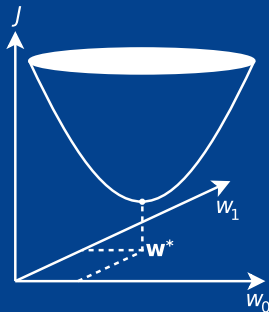




LESSON 5: Training (Regression, GD and SGD)

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FALL 2023



L05: Training (Regression, GD and SGD)

Agenda

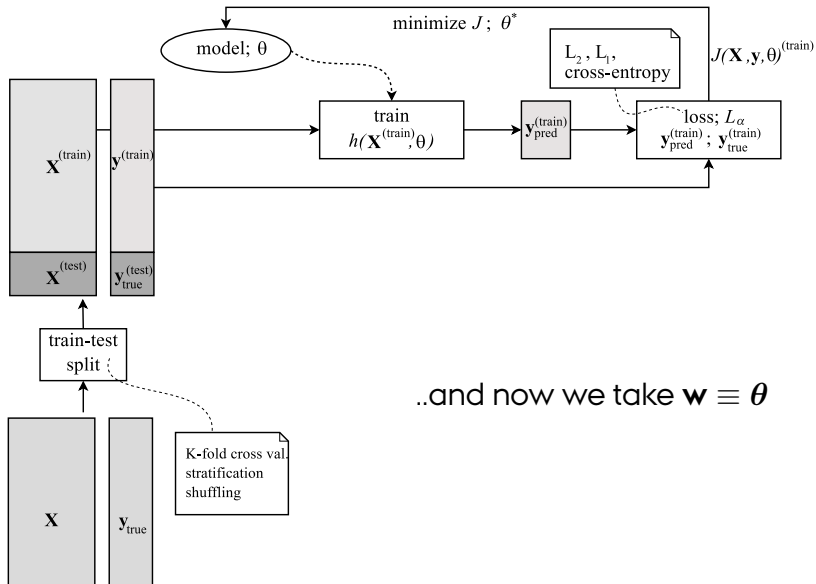
- ▶ Training a linear regression model,
 - ▶ (and intro to GD)
- ▶ Cost function in closed-form vs. numerical solutions.
 - ▶ Opgave: [L05/linear_regression_1.ipynb](#)
 - ▶ Opgave: [L05/linear_regression_2.ipynb](#) [OPTIONAL]
- ▶ Gradient Descent (GD),
 - ▶ Learning rates,
 - ▶ Batch Gradient Descent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



Training a Linear Regressor

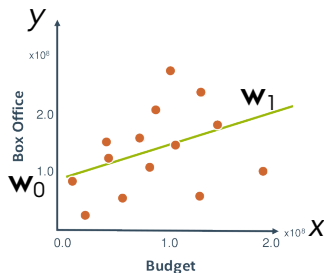
Linear Regression: In one dimension

The well know linear equation

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

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

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



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

Training a Linear Regressor

Linear Regression: Hypothesis Function in N -dimensions

For 1-D:

$$h(x^{(i)}; \mathbf{w}) = w_0 + w_1 x^{(i)}, \quad \text{with } \mathbf{w} = \begin{bmatrix} w_0 \\ w_1 \end{bmatrix}$$

The same for N -D:

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

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

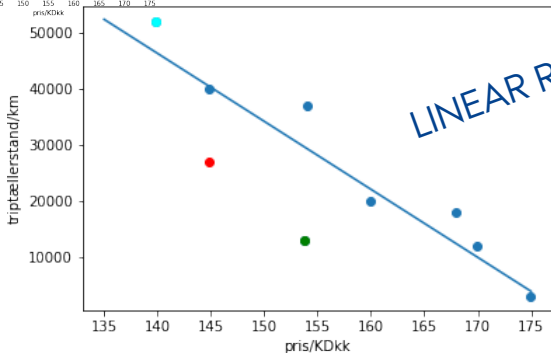
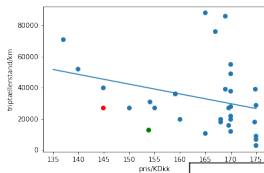
$$h(\mathbf{x}^{(i)}; \mathbf{w}) = \mathbf{w}^\top \mathbf{x}^{(i)}$$

Training a Linear Regressor

Case study: a new car..

Scrobe [bilbasen.dk], for particular e-Golf.

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



LINEAR REGRESSOR

Training a Linear Regressor

Linear Regression: Loss Function (or Cost/Objective Fun.)

