

# \*\*\* Applied Machine Learning Fundamentals \*\*\*

## Regression

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SAP SE

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# Lecture Overview

Unit I	Machine Learning Introduction
Unit II	Mathematical Foundations
Unit III	Bayesian Decision Theory
Unit IV	Probability Density Estimation
<b>Unit V</b>	<b>Regression</b>
Unit VI	Classification I
Unit VII	Evaluation
Unit VIII	Classification II
Unit IX	Clustering
Unit X	Dimensionality Reduction

# Agenda for this Unit

## ① Introduction

- What is Regression?
- Least Squares Error Function

## ② Solutions to Regression

- Closed-Form Solutions and Normal Equation
- Gradient Descent

## ③ Probabilistic Regression

- Underlying Assumptions
- Maximum Likelihood Solution

## ④ Basis Function Regression

- General Idea
- Polynomial Basis Functions
- Radial Basis Functions
- Regularization Techniques

## ⑤ Wrap-Up

- Summary
- Self-Test Questions
- Lecture Outlook
- Recommended Literature and further Reading
- Meme of the Day

Section:  
**Introduction**



# Regression

Type of target variable

Continuous

Type of training information

Supervised

Example Availability

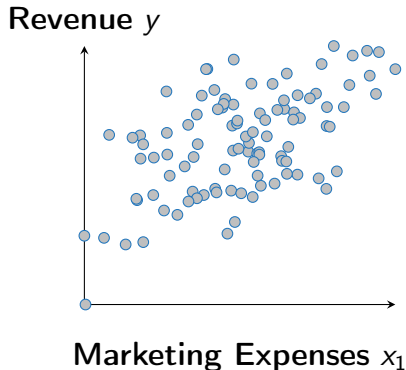
Batch learning

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

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

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

## Example Data Set: Revenues



- Find a linear function:

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

- Usually:  $x_0 = 1$ :

$$\hat{\mathbf{x}} \in \mathbb{R}^{m+1} = [1 \ \mathbf{x}]^T$$

$$h_{\theta}(\hat{\mathbf{x}}) = \sum_{j=0}^m \theta_j x_j = \boldsymbol{\theta}^T \hat{\mathbf{x}}$$

## Error Function for Regression

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

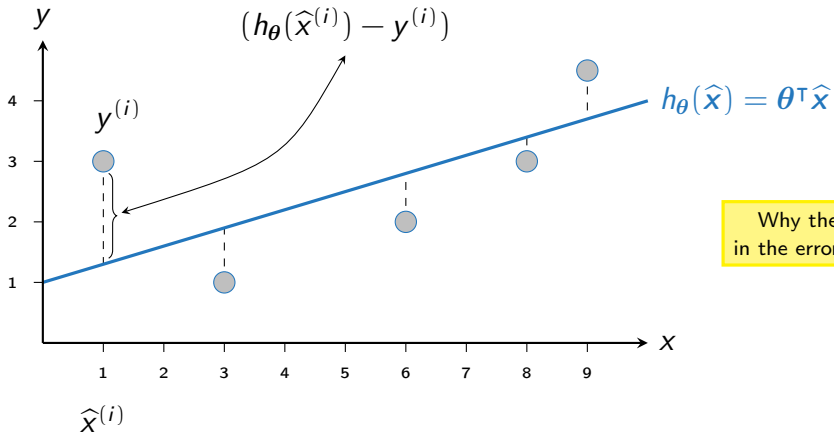
$$\mathcal{J}(\boldsymbol{\theta}) = \frac{1}{2n} \sum_{i=1}^n (h_{\boldsymbol{\theta}}(\hat{\mathbf{x}}^{(i)}) - y^{(i)})^2 \quad (2)$$

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

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

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

# Error Function Intuition



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



Section:  
**Solutions to Regression**



## Closed-Form Solutions

- Usual approach (for two unknowns): Calculate  $\theta_0$  and  $\theta_1$  according to

sample mean  $\bar{x}$

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

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

$$\theta = \underbrace{(\hat{X}^\top \hat{X})^{-1} \hat{X}^\top}_{\text{Moore-Penrose pseudo-inverse}} y \quad (4)$$

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

# Design Matrix / Regressor Matrix

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

In the following

$$\hat{\mathbf{X}} \equiv \mathbf{X}$$

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

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

$$\mathbf{y} = (y^{(1)}, y^{(2)}, y^{(3)}, \dots, y^{(n)})^T$$



# Derivation of the Normal Equation

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

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

- To be continued...



