*** Applied Machine Learning Fundamentals *** Mathematical Foundations

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SAP SE

Winter term 2019/2020

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Lecture Overview

Agenda for this Unit

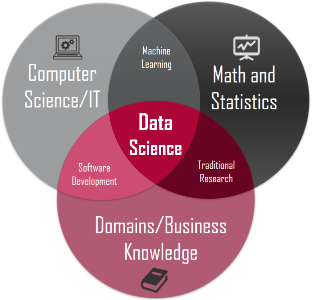
Section:

Introduction

DHBW
Duale Hochschule
Baden-Württemberg

Introduction

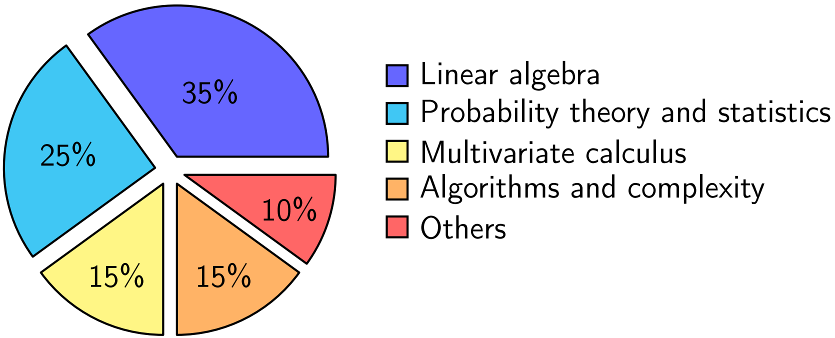
Math is a significant portion of data science / machine learning!



You will need it to understand:

- **Statistical** machine learning
- How optimization for learning / empirical risk minimization works
- How linear algebra, calculus and statistics are used to make learning and inference more efficient

Math is important!



Section:

Linear Algebra

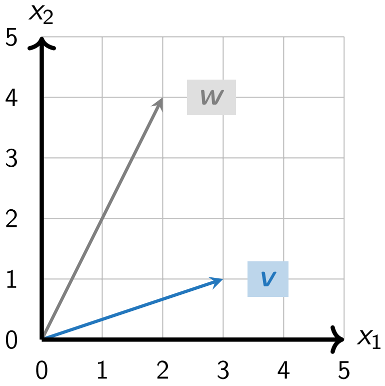
Duale Hochschule Baden-Württemberg

What is a Vector?

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$\boldsymbol{v} = \begin{bmatrix} 3 \\ 1 \end{bmatrix}$$

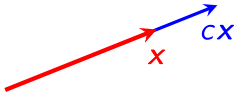
$$\boldsymbol{w} = \begin{bmatrix} 2 \\ 4 \end{bmatrix}$$



Multiplication by a Scalar

$$c\boldsymbol{x} = c\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} cx_1 \\ cx_2 \end{bmatrix}$$

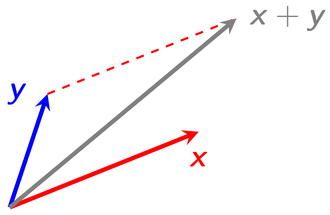
$$2\boldsymbol{v} = 2\begin{bmatrix} 3 \\ 1 \end{bmatrix} = \begin{bmatrix} 6 \\ 2 \end{bmatrix}$$



Addition of Vectors

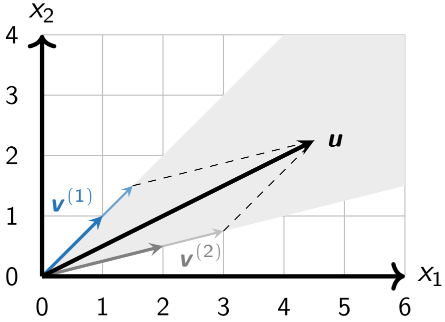
$$\boldsymbol{x} + \boldsymbol{y} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} x_1 + y_1 \\ x_2 + y_2 \end{bmatrix}$$

$$\boldsymbol{v} + \boldsymbol{w} = \begin{bmatrix} 3 \\ 1 \end{bmatrix} + \begin{bmatrix} 2 \\ 4 \end{bmatrix} = \begin{bmatrix} 5 \\ 5 \end{bmatrix}$$



Linear Combination of Vectors

$$\boldsymbol{u} = c_1 \boldsymbol{v}^{(1)} + c_2 \boldsymbol{v}^{(2)} + \cdots + c_n \boldsymbol{v}^{(n)} \tag{1}$$



Vector Transpose, inner and outer Product

- Vector transpose:

$$\boldsymbol{v} = \begin{bmatrix} 3 \\ 1 \end{bmatrix} \qquad \boldsymbol{v}^\intercal = \begin{bmatrix} 3 & 1 \end{bmatrix}$$

- Inner product / dot product / scalar product:

$$\boldsymbol{v} \cdot \boldsymbol{w} \equiv \boldsymbol{v}^\intercal \boldsymbol{w} \equiv \langle \boldsymbol{v}, \boldsymbol{w} \rangle = \sum_{j=1}^{m} v_j w_j \tag{2}$$

$$= \begin{bmatrix} 3 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \end{bmatrix} = (3 \cdot 2) + (1 \cdot 4) = 10$$

Important

Vector Transpose and inner and outer Product (Ctd.)

- Outer product:

$$\boldsymbol{v}\boldsymbol{w}^{\mathsf{T}} = \begin{bmatrix} 3 \\ 1 \end{bmatrix} \begin{bmatrix} 2 & 4 \end{bmatrix} = \begin{bmatrix} 6 & 12 \\ 2 & 4 \end{bmatrix}$$

The inner product yields a scalar value, the results of an outer product is a matrix!

