*** Applied Machine Learning Fundamentals *** Regression

Daniel Wehner, M.Sc.

SAP SE / DHBW Mannheim

Winter term 2023/2024

Find all slides on GitHub (DaWe1992/Applied_ML_Fundamentals)

Lecture Overview

Unit I	Machine Learning Introduction
Unit II	Mathematical Foundations
Unit III	Bayesian Decision Theory
Unit IV	**Regression**
Unit V	Classification I
Unit VI	Evaluation
Unit VII	Classification II
Unit VIII	Clustering
Unit IX	Dimensionality Reduction

Agenda for this Unit

Section:
Introduction

Regression

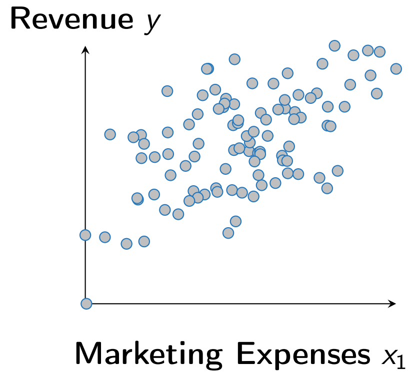
Type of target variable	Continuous
Type of training information	Supervised
Example Availability	Batch learning

Algorithm sketch: Given the training data $\mathcal{D}$, the algorithm derives a function of the type

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \theta_0 + \theta_1 x_1 + \cdots + \theta_m x_m \qquad \boldsymbol{x} \in \mathbb{R}^m, \boldsymbol{\theta} \in \mathbb{R}^{m+1} \tag{1}$$

from the data. $\boldsymbol{\theta}$ is the parameter vector containing the coefficients to be estimated by the regression algorithm. Once $\boldsymbol{\theta}$ is learned, it can be used for prediction.

Example Data Set: Revenues



- Find a linear function:

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \theta_0 + \theta_1 x_1 + \cdots + \theta_m x_m$$

- Usually: $x_0 = 1$:

$$\widehat{\boldsymbol{x}} \in \mathbb{R}^{m+1} = [1 \ \boldsymbol{x}]^\intercal$$

$$h_{\boldsymbol{\theta}}(\widehat{\boldsymbol{x}}) = \sum_{j=0}^{m} \theta_j x_j = \boldsymbol{\theta}^\intercal \widehat{\boldsymbol{x}}$$

Error Function for Regression

- We need an error function $\mathcal{J}(\boldsymbol{\theta})$ in order to know how good the function fits:

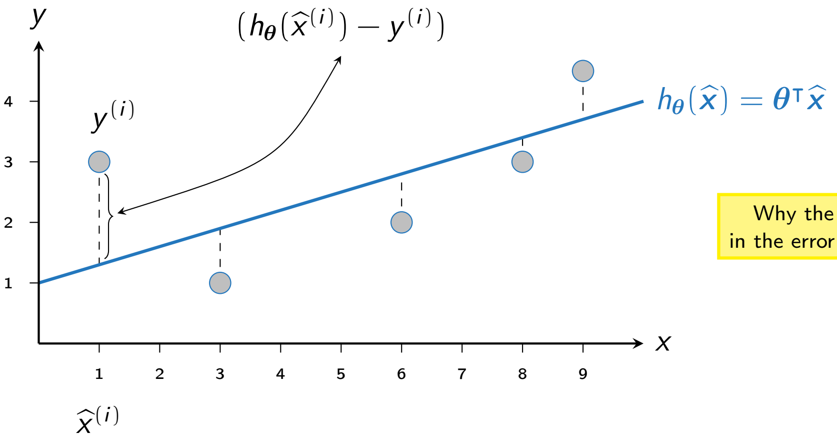
$$\mathcal{J}(\boldsymbol{\theta}) = \frac{1}{2n} \sum_{i=1}^{n} (h_{\boldsymbol{\theta}}(\widehat{\boldsymbol{x}}^{(i)}) - y^{(i)})^2 \tag{2}$$

- We want to minimize $\mathcal{J}(\boldsymbol{\theta})$:

$$\min_{\boldsymbol{\theta}} \frac{1}{2n} \sum_{i=1}^{n} (h_{\boldsymbol{\theta}}(\widehat{\boldsymbol{x}}^{(i)}) - y^{(i)})^2$$

- This is **ordinary least squares (OLS)**

Error Function Intuition



Why the **square** in the error function?

