



### **LESSON 2: Classification**

Cost function, Supervised classification, Performance metrics

### CARSTEN EIE FRIGAARD

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$$\mathbf{X} = \begin{bmatrix} x_1^{(1)} & x_2^{(1)} & \cdots & x_d^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \cdots & x_d^{(2)} \\ \vdots & & & \vdots \\ x_1^{(n)} & x_2^{(n)} & \cdots & x_d^{(n)} \end{bmatrix} = \begin{bmatrix} (\mathbf{x}^{(1)})^T \\ (\mathbf{x}^{(2)})^T \\ \vdots \\ (\mathbf{x}^{(n)})^T \end{bmatrix}$$



## Agenda

#### Supervised classification, Cost function, Performance metrics

- 1. Admin (afleveringer, grupper, etc.)
- 2. Resume
  - kort om Python libs
  - supervised learning: en oversigt
- 3. Linær algebra og cost funktionen, J
  - ▶ matricer, vektors, norms og NumPy,
  - MSE, MAE,
  - ► Jupyter notebook: L02/cost\_function.ipynb
- 4. Supervised binær klassifikation
  - 'demo' datasæt,
  - fundamental ML supervised lærings-proces,
  - Scikit-learn fit-predict interface,
  - Jupyter notebook: L02/dummy\_classifier.ipynb
- Performace metrics
  - $\triangleright$  precision, recall, accuracy,  $F_1$ -score,
  - confusion matrix.
  - ► Jupyter notebook: L02/performance\_metrics.ipynb

### The toolset for ML

#### A list of our toolbox

- Python: our prefeered language for ML,
- Anaconda: a particular distibution of python, that we will use,
- Jupyter notebooks: interactive coding and visualization for python (alt: Spider, PyCharm),
- NumPy, SciPy, Pandas, Matplotlib, Seaborn: numerical computation and data visualization libraries for python,
- Scikit-learn: machine learning tools.

# Jupyter Crash Couse

### Jupyter need-to-know:

- Ctrl+Enter: executes cell,
- Shift+Tab: help for function under cusor,
- Shift+Tab repeated: extended help,
- Tab: 'tab'-completion??

### Jupyter magic commands:

- %matplotlib inline: pull in the matplotlib,
- %reset -f: reset all vars (or -sf),
- %run filename.ipynb; execute code from another notebook or python file,
- %load filename.py: copy contents of the file and paste into the cell,
- ! dir: executes a shell command.

# Jupyter Crash Course

### Jupyter shortcuts:

To modes: command mode (blue) and edit-mode (green),

In [ ]: a=1

ESC: goto command mode (from edit mode),

#### Keyboard shortcuts

The Jupyter Notebook has two different keyboard input modes. **Edit mode** allows you to type code/text into a cell and is indicated by a green cell border. **Command mode** binds the keyboard to notebook level actions and is indicated by a grey cell border with a blue left margin.

### Command Mode (press Esc to enable)

E: find and replace

Ctrl-Shift-P: open the command palette

Enter: enter edit mode

Shift-Enter: run cell, select below

Ctrl-Enter: run selected cells

Alt-Enter: run cell, insert below

Shift-J: extend selected cells below

A: insert cell above
B: insert cell below
X: cut selected cells
C: copy selected cells
Shift-V: paste cells above

## Python Libraries Crash Course

A lot of modules/libraries are available for python, here we will use:

- numpy: numerical data representation module, for say vectors, matrices etc,
- matplotlib: Matplotlib is a Python 2D plotting library which produces publication quality figures.

### Other libraries, typically used in ML, are:

- pandas: python data analysis library, a module for loading/saving and handling large data set,
- scipy: python library used for scientific computing and technical computing.

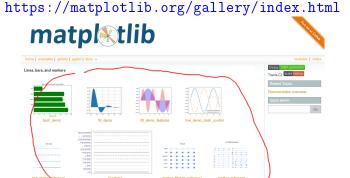
but we try to stick to numpy in this course, ...and note that numpy .matrix is depricated!