Length of a Vector

- Length of a vector (Frobenius norm):

$$\|\boldsymbol{x}\| = \sqrt{\boldsymbol{x}^\intercal \boldsymbol{x}} \tag{3}$$

$$\|c\boldsymbol{x}\| = |c| \cdot \|\boldsymbol{x}\| \tag{4}$$

$$\|\boldsymbol{x} + \boldsymbol{y}\| \leqslant \|\boldsymbol{x}\| + \|\boldsymbol{y}\| \tag{5}$$

- Example:

$$\|\boldsymbol{v}\| = \sqrt{3^2 + 1^2} = \sqrt{10}$$

Angle between Vectors

- The angle between two vectors is given by:

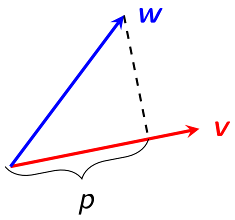
$$\cos \measuredangle(\boldsymbol{x}, \boldsymbol{y}) = \frac{\boldsymbol{x} \cdot \boldsymbol{y}}{\|\boldsymbol{x}\| \cdot \|\boldsymbol{y}\|} = \frac{\sum_{j=1}^{m} x_j \cdot y_j}{\sqrt{\sum_{j=1}^{m} (x_j)^2} \cdot \sqrt{\sum_{j=1}^{m} (y_j)^2}} \tag{6}$$

$$\cos \measuredangle(\boldsymbol{v}, \boldsymbol{w}) = \frac{\boldsymbol{v} \cdot \boldsymbol{w}}{\|\boldsymbol{v}\| \cdot \|\boldsymbol{w}\|} = \frac{10}{\sqrt{10} \cdot \sqrt{20}} \approx 0.71$$

- Inner product: $\boldsymbol{x} \cdot \boldsymbol{y} = \|\boldsymbol{x}\| \cdot \|\boldsymbol{y}\| \cdot \cos \measuredangle(\boldsymbol{x}, \boldsymbol{y})$

Projection of Vectors

- How is the projection of $\boldsymbol{w}$ onto $\boldsymbol{v}$ defined?
- Formally, we have:



$$\begin{aligned} p &= \|\boldsymbol{v}\| \cos \measuredangle(\boldsymbol{v}, \boldsymbol{w}) \\ &= \|\boldsymbol{v}\| \frac{\boldsymbol{v} \cdot \boldsymbol{w}}{\|\boldsymbol{v}\| \cdot \|\boldsymbol{w}\|} \\ &= \frac{\boldsymbol{v} \cdot \boldsymbol{w}}{\|\boldsymbol{w}\|} \end{aligned} \tag{7}$$

- Note that p is **not a vector!**

What is a Matrix?

General case ($\mathbb{R}^{n \times m}$):

$$\boldsymbol{X} = \begin{bmatrix} X_{11} & X_{12} & \dots & X_{1m} \\ X_{21} & X_{22} & \dots & X_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ X_{n1} & X_{n2} & \dots & X_{nm} \end{bmatrix}$$

$$\boldsymbol{M} = \begin{bmatrix} 3 & 4 & 5 \\ 1 & 0 & 1 \end{bmatrix} \qquad \mathbb{R}^{2 \times 3}$$

$$\boldsymbol{N} = \begin{bmatrix} 3 & 0 & 0 \\ 0 & 7 & 0 \\ 0 & 0 & 1 \end{bmatrix} \qquad \mathbb{R}^{3 \times 3}$$

$$\boldsymbol{P} = \begin{bmatrix} 10 & 1 \\ 11 & 2 \end{bmatrix} \qquad \mathbb{R}^{2 \times 2}$$

Matrix Transpose and Addition

- Transpose of a matrix:

$$\boldsymbol{M}^{\intercal} = \begin{bmatrix} 3 & 4 & 5 \\ 1 & 0 & 1 \end{bmatrix}^{\intercal} = \begin{bmatrix} 3 & 1 \\ 4 & 0 \\ 5 & 1 \end{bmatrix} \tag{8}$$

- Addition of matrices:

$$\boldsymbol{X} + \boldsymbol{Y} = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} + \begin{bmatrix} Y_{11} & Y_{12} \\ Y_{21} & Y_{22} \end{bmatrix} = \begin{bmatrix} X_{11} + Y_{11} & X_{12} + Y_{12} \\ X_{21} + Y_{21} & X_{22} + Y_{22} \end{bmatrix} \tag{9}$$

Important

Matrix Multiplication

- Multiplication by scalars:

$$c\boldsymbol{X} = c\begin{bmatrix} X_{11} & X_{12} & X_{13} \\ X_{21} & X_{22} & X_{23} \end{bmatrix} = \begin{bmatrix} c \cdot X_{11} & c \cdot X_{12} & c \cdot X_{13} \\ c \cdot X_{21} & c \cdot X_{22} & c \cdot X_{23} \end{bmatrix} \tag{10}$$

- Matrix-vector multiplication:

$$\boldsymbol{z} = \boldsymbol{X}\boldsymbol{y} = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} X_{11} \cdot y_1 + X_{12} \cdot y_2 \\ X_{21} \cdot y_1 + X_{22} \cdot y_2 \end{bmatrix} \tag{11}$$

Important

Matrix Multiplication (Ctd.)

