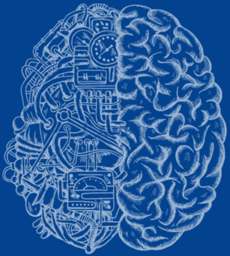
AARHUS
UNIVERSITY
SCHOOL OF ENGINEERING

MACHINE LEARNING

LESSON 4: Training I

CARSTEN EIE FRIGAARD

SPRING 2019



LESSON:4 Training I

Agenda

- Exercise from L03:
  Exercise: `L03/metrics.ipynb`
- L04 Training I: *Training a linear regression model*
  Exercise: `L04/linear_regression_1.ipynb`
  Exercise: `L04/linear_regression_2.ipynb`
- After the class:
  yet another WIKI page,
  deadline *L06*, 05-03-2019 (in two weeks).
- Next lesson: L05 Training II:
  Training and model concepts
- NOTE: on page # in [HOML]
  ...up to 7 editions.

Editor: Nicole Tache
Production Editor: Nicholas Adams
Copyeditor: Rachel Monaghan
Proofreader: Charles Roumeliotis

March 2017: First Edition

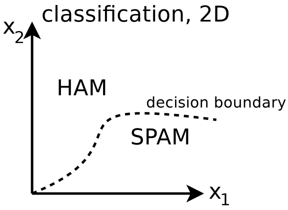
Revision History for the First Edition
2017-03-10: First Release

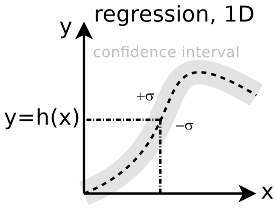
RESUMÉ: Classification vs. Regression

Given the following

$$h : \mathbf{x} \rightarrow y$$

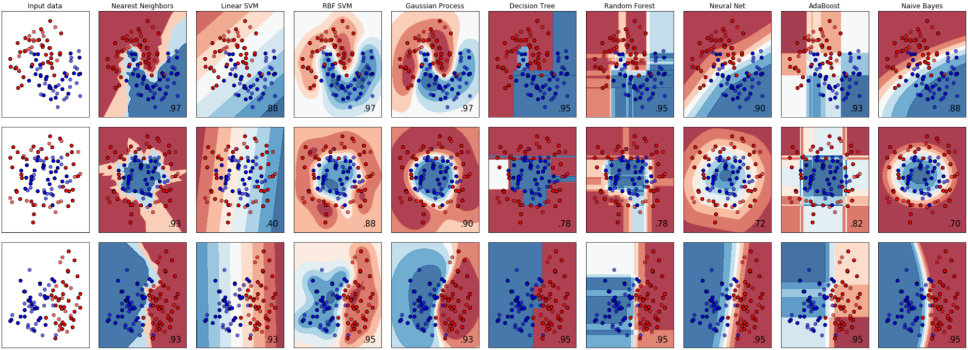
- if y is discrete/categorical variable, then this is **classification** probl
- if y is real number/continuous, then this is a **regression** problem.





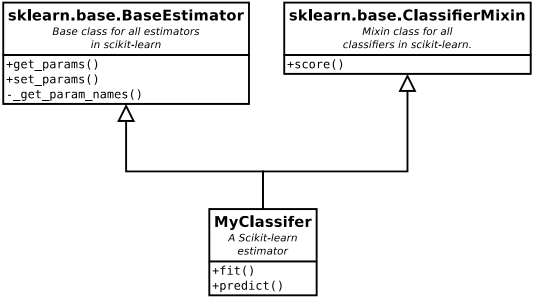
RESUMÉ: Classification

Decision Boundaries for different Models and Datasets



Souce code: `L03/Extra/plot_classifier_comparison.ipynb` in [GITMAL].

RESUMÉ: 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`

RESUMÉ: Exercise:

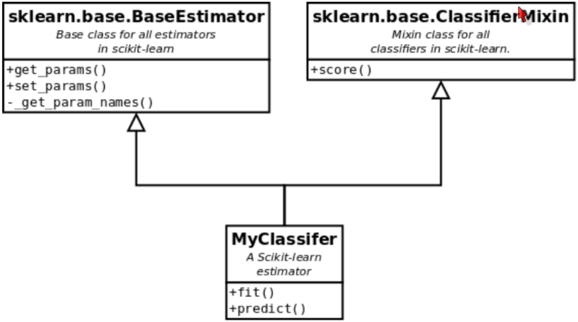
`L03/dummy_classifier.ipynb`

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

Qb Implement a dummy binary classifier

Follow the code found in [HOML], p84, but name you estimator `DummyClassifier` instead of `Never5Classifyer`.