## Derivation of the Normal Equation (Ctd.)

- Step ②: Calculate the derivative of  $\mathcal{J}(\theta)$  and set it to zero:

$$\begin{aligned}\nabla_{\theta} \mathcal{J}(\theta) &= 1/2(2\mathbf{X}^T \mathbf{X} \theta - 2\mathbf{X}^T \mathbf{y}) \stackrel{!}{=} \mathbf{0} \\ \Leftrightarrow \mathbf{X}^T \mathbf{X} \theta &= \mathbf{X}^T \mathbf{y}\end{aligned}$$

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

Normal equation:

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

# Problems with Matrix Inversion?

- What if  $(\mathbf{X}^\top \mathbf{X})^{-1}$  does not exist?
- Problems and solutions:
  - ① Linearly dependent (redundant) features or design matrix does not have full rank? (E. g. size in  $\text{m}^2$  and size in  $\text{feet}^2$ )  
 $\Rightarrow$  **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  $\mathcal{J} : \mathbb{R}^{m+1} \rightarrow \mathbb{R}$ :

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

- Update the parameters iteratively:

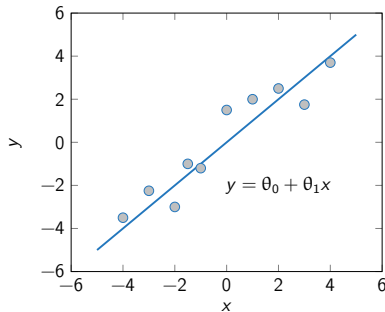
$$\boldsymbol{\theta}^{(t+1)} \longleftarrow \boldsymbol{\theta}^{(t)} - \alpha \nabla_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta}^{(t)}) \quad (6)$$

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

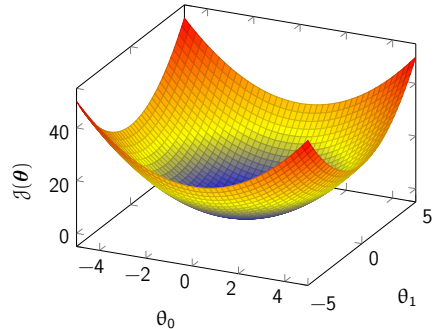
$$\nabla_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta}) = \left( \frac{\partial \mathcal{J}(\boldsymbol{\theta})}{\partial \theta_0}, \frac{\partial \mathcal{J}(\boldsymbol{\theta})}{\partial \theta_1}, \dots, \frac{\partial \mathcal{J}(\boldsymbol{\theta})}{\partial \theta_m} \right)^\top$$

# Data Input Space vs. Hypothesis Space

## Data input space



## Hypothesis space $\mathcal{H}$

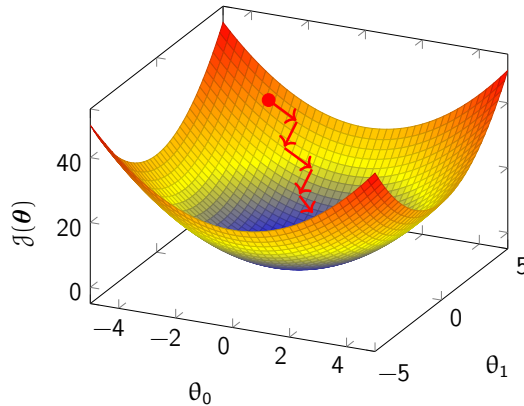




# Data Input Space vs. Hypothesis Space (Ctd.)

- **Data input space**
  - Determined by the  $m + 1$  **attributes** of the data set  $x_0, x_1, x_2, \dots, x_m$
  - 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  $\mathcal{H}$**

