



LESSON 2: Classification

Cost function, Supervised classification, Performance metrics

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SPRING 2020

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



Agenda

Supervised classification, Cost function, Performance metrics

1. Admin (afleveringer, grupper, etc.)
2. Resume
 - ▶ kort om Python libs
 - ▶ supervised learning: en oversigt
3. Lineær 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](#)
5. Performance metrics
 - ▶ 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 preferred language for ML,
- ▶ **Anaconda:** a particular distribution 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 Course

Jupyter need-to-know:

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

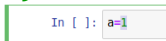
Jupyter magic commands:

- ▶ `%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)

F: 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 deprecated!*

Matplotlib Crash Course

Visualizations can be created in multiple ways:

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

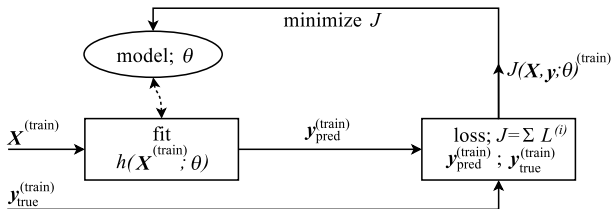
And we will stick to `matplotlib`, don't re-invent the wheel;
find demos here

<https://matplotlib.org/gallery/index.html>



RESUMÉ

Data-flow model for supervised learning



$\mathbf{X}^{(\text{train})}$: trænings data input,

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

θ : model parametre,

h : hypothesis function; types of ML algos,

$\mathbf{y}_{\text{true}}^{(\text{train})}$: 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 \mathbf{X} and \mathbf{y} are sometimes concatenated 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

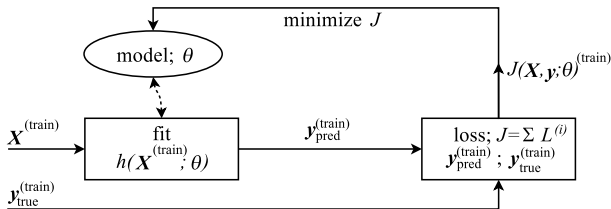
$$\begin{aligned} d(\mathbf{x}, \mathbf{y}) &= ||\mathbf{x} - \mathbf{y}||_2 \\ &= \left(\sum_{i=1}^n |x_i - y_i|^2 \right)^{1/2} \end{aligned}$$

The general \mathcal{L}_p norm is given by

$$\mathcal{L}_p : ||\mathbf{x}||_p = \left(\sum_i |x_i|^p \right)^{1/p} ; \text{ norm: } \begin{cases} \mathcal{L}_p(\mathbf{x}) = 0, \Rightarrow \mathbf{x} = \mathbf{0} \\ \mathcal{L}_p(\mathbf{x} + \mathbf{y}) \leq \mathcal{L}_p(\mathbf{x}) + \mathcal{L}_p(\mathbf{y}), \\ \quad \quad \quad \text{(triangle inequality)} \\ \mathcal{L}_p(\alpha \mathbf{x}) = |\alpha| \mathcal{L}_p(\mathbf{x}) \end{cases}$$

Exercise: L02/cost_function.ipynb

Data-flow model for supervised learning



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

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

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

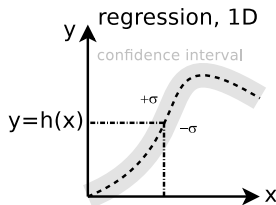
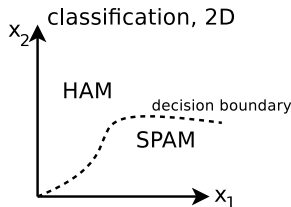
$$\text{cost function: } J(\mathbf{X}, \mathbf{y}_{true}; \theta) \propto \frac{1}{2} \|\mathbf{y}_{pred} - \mathbf{y}_{true}\|_2^2 \propto \text{MSE}$$