Here our Python class knowledge comes into play. The estimator class hierarchy looks like



All Scikit-learn classifiers inherit form `BaseEstimator` (and possible also `ClassifierMixin`), and they must have a `fit-predict` function pair (strangely not in the

Exercise: `L03/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

Exercise: `L03/metrics.ipynb`

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

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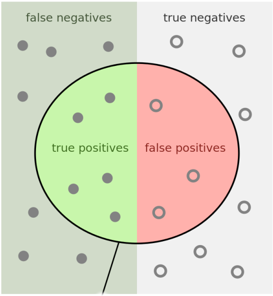

[https://en.wikipedia.org/wiki/Precision_and_recall]

Exercise: `L03/metrics.ipynb`

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

$$
\begin{aligned}
&\text{precision,} && p && = \frac{TP}{TP+FP} \\
&\text{recall (or sensitivity),} && r && = \frac{TP}{TP+FN} \\
&\text{accuracy,} && a && = \frac{TP+TN}{TP+TN+FP+FN} \\
&F_1\text{-score,} && F_1 && = \frac{2pr}{p+r}
\end{aligned}
$$

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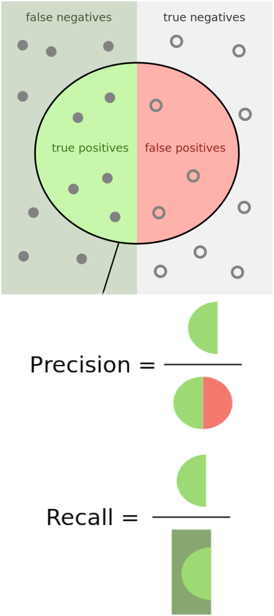

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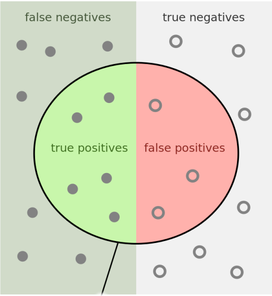

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$$

Precision =

Recall =

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

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

NOTE$_0$: you can *compare* precision...F_1-score, but not necessarily the cost, J.
NOTE$_1$: beware of matrix transpose and interpretation of *'TP/TN'*!

Exercise: `L03/metrics.ipynb`

Nomenclature for the Confusion Matrix

		True condition				
	Total population	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) $= \frac{\text{LR+}}{\text{LR}-}$	F_1 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−) $= \frac{\text{FNR}}{\text{TNR}}$		

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Mr. Itmal (): *prevalence, positive predictive value*, etc. not important to know in detail!

Exercise: `L03/metrics.ipynb`

Accuracy Paradox...

```python
class ParadoxClassifier(BaseEstimator):
    def fit(self, X, y=None):
        pass
    def predict(self, X):
        return np.ones(len(X),dtype=bool)
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Test via the breast cancer Wisconsin dataset...

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```python
X, y_true = load_breast_cancer(return_X_y=True)

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()
clf.fit(X_train, y_train)
y_pred = clf.predict(X_test)

a = accuracy_score(y_pred, y_test)
print('  acc=', a, ', N=', y_pred.shape[0])
```

Exercise: L03/metrics.ipynb

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```

prints: `acc= 0.6228070175438597 , N= 114`

NOTE$_0$: for MNIST, a dum classify as '5' $\sim a = 10\%$

NOTE$_1$: for MNIST, a dum classify not-as '5' $\sim a = 90\%$

Training a Linear Regressor

Linear Regression: In one dimension

The well know linear equation

$$y(x) = \alpha x + \beta$$

or changing some of the symbol names, so that $h(\mathbf{x}; \mathbf{w})$ means the **predicted** value from x for a parameter set $\mathbf{w}$, via the hypothesis function

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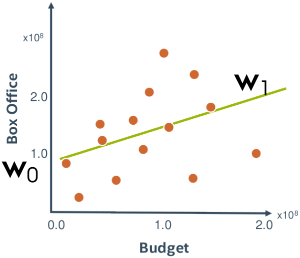

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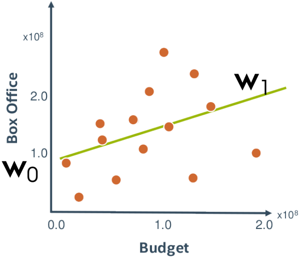

Question: how do we find the $\mathbf{w}_n$'s?