Section:

Solutions to Regression

DHBW
Duale Hochschule
Baden-Württemberg

Closed-Form Solutions

- Usual approach (for two unknowns): Calculate θ_0 and θ_1 according to

sample mean $\overline{x}$

$$\theta_0 = \overline{y} - \theta_1 \overline{x} \qquad \theta_1 = \frac{\sum_{i=1}^{n} (x^{(i)} - \overline{x}) \cdot (y^{(i)} - \overline{y})}{\sum_{i=1}^{n} (x^{(i)} - \overline{x})^2} \tag{3}$$

- '**Normal equation**' (scales to arbitrary dimensions):

$$\boldsymbol{\theta} = \underbrace{(\widehat{\boldsymbol{X}}^\intercal \widehat{\boldsymbol{X}})^{-1} \widehat{\boldsymbol{X}}^\intercal}_{\text{Moore-Penrose pseudo-inverse}} \boldsymbol{y} \tag{4}$$

$\widehat{\boldsymbol{X}}$ is called 'design matrix' or 'regressor matrix'

Design Matrix / Regressor Matrix

- The design matrix $\widehat{\boldsymbol{X}} \in \mathbb{R}^{n \times (m+1)}$ looks as follows:

In the following
$\widehat{\boldsymbol{X}} \equiv \boldsymbol{X}$

$$\widehat{\boldsymbol{X}} = \begin{pmatrix} 1 & x_1^{(1)} & x_2^{(1)} & \cdots & x_m^{(1)} \\ 1 & x_1^{(2)} & x_2^{(2)} & \cdots & x_m^{(2)} \\ 1 & x_1^{(3)} & x_2^{(3)} & \cdots & x_m^{(3)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{(n)} & x_2^{(n)} & \cdots & x_m^{(n)} \end{pmatrix} \tag{5}$$

- And the $n \times 1$ label vector:

$$\boldsymbol{y} = \left(y^{(1)}, y^{(2)}, y^{(3)}, \ldots, y^{(n)}\right)^{\mathsf{T}}$$

Derivation of the Normal Equation

- The derivation involves a bit of linear algebra
- Step ❶: Rewrite $\mathcal{J}(\boldsymbol{\theta})$ in matrix-vector notation:

$$\begin{aligned}
\mathcal{J}(\boldsymbol{\theta}) &= 1/2(\boldsymbol{X}\boldsymbol{\theta} - \boldsymbol{y})^\intercal(\boldsymbol{X}\boldsymbol{\theta} - \boldsymbol{y}) \\
&= 1/2((\boldsymbol{X}\boldsymbol{\theta})^\intercal - \boldsymbol{y}^\intercal)(\boldsymbol{X}\boldsymbol{\theta} - \boldsymbol{y}) \\
&= 1/2((\boldsymbol{X}\boldsymbol{\theta})^\intercal\boldsymbol{X}\boldsymbol{\theta} - (\boldsymbol{X}\boldsymbol{\theta})^\intercal\boldsymbol{y} - \boldsymbol{y}^\intercal(\boldsymbol{X}\boldsymbol{\theta}) + \boldsymbol{y}^\intercal\boldsymbol{y}) \\
&= 1/2(\boldsymbol{\theta}^\intercal\boldsymbol{X}^\intercal\boldsymbol{X}\boldsymbol{\theta} - 2(\boldsymbol{X}\boldsymbol{\theta})^\intercal\boldsymbol{y} + \boldsymbol{y}^\intercal\boldsymbol{y})
\end{aligned}$$

- To be continued...

Derivation of the Normal Equation (Ctd.)

