AARHUS UNIVERSITY
SCHOOL OF ENGINEERING

LESSON 5: Regression og SGD (and Training)

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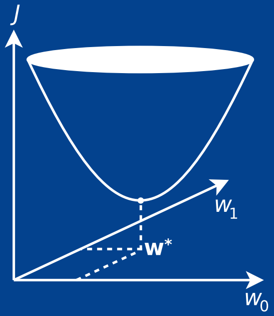
SPRING 2022



L05: Regression og SGD (and Training)

Agenda

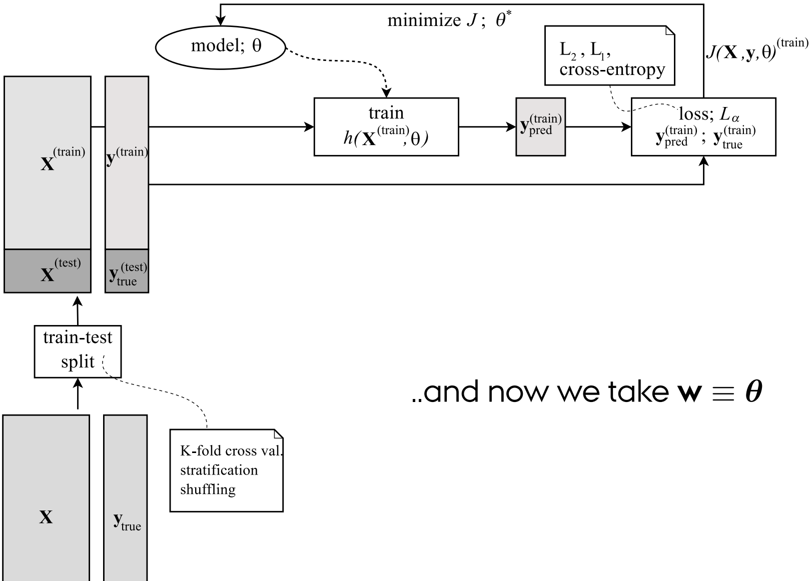
- Training a linear regression model,
  - (and intro to GD)
- Cost function in closed-form vs. numerical solutions.
  - Opgave: `L05/linear_regression_1.ipynb`
  - Opgave: `L05/linear_regression_2.ipynb` [OPTIONAL]
- Gradient Descent (GD),
  - Learning rates,
  - Batch Gradient Descent (GD),
  - Stochastic Gradient Descent (SGD),
  - Mini-batch Gradient Descent.

  - Opgave: `L05/gradient_descent.ipynb`

TRAINING A LINEAR REGRESSOR

Training in General

Training is minimization of J (optimization)



..and now we take $\mathbf{w} \equiv \boldsymbol{\theta}$

Training a Linear Regressor

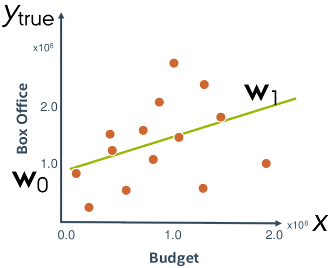
Linear Regression: In one dimension

The well know linear equation

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

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

$$h(x; \mathbf{w}) \quad \stackrel{1D}{=} w_0 + w_1 x$$



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

Training a Linear Regressor

Linear Regression: Hypotheis Function in N-dimensions

For 1-D:

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

The same for N-D:

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

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

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

yielding the vector form of the hypothesis function

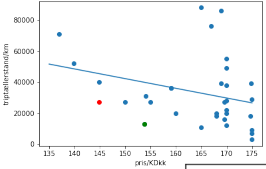
$$\boxed{h(\mathbf{x}^{(i)}; \mathbf{w}) = \mathbf{w}^\top \mathbf{x}^{(i)}}$$

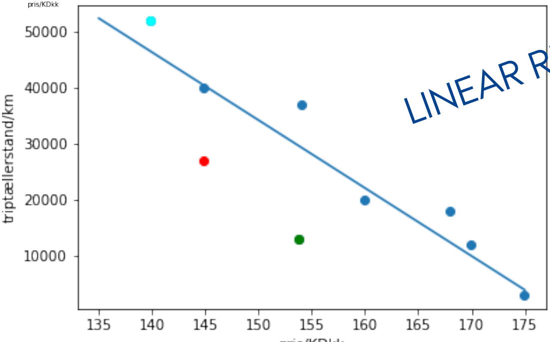
Training a Linear Regressor

Case study: a new car..