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

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

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

only when y is 1D

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

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

Ignoring constant factors, this yields our linear regression cost function

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

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

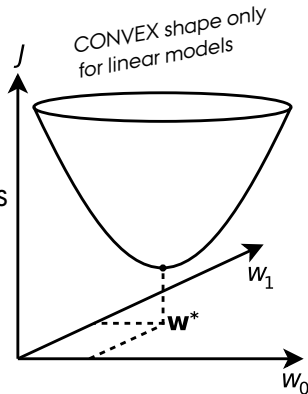
$$\begin{aligned}\mathbf{w}^* &= \operatorname{argmin}_{\mathbf{w}} J(\mathbf{X}, \mathbf{y}; \mathbf{w}) \\ &= \operatorname{argmin}_{\mathbf{w}} \frac{1}{2} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2\end{aligned}$$

and by minima, we naturally hope for

- ▶ the global minimum

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

- ▶ local minimum



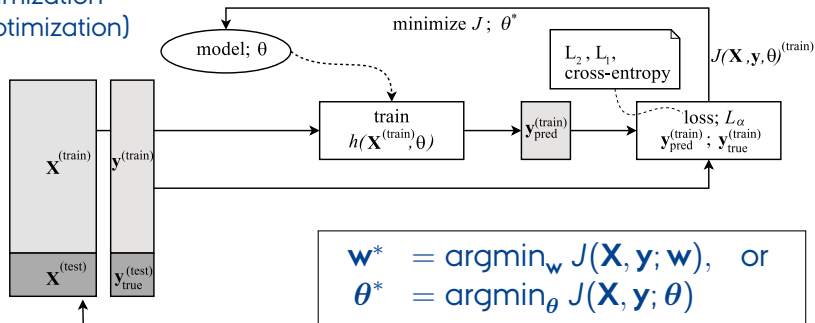
COST FUNCTION MINIMIZATION IN CLOSED-FORM

The Closed-form Linear-Least-Squares Solution

$$(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{y}$$

Training in General

Minimization
(optimization)



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}

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

Taking the partial derivative $\partial/\partial_{\mathbf{w}}$ of the J via the gradient (nabla) operator (*with a large amount of matrix algebra*)

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

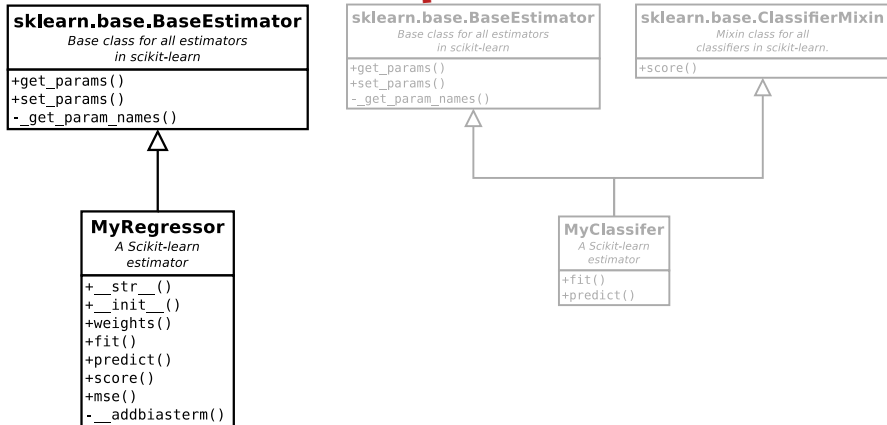
with a *small amount of matrix algebra*, this gives the **normal equation**

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

Exercise: L05/linear_regression_2.ipynb

Python class: `MyRegressor`

[OPTIONAL Exercise]

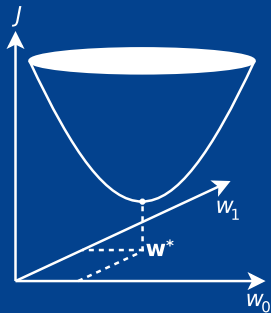


Exercise: create a linear regressor, inheriting from `BaseEstimator` and implement `score()` and `mse()`.

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

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

$$\nabla_{\mathbf{w}} J(\mathbf{X}, \mathbf{y}; \mathbf{w}) = \frac{1}{n} \mathbf{X}^T (\mathbf{X}\mathbf{w} - \mathbf{y}),$$

only when $J \propto \text{MSE}$

$$\mathbf{w}^{\text{next step}} = \mathbf{w} - \eta \nabla_{\mathbf{w}} J(\mathbf{X}, \mathbf{y}; \mathbf{w})$$

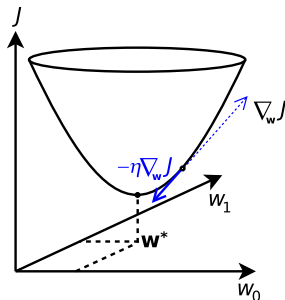
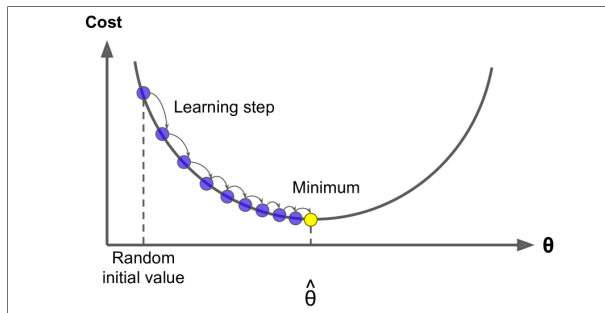


Figure 4-3. Gradient Descent

Gradient Descent (GD)