- Step ❷: Calculate the derivative of $\mathcal{J}(\boldsymbol{\theta})$ and set it to zero:

$$\nabla_{\boldsymbol{\theta}}\mathcal{J}(\boldsymbol{\theta}) = {}^1\!/_2(2\boldsymbol{X}^\intercal\boldsymbol{X}\boldsymbol{\theta} - 2\boldsymbol{X}^\intercal\boldsymbol{y}) \stackrel{!}{=} 0$$
$$\Leftrightarrow \boldsymbol{X}^\intercal\boldsymbol{X}\boldsymbol{\theta} = \boldsymbol{X}^\intercal\boldsymbol{y}$$

- If $\boldsymbol{X}^\intercal\boldsymbol{X}$ is invertible, we can multiply both sides by $(\boldsymbol{X}^\intercal\boldsymbol{X})^{-1}$:

Normal equation:

$$\boldsymbol{\theta} = (\boldsymbol{X}^\intercal\boldsymbol{X})^{-1}\boldsymbol{X}^\intercal\boldsymbol{y}$$

Problems with Matrix Inversion?

- What if $(\boldsymbol{X}^\intercal \boldsymbol{X})^{-1}$ does not exist?
- Problems and solutions:
  1. Linearly dependent (redundant) features or design matrix does not have full rank? (E. g. size in m^2 and size in feet^2)
     $\Rightarrow$ **Delete correlated features**
  2. Too many features ($m > n$)?
     $\Rightarrow$ **Delete features (e. g. using PCA) / add training examples**
  3. Other numerical instabilities?
     $\Rightarrow$ **Add a regularization term** (later)
  4. Computationally too expensive?
     $\Rightarrow$ **Use gradient descent**

Gradient Descent

- We want to minimize a smooth function $\mathcal{J} : \mathbb{R}^{m+1} \to \mathbb{R}$:

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^{m+1}} \mathcal{J}(\boldsymbol{\theta})$$

- Update the parameters iteratively:

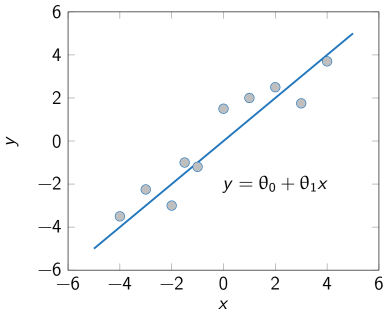
$$\boldsymbol{\theta}^{(t+1)} \longleftarrow \boldsymbol{\theta}^{(t)} - \alpha \nabla_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta}^{(t)}) \tag{6}$$

- where $\alpha > 0$ (learning rate) and $\nabla_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta})$ is the gradient of $\mathcal{J}(\boldsymbol{\theta})$ w. r. t. $\boldsymbol{\theta}$:

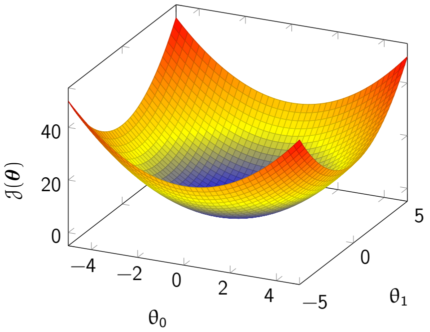
$$\nabla_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta}) = \left(\frac{\partial \mathcal{J}(\boldsymbol{\theta})}{\partial \theta_0}, \frac{\partial \mathcal{J}(\boldsymbol{\theta})}{\partial \theta_1}, \ldots, \frac{\partial \mathcal{J}(\boldsymbol{\theta})}{\partial \theta_m} \right)^{\intercal}$$

