AARHUS
UNIVERSITY
SCHOOL OF ENGINEERING

MACHINE LEARNING

LESSON 5: Training II

CARSTEN EIE FRIGAARD

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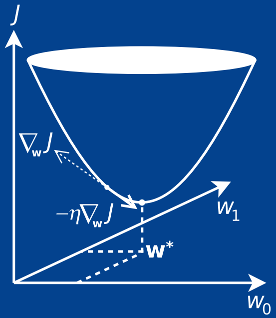


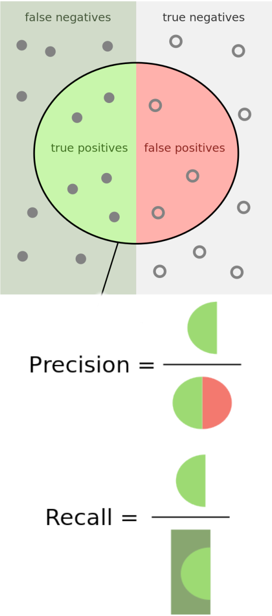
L05: Training II

Agenda

- Important: your feedback (positive as well as negative)...
- Course modification i): *more OPTIONAL* exercices
- Course modification ii): revision to 'Microlearning'
  (only one lecure session, beginning of class)
- Installing `keras` is slow/buggy, see WIKI..
- L04 Training I: Training a linear regression model
  OPTIONAL: Exercise: `L04/linear_regression_1.ipynb`
  OPTIONAL: Exercise: `L04/linear_regression_2.ipynb`
- L05 Training II: **Training and model concepts**
  Exercise: `L05/gradient_descent.ipynb`
  Exercise: `L05/capacity_under_overfitting.ipynb`
  Exercise: `L05/generalization_error.ipynb`
  OPTIONAL: Exercise: `L05/train_test_split.ipynb`

RESUMÉ: Metrics

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



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

Confusion Matrix, binary-class data,

$\mathbf{M}_{\text{confusion}} =$

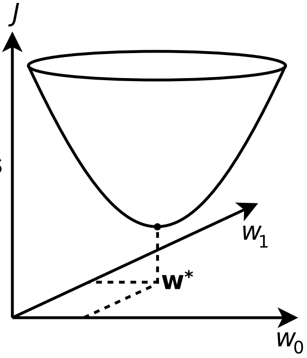
	actual true	actual false
predicted true	TP	FP
predicted false	FN	TN

RESUMÉ: Training a Linear Regressor

Minimizing the Linear Regression: The `argmin` concept

Our linear regression cost function was

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



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

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

and by minima, we naturally hope for

- the global minumum

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

- local minimum

RESUMÉ: `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 $\mathbf{w}$

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

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 algebra, this gives the *normal equation*

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

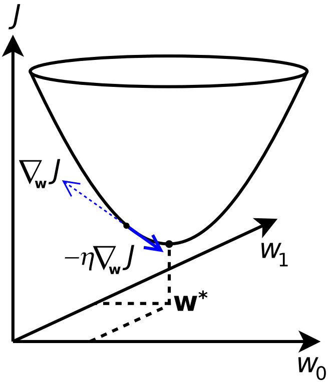
Numerically Solution: Gradient Descent (GD)

The GD Algorithm

First, find the deriverty of J, via $\nabla_{\mathbf{w}} J$, that after some matrix algebra gives

$$\nabla_{\mathbf{w}} J(\mathbf{w}) = \frac{2}{m}\mathbf{X}^{\top}\left(\mathbf{X}\mathbf{w} - \mathbf{y}^{(i)}\right)$$

Then move along in the *opposite* direction of this gradient, taking a step of size η



$$\mathbf{w}^{(step\ N+1)} = \mathbf{w}^{(step\ N)} - \eta\nabla_{\mathbf{w}} J(\mathbf{w})$$

The SG-algo in python code

```
for iteration in range(n_iterations):
    gradients=2/m*X_b.T.dot(X_b.dot(theta)-y)
    theta=theta - eta * gradients
```

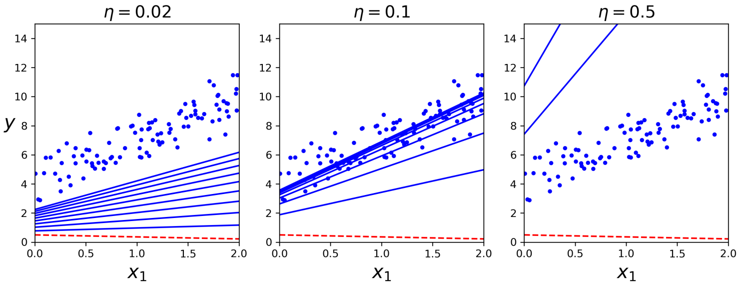
NOTE: The `X_b` is a `X` with a all-1 column prepended, and using the contant factor $2/m$ instead of just $1/2$ and with $\mathbf{w} = \boldsymbol{\theta}$