Classification vs. Regression

Given the following hypothesis function

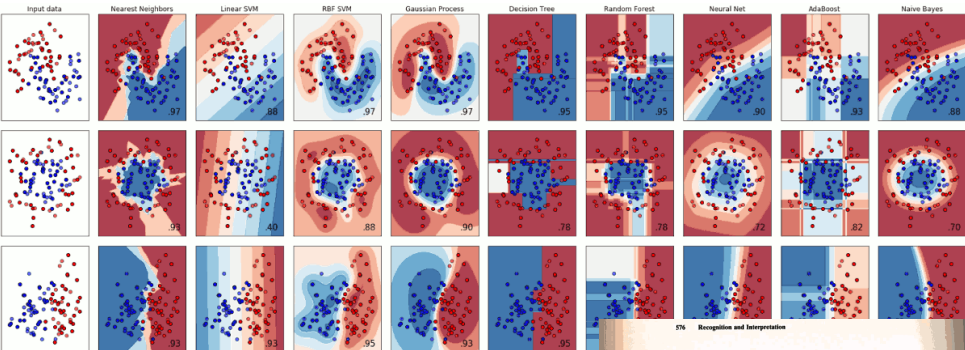
$$h(\mathbf{x}) \rightarrow y$$

- ▶ 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



576 Recognition and Interpretation

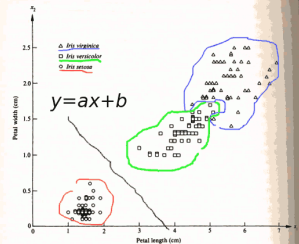


Figure 9.2 Two measurements performed on three types of iris. (Adapted from Duda et al., 1997)

'Demo' datasæt

MNIST, Iris og Moon

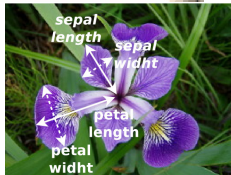
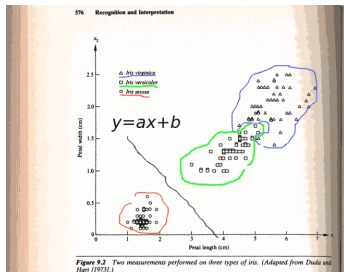
Iris:

Sepal/petal længde/bredde,

Mr. Fisher, 1936,

"Anderson's Iris data set"

`sklearn.datasets.load_iris(..)`



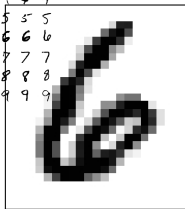
MNIST:

Håndskrevne tal,

preprocesseret, centrerede,

`sklearn.datasets.fetch_openml('mnist_784'..)`

0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
4 4 4 4 4 4 4 4 4 4 4 4 4 4 4
5 5 5 5 5 5 5 5 5 5 5 5 5 5 5
6 6 6 6 6 6 6 6 6 6 6 6 6 6 6
7 7 7 7 7 7 7 7 7 7 7 7 7 7 7
8 8 8 8 8 8 8 8 8 8 8 8 8 8 8
9 9 9 9 9 9 9 9 9 9 9 9 9 9 9

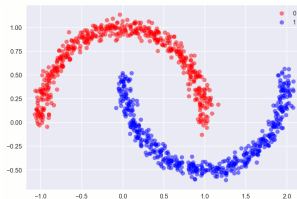


Moon:

'XOR' lign.,

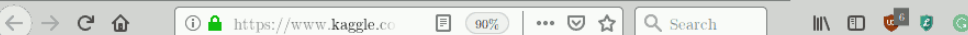
non-linear decision boundary,

`sklearn.datasets.make_moons(..)`



'Dit' datasæet

Fra <https://www.kaggle.com...>



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Competitions

Datasets

Kernels

Discussion

Learn



Sign i

Dataset

Beer Consumption - Sao Paulo

Predict beer consumption



Don George · updated 3 months ago (Version 2)

Data

Overview

Kernels (8)

Discussion (1)

Activity

Download (5 KB)

New Kernel



Data (5 KB)



Data Sources

Consumo_cerveja.csv 941 x 7

About this file

Beer is one of the most democratic and consumed drinks in the world. Not without reason, it is perfect for almost every situation, from happy hour to