# Visualization of Gradient Descent in 3 Dimensions



## Versions of Gradient Descent

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

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

- 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

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

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

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

# Solving linear Regression using Gradient Descent

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

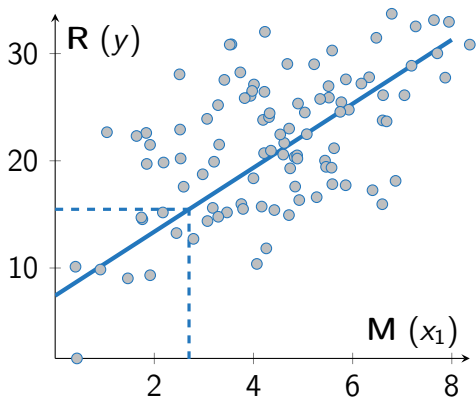
$$\theta^{(t+1)} \longleftarrow \theta^{(t)} - \alpha \nabla_{\theta} \mathcal{J}(\theta^{(t)}) \quad (9)$$

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

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

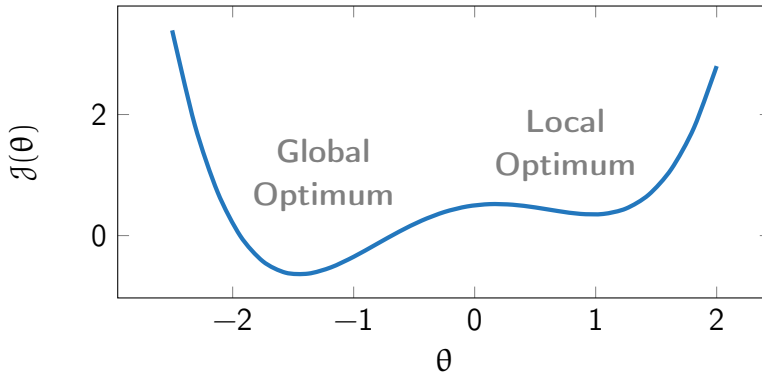
$$= (h_{\theta}(\mathbf{x}) - y) \cdot \frac{\partial}{\partial \theta_j} (\theta_0 x_0 + \dots + \theta_m x_m - y) = \boxed{(h_{\theta}(\mathbf{x}) - y) x_j} \quad (11)$$

# Solving the introductory Example



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

# Disadvantage of Gradient Descent



Section:  
**Probabilistic Regression**





# Probabilistic Regression

- **Assumption 1:** The target function values are generated by adding noise the true function's estimate:

$$y = f(\mathbf{x}, \boldsymbol{\theta}) + \varepsilon \quad (12)$$

- **Assumption 2:** The noise is a Gaussian random variable:

$$\begin{aligned} \beta &\equiv \text{precision} \\ \beta &= 1/\sigma^2 \end{aligned}$$

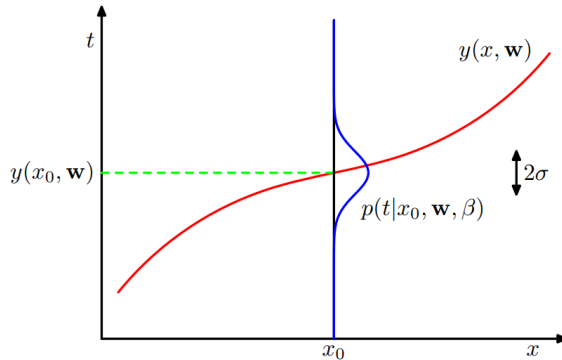
$$\varepsilon \sim \mathcal{N}(0, \beta^{-1}) \quad (13)$$

$$p(y|\mathbf{x}, \boldsymbol{\theta}, \beta) = \mathcal{N}(y|f(\mathbf{x}, \boldsymbol{\theta}), \beta^{-1}) \quad (14)$$