## Matplotlib Crash Course

Visualizations can be created in multiple ways:

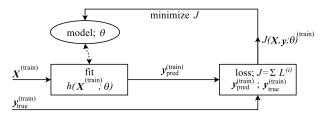
- ▶ matplotlib
- pandas: (via matplotlib),
- seaborn: statistically-focused plotting methods.

And we will stick to matplotlib, don't re-invent the wheel; find demos here



### RESUMÉ

### Data-flow model for supervised learning



```
X<sup>(train)</sup>: trænings data input,
```

loose notation:  $\mathbf{X}^{(\text{train})} = \mathbf{X}^{(i)}$  for  $\forall i \in \text{train set}$ 

 $\theta$ : model parametre,

h: hypothesis function; types of ML algos,

**y**(train): training data output,

 $\mathbf{y}_{\text{pred}}^{(\text{train})}$ : predicted (train) data output,

 $L^{(i)}$ : individual loss (distance),

J: loss/cost/error/objective function (summeret)

## Exercise: L02/cost\_function.ipynb

#### Matrix notation

Say, we have d features for a given sample point. This d-sized feature column vector for a data-sample i is then given by

$$\mathbf{x}^{(i)} = \begin{bmatrix} x_1^{(i)} & x_2^{(i)} & \cdots & x_d^{(i)} \end{bmatrix}^T$$

The full data matrix  $\mathbf{X}$  and target column vector  $\mathbf{y}$  are then constructed out of n samples of these feature vectors

$$\mathbf{X} = \begin{bmatrix} x_1^{(1)} & x_2^{(1)} & \cdots & x_d^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \cdots & x_d^{(2)} \\ \vdots & & & \vdots \\ x_1^{(n)} & x_2^{(n)} & \cdots & x_d^{(n)} \end{bmatrix} = \begin{bmatrix} (\mathbf{x}^{(1)})^T \\ (\mathbf{x}^{(2)})^T \\ \vdots \\ (\mathbf{x}^{(n)})^T \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} y^{(1)} \\ y^{(2)} \\ \vdots \\ y^{(n)} \end{bmatrix}$$

(and **X** and **y** are sometimes concantenated into a single matrix!)

# Exercise: L02/cost\_function.ipynb

Distance/norms

The  $\mathcal{L}_2$  Euclidian norm for a vector of size n is defined as

$$\mathcal{L}_2: ||\mathbf{x}||_2 = \left(\sum_{i=1}^n |x_i|^2\right)^{1/2}$$

and thus via linear algebra and vector inner-dot product

$$\mathcal{L}_{2}^{2}: ||\mathbf{x}||_{2}^{2} = \mathbf{x}^{\top}\mathbf{x}$$

The distance between two vectors is given by

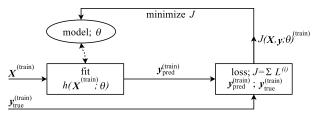
$$d(\mathbf{x}, \mathbf{y}) = ||\mathbf{x} - \mathbf{y}||_2$$
  
=  $\left(\sum_{i=1}^{n} |x_i - y_i|^2\right)^{1/2}$ 

The general  $\mathcal{L}_{p}$  norm is given by

$$\mathcal{L}_{p}: \ ||\mathbf{x}||_{p} = \left(\sum_{i} |x_{i}|^{p}\right)^{1/p}; \ \text{norm:} \left\{ \begin{array}{l} \mathcal{L}_{p}(\mathbf{x}) = \mathbf{0}, \ \Rightarrow \mathbf{x} = \mathbf{0} \\ \mathcal{L}_{p}(\mathbf{x} + \mathbf{y}) \leq \mathcal{L}_{p}(\mathbf{x}) + \mathcal{L}_{p}(\mathbf{y}), \\ \text{(triangle inequality)} \\ \mathcal{L}_{p}(\alpha \mathbf{x}) = |\alpha| \mathcal{L}_{p}(\mathbf{x}) \end{array} \right.$$