Training a Linear Regressor

Linear Regression: Hypotheis Function in N-dimensions

For 1-D:

$$h(x^{(i)}; w) = w_0 + w_1 x^{(i)}$$

Training a Linear Regressor

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The same for N-D:

$$\begin{aligned} h(\mathbf{x}^{(i)}; \mathbf{w}) &= \mathbf{w}^\top \begin{bmatrix} 1 \\ \mathbf{x}^{(i)} \end{bmatrix} \\ &= w_0 + w_1 x_1^{(i)} + w_2 x_2^{(i)} + \cdots + w_d x_d^{(i)} \end{aligned}$$

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and to ease notation we always prepend $\mathbf{x}$ with a 1 as

$$\begin{bmatrix} 1 \\ \mathbf{x}^{(i)} \end{bmatrix} \mapsto \mathbf{x}^{(i)}, \quad \text{by convention in the following...}$$

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$$\begin{bmatrix} 1 \\ \mathbf{x}^{(i)} \end{bmatrix} \mapsto \mathbf{x}^{(i)}, \quad \text{by convention in the following...}$$

yielding the vector form of the hypothesis function

$$h(\mathbf{x}^{(i)}; \mathbf{w}) = \mathbf{w}^\top \mathbf{x}^{(i)}$$

Training a Linear Regressor

Linear Regression: Loss or Objective Function

Individual loss, via a square difference

$$\begin{aligned} L^{(i)} &= \left(h(\mathbf{x}^{(i)}; \mathbf{w}) - y^{(i)}\right)^2 \\ &= \left(\mathbf{w}^\top \mathbf{x}^{(i)} - y^{(i)}\right)^2 \end{aligned}$$

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and to minimize all the $L^{(i)}$ losses (or indirectly also the MSE or RMSE) is to minimize the sum of all the individual costs, via the total cost function J

$$\begin{aligned} \text{MSE}(\mathbf{X}, \mathbf{y}; \mathbf{w}) &= \frac{1}{n} \sum_{i=1}^{n} L^{(i)} \\ &= \frac{1}{n} \sum_{i=1}^{n} \left(\mathbf{w}^\top \mathbf{x}^{(i)} - y^{(i)}\right)^2 \\ &= \frac{1}{n} ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2 \end{aligned}$$

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&= \frac{1}{n} ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2
\end{aligned}
$$

Ignoring constant factors, this yields our linear regression cost function

$$
\begin{aligned}
J &= \frac{1}{2} ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2 \\
&\propto \mathrm{MSE}
\end{aligned}
$$

Training a Linear Regressor

Minimizing the Linear Regression: The `argmin` concept

Our linear regression cost function was

$$J(\mathbf{X}, \mathbf{y}; \mathbf{w}) = \frac{1}{2} \left|\left|\mathbf{X}\mathbf{w} - \mathbf{y}\right|\right|_2^2$$

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$$J(\mathbf{X}, \mathbf{y}; \mathbf{w}) = \frac{1}{2} \, ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2$$

and training amounts to finding a value of $\mathbf{w}$, that minimizes J. This is denoted as

$$\begin{aligned} \mathbf{w}^* &= \mathrm{argmin}_{\mathbf{w}} \, J(\mathbf{X}, \mathbf{y}; \mathbf{w}) \\ &= \mathrm{argmin}_{\mathbf{w}} \, \tfrac{1}{2} \, ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2 \end{aligned}$$