- **$y$  is now a random variable!**

# Probabilistic Regression (Ctd.)

$$\mathbf{w} \equiv \boldsymbol{\theta}$$



cf. [1], p. 29; probabilistic regression

# Maximum Likelihood Regression

- **Given:** A labeled set of training data points  $\{(\mathbf{x}^{(i)}, y^{(i)})\}_{i=1}^n$
- **Conditional likelihood** (assuming the data is i. i. d.):

$$p(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta}, \beta) = \prod_{i=1}^n \mathcal{N}(y^{(i)} | f(\mathbf{x}^{(i)}), \beta^{-1}) \quad (15)$$

$$= \prod_{i=1}^n \mathcal{N}(y^{(i)} | \boldsymbol{\theta}^\top \mathbf{x}^{(i)}, \beta^{-1}) \quad (16)$$

- Maximize the likelihood w. r. t.  $\boldsymbol{\theta}$  and  $\beta$

# Maximum Likelihood Regression (Ctd.)

Simplify using the **log**-likelihood:

$$\log p(\mathbf{y}|\mathbf{X}, \boldsymbol{\theta}, \beta) = \sum_{i=1}^n \log \mathcal{N}(y^{(i)}|\boldsymbol{\theta}^\top \mathbf{x}^{(i)}, \beta^{-1}) \quad (17)$$

$$= \sum_{i=1}^n \left[ \log \left( \frac{\sqrt{\beta}}{\sqrt{2\pi}} \right) - \frac{\beta}{2} (y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)})^2 \right] \quad (18)$$

Remember log-rules?

$$= \frac{n}{2} \log \beta - \frac{n}{2} \log(2\pi) - \frac{\beta}{2} \sum_{i=1}^n (y^{(i)} - \boldsymbol{\theta}^\top \mathbf{x}^{(i)})^2 \quad (19)$$

# Maximum Likelihood Regression (Ctd.)

- Compute the gradient w. r. t.  $\theta$ :

$$\begin{aligned}\nabla_{\theta} \log p(\mathbf{y}|\mathbf{X}, \theta, \beta) &= \mathbf{0} \\ -\beta \sum_{i=1}^n (y^{(i)} - \theta^{\top} \mathbf{x}^{(i)}) \mathbf{x}^{(i)} &= \mathbf{0} \\ \dots \\ \theta_{ml} &= (\mathbf{X}^{\top} \mathbf{X})^{-1} \mathbf{X}^{\top} \mathbf{y}\end{aligned}$$

- Same result as in least squares regression



# We have derived the squared Error!

Minimizing the squared error gives the maximum likelihood solution for the parameters  $\theta$  assuming Gaussian noise.

- The maximum likelihood approach gives rise to the squared error
- But it is much more powerful than regular least squares  $\Rightarrow$  **We can estimate the uncertainty  $\beta$**

$$\beta_{ml} = \left( \frac{1}{n} \sum_{i=1}^n (y^{(i)} - \theta_{ml}^T \mathbf{x}^{(i)})^2 \right)^{-1} \quad (20)$$

Section:  
**Basis Function Regression**

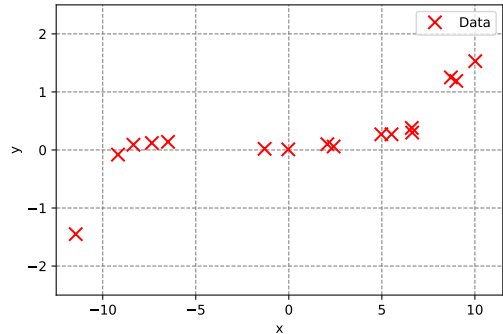


# What if the Data is non-linear?

- 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**  $\varphi$ :