Scrabe `[bilbasen.dk]`, for particuar e-Golf.

Features: total tripdistance/km and price/KDkk..





LINEAR REGRESSOR

Training a Linear Regressor

Linear Regression: Loss or Objective Function

Individual loss, via a square difference ($L = \mathcal{L}_2^2$)

$$
\begin{aligned}
L^{(i)} &= ||y_{\text{pred}}^{(i)} - y^{(i)}||_2^2 \\
&= \left(h(\mathbf{x}^{(i)}; \mathbf{w}) - y^{(i)}\right)^2 \\
&= \left(\mathbf{w}^\top \mathbf{x}^{(i)} - y^{(i)}\right)^2
\end{aligned}
$$

$y \equiv y_{\text{true}}$ in the following

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

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

Ignoring constant factors, this yields our linear regression cost function

$$
\boxed{J = \frac{1}{2} ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2 \ \propto \text{MSE}}
$$

Training a Linear Regressor

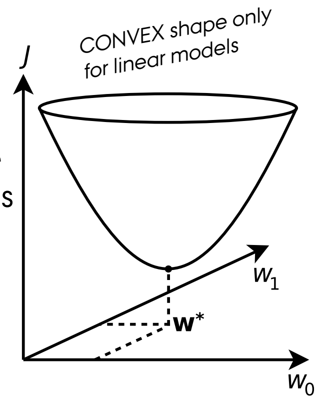
Minimizing the Linear Regression: The `argmin` concept

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

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



and by minima, we naturally hope for

- the global minumum

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

- local minimum

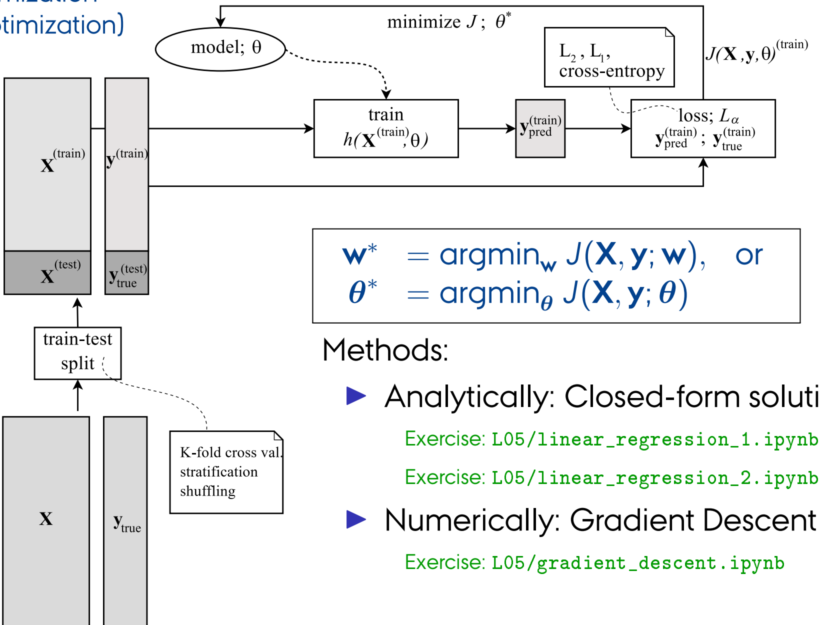
COST FUNCTION MINIMIZATION IN CLOSED-FORM

The Closed-form Linear-Least-Squares Solution

$$\left(\mathbf{X}^\top\mathbf{X}\right)^{-1}\mathbf{X}^\top\mathbf{y}$$

Training in General

Minimization (optimization)



$$
\begin{aligned}
\mathbf{w}^* &= \mathrm{argmin}_{\mathbf{w}}\, J(\mathbf{X},\mathbf{y};\mathbf{w}), \quad \text{or} \\
\boldsymbol{\theta}^* &= \mathrm{argmin}_{\boldsymbol{\theta}}\, J(\mathbf{X},\mathbf{y};\boldsymbol{\theta})
\end{aligned}
$$

Methods:

- Analytically: Closed-form solution

  Exercise: `L05/linear_regression_1.ipynb`

  Exercise: `L05/linear_regression_2.ipynb`

- Numerically: Gradient Descent

  Exercise: `L05/gradient_descent.ipynb`

Exercise: `L05/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

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

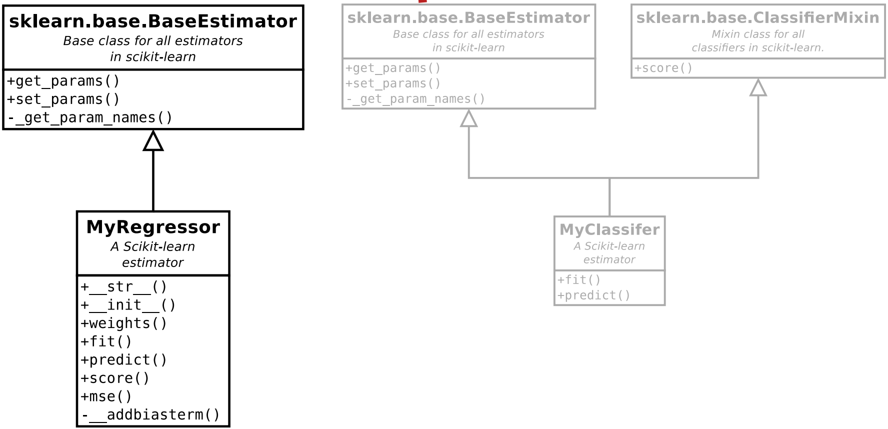
with a small amount of matrix algegra, this gives the *normal equation*

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

Exercise: L05/linear_regression_2.ipynb

[OPTIONAL Exercise]

Python class: MyRegressor

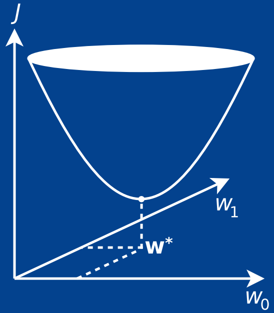


Exercise: create a linear regressor, inheriting from `BaseEstimator` and implement `score()` and `mse()`.

NOTE: no inhering from `ClassifierMixin`.

COST FUNCTION MINIMIZATION VIA NUMERICAL SOLUTIONS

Gradient Descent



(Full) Batch Gradient Descent (GD)

The nabla matrix differentiation, $\nabla_{\mathbf{w}}$, and the learning rate, η

$$
\begin{aligned}
J(\mathbf{X},\mathbf{y};\mathbf{w}) &= \tfrac{1}{2}||\mathbf{X}\mathbf{w}-\mathbf{y}||_2^2 \;\propto \mathrm{MSE}(\mathbf{X},\mathbf{y};\mathbf{w})\\
\nabla_{\mathbf{w}} J(\mathbf{X},\mathbf{y};\mathbf{w}) &= \tfrac{1}{n}\mathbf{X}^\top(\mathbf{X}\mathbf{w}-\mathbf{y}), \qquad \text{only when } J \propto \mathrm{MSE}\\
\mathbf{w}^{\text{next step}} &= \mathbf{w} - \eta\nabla_{\mathbf{w}} J(\mathbf{X},\mathbf{y};\mathbf{w})
\end{aligned}
$$

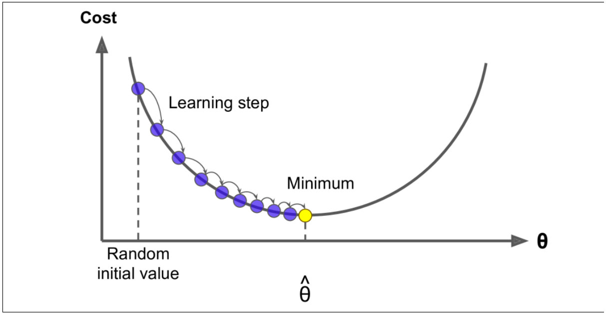
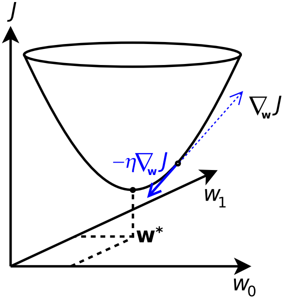


Figure 4-3. Gradient Descent



Gradient Descent (GD)