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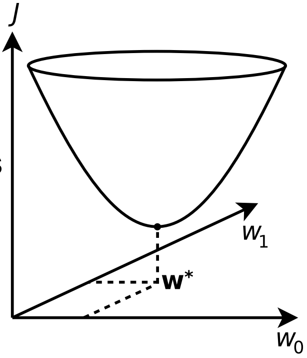

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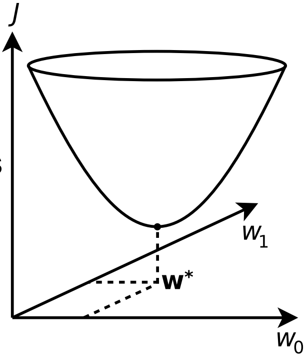

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and by minima, we naturally hope for

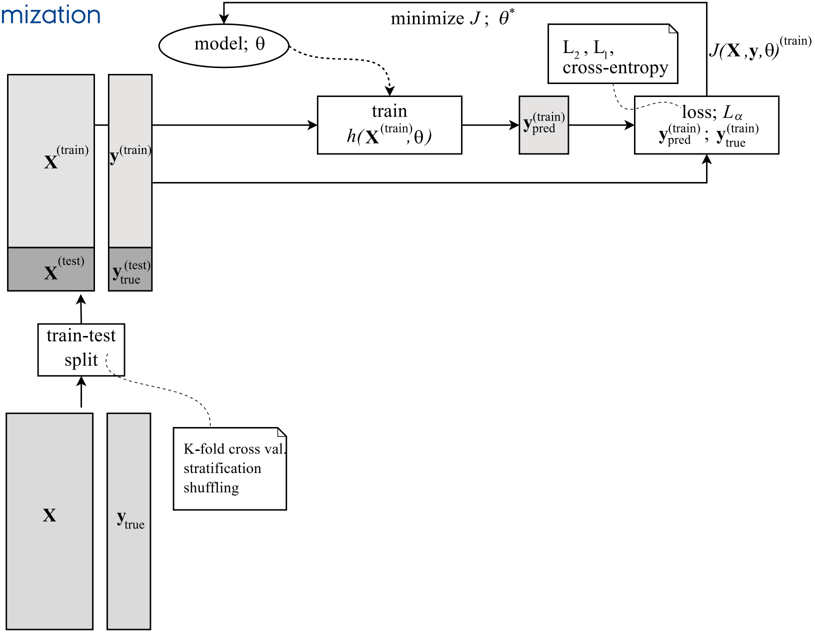
- the global minumum

thought for non-linear models this cannot be guarantied, hitting some

- local minimum

Training in General

Minimization



Training in General

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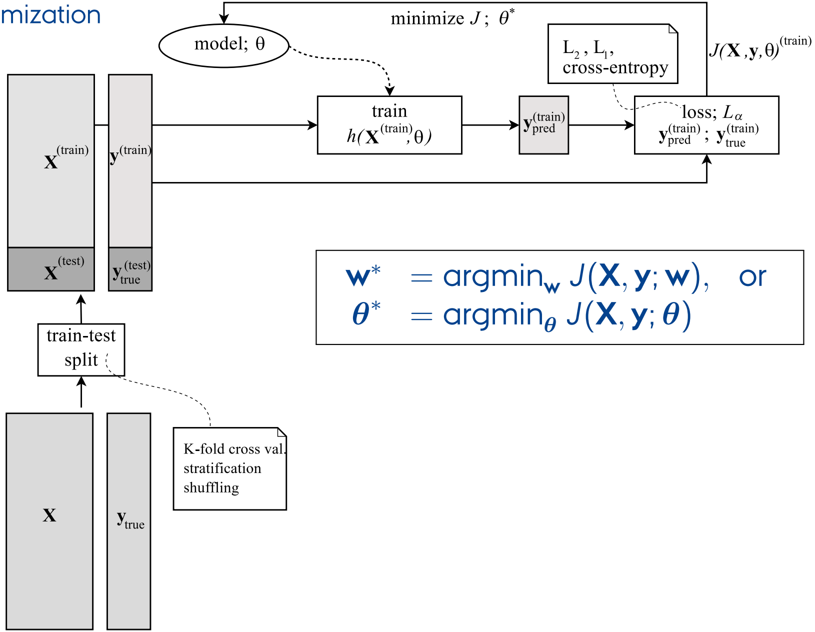