We assume 1-D data

$$h_{\theta}(x) = \sum_{j=0}^p \theta_j \varphi_j(x) \quad (21)$$

- 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  $\mathbf{X}$  we get the new design matrix  $\Phi$ :

$$\Phi = \begin{pmatrix} \varphi_0(x^{(1)}) & \varphi_1(x^{(1)}) & \varphi_2(x^{(1)}) & \dots & \varphi_p(x^{(1)}) \\ \varphi_0(x^{(2)}) & \varphi_1(x^{(2)}) & \varphi_2(x^{(2)}) & \dots & \varphi_p(x^{(2)}) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \varphi_0(x^{(n)}) & \varphi_1(x^{(n)}) & \varphi_2(x^{(n)}) & \dots & \varphi_p(x^{(n)}) \end{pmatrix} \quad (22)$$

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!

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

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

# Basis Functions: Radial Basis Functions

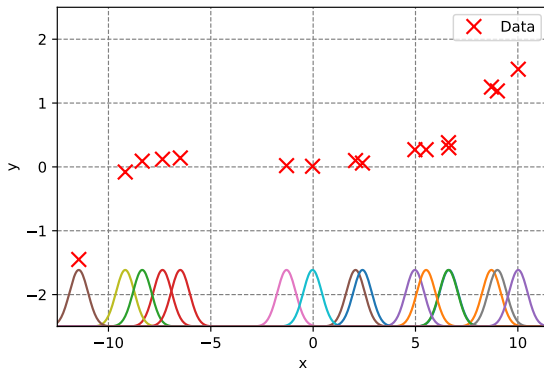
- Yet another possible choice of basis function: **Radial basis functions**

$$\varphi_0(x) = 1 \quad (23)$$

$$\varphi_j(x) = \exp \left\{ -1/2 \|x - z_j\|^2 / 2\sigma^2 \right\} \quad (24)$$

- $\{z_j\}$  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.)

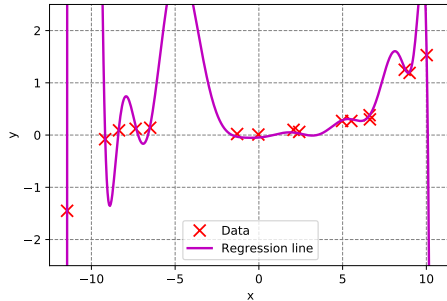




# The Danger of too expressive Models...

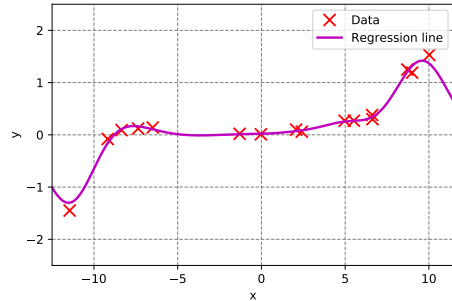
Polynomial of degree  $p = 16$

(☠️ **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**

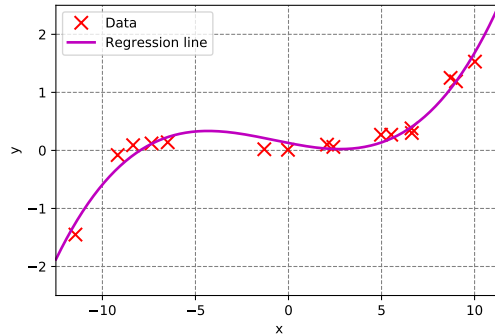
- The model predicts the training data perfectly
- But it **fails to generalize** to unseen instances  $\Rightarrow$  **High variance**
- Decrease the degree of freedom or add more training examples
- Also: Try **regularization**

- **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  $\theta_j$  are prevented)
- Two forms of regularization, **L1** and **L2**:

$$\min_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta}) + \lambda |\boldsymbol{\theta}| \rightarrow (\text{L1})$$

$$\min_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta}) + \lambda \|\boldsymbol{\theta}\|^2 \rightarrow (\text{L2})$$