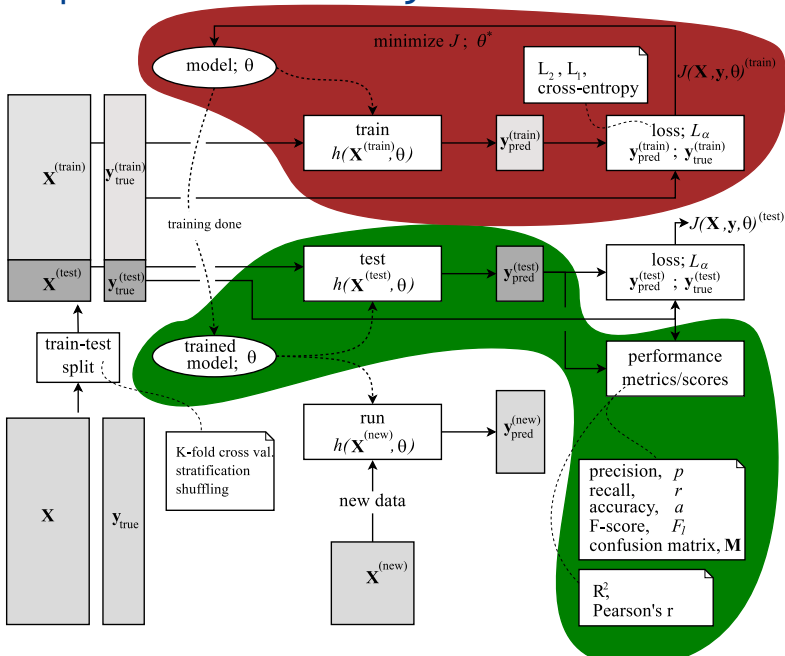
Columns

Data

Temperatura Media (C)

Temperatura Minima (C)

ML Supervised Learning, Train/Test



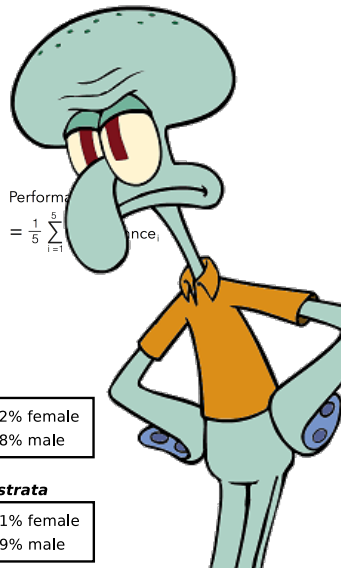
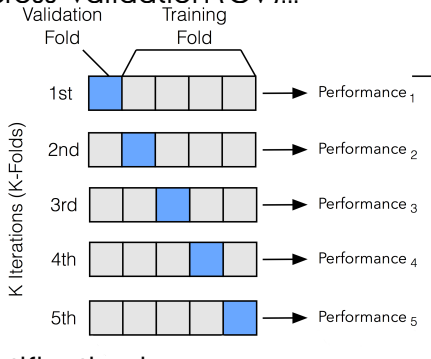
Fundamental supervised learning-proces

- i) Forbered data:
 - ▶ manuel preprocessing + visualisering (støj, outliers..)
 - ▶ label \mathbf{y}_{true} 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

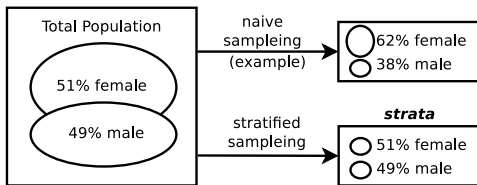
Bemærk: mere preprocess og k-fold cross-validation i L06, koncepter II..

K-fold cross-validation (CV)...



$$\text{Performance} = \frac{1}{5} \sum_{i=1}^5 \text{Performance}_i$$

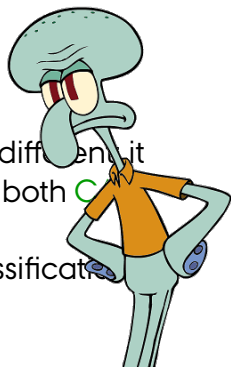
and stratification is...



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 different, it can categorize item into more classes, say both CAT and DOG!
- ▶ ...and Multioutput/multilabel multiclass classification



The Scikit-learn Fit-Predict Interface



Supervised Classification in practice

*The API has one predominant object: **the estimator**.*

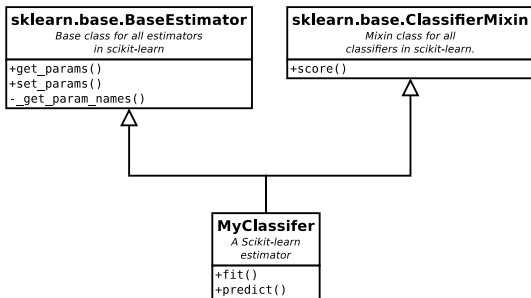


An estimator is an object that fits a model based on some training data and is capable of inferring some properties on new data. It can be, for instance, a classifier or a regressor.

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 funcs can still be accessed via a hack?!

...src file: `/opt/anaconda3/pkgs/.../sklearn/base.py`

The Scikit-learn Fit-Predict Interface



Demo..