### Exercise: L02/cost\_function.ipynb

Data-flow model for supervised learning



Express J in terms of vectors and matrices using the  $\mathcal{L}_2$ 

$$\begin{array}{ll} J(\mathbf{X},\mathbf{y};\boldsymbol{\theta}) &= \frac{1}{n} \sum_{i=1}^{n} L^{(i)} \\ &= \frac{1}{n} \sum_{i=1}^{n} d(h(\mathbf{X}^{(i)}) - \mathbf{y}_{\text{true}}^{(i)})^2 \\ &= \frac{1}{n} ||h(\mathbf{X}) - \mathbf{y}_{\text{true}}||_2^2 \\ &= \frac{1}{n} ||\mathbf{y}_{\text{pred}} - \mathbf{y}_{\text{true}}||_2^2 \end{array}$$

arriving at a J proportional to the MSE or  $\mathcal{L}_2$  metric

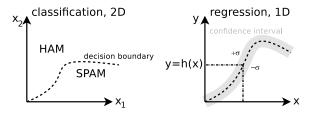
cost function: 
$$J(\mathbf{X},\mathbf{y}_{true};m{ heta})\propto rac{1}{2}||\mathbf{y}_{pred}-\mathbf{y}_{true}||_2^2\propto \mathit{MSE}$$

## Classification vs. Regression

Given the following hypothesis function

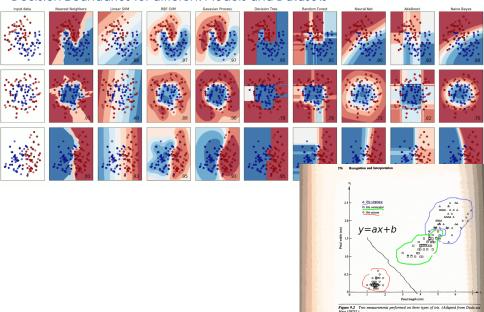
$$h(\mathbf{x}) \rightarrow y$$

- if y is discrete/categorical variable, then this is classification problem.
- if y is real number/continuous, then this is a regression problem.



### Classification

#### Decision Boundaries for different Models and Datasets

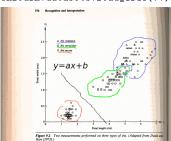


### 'Demo' datasæt

### MNIST, Iris og Moon

### Iris:

Sepal/petal længde/bredde, Mr. Fisher, 1936, "Anderson's Iris data set" sklearn.datasets.load\_iris(...)







### MNIST:

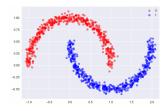
Håndskrevne tal,
preprocesseret, centrerede,
sklearn.datasets.fetch\_openml('mnist\_784'...



### Moon:

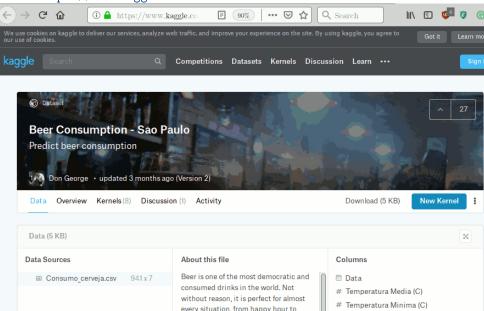
'XOR' lign.,

non-linear decision boundary, sklearn.datasets.make\_moons(..)

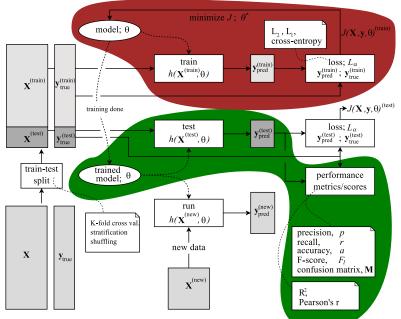


### 'Dit' datasæt

Fro https://www.kaggle.com...



