fitting Protocol

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



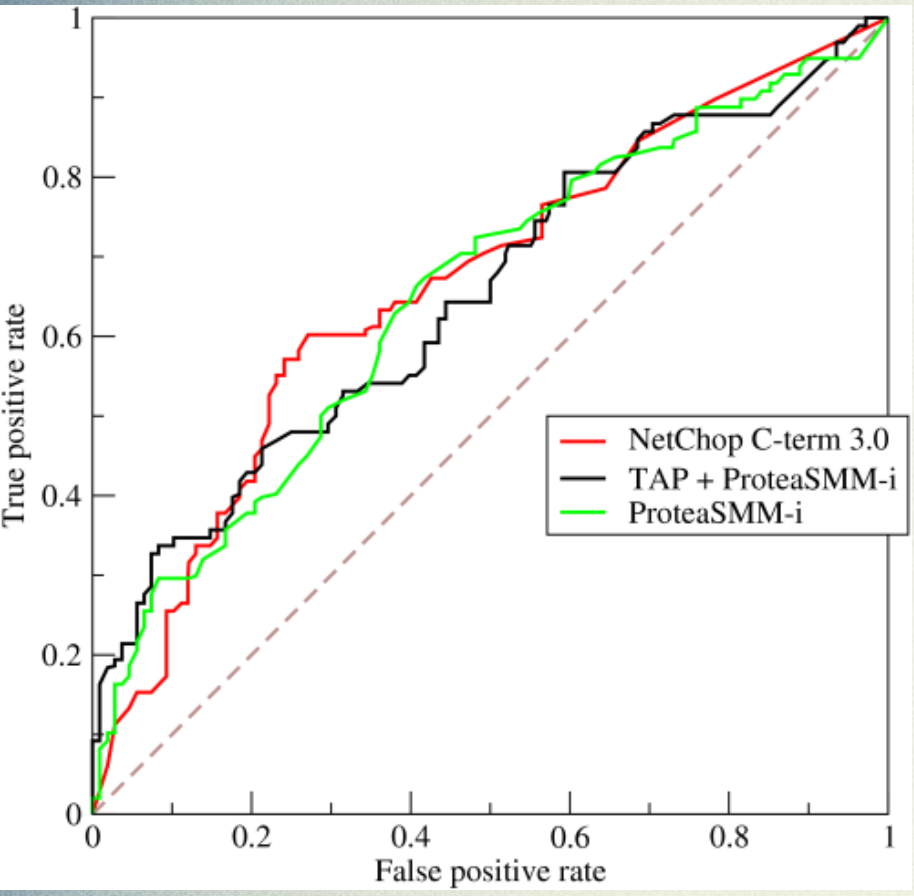
accuracy =
true positives + true negatives / total

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 $\in$ [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

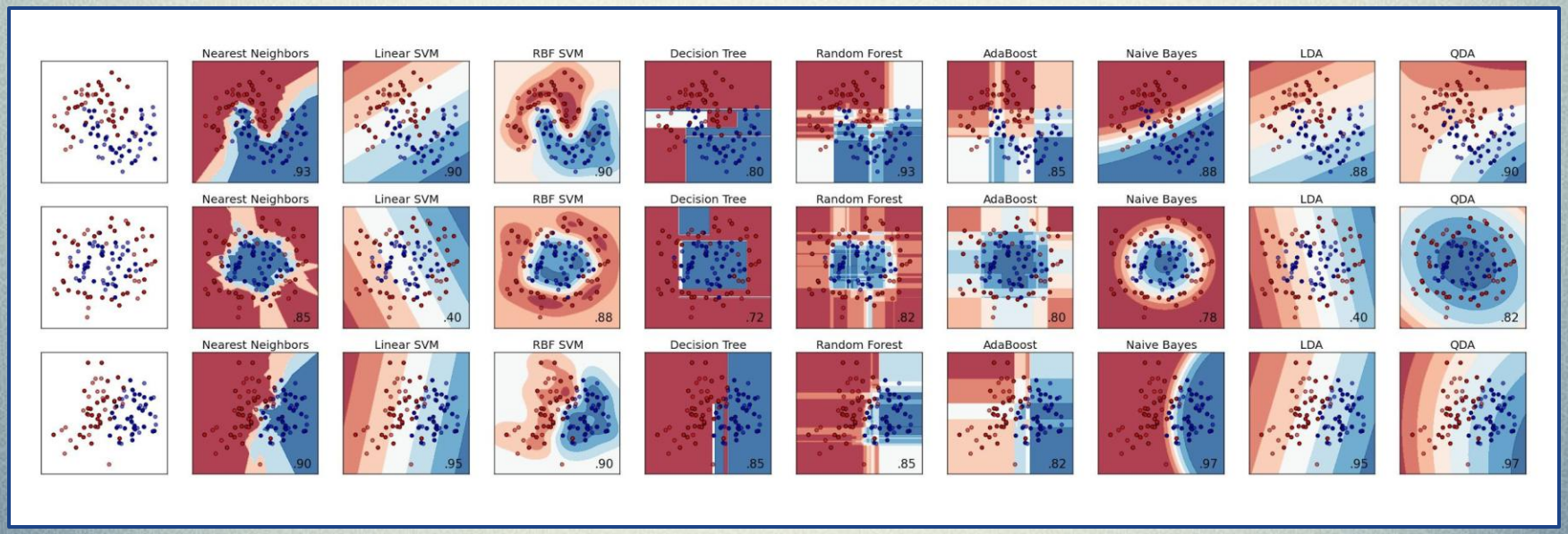
Clustering
Pairwise
- cosine / euklidean distance, …
…
-http://scikit-learn.org/stable/modules/classes.html#module-sklearn.metrics

```
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)
0.97090576345108104
```

Pipelined Model

Task 7

Select dataset (wines / student performance)

- Run train_test_split() @ 20% test set
- Select learning method
  - Select best hyperparameters based on cross-validation

Return R^2, MAE and RMSE based on scipy methods

- vizualize CDF and independent/dependent vars

-try, e.g. StandardScaler() and PolynomialFeatures() for extraction

- http://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.PolynomialFeatures.html

Semestrální projekt – varianta 3

- Identifikace / autentizace osob dle keystroke dynamics
  - Vzdělávací servery / online výuka atp.
  - Soutěž na http://biointelligence.hu/typing-challenge/index.php
    - dataset není v současné době veřejný (GDPR), zájemcům bude předán
    - malý dataset (12 osob, 5 trénovacích a 50 testovacích vzorků / osobu)
    - JavaScript events keyup/down/press, keycode, timestamp
    - Autentizace (potvrzení očekávané osoby)
    - Identifikace (která z osob odpovídá danému vzorku)
  - Evaluace:
    - Odeslat řešení v daném formátu na web soutěže
    - Accuracy (TP+TN)/ALL
    - „Rozumné“ výsledky alespoň okolo ECKNN
  - Typické algoritmy:
    - Dynamic Time Warping (https://en.wikipedia.org/wiki/Dynamic_time_warping)
    - Rychlosti lokálních přechodů / dimensionality reduction
    - RNN? asi příliš malý dataset. Možná document2vec.
  - http://biointelligence.hu/typing.html