Data Input Space vs. Hypothesis Space

Data input space



Hypothesis space $\mathcal{H}$

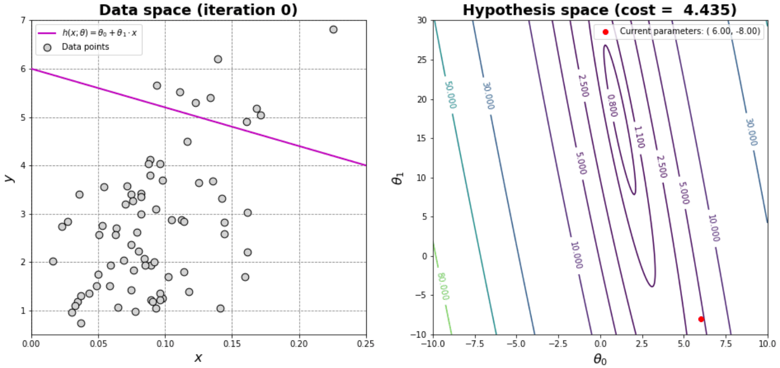


Data Input Space vs. Hypothesis Space (Ctd.)

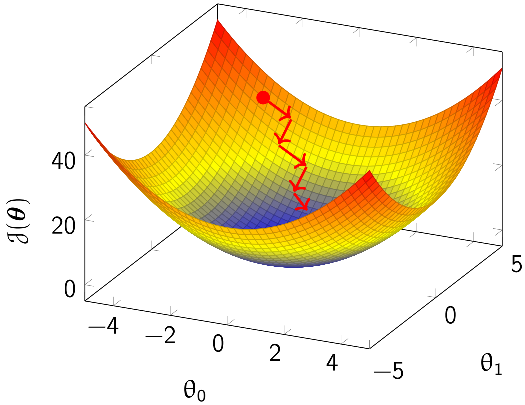
- **Data input space**
  - Determined by the $m + 1$ **attributes** of the data set $x_0, x_1, x_2, \ldots, x_m$
  - Often high-dimensional
- **Hypothesis space $\mathcal{H}$**
  - Determined by the **number of parameters** of the model
  - Each point in the hypothesis space corresponds to a **specific assignment of model parameters**
  - The error function gives information about how good this assignment is
  - **Gradient descent is applied in the hypothesis space $\mathcal{H}$**

Important

Data Input Space vs. Hypothesis Space (Ctd.)



Visualization of Gradient Descent in 3 Dimensions



Versions of Gradient Descent

- Assume some training data $\mathcal{D}$: $\{\boldsymbol{x}^{(i)}, y^{(i)}\}_{i=1}^{n}$
- Squared error for a **single** example: $\ell(y_{pred}, y_{true}) = (y_{pred} - y_{true})^2$
- Our objective is to minimize the **total** error:

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^{m+1}} \mathcal{J}(\boldsymbol{\theta}) = \min_{\boldsymbol{\theta} \in \mathbb{R}^{m+1}} \sum_{i=1}^{n} \ell(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}), y^{(i)})$$

- Three versions of gradient descent:
  1. Batch gradient descent
  2. Stochastic gradient descent
  3. Mini-batch gradient descent

Versions of Gradient Descent (Ctd.)

- **Batch gradient descent**: Compute gradient based on **ALL** data points

$$\boldsymbol{\theta}^{(t+1)} \longleftarrow \boldsymbol{\theta}^{(t)} - \alpha \sum_{i=1}^{n} \nabla \ell(h_{\boldsymbol{\theta}^{(t)}}(\boldsymbol{x}^{(i)}), y^{(i)}) \tag{7}$$

- **Stochastic gradient descent**: Compute gradient based on a **SINGLE** data point **(pick training example randomly and not sequentially!)**
- For $i \in \{1, \ldots, n\}$ do:

$$\boldsymbol{\theta}^{(t+1)} \longleftarrow \boldsymbol{\theta}^{(t)} - \alpha \nabla \ell(h_{\boldsymbol{\theta}^{(t)}}(\boldsymbol{x}^{(i)}), y^{(i)}) \tag{8}$$

Solving linear Regression using Gradient Descent

- Randomly initialize $\boldsymbol{\theta}$
- To minimize the error, keep changing $\boldsymbol{\theta}$ according to:

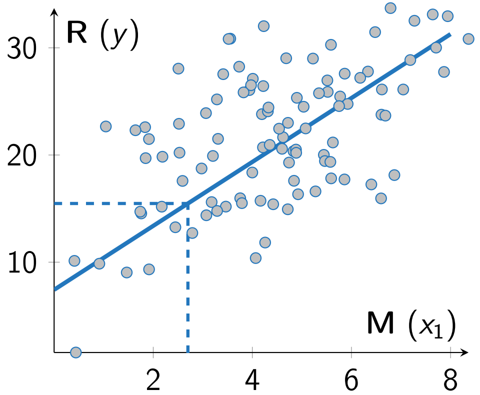
$$\boldsymbol{\theta}^{(t+1)} \longleftarrow \boldsymbol{\theta}^{(t)} - \alpha \nabla_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta}^{(t)}) \tag{9}$$

- We need to calculate $\nabla_{\theta_j} \mathcal{J}(\boldsymbol{\theta}^{(t)})$: (based on a single example)

$$\frac{\partial}{\partial \theta_j} \mathcal{J}(\boldsymbol{\theta}) = \frac{\partial}{\partial \theta_j} \frac{1}{2} (h_{\boldsymbol{\theta}}(\boldsymbol{x}) - y)^2 = 2 \cdot \frac{1}{2} (h_{\boldsymbol{\theta}}(\boldsymbol{x}) - y) \cdot \frac{\partial}{\partial \theta_j} (h_{\boldsymbol{\theta}}(\boldsymbol{x}) - y) \tag{10}$$

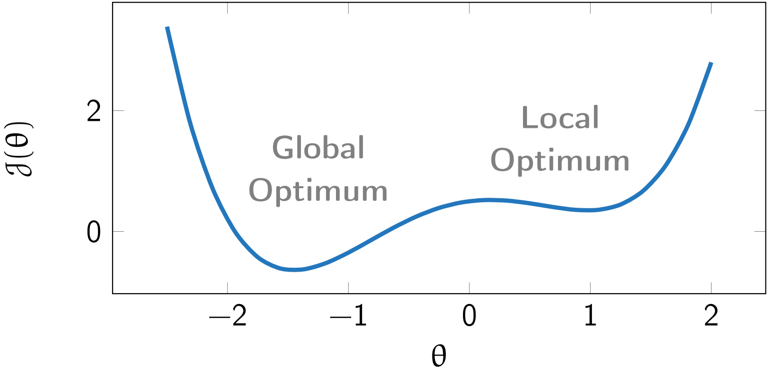
$$= (h_{\boldsymbol{\theta}}(\boldsymbol{x}) - y) \cdot \frac{\partial}{\partial \theta_j} (\theta_0 x_0 + \cdots + \theta_m x_m - y) = \boxed{(h_{\boldsymbol{\theta}}(\boldsymbol{x}) - y) x_j} \tag{11}$$

Solving the introductory Example



- $\theta_0 \approx 7.4218$
- $\theta_1 \approx 2.9827$
- $\mathcal{J}(\boldsymbol{\theta}) \approx 446.9584$
- $h_{\boldsymbol{\theta}}(\boldsymbol{x}) = 7.4218 + 2.9827 \cdot x_1$
- $R = h_{\boldsymbol{\theta}}(2.7) = \underline{\underline{15.4750}}$

Disadvantage of Gradient Descent



Section:

Basis Function Regression

DHBW

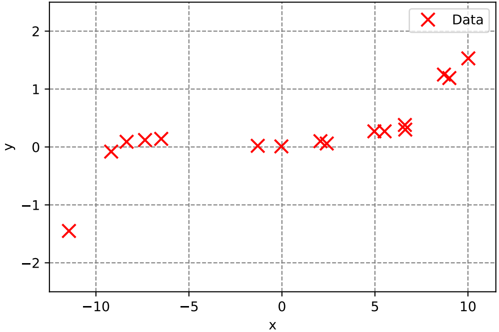
Duale Hochschule
Baden-Württemberg

What if the Data is non-linear?

- So far we have fitted straight lines
- **What if the data is not linear...?**

The best-fitting function is obviously **not a straight line**!

What would you do?