# ML Supervised Learning, Train/Test

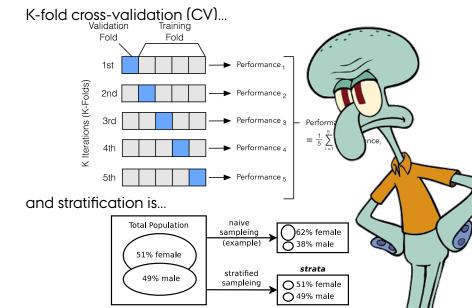


## Fundamental supervised learning-proces

- i) Forbered data:
  - manuel preprocessering + visualisering (støj, outliers..)
  - ▶ label y<sub>true</sub> data!!!
  - normalization, skalering
  - shuffle,
  - (stratification, K-fold cross-validation).
- ii) Split data i train/test.
  - analogi: skriftlig eksamenssæt på ASE: test-træningssæt (eksamen) udleveres ikke til træning inden!
- iii) Træn på trænings-data (fit)
  - ► ML træning via J,
- iv) Evaluér på test-data (predict)
  - performance metrics/scores

### Forbered data: cross-validation, stratification

Bemærk: mere preprocess og k-fold cross-validation i L06, koncepter II..



### Multiclass/Multinomial Classification

And Introduction to Multilabel Classification

- Many classifiers are binary (HAM/SPAM)
- What to do for say a three category, like CAT/DOG/TURTLE problem?
- Divide into three CAT/NON-CAT, etc, binary classifiers and solve!
- Aka.: one-vs-rest/one-vs-all (OvA), one-against-all (OAA).
- Or the one-vs-one (OvO) method.
- NOTE: Multilabel classification is yet again differentity can categorize item into more classes, say both cand DOG!
- ...and Multioutput/multilabel multiclass classificate

### The Scikit-learn Fit-Predict Interface



Supervised Classification in practice

The API has one predominant object: the estimator.



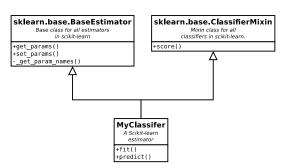
An estimator is an object that fits a model based on some training data and is capable of inferring some properties on new data. It can be, for instance, a classifier or a regressor.

All estimators implement the fit method: estimator.fit(X,y) All built-in estimators also have a  $set\_params$  method, which sets data-independent parameters (overriding previous parameter values passed to  $\_init\_$ .

All estimators in the main scikit-learn codebase should inherit from sklearn, base, BaseEstimator.

### The Scikit-learn Fit-Predict Interface





Python module and class function and member encapsulation:

- module private: one underscore
- class-private: two underscores

via mangled names.

- ...NOTE: no virtual void fit() = 0; declaration in python!
- ...for modules, private funs can still be accessed via a hack?!
- ...src file: /opt/anaconda3/pkgs/.../sklearn/base.py

# The Scikit-learn Fit-Predict Interface



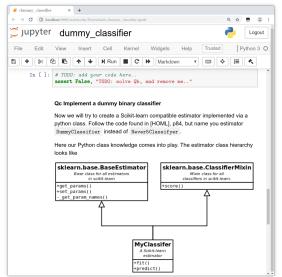
Demo..

Implementing an estimater via a python class as simple as

```
class ParadoxClassifier(BaseEstimator, ClassifierMixin):
    def fit(self, X, y=None):
        pass
    def predict(self, X):
        assert X.ndim==2
    return np.ones(X.shape[0],dtype=bool)
```

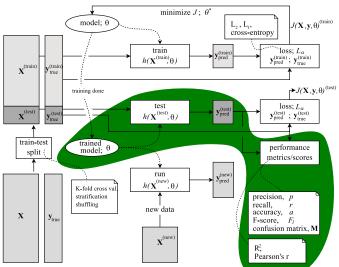
### Exercise: L02/dummy\_classifier.ipynb

A dummy classifier for the fit-predict interface, plus intro to a Stochastic Gradient Decent method (SGD) and introduction to the accuracy-paradox.