Learning rate, η

And understanding Scikit-learn's `SGDRegressor`

Scikit-learn η updating schemes:

constant, adaptive, invscaling, optimal



The `SGDRegressor` in Scikit-learn has a *hyperparameter* for this

```
learning_rate:  string, optional
'invscaling':[default], eta=eta0/pow(t,power_t)
```

Learning rate, η

And understanding Scikit-learn's `SGDRegressor`

The `SGDRegressor` constructor in Scikit-learn

```
class sklearn.linear_model.SGDRegressor(
  loss     ='squared_loss', penalty      ='l2',
  alpha    =0.0001,         l1_ratio     =0.15,
  tol      =None,           shuffle      =True,
  verbose  =0,              epsilon      =0.1,
  eta0     =0.01,           power_t      =0.25,
  n_iter_no_change=5,       warm_start   =False,
  fit_intercept   =True,    max_iter     =None,
  average         =False,   n_iter       =None
  random_state    =None,    learning_rate='invscaling',
  early_stopping =False,    validation_fraction=0.1
)
```

Important for now...

- `loss`, `penalty` (our MSE and $\mathcal{L}_2$ norm),
- `eta`, `learning_rate`,
- `shuffle` `early_stopping`,
- and perhaps `random_state`.

Stochastic Gradient Descent (SGD) Method

Exercise: `gradient_descent.ipynb`

The problem with the GD Algorithm, it takes $\mathbf{X}$ as input, the complete dataset

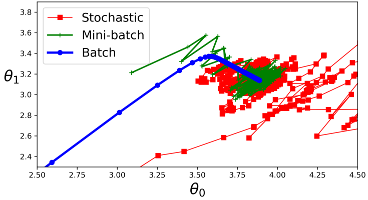
$$\nabla_{\mathbf{w}} J(\mathbf{w}) = \frac{2}{m}\mathbf{X}^{\top}\left(\mathbf{X}\mathbf{w} - \mathbf{y}\right)$$

That's a big mouthful to matrix transpose and multiply!

Introducing a per-data-sample, or stochastic, method

$$\nabla_{\mathbf{w}} J(\mathbf{w})^{(i)} = \frac{2}{m}\mathbf{x}^{(i)\top}\left(\mathbf{x}^{(i)}\mathbf{w} - \mathbf{y}\right)$$

```
for epoch in range(n_epochs):
  for i in range(m):
    .
    .
    .
    grads = 2*xi.T.dot(xi.dot(theta)-yi)
    eta   = ...
    theta = ...
```



Model capacity and under/overfitting

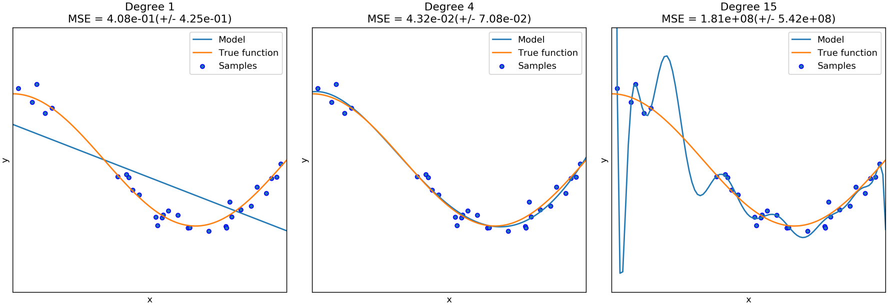
Exercise: `capacity_under_overfitting.ipynb`

Dummy and Paradox classifier:

capacity fixed ~ 0, cannot generalize at all!

Linear regression for a polynomial model:

capacity $\sim$ degree of polynomial, x^n

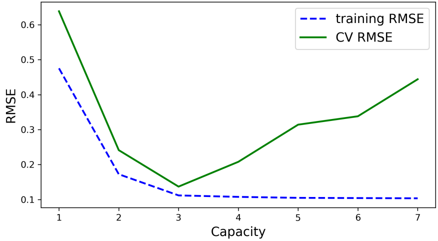


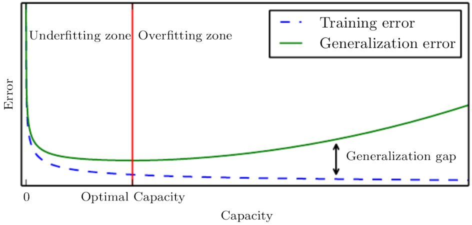
- underfitting: capacity of model too low,
- overfitting: capacity to high.

Generalization Error

Exercise: `generalization_error.ipynb`

RMSE-capacity plot for lin. reg. with polynomial features
(capacity = degree of poly)





Inspecting the plots from [HOML] and [DL], extracting the concepts

- training/generalization error,
- underfit/overfit zone,
- generalization gab,
- optimal capacity (best-model, early stop).