Implementing an estimator via a python class as simple as

```
1 class ParadoxClassifier(BaseEstimator, ClassifierMixin):
2     def fit(self, X, y=None):
3         pass
4     def predict(self, X):
5         assert X.ndim==2
6         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.

The screenshot shows a Jupyter Notebook interface with the title 'dummy_classifier'. The browser address bar indicates the file is located at 'localhost:8889/notebooks/Downloads/dummy_classifier.ipynb'. The notebook has a code cell with the following content:

```
In [ ]: # TODO: add your code here..
        assert False, "TODO: solve Qb, and remove me.."
```

Below the code cell, the text reads: **Qc Implement a dummy binary classifier**. This is followed by an explanation: "Now we will try to create a Scikit-learn compatible estimator implemented via a python class. Follow the code found in [HOML], p84, but name you estimator `DummyClassifier` instead of `Never5Classifier`."

Then, it states: "Here our Python class knowledge comes into play. The estimator class hierarchy looks like".

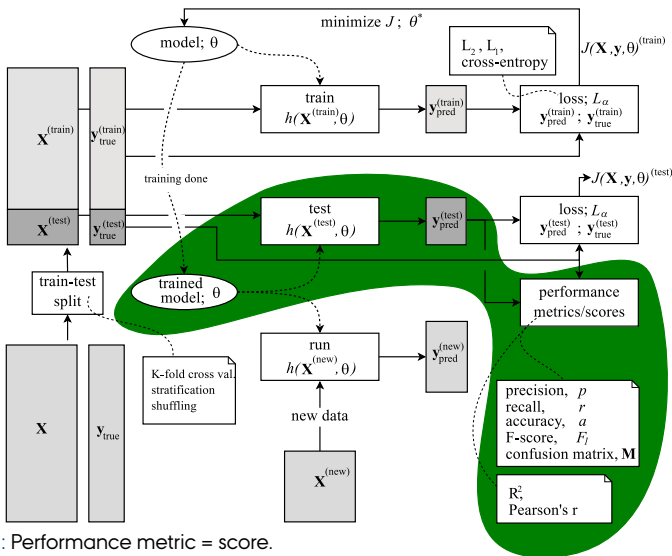
A class hierarchy diagram is shown below the text. It consists of three boxes representing classes:

- sklearn.base.BaseEstimator**: Base class for all estimators in scikit-learn. Methods: `+get_params()`, `+set_params()`, `- get_param_names()`.
- sklearn.base.ClassifierMixin**: Mixin class for all classifiers in scikit-learn. Method: `+score()`.
- MyClassifier**: A Scikit-learn estimator. Methods: `+fit()`, `+predict()`.

Arrows indicate the inheritance relationships: `MyClassifier` inherits from both `BaseEstimator` and `ClassifierMixin`.

Evaluér på test-data: Performance metrics

Kort intro til konceptet *performance metrics*.



NOTE₀: Performance metric = score.

NOTE₁: 'Performance measure' begreb bruges ikke, kun score eller perf. metric.

NOTE₂: Loss er ML algo'ens 'performance mål', score er vores evalueringsmål.

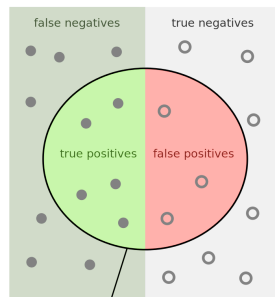
Exercise: L02/performance_metrics.ipynb

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]

Exercise: L02/performance_metrics.ipynb

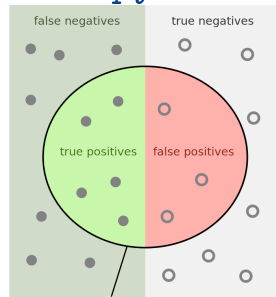
Precision, recall and accuracy, F_1 -score, and confusion matrix

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



Precision = $\frac{\text{true positives}}{\text{true positives} + \text{false positives}}$

Recall = $\frac{\text{true positives}}{\text{true positives} + \text{false negatives}}$

Confusion Matrix, $\mathbf{M}_{\text{confusion}} =$

	actual true	actual false
predicted true	TP	FP
predicted false	FN	TN


NOTE₀: you can compare precision... F_1 -score, but not necessarily the cost, J .

NOTE₁: beware of matrix transpose and interpretation of 'TP/TN'!

Exercise: L02/performance_metrics.ipynb

Nomenclature for the Confusion Matrix

		True condition			
		Condition positive	Condition negative	Prevalence $= \frac{\Sigma \text{Condition positive}}{\Sigma \text{Total population}}$	Accuracy (ACC) = $\frac{\Sigma \text{True positive} + \Sigma \text{True negative}}{\Sigma \text{Total population}}$
Predicted condition	Predicted condition positive	True positive, Power	False positive, Type I error	Positive predictive value (PPV), Precision = $\frac{\Sigma \text{True positive}}{\Sigma \text{Predicted condition positive}}$	False discovery rate (FDR) = $\frac{\Sigma \text{False positive}}{\Sigma \text{Predicted condition positive}}$
	Predicted condition negative	False negative, Type II error	True negative	False omission rate (FOR) $= \frac{\Sigma \text{False negative}}{\Sigma \text{Predicted condition negative}}$	Negative predictive value (NPV) = $\frac{\Sigma \text{True negative}}{\Sigma \text{Predicted condition negative}}$
		True positive rate (TPR), Recall, Sensitivity, probability of detection $= \frac{\Sigma \text{True positive}}{\Sigma \text{Condition positive}}$	False positive rate (FPR), Fall-out, probability of false alarm $= \frac{\Sigma \text{False positive}}{\Sigma \text{Condition negative}}$	Positive likelihood ratio (LR+) $= \frac{\text{TPR}}{\text{FPR}}$	Diagnostic odds ratio (DOR) $= \frac{\text{LR+}}{\text{LR-}}$ F1 score = $\frac{2}{\frac{1}{\text{Recall}} + \frac{1}{\text{Precision}}}$
		False negative rate (FNR), Miss rate $= \frac{\Sigma \text{False negative}}{\Sigma \text{Condition positive}}$	True negative rate (TNR), Specificity (SPC) $= \frac{\Sigma \text{True negative}}{\Sigma \text{Condition negative}}$	Negative likelihood ratio (LR-) $= \frac{\text{FNR}}{\text{TNR}}$	

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

Exercise: L02/performance_metrics.ipynb

Accuracy Paradox...

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

Test via the breast cancer Wisconsin dataset..