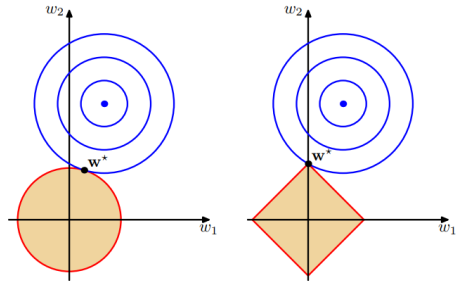
$$|\boldsymbol{\theta}| = \sum_{j=1}^m |\theta_j|$$

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

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

# Regularization visualized

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



cf. [1], p. 146; left: L2, right: L1

# Incorporating Regularization

- Normal equation with regularization:  
(ridge regression)

The regularization also helps to overcome numerical issues!

$$\boldsymbol{\theta} = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})^{-1} \mathbf{X}^T \mathbf{y} \quad (25)$$

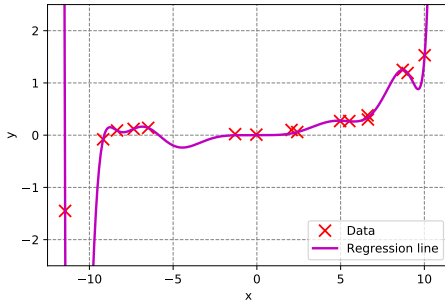
- Regularized gradient descent update rule:

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

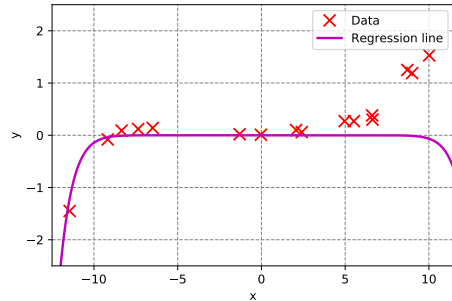
$$\frac{\partial}{\partial \theta_j} \mathcal{J}(\boldsymbol{\theta}) = (h_{\boldsymbol{\theta}}(\mathbf{x}) - y) x_j + \lambda \theta_j$$

# Polynomial Regression with Regularization

At least better



Way too much regularization



Section:  
**Wrap-Up**



# 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



# 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 What is the advantage of probabilistic regression?
- 6 What are basis functions? Why use them? State some examples.
- 7 What is overfitting / 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
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<b>Unit VI</b>	<b>Classification I</b>
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# Recommended Literature and further Reading I



## [1] Pattern Recognition and Machine Learning

*Christopher Bishop. Springer. 2006.*

→ [Link](#), cf. chapter 3.1 'Linear Models for Regression'



## [2] Machine Learning: A Probabilistic Perspective

*Kevin Murphy. MIT Press. 2012.*

→ [Link](#), cf. chapters 1.4.5 'Linear Regression' and 1.4.7 'Overfitting'



## [3] Stanford CS229 course notes

*Andrew Ng. Stanford University. 2019.*

→ [Link](#)

## Recommended Literature and further Reading II

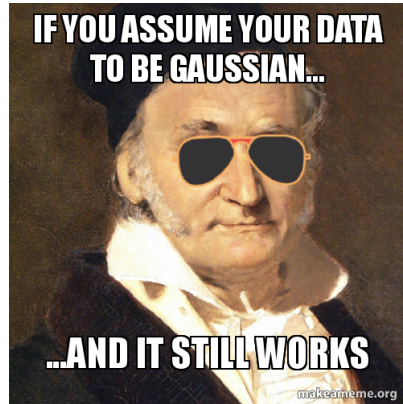


### [4] Stanford CS229 course recording

*Andrew Ng. Stanford University. 2008.*

→ [Link](#)

## Meme of the Day



Thank you very much for the attention!

**Topic:** \*\*\* Applied Machine Learning Fundamentals \*\*\* Regression

**Term:** Winter term 2019/2020

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Do you have any questions?