GD pitfalls

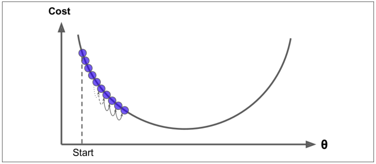


Figure 4-4. Learning rate too small

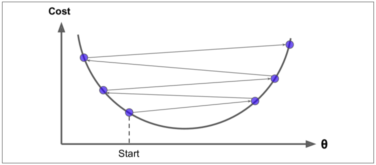


Figure 4-5. Learning rate too large

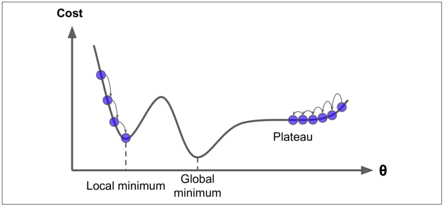


Figure 4-6. Gradient Descent pitfalls

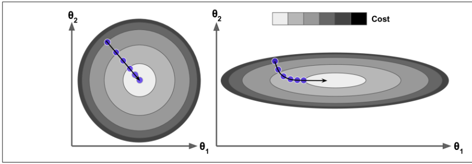
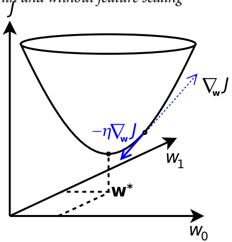


Figure 4-7. Gradient Descent with and without feature scaling



Stochastic Gradient Descent (SGD)

$$\mathbf{X}_{\text{SGD}} <= \text{one random sample } \mathbf{x}^{(i)}\text{'s from } \mathbf{X}$$

and this lowers the cost of calculating the gradient in each iteration

$$\nabla_{\mathbf{w}} J_{\text{SGD}}(\mathbf{X}_{\text{SGD}}, \mathbf{y}; \mathbf{w}) = \frac{1}{n}\mathbf{X}_{\text{SGD}}^{\top}(\mathbf{X}_{\text{SGD}}\mathbf{w} - \mathbf{y})$$

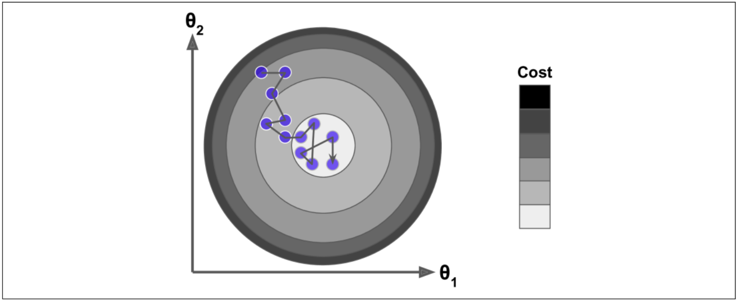


Figure 4-9. Stochastic Gradient Descent

Mini-batch (stochastic) Gradient Descent (SGD)

$$\mathbf{X}_{\text{mini}} <= \text{a set of random samples } \mathbf{x}^{(i)}\text{'s from } \mathbf{X}$$

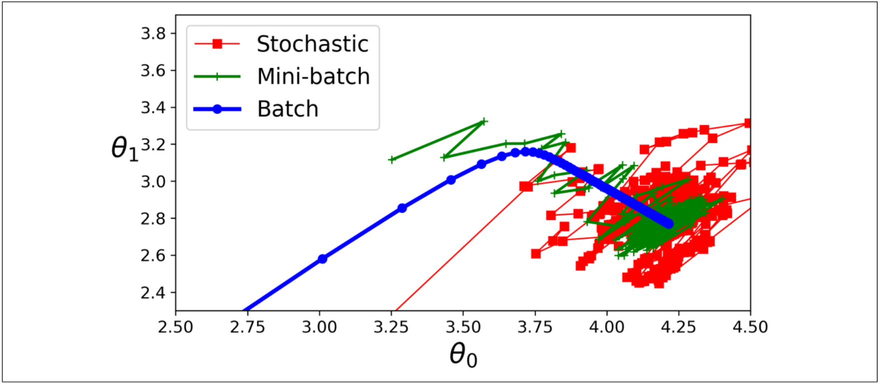


Figure 4-11. Gradient Descent paths in parameter space