- Matrix-matrix multiplication:

$$
\begin{aligned}
Z &= XY \\
&= \begin{bmatrix} X_{11} & X_{12} & X_{13} \\ X_{21} & X_{22} & X_{23} \end{bmatrix} \begin{bmatrix} Y_{11} & Y_{12} \\ Y_{21} & Y_{22} \\ Y_{31} & Y_{32} \end{bmatrix} \\
&= \begin{bmatrix} X_{11}Y_{11} + X_{12}Y_{21} + X_{13}Y_{31} & X_{11}Y_{12} + X_{12}Y_{22} + X_{13}Y_{32} \\ X_{21}Y_{11} + X_{22}Y_{21} + X_{23}Y_{31} & X_{21}Y_{12} + X_{22}Y_{22} + X_{23}Y_{32} \end{bmatrix} \quad (12)
\end{aligned}
$$

Matrix Inversion

- Matrix inversion is defined for **square matrices** $\boldsymbol{X} \in \mathbb{R}^{n \times n}$
- A matrix $\boldsymbol{X}$ multiplied by its inverse $\boldsymbol{X}^{-1}$ gives the identity matrix:

$$\boldsymbol{X}^{-1}\boldsymbol{X} = \boldsymbol{X}\boldsymbol{X}^{-1} = \boldsymbol{I} \tag{13}$$

$$\boldsymbol{I} = \begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 \end{bmatrix} \tag{14}$$

- If $\boldsymbol{X}^{-1}$ exists, we say that $\boldsymbol{X}$ is non-singular

Matrix Inversion (Ctd.)

- It holds that (C is the cofactor matrix):

$$X^{-1} = \frac{1}{\det(X)} C^\intercal \tag{15}$$

- A condition for invertability is that **the determinant has to be different from zero**
- **Example:**

$$X = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \qquad \det(X) = 0 \qquad X^{-1} = ?$$

Matrix Inversion Example

$$\boldsymbol{X} = \begin{bmatrix} 1 & 1/2 \\ -1 & 1 \end{bmatrix} \qquad \boldsymbol{X}^{-1} = \begin{bmatrix} 2/3 & -1/3 \\ 2/3 & 2/3 \end{bmatrix}$$

Please verify!

$$\boldsymbol{X}\boldsymbol{X}^{-1} = \boldsymbol{I} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \boldsymbol{X}^{-1}\boldsymbol{X}$$

Use for example the Gauss-Jordan algorithm to find the inverse!

Matrix Pseudoinverse

- **Question:** How can we invert a matrix $\boldsymbol{X} \in \mathbb{R}^{n \times m}$ which is not squared?
- **Left pseudoinverse $\boldsymbol{X}^{\#}\boldsymbol{X}$:**

$$\boldsymbol{X}^{\#}\boldsymbol{X} = \underbrace{(\boldsymbol{X}^{\intercal}\boldsymbol{X})^{-1}\boldsymbol{X}^{\intercal}}_{\text{left-multiplied}}\boldsymbol{X} = \boldsymbol{I}_m \tag{16}$$

- **Right pseudoinverse $\boldsymbol{X}\boldsymbol{X}^{\#}$:**

$$\boldsymbol{X}\boldsymbol{X}^{\#} = \boldsymbol{X}\underbrace{\boldsymbol{X}^{\intercal}(\boldsymbol{X}\boldsymbol{X}^{\intercal})^{-1}}_{\text{right-multiplied}} = \boldsymbol{I}_n \tag{17}$$

Important

Eigenvectors and Eigenvalues

- Some vectors $\boldsymbol{v}$ only change their length when multiplied by a matrix $\boldsymbol{X}$
- **Example:**

$$\begin{bmatrix} 4 & -1 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \end{bmatrix} = 2 \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

- These vectors are called eigenvectors, the scaling factors are known as eigenvalues
- More general:

$$\boldsymbol{W}\boldsymbol{v} = \lambda \boldsymbol{v} \tag{18}$$

Eigenvectors form a Basis

- Let us assume that there are n eigenvectors with corresponding eigenvalues:

$$\boldsymbol{v}^{(1)}, \boldsymbol{v}^{(2)}, \ldots, \boldsymbol{v}^{(n)}$$

$$\lambda_1, \lambda_2, \ldots, \lambda_n$$

- **Theorem:**
  - For an $n \times n$ matrix with eigenvectors $\boldsymbol{v}^{(1)}, \boldsymbol{v}^{(2)}, \ldots, \boldsymbol{v}^{(n)}$, if they correspond to **distinct** eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, then the set $\{\boldsymbol{v}^{(1)}, \boldsymbol{v}^{(2)}, \ldots, \boldsymbol{v}^{(n)}\}$ is linearly independent
  - Hence, any vector can be expressed as a linear combination of eigenvectors:

$$\boldsymbol{v} = c_1\boldsymbol{v}^{(1)} + c_2\boldsymbol{v}^{(2)} + \cdots + c_n\boldsymbol{v}^{(n)}$$

Symmetric Matrices

- A squared $n \times n$ matrix $\boldsymbol{X}$ is **symmetric**, iff

$$\forall i, j: \quad X_{ij} = X_{ji} \tag{19}$$

$$\boldsymbol{X} = \boldsymbol{X}^\intercal \tag{20}$$

- Some properties:
  - The inverse $\boldsymbol{X}^{-1}$ is also symmetric
  - **Eigen-decomposition:** $\boldsymbol{X}$ can be decomposed into $\boldsymbol{X} = \boldsymbol{Q}\boldsymbol{D}\boldsymbol{Q}^\intercal$, where the columns of $\boldsymbol{Q}$ are the eigenvectors of $\boldsymbol{X}$, and $\boldsymbol{D}$ is a diagonal matrix whose entries are the corresponding eigenvalues

Positive (semi-)definite Matrices

- A **squared symmetric** matrix $\boldsymbol{X}^{n \times n}$ is positive definite, iff for any vector $\boldsymbol{y} \in \mathbb{R}^n$:

$$\boldsymbol{y}^\intercal \boldsymbol{X} \boldsymbol{y} > 0 \tag{21}$$

- Or positive semi-definite, iff $\boldsymbol{y}^\intercal \boldsymbol{X} \boldsymbol{y} \geqslant 0$

Such matrices are important in machine learning. For instance, the covariance matrix is always positive semi-definite.