Basis Functions

- Remember: '**When stuck switch to a different perspective**'
- We can add **higher-order** features using **basis functions** φ:

We assume 1-D data

$$h_{\theta}(x) = \sum_{j=0}^{p} \theta_j \varphi_j(x) \tag{12}$$

- There exist several types of basis functions:
  - **linear:** $\varphi_0(x) = 1$ and $\varphi_1(x) = x$
  - **polynomial** $\Rightarrow$ see below
  - **radial basis functions (RBFs)** $\Rightarrow$ see below
  - **Fourier basis**

New Design Matrix

Applying the basis functions to $\boldsymbol{X}$ we get the new design matrix $\boldsymbol{\Phi}$:

$$\boldsymbol{\Phi} = \begin{pmatrix} \varphi_0(x^{(1)}) & \varphi_1(x^{(1)}) & \varphi_2(x^{(1)}) & \dots & \varphi_p(x^{(1)}) \\ \varphi_0(x^{(2)}) & \varphi_1(x^{(2)}) & \varphi_2(x^{(2)}) & \dots & \varphi_p(x^{(2)}) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \varphi_0(x^{(n)}) & \varphi_1(x^{(n)}) & \varphi_2(x^{(n)}) & \dots & \varphi_p(x^{(n)}) \end{pmatrix} \tag{13}$$

The model is still linear in the parameters, so we can still use the same algorithm as before. This is still linear regression (!!!)

Polynomial Basis Functions

- A quite frequently used basis function: The **polynomial basis**

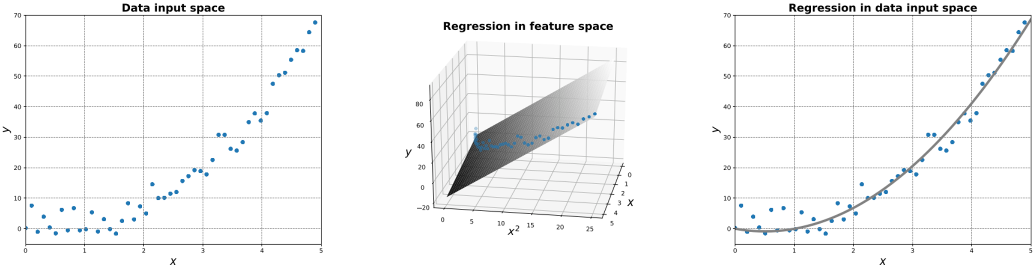
$$\varphi_0(x) = 1$$
$$\varphi_j(x) = x^j$$

For N-D data we would also include cross-terms!

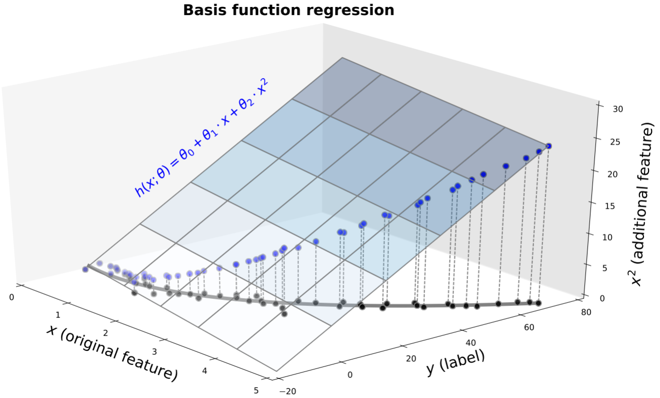
$$h_{\boldsymbol{\theta}}(x) = \sum_{j=0}^{p} \theta_j \varphi_j(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_p x^p$$

- Here, p is the degree of the polynomial
- Here: $\varphi(x) = [1, x, x^2, x^3, \ldots, x^p]$

It is still linear!



It is still linear! (Ctd.)