GD pitfalls

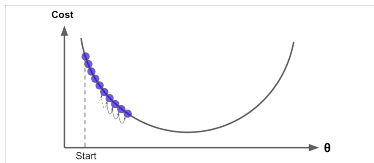


Figure 4-4. Learning rate too small

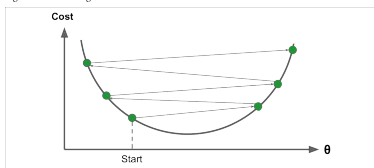


Figure 4-5. Learning rate too large

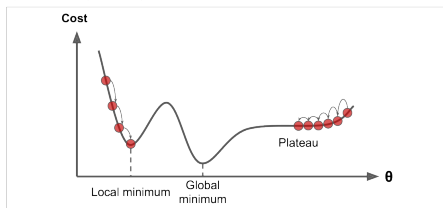


Figure 4-6. Gradient Descent pitfalls

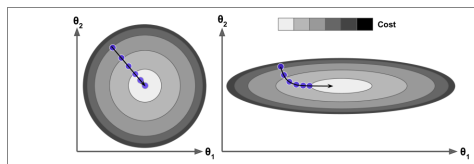
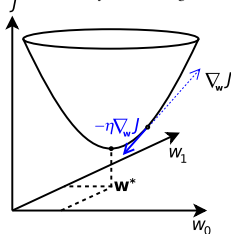


Figure 4-7. Gradient Descent with and without feature scaling



Learning Curve for GD

Plot J for Fig 4-4, 4.5 and 4.6 over 'time' or iteration in the numerical gradient descent algorithm..

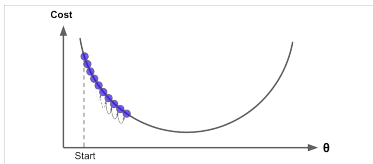


Figure 4-4. Learning rate too small

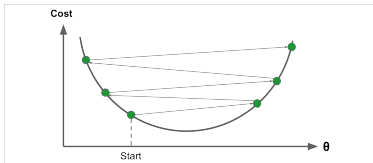


Figure 4-5. Learning rate too large

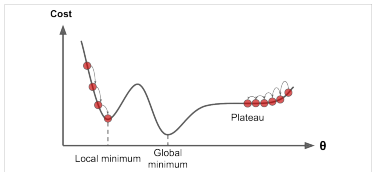
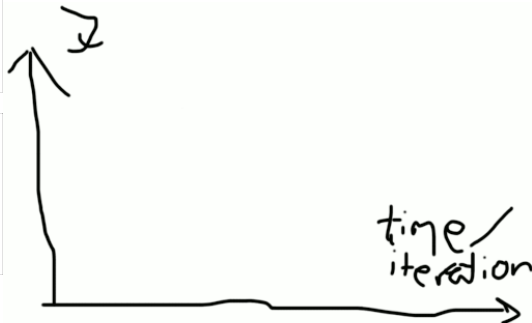


Figure 4-6. Gradient Descent pitfalls



Stochastic Gradient Descent (SGD)

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

and this lowers the computational effort of calculating the gradient in each iteration

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

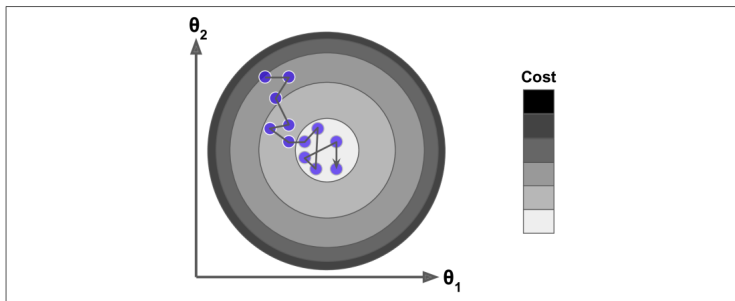


Figure 4-9. Stochastic Gradient Descent

Mini-batch (stochastic) Gradient Descent (SGD)

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

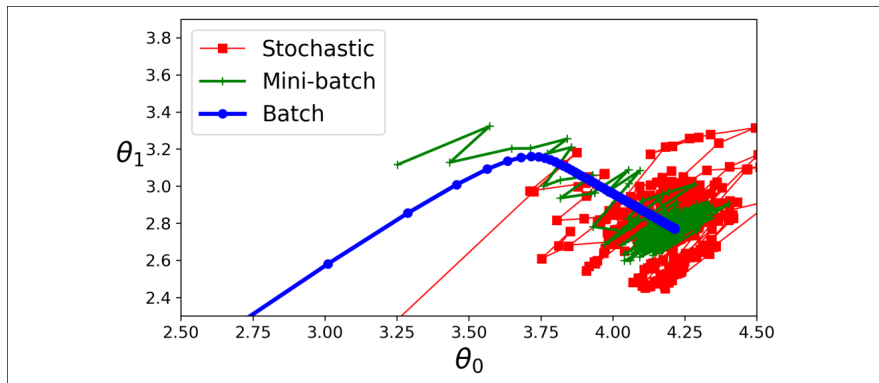


Figure 4-11. Gradient Descent paths in parameter space