Section:

Statistics

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Random Variables

- What is a random variable?

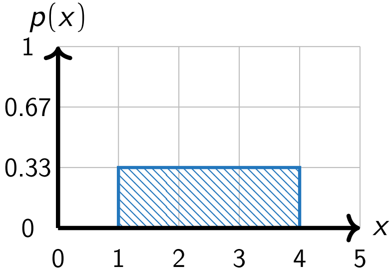
Random Variables

- What is a **random variable**?
  - It's a random number determined by chance (according to a distribution)
  - Random variables in machine learning: input data, output data, noise
- What is a **probability distribution**?

Random Variables

- What is a **random variable**?
  - It's a random number determined by chance (according to a distribution)
  - Random variables in machine learning: input data, output data, noise
- What is a **probability distribution**?
  - Describes the probability that a random variable is equal to a certain value
  - It can be given by the physics of an experiment (e. g. throwing dice)
  - **Discrete** vs. **continuous** distributions

Uniform Distribution



Every outcome is equally probable within a bounded region $\mathcal{R}$

$$p(x) = {}^1\!/_{\mathcal{R}} \tag{22}$$

Discrete Distributions

The random variables take on **discrete values**

Examples:

- When throwing a die, the possible values are given by a countably finite set:

$$x_i \in \{1, 2, 3, 4, 5, 6\}$$

- The number of sand grains at the beach (countably infinite set):

$$x_i \in \mathbb{N}$$

Discrete Distributions (Ctd.)

- All probabilities sum up to 1:

$$\sum_i p(x_i) = 1$$

- Discrete distributions are particularly important in classification
- A discrete distribution is described by a **probability mass function** (also called frequency function)

Bernoulli Distribution

- A **Bernoulli random variable** only takes on two values (e. g. 0 and 1):

$$x \in \{0, 1\} \tag{23}$$

$$p(x = 1|\mu) = \mu \tag{24}$$

$$\mathrm{Bern}(x|\mu) = \mu^x (1 - \mu)^{1-x} \tag{25}$$

$$\mathbb{E}\{x\} = \mu \tag{26}$$

$$\mathrm{var}\{x\} = \mu(1 - \mu) \tag{27}$$

- The only parameter is μ, i. e. the distribution is completely defined by this parameter

Binomial Distribution

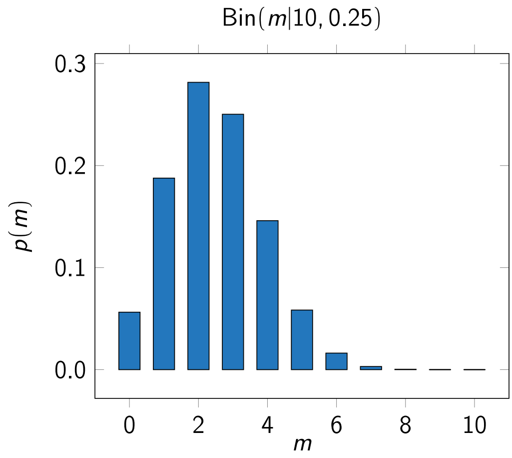
- **Binomial variables** are a sequence of n repeated Bernoulli variables
- **Example:** What is the probability of getting $m \in \mathbb{N}$ heads in n trials?

$$\mathrm{Bin}(m|n, \mu) = \binom{n}{m} \mu^m (1-\mu)^{n-m} \tag{28}$$

$$\mathbb{E}\{m\} = n\mu \tag{29}$$

$$\mathrm{var}\{m\} = n\mu(1-\mu) \tag{30}$$

Binomial Distribution (Ctd.)



Continuous Distributions

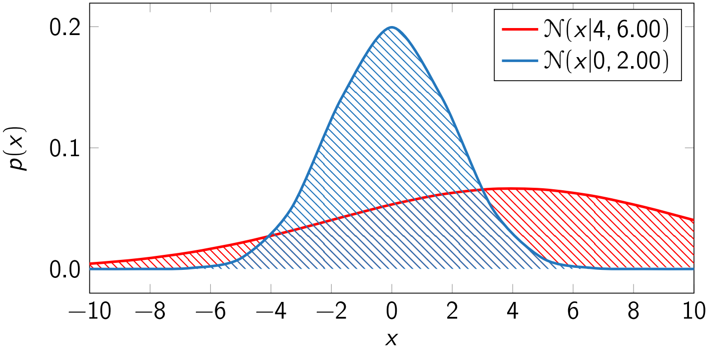
The random variables take on **continuous values**

- Continuous distributions are discrete distributions where the **number of discrete values goes to infinity** while the **probability of each value goes to zero**
- It's described by a probability density function which integrates to 1:

$$\int_{-\infty}^{+\infty} p(x)\,\mathrm{d}x = 1$$

Important

Gaussian Distribution



$$p(x) = \mathcal{N}(x|\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{-\frac{(x-\mu)^2}{2\sigma^2}\right\} \tag{31}$$

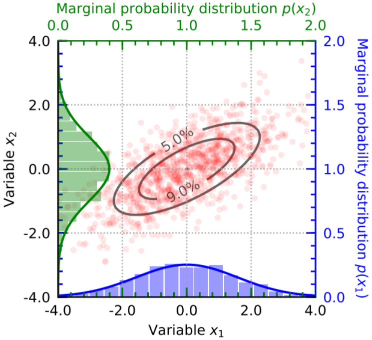
Central Limit Theorem

Central Limit Theorem:
The distribution of the sum of n i. i. d. (independent and identically distributed) random variables becomes increasingly Gaussian as n increases.