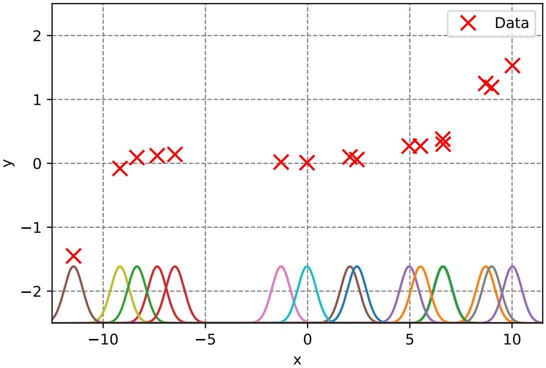
Basis Functions: Radial Basis Functions

- Yet another possible choice of basis function: **Radial basis functions**

$$\varphi_0(x) = 1 \tag{14}$$
$$\varphi_j(x) = \exp\left\{-{}^1\!/_2\|x - z_j\|^2/2\sigma^2\right\} \tag{15}$$

- $\{z_j\}$ are the centers of the radial basis functions
- p denotes the number of centers / number of radial basis functions
- Often we take each data point as a center, so $p = n$

Radial Basis Functions (Ctd.)



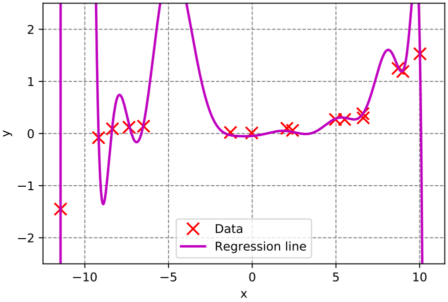
Section:

Regularization Techniques

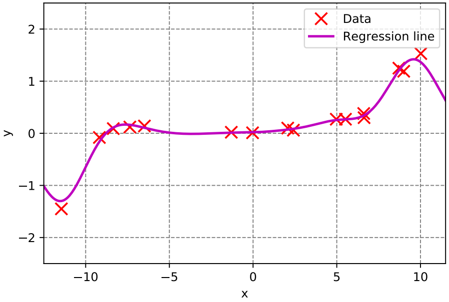
Important

The Danger of too expressive Models...

Polynomial of degree $p = 16$
(☠ **severe overfitting** ☠)



RBF with $\sigma = 1.00$, $p = n$
(About right)



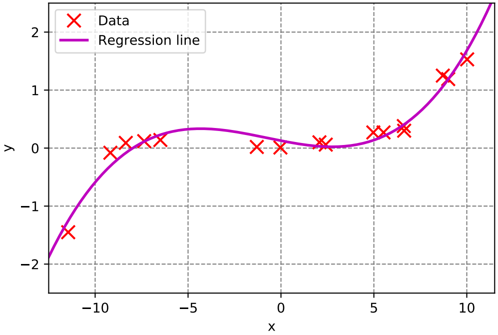
Overfitting vs. Underfitting

- **Underfitting**
  - The model is not complex enough to fit the data well $\Rightarrow$ High bias
  - Make the model more complex; adding new examples does not help
- **Overfitting**
  - The model predicts the training data perfectly
  - But it fails to generalize to unseen instances $\Rightarrow$ High variance
  - Decrease the degree of freedom or add more training examples
  - Also: Try regularization
- **Bias-Variance trade-off**

First Solution: Smaller Degree

One solution: Use a **smaller degree** (here: $p = 3$)

Much better :)



Second Solution: Regularization

- Enrich $\mathcal{J}(\boldsymbol{\theta})$ with a **regularization term**
- This can **prevent overfitting** and results in a smoother function (large values for θ_j are prevented)
- Two forms of regularization, **L1** and **L2**:

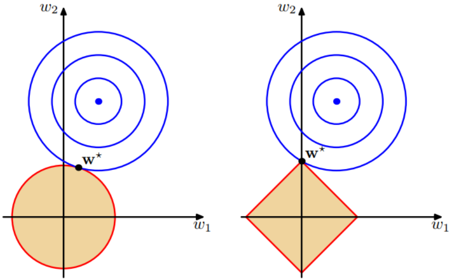
$$\min_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta}) + \lambda|\boldsymbol{\theta}| \quad \to \textbf{(L1)} \qquad\qquad \min_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta}) + \lambda\|\boldsymbol{\theta}\|^2 \quad \to \textbf{(L2)}$$

$$|\boldsymbol{\theta}| = \sum_{j=1}^{m} |\theta_j| \qquad\qquad \|\boldsymbol{\theta}\|^2 = \sum_{j=1}^{m} \theta_j^2$$