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\mathbf{w}^* &= \operatorname{argmin}_{\mathbf{w}} J(\mathbf{X}, \mathbf{y}; \mathbf{w}), \quad \text{or} \\
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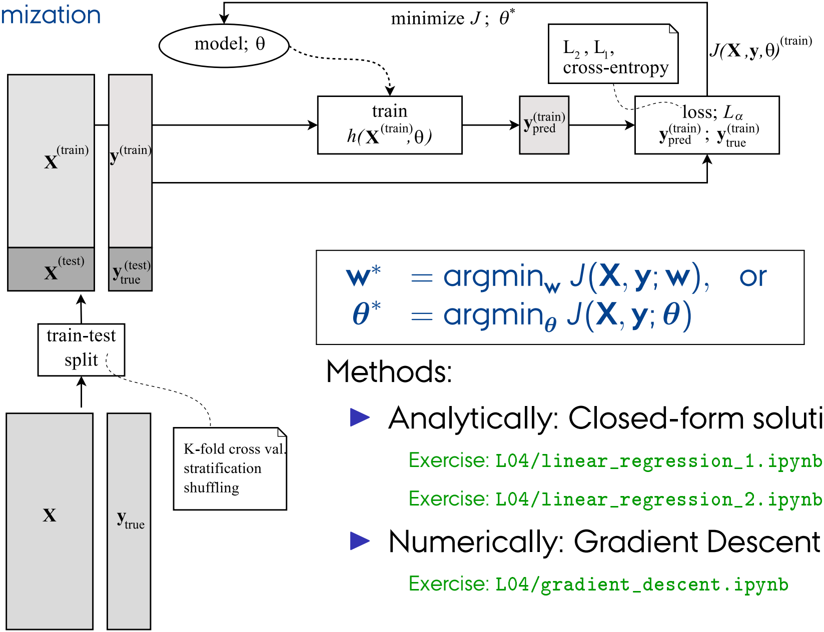
Training in General

Minimization



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Methods:

- Analytically: Closed-form solution

  Exercise: `L04/linear_regression_1.ipynb`

  Exercise: `L04/linear_regression_2.ipynb`

- Numerically: Gradient Descent

  Exercise: `L04/gradient_descent.ipynb`

Exercise: `L04/linear_regression_1.ipynb`

Training: The Closed-form Linear-Least-Squares Solution

To solve for $\mathbf{w}^*$ in closed form, we find the gradient of J with respect to $\mathbf{w}$

$$\nabla_{\mathbf{w}} J = \left[\frac{\partial J}{\partial w_1}, \frac{\partial J}{\partial w_2}, \ldots, \frac{\partial J}{\partial w_m}\right]^\top$$

Exercise: `L04/linear_regression_1.ipynb`

Training: The Closed-form Linear-Least-Squares Solution

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$$\nabla_{\mathbf{w}} J = \left[\frac{\partial J}{\partial w_1}, \frac{\partial J}{\partial w_2}, \ldots, \frac{\partial J}{\partial w_m}\right]^\top$$

Taking the partial deriverty $\partial/\partial_{\mathbf{w}}$ of the J via the gradient (nabla) operator

$$\begin{aligned}\nabla_{\mathbf{w}} J(\mathbf{X}, \mathbf{y}; \mathbf{w}) &= \mathbf{X}^\top (\mathbf{X}\mathbf{w} - \mathbf{y}) \; = \; 0 \\ 0 &= \mathbf{X}^\top \mathbf{X}\mathbf{w} - \mathbf{X}^\top \mathbf{y}\end{aligned}$$

Exercise: `L04/linear_regression_1.ipynb`

Training: The Closed-form Linear-Least-Squares Solution

To solve for $\mathbf{w}^*$ in closed form, we find the gradient of J with respect to $\mathbf{w}$

$$\nabla_{\mathbf{w}} J = \left[\frac{\partial J}{\partial w_1}, \frac{\partial J}{\partial w_2}, \ldots, \frac{\partial J}{\partial w_m}\right]^\top$$

Taking the partial deriverty $\partial/\partial_{\mathbf{w}}$ of the J via the gradient (nabla) operator