- The Gaussian distribution is one among the most important distributions
- Gaussians are often a good model
- Working with Gaussians leads to **analytical solutions for complex operations**

Multivariate Gaussian Distribution

$$p_D(\boldsymbol{x}) = \mathcal{N}_D(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{\sqrt{(2\pi)^D|\boldsymbol{\Sigma}|}} \exp\left\{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^\intercal \boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right\} \quad (32)$$



For clarification: $\boldsymbol{x}$ and $\boldsymbol{\mu}$ are vectors, while $\boldsymbol{\Sigma}$ is a matrix. The probability given by $\mathcal{N}_D(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) \in [0; 1]$ is still a scalar value!

Basic Rules of Probability

- **Joint distribution:**

$$p(x, y) \tag{33}$$

- **Marginal distribution:**

$$p(y) = \int_x p(x, y)\,\mathrm{d}x \tag{34}$$

- **Conditional distribution:**

$$p(y|x) = \frac{p(x, y)}{p(x)} \tag{35}$$

Basic Rules of Probability (Ctd.)

- **Probabilistic independence:**

$$p(x, y) = p(x)p(y) \tag{36}$$

- **Chain rule of probabilities:**

$$\begin{aligned} p(x_1, \dots, x_n) &= p(x_1|x_2, \dots, x_n)p(x_2, \dots, x_n) \\ &= p(x_1|x_2, \dots, x_n)p(x_2|x_3, \dots, x_n) \dots p(x_{n-1}|x_n)p(x_n) \end{aligned} \tag{37}$$

- **Bayes' rule:**

$$p(y|x) = \frac{p(x|y)p(y)}{p(x)} \tag{38}$$

Expectation

$$\mathbb{E}_{x \sim p(x)}\{f(x)\} = \mathbb{E}_x\{f\} = \mathbb{E}\{f\} = \sum_x p(x) f(x) \qquad \text{discrete case} \tag{39}$$

$$= \int_x p(x) f(x) \, \mathrm{d}x \qquad \text{continuous case} \tag{40}$$

Approximate expectation:

$$\mathbb{E}\{f\} = \int_x p(x) f(x) \, \mathrm{d}x \approx \frac{1}{n} \sum_{i=1}^{n} f(x_i) \tag{41}$$

Expectation (Ctd.)

- Some rules of expectations:
  - $\mathbb{E}\{a\boldsymbol{x}\} = a\mathbb{E}\{\boldsymbol{x}\}$
  - $\mathbb{E}\{\boldsymbol{x} + \boldsymbol{y}\} = \mathbb{E}\{\boldsymbol{x}\} + \mathbb{E}\{\boldsymbol{y}\}$
  - $\mathbb{E}\{\boldsymbol{x}\boldsymbol{y}\} = \mathbb{E}\{\boldsymbol{x}\}\mathbb{E}\{\boldsymbol{y}\}$ (if $\boldsymbol{x}$ and $\boldsymbol{y}$ are independent)
  - $\mathbb{E}\{\sum_i a_i x_i\} = \sum_i a_i \mathbb{E}\{x_i\}$
- Expectations of functions:
  - $\mathbb{E}\{g(\boldsymbol{x})\} = \int_{\boldsymbol{x}} p(\boldsymbol{x}) g(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}$
  - In general: $\mathbb{E}\{g(\boldsymbol{x})\} \neq g(\mathbb{E}\{\boldsymbol{x}\})$

Variance and Covariance

- Covariances give a measure of correlation: (how much variables change together)
- Scalars:

$$\begin{aligned} \operatorname{cov}\{x, y\} &= \mathbb{E}_{x,y}\{(x - \mathbb{E}_x\{x\})(y - \mathbb{E}_y\{y\})\} \\ &= \mathbb{E}_{x,y}\{xy\} - \mathbb{E}_x\{x\}\mathbb{E}_y\{y\} \end{aligned} \tag{42}$$

- Vector notation:

$$\operatorname{cov}\{\boldsymbol{x}, \boldsymbol{y}\} = \mathbb{E}_{\boldsymbol{x},\boldsymbol{y}}\{(\boldsymbol{x} - \mathbb{E}_{\boldsymbol{x}}\{\boldsymbol{x}\})(\boldsymbol{y} - \mathbb{E}_{\boldsymbol{y}}\{\boldsymbol{y}\})^\intercal\} \tag{43}$$

Kullback-Leibler Divergence

- The **Kullback-Leibler (KL) divergence** is a similarity measure between two distributions p and q:

$$\mathrm{KL}(p||q) = \sum_x p(x) \cdot \log \frac{p(x)}{q(x)} \tag{44}$$

- Some properties:
  - It is not a distance metric: $\mathrm{KL}(p||q) \neq \mathrm{KL}(q||p)$
  - It is non-negative: $\mathrm{KL}(p||q) \geqslant 0$
  - If $\forall x : p(x) = q(x) \Rightarrow \mathrm{KL}(p||q) = 0$

Section:

Optimization

Motivation

- In every machine learning problem, you will have:
  1. An **objective function** you want to optimize
  2. **Data** you want to learn from
  3. **Parameters** which need to be learned
  4. Assumptions about the problem and the data
- We would like to have general solutions to the problem of learning
- Different algorithms embody different objective functions and assumptions

Every machine learning problem is an optimization problem!