## Evaluér på test-data: Perfomance metrics

Kort intro til konceptet performance metrics..



 $NOTE_0$ : Performance metric = score.

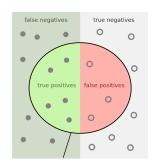
NOTE<sub>1</sub>: 'Performance measure' begreb bruges ikke, kun score eller perf. metric. NOTE<sub>2</sub>: Loss er ML algo'ens 'performance mål', score er vores evalueringsmål.

#### Nomenclature

For a binary classifier

NAME	SYMBOL	ALIAS
true positives	TP	
true negatives	TN	
false positives	FP	type I error
false negatives	FN	type II error

and  $N = N_P + N_N$  being the total number of samples and the number of positive and negative samples respectively.



[https://en.wikipedia.org/wiki/Precision\_and\_recall]

Precision, recall and accuracy,  $F_1$ -score, and confusion matrix

precision, 
$$p = \frac{TP}{TP+FP}$$
recall (or sensitivity), 
$$r = \frac{TP}{TP+FN}$$
accuracy, 
$$a = \frac{TP+TN}{TP+TN+FP+FN}$$

$$F_1\text{-score}, \qquad F_1 = \frac{2pr}{p+r}$$

false negatives	true negatives	
• • •	0 0	
• (•	0 0	
true positives	false positives	
	0 0	
• • ]	0 0	
,		

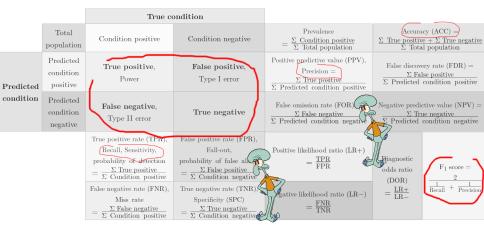
Precision = -

Confusion Matrix,				
	actual	actual		
	true	false		
predicted true	TP	FP		
predicted false	• FN	TN		



NOTE<sub>0</sub>: you can *compare* precision... $F_1$ -score, but not necessarily the cost, J.

#### Nomenclature for the Confusion Matrix





prevalence, positive predictive value, etc. not important to know at all!

Accuracy Paradox...

```
class ParadoxClassifier(BaseEstimator, ClassifierMixin):
        def fit(self, X, y=None):
             pass
        def predict(self, X):
             assert X.ndim==2
5
             return np.ones(X.shape[0],dtype=bool)
    Test via the breast cancer Wisconsin dataset...
    print(f" X.shape={X.shape}, y_true.shape={y_true.shape}")
    X_train, X_test, y_train, y_test = train_test_split(
        X, y_true, test_size=0.2, shuffle=True,random_state= 42)
    clf = ParadoxClassifier()
                                         prints: acc=0.6228070175438597,
    clf.fit(X_train, y_train)
                                                 N = 114
    y_pred = clf.predict(X_test)
8
    acc = accuracy_score(y_test, y_pred)
9
    print(f' acc={acc}, N={y_pred.shape[0]}')
    score = clf.score(X_test, y_test)
    print(f' clf.score()={score} (same as accuracy_score)')
12
    NOTE<sub>0</sub>: for MNIST, a dum classify as '5' \sim a = 10\%
    NOTE<sub>1</sub>: for MNIST, a dum classify not-as '5' \sim a = 90\%
```

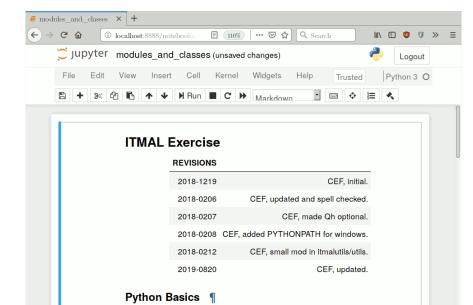
More on metrics, oh-so-many!