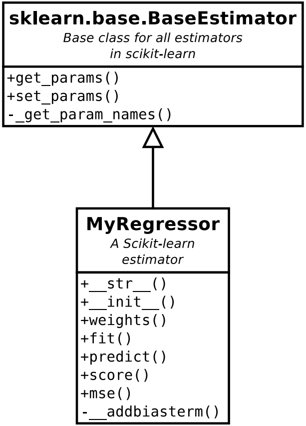
$$\begin{aligned} \nabla_{\mathbf{w}} J(\mathbf{X}, \mathbf{y}; \mathbf{w}) &= \mathbf{X}^\top (\mathbf{X}\mathbf{w} - \mathbf{y}) \; = \; 0 \\ 0 &= \mathbf{X}^\top \mathbf{X}\mathbf{w} - \mathbf{X}^\top \mathbf{y} \end{aligned}$$

with a small amount of matrix algegra, this gives the closed-form solution

$$\begin{aligned} \mathbf{w}^* &= \mathrm{argmin}_{\mathbf{w}} \tfrac{1}{2} ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2 \\ &= \left(\mathbf{X}^\top \mathbf{X}\right)^{-1} \mathbf{X}^\top \mathbf{y} \end{aligned}$$

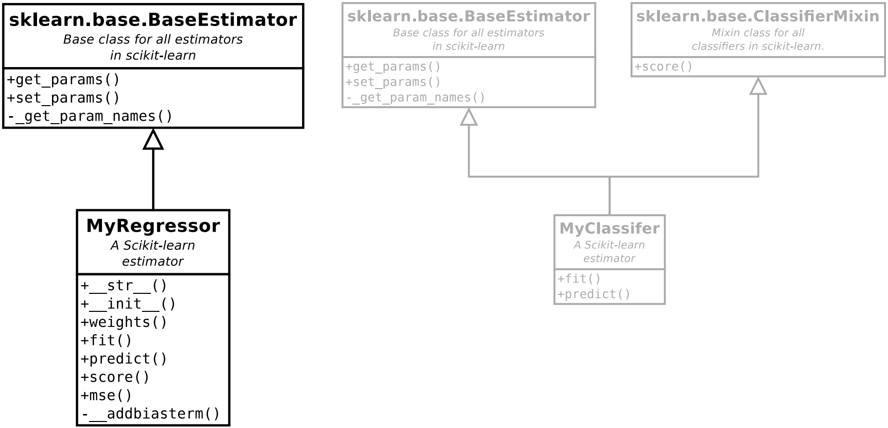
Exercise: L04/linear_regression_2.ipynb

Python class: MyRegressor



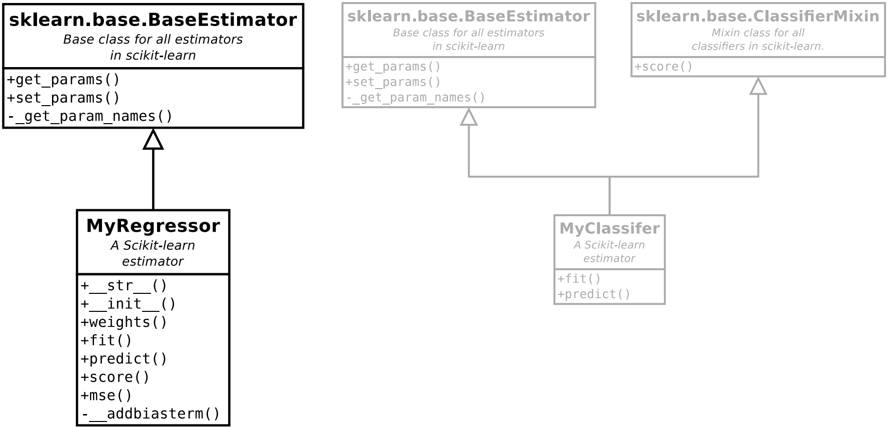
Exercise: `L04/linear_regression_2.ipynb`

Python class: `MyRegressor`



Exercise: `L04/linear_regression_2.ipynb`

Python class: `MyRegressor`



Exercise: create a linear regressor, inheriting from `BaseEstimator` and implement `score()` and `mse()`.

NOTE: no inhering from `ClassifierMixin`.