Unconstrained Optimization

You know how to do that, don't you?

Constrained Optimization

Formalization:

$$\begin{aligned}
\min_{\boldsymbol{\theta}} \mathcal{J}(\theta) &= \dots && \longleftarrow \text{cost function / objective} \\
\text{s.t. } f(\theta) &= 0 && \longleftarrow \text{equality constraints} \\
g(\theta) &\geqslant 0 && \longleftarrow \text{inequality constraints}
\end{aligned}$$

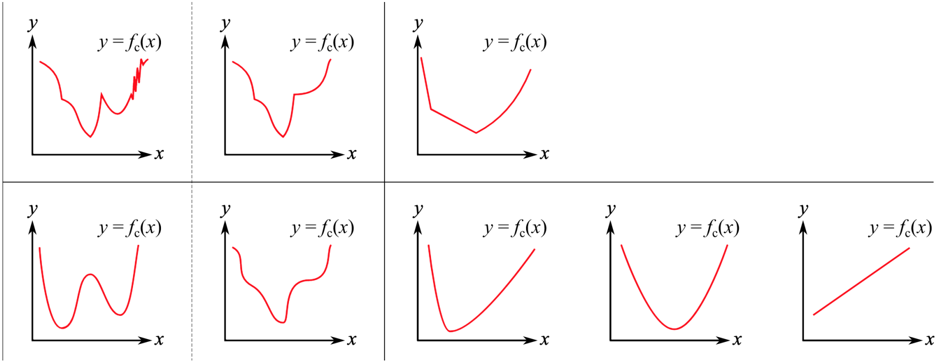
What should an ideal optimization problem, i.e. the cost function and constraints look like?

Constrained Optimization (Ctd.)

$$\begin{aligned} \min_{\boldsymbol{\theta}} \mathcal{J}(\theta) &= \dots && \longleftarrow \text{convex function} \\ \text{s.t.}\ \ f(\theta) &= 0 && \longleftarrow \text{linear function} \\ g(\theta) &\geqslant 0 && \longleftarrow \text{convex set} \end{aligned}$$

Cost Functions

non-convex | convex

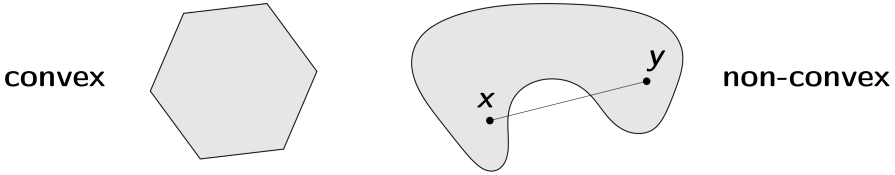


Convexity – Convex Sets

- A set $C \subseteq \mathbb{R}^n$ is convex, if $\forall \boldsymbol{x}, \boldsymbol{y} \in C$ and $\forall \alpha \in [0, 1]$

$$\alpha \boldsymbol{x} + (1 - \alpha) \boldsymbol{y} \in C \tag{45}$$

- This is the equation line segment between $\boldsymbol{x}$ and $\boldsymbol{y}$

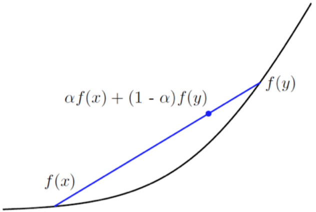


Convexity – Convex Functions

- A function $f : \mathbb{R}^n \mapsto \mathbb{R}$ is convex, if $\forall \boldsymbol{x}, \boldsymbol{y} \in \mathrm{dom}(f)$ and $\forall \alpha \in [0, 1]$

$$f(\alpha \boldsymbol{x} + (1 - \alpha)\boldsymbol{y}) \leqslant \alpha f(\boldsymbol{x}) + (1 - \alpha) f(\boldsymbol{y}) \tag{46}$$

- Examples are linear functions $f(\boldsymbol{x}) = \boldsymbol{a}^\intercal \boldsymbol{x} + b$ and quadratic functions $f(\boldsymbol{x}) = \boldsymbol{x}^\intercal \boldsymbol{A}\boldsymbol{x} + \boldsymbol{b}^\intercal \boldsymbol{x} + c$



Convexity (Ctd.)

- **Why are convex cost functions so appealing?**
- Local solutions are global optima
- Efficient implementations of optimizers are available

Important

Constrained Optimization

- **How to solve this optimization problem?**

$$\min_{x,y} \mathcal{J}(x, y) = 2y + x$$

subject to (s. t.):

$$f(x, y) = y^2 + xy - 1 = 0$$

- Convert the problem to an unconstrained one
- This is done using Lagrange multipliers α

Important

The Concept of Lagrange Multipliers

General Lagrange function: $\mathcal{L}(x, y, \lambda) = \mathcal{J}(x, y) + \lambda f(x, y)$

$$\min_{x,y} \mathcal{J}(x, y) = 2y + x$$

s. t.:

$$f(x, y) = y^2 + xy - 1 = 0$$

Step ❶: Differentiate w. r. t. x, y and λ:

I. $\nabla_x \mathcal{L} = 1 + \lambda y$

II. $\nabla_y \mathcal{L} = 2 + 2\lambda y + \lambda x$

III. $\nabla_\lambda \mathcal{L} = y^2 + xy - 1$

The Concept of Lagrange Multipliers (Ctd.)