[https://scikit-learn.org/stable/modules/classes.html#sklearn-metrics-metrics]

Classification metrics	
See the Classification metrics section of the user guide for furti	her detalls.
metrics.accuracy_score(y_true, y_pred[,])	Accuracy classification score.
metrics.auc(x, y[, reorder])	Compute Area Under the Curve (AUC) using the trapezoidal rule
metrics.average_precision_score(y_true, y_score)	Compute average precision (AP) from prediction scores
metrics.balanced_accuracy_score(y_true, y_pred)	Compute the balanced accuracy
metrics.brier_score_loss(y_true, y_prob[,])	Compute the Brier score.
metrics.classification_report(y_true, y_pred)	Build a text report showing the main classification metrics
metrics.cohen_kappa_score(y1, y2[, labels,])	Cohen's kappa: a statistic that measures inter-annotator agreement.
metrics.confusion_matrix(y_true, y_pred[,])	Compute confusion matrix to evaluate the accuracy of a classification
metrics.fl_score (y_true, y_pred[, labels,])	Compute the F1 score, also known as balanced F-score or F-measure
metrics.fbeta_score(y_true, y_pred, beta[,])	Compute the F-beta score
metrics.hamming_loss(y_true,y_pred[,])	Compute the average Hamming loss.
metrics.hinge_loss (y_true, pred_decision[,])	Average hinge loss (non-regularized)
metrics.jaccard_similarity_score(y_true, y_pred)	Jaccard similarity coefficient score
metrics.log_loss (y_true, y_pred[, eps,])	Log loss, aka logistic loss or cross-entropy loss.
metrics.matthews_corrcoef(y_true, y_pred[,])	Compute the Matthews correlation coefficient (MCC)
metrics.precision_recall_curve(y_true,)	Compute precision-recall pairs for different probability thresholds
metrics.precision_recall_fscore_support()	Compute precision, recall, F-measure and

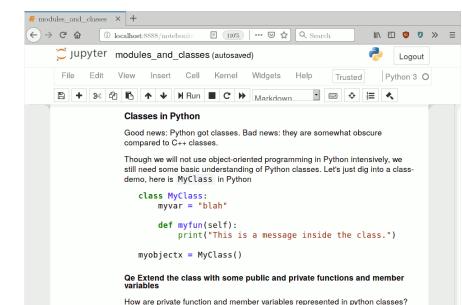
# Exercise: L02/modules\_and\_classes.ipynb

Modules and Packages...



# Exercise: L02/modules\_and\_classes.ipynb

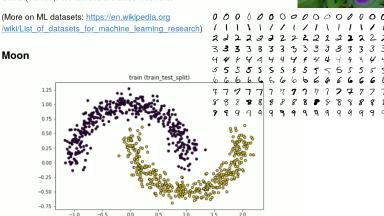
Python classes...



### Exercise: L02/datasets.ipynb

#### Vanilla Datasets

There are a number of popular datasets out-there, that are used again and again for small scale testing in ML: most popular are Moon, MNIST, Iris and CIFAR(10/100). We will use the three first here.

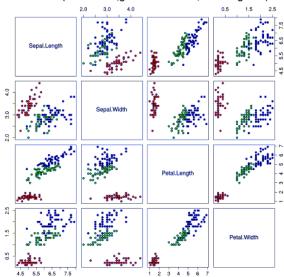


Vanilla/ML hello-world datasets: Moon, MNIST, iris...

# Exercise: L02/datasets.ipynb

Feature scatterplot...





## Exercise: L02/datasets.ipynb

Your dataset, from https://www.kaggle.com...