- $\lambda \geqslant 0$ controls the **degree of regularization**

Regularization visualized

- Here: $\boldsymbol{w} \equiv \boldsymbol{\theta}$
- L1-Regularization
  $\Rightarrow$ **Lasso regression**
  (least abs. shrinkage and select. operator)
- L2-Regularization
  $\Rightarrow$ **Ridge regression**
  (Tikhonov regularization)
- The combination of both is called **elastic net**



cf. [?], p. 146; left: L2, right: L1

Incorporating Regularization

Regularization also helps to overcome numerical issues!

- Normal equation with regularization: (ridge regression)

$$\boldsymbol{\theta} = (\boldsymbol{X}^\intercal \boldsymbol{X} + \lambda \boldsymbol{I})^{-1} \boldsymbol{X}^\intercal \boldsymbol{y} \tag{16}$$

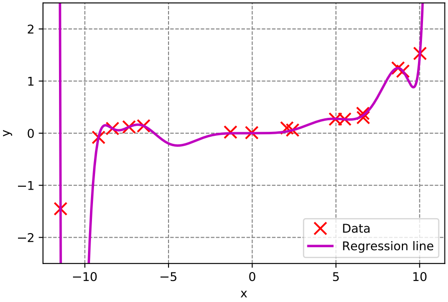
- Regularized gradient descent update rule:

$$\boldsymbol{\theta}^{(t+1)} \longleftarrow \boldsymbol{\theta}^{(t)} - \alpha \nabla_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta}^{(t)})$$

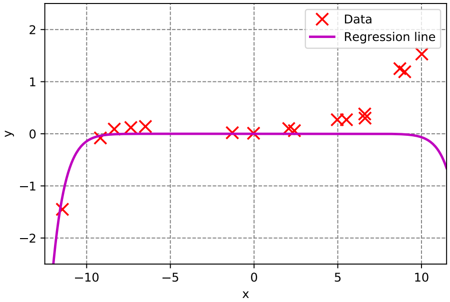
$$\frac{\partial}{\partial \theta_j} \mathcal{J}(\boldsymbol{\theta}) = (h_{\boldsymbol{\theta}}(\boldsymbol{x}) - y) x_j + \lambda \theta_j$$

Polynomial Regression with Regularization

At least better



Way too much regularization



Section:

Wrap-Up

DHBW
Duale Hochschule
Baden-Württemberg

Summary

- Regression predicts **continuous target variables**
- The algorithm minimizes the **(mean) squared error**
- Minimizing the squared error gives the **maximum likelihood solution**
- **Two approaches:**
  1. Normal equation
  2. (Batch / stochastic / mini-batch) gradient descent
- Probabilistic regression allows to **quantify the uncertainty of the model**
- Use **basis functions** to fit non-linear regression lines
- **Regularization** is important

Important

Self-Test Questions

1. What is the goal of regression?
2. What can you do if matrix inversion fails for the normal equation?
3. What is a suitable cost function for regression? Where does it come from?
4. Does gradient descent give the exact solution?
5. Which versions of gradient descent do you know?
6. What are basis functions? Why use them? State some examples.
7. What is overfitting and underfitting?
8. What is regularization? Why should you apply it?

What's next...?

Unit I	Machine Learning Introduction
Unit II	Mathematical Foundations
Unit III	Bayesian Decision Theory
Unit IV	Regression
Unit V	**Classification I**
Unit VI	Evaluation
Unit VII	Classification II
Unit VIII	Clustering
Unit IX	Dimensionality Reduction

Thank you very much for the attention!

Topic: *** Applied Machine Learning Fundamentals *** Regression
Term: Winter term 2023/2024

Contact:
Daniel Wehner, M.Sc.
SAP SE / DHBW Mannheim
daniel.wehner@sap.com

Do you have any questions?