Step ❷: Set equations to zero:

$$\begin{aligned} \text{I.} \quad & 1 + \lambda y && \overset{!}{=} 0 \\ \text{II.} \quad & 2 + 2\lambda y + \lambda x && \overset{!}{=} 0 \\ \text{III.} \quad & y^2 + xy - 1 && \overset{!}{=} 0 \end{aligned}$$

Step ❸: Substitute:

$$\begin{aligned} \text{I.} \quad & \lambda = -\frac{1}{y} \\ \text{I.} \rightarrow \text{II.} \quad & x = 0 \\ \text{II.} \rightarrow \text{III.} \quad & y = \pm 1 \end{aligned}$$

Exercise

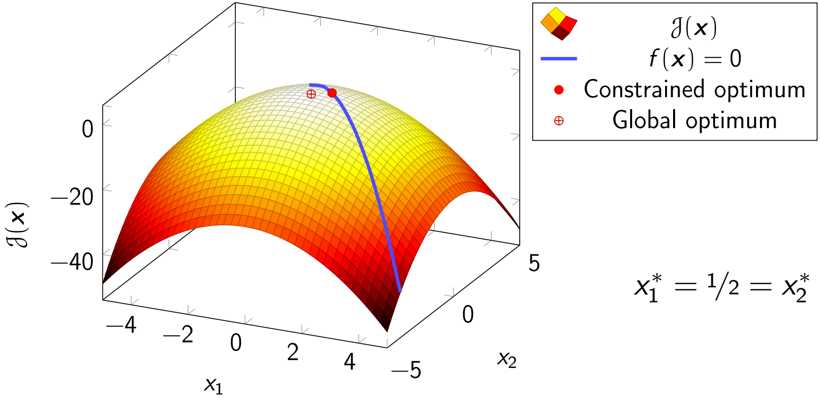
Optimize the following function:

$$\min_{x_1, x_2} \mathcal{J}(x_1, x_2) = 1 - x_1^2 - x_2^2$$

s. t.:

$$f(x_1, x_2) = x_1 + x_2 - 1 = 0$$

Exercise Solution



$$x_1^* = 1/2 = x_2^*$$

Important

Numerical Optimization

- Different numerical optimization algorithms exist for optimizing a function numerically on a computer if we can't solve it analytically
- **Gradient descent:** Incrementally update an estimate of the parameters:

$$\boldsymbol{\theta}_{new} \longleftarrow \boldsymbol{\theta}_{old} + \alpha \delta \boldsymbol{\theta} \tag{47}$$

- After each update: $\mathcal{J}(\boldsymbol{\theta}_{new}) < \mathcal{J}(\boldsymbol{\theta}_{old})$
- The algorithms differ in the number of iterations required, the computational cost, the convergence guarantees, the robustness with noisy cost functions and their memory usage

Numerical Optimization Algorithms

- **Gradient-based methods:**
  - Gradient descent (with constant, variable step size α)
  - (L-)BFGS (Broyden-Fletcher-Goldfarb-Shanno)
  - Conjugate gradient descent
- **Non-gradient based methods:**
  - Genetic algorithms
  - Non-Linear simplex
  - Nelder-Mead

Numerical techniques may not find the global optimum!

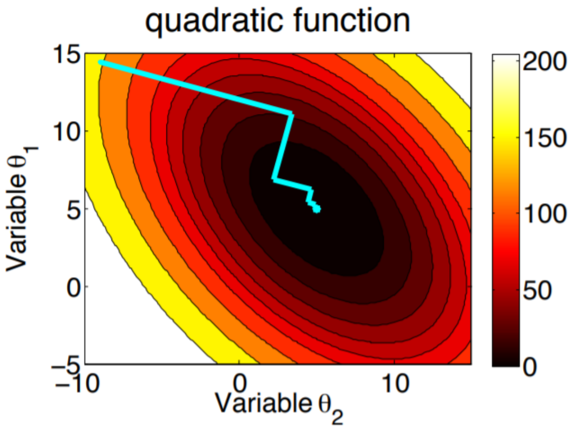
Gradient Descent

- Most basic algorithm (and most commonly used)
- Go into the direction of the **steepest descent**
- The gradient points in the direction of the maximum ($\rightarrow$ subtract gradient)

$$\boldsymbol{\theta}^{(new)} \longleftarrow \boldsymbol{\theta}^{(old)} - \alpha \nabla_{\boldsymbol{\theta}} \mathcal{J}(\boldsymbol{\theta}^{(old)}) \tag{48}$$

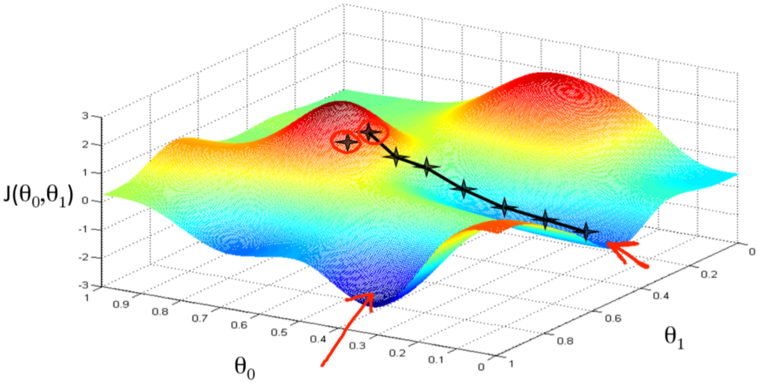
- The parameter updates tend to 'zig-zag' down the valley (see next slide)
- Gradient descent is a 1st-order method

Gradient Descent (Ctd.)