```
1 print(f" X.shape={X.shape}, y_true.shape={y_true.shape}")
2 X_train, X_test, y_train, y_test = train_test_split(
3     X, y_true, test_size=0.2, shuffle=True, random_state= 42)
```

```
4
5 clf = ParadoxClassifier()
6 clf.fit(X_train, y_train)
7 y_pred = clf.predict(X_test)
```

prints: acc=0.6228070175438597,
N=114

```
8
9 acc = accuracy_score(y_test, y_pred)
10 print(f' acc={acc}, N={y_pred.shape[0]}')
11 score = clf.score(X_test, y_test)
12 print(f' clf.score()={score} (same as accuracy_score)')
```

NOTE₀: for MNIST, a dum classify as '5' $\sim a = 10\%$

NOTE₁: for MNIST, a dum classify not-as '5' $\sim a = 90\%$

Exercise: L02/performance_metrics.ipynb

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 further details.

<code>metrics.accuracy_score(y_true, y_pred[, ...])</code>	Accuracy classification score.
<code>metrics.auc(x, y[, reorder])</code>	Compute Area Under the Curve (AUC) using the trapezoidal rule
<code>metrics.average_precision_score(y_true, y_score)</code>	Compute average precision (AP) from prediction scores
<code>metrics.balanced_accuracy_score(y_true, y_pred)</code>	Compute the balanced accuracy
<code>metrics.brier_score_loss(y_true, y_prob[, ...])</code>	Compute the Brier score.
<code>metrics.classification_report(y_true, y_pred)</code>	Build a text report showing the main classification metrics
<code>metrics.cohen_kappa_score(y1, y2[, labels, ...])</code>	Cohen's kappa: a statistic that measures Inter-annotator agreement.
<code>metrics.confusion_matrix(y_true, y_pred[, ...])</code>	Compute confusion matrix to evaluate the accuracy of a classification
<code>metrics.f1_score(y_true, y_pred[, labels, ...])</code>	Compute the F1 score, also known as balanced F-score or F-measure
<code>metrics.fbeta_score(y_true, y_pred, beta[, ...])</code>	Compute the F-beta score
<code>metrics.hamming_loss(y_true, y_pred[, ...])</code>	Compute the average Hamming loss.
<code>metrics.hinge_loss(y_true, pred_decision[, ...])</code>	Average hinge loss (non-regularized)
<code>metrics.jaccard_similarity_score(y_true, y_pred)</code>	Jaccard similarity coefficient score
<code>metrics.log_loss(y_true, y_pred[, eps, ...])</code>	Log loss, aka logistic loss or cross-entropy loss.
<code>metrics.matthews_corrcoef(y_true, y_pred[, ...])</code>	Compute the Matthews correlation coefficient (MCC)
<code>metrics.precision_recall_curve(y_true, ...)</code>	Compute precision-recall pairs for different probability thresholds
<code>metrics.precision_recall_fscore_support(...)</code>	Compute precision, recall, F-measure and support for each class