Initialization

Initialization also matters...



Newton's Method

- We want to solve: ($\boldsymbol{H}$ is the **Hessian**, $\boldsymbol{g}$ the **Jacobian**)

$$\delta\boldsymbol{\theta} = \arg\min_{\delta\boldsymbol{\theta}} \Big[\underbrace{c + \boldsymbol{g}^\intercal \delta\boldsymbol{\theta} + \frac{1}{2}\delta\boldsymbol{\theta}^\intercal \boldsymbol{H} \delta\boldsymbol{\theta}}_{\text{Taylor series expansion}} \Big] \tag{49}$$

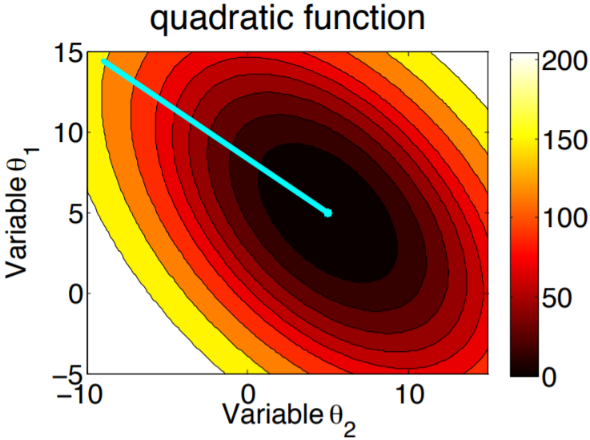
- We have to differentiate and set to zero:

$$\nabla_{\delta\boldsymbol{\theta}} \left[c + \boldsymbol{g}^\intercal \delta\boldsymbol{\theta} + \frac{1}{2}\delta\boldsymbol{\theta}^\intercal \boldsymbol{H} \delta\boldsymbol{\theta} \right] = \boldsymbol{g} + \boldsymbol{H}\delta\boldsymbol{\theta} \stackrel{!}{=} \boldsymbol{0} \tag{50}$$

- Which yields the solution:

$$\delta\boldsymbol{\theta} = -\boldsymbol{H}^{-1}\boldsymbol{g} \tag{51}$$

Newton's Method (Ctd.)



Section:

Wrap-Up

DHBW
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Summary I

- Machine learning is math!
- **Linear algebra:**
  - You should know what vectors are and what you can do with them (addition, multiplication, transpose, ...)
  - The same applies to matrices
  - Matrix inversion and pseudoinverse
  - Eigenvectors and eigenvalues are important, **eigenvectors form a basis**

Summary II

- **Statistics:**
  - Random variables are numbers **determined by chance**
  - Probability distributions describe a **probability mass** or **density**
  - Discrete distributions: Bernoulli, Binomial, Poisson (not covered)
  - Continuous distributions: Gaussian, Student-t (not covered)
  - Gaussians are important in machine learning and have appealing properties
  - Terms: Joint-, marginal- and conditional distribution, chain rule, probabilistic independence, Bayes' rule
  - You should know what expectation and variance is

Summary III

- **Optimization:**
  - **Every machine learning problem is an optimization problem!**
  - Good cost functions are **convex**
  - Unconstrained and constrained optimization (Lagrange multipliers)
  - Closed-form solutions are not always possible $\rightarrow$ **numerical optimization**
  - The most prominent numerical technique is called **gradient descent**

Self-Test Questions

1. What is a vector and what is a matrix?
2. What is the result of an inner product / outer product?
3. How can you invert matrices? Is this always possible?
4. What is an eigenvalue problem? Where do they play a role?
5. What are random variables and probability distributions?
6. Why is the Gaussian distribution so important?
7. What is Bayes' rule? Explain its components!
8. What is convexity? Why should cost functions be convex?
9. What can you do if no analytical solution to optimization problems exists?

What's next...?

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

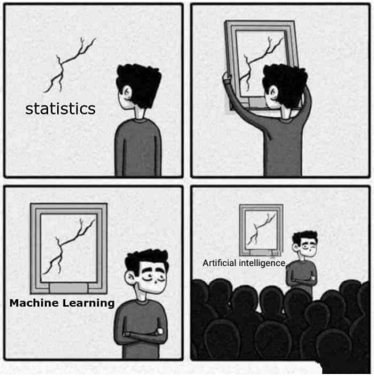
Recommended Literature and further Reading I

- **[1] Mathematics for Machine Learning**
  Deisenroth et al. Cambridge University Press. 2019.
  → Link
- **[2] Deep Learning**
  Ian Goodfellow et al. MIT Press. 2016.
  → Link, cf. chapters 4.3, 4.4, 8
- **[3] Convex Optimization**
  Stephen Boyd et al. Cambridge University Press. 2004.
  → Link

Recommended Literature and further Reading II

[4] Lecture slides 'Convex Optimization'
Stephen Boyd. Stanford University. 2019.
→ Link

Meme of the Day



Thank you very much for the attention!

Topic: *** Applied Machine Learning Fundamentals *** Mathematical Foundations
Term: Winter term 2019/2020

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Do you have any questions?