Forecasting and Simulation

Ulf Brefeld & Yannick Rudolph
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Machine Learning Group
Leuphana University of Lüneburg

Course General Information

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Lecturers

- Ulf Brefeld (Lecture)
- Yannick Rudolph (Exercise)

- brefeld@leuphana.de
- yannick.rudolph@leuphana.de

Grading and Tutorial

- Written exam (see myStudy)
- Tutorials
  - Regular exercise sheets ($\sim$ weekly)
  - Practical questions
  - Discussions
- Each tutorial
  - You mark all tasks you worked on (solved or tried to solve)
  - We discuss solutions together
- You need 50% of the marks to pass the tutorial

Recap Overview

- Calculus
- Linear Algebra
- Probability Theory
- Supervised Machine Learning

Calculus Recap

Sum and Product

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  - $\sum_{i \in I} a_i$ for $I = \{1, 2, \dots, n\}$
  - $\sum_{a \in A} a$, for $A = \{a_1, a_2, \dots, a_n\}$
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- Product: $a_1 \cdot a_2 \cdot \ldots \cdot a_n$
  - $\prod_{i=1}^n a_i = a_1 \cdot a_2 \cdot a_3 \cdot \ldots \cdot a_n$
- For $I = \emptyset$ or $A = \emptyset$, the product is equal to one

Binomial Coefficient

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  - $\binom{n}{k}$ = number of combinations with k elements from a set with n elements

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$$\begin{aligned} f'(x) &= \left(a \cdot x^2 + b \cdot x + c\right)' \\ &= \left(a \cdot x^2\right)' + (b \cdot x)' + c' \\ &= a \cdot \left(x^2\right)' + b \cdot x' + c' \\ &= 2ax + b \end{aligned}$$

Integration Rules

- Linearity

$$\int (f+g)(x)\mathrm{d}x = \int f(x)\mathrm{d}x + \int g(x)\mathrm{d}x$$

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  - Primitive (antiderivative) function: $F' = f$

$$\int_a^b f(x)\mathrm{d}x = [F(x)]_a^b = F(b) - F(a)$$

Integration Rules – Example

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\begin{aligned}
\int_u^v f(x)\mathrm{d}x &= \int_u^v \left(a \cdot x^2 + b \cdot x + c\right) \mathrm{d}x \\
&= \int_u^v a \cdot x^2 \mathrm{d}x + \int_u^v b \cdot x \mathrm{d}x + \int_u^v c \mathrm{d}x \\
&= a \cdot \int_u^v x^2 \mathrm{d}x + b \cdot \int_u^v x \mathrm{d}x + c \cdot \int_u^v 1 \mathrm{d}x \\
&= a \cdot \left[\frac{1}{3}x^3\right]_u^v + b \cdot \left[\frac{1}{2}x^2\right]_u^v + c \cdot [x]_u^v \\
&= \frac{a}{3}\left(v^3 - u^3\right) + \frac{b}{2}\left(v^2 - u^2\right) + c\left(v - u\right)
\end{aligned}
$$

Exponential Function

$a, b, x, y \in \mathbb{R}$

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- $\exp(x)' = \exp(x)$

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- $\log'(x) = \frac{1}{x}$
- Natural logarithm: $\ln(x) = \log_a(x)$ when $a = e$

Linear Algebra Recap

Vectors

$$\mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_d \end{pmatrix} \in \mathbb{R}^d$$

Vectors

- Multiplication by a scalar $c \in \mathbb{R}$

$$c\mathbf{x} = \begin{pmatrix} cx_1 \\ cx_2 \\ \vdots \\ cx_d \end{pmatrix}$$

- Addition of two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$

$$\mathbf{x} + \mathbf{y} = \begin{pmatrix} x_1 + y_1 \\ x_2 + y_2 \\ \vdots \\ x_d + y_d \end{pmatrix}$$

- Transpose

$$\mathbf{x}^\top = \begin{pmatrix} x_1 & x_2 & \dots & x_d \end{pmatrix}$$

Vectors

- Inner product of two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$

$$\mathbf{x}^\top \mathbf{y} = \langle \mathbf{x}, \mathbf{y} \rangle = x_1 y_1 + x_2 y_2 + \ldots + x_d y_d = \sum_{i=1}^{d} x_i y_i \in \mathbb{R}$$

- Outer product of two vectors $\mathbf{x} \in \mathbb{R}^{d_1}, \mathbf{y} \in \mathbb{R}^{d_2}$

$$\mathbf{x}\mathbf{y}^\top = \begin{pmatrix} x_1 y_1 & \cdots & x_1 y_{d_2} \\ \vdots & \ddots & \vdots \\ x_{d_1} y_1 & \cdots & x_{d_1} y_{d_2} \end{pmatrix} \in \mathbb{R}^{d_1 \times d_2}$$

Vectors

- Length of a vector $\mathbf{x} \in \mathbb{R}^d$

$$\mathbf{x} = \|\mathbf{x}\|_2 = \sqrt{\mathbf{x}^\top \mathbf{x}} = \sqrt{x_1^2 + \ldots + x_d^2} \in \mathbb{R}$$

- Angle between vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$

$$\cos(\theta) = \frac{\mathbf{x}^\top \mathbf{y}}{\|\mathbf{x}\|_2 \cdot \|\mathbf{y}\|_2}$$

Matrices

A matrix can be seen as a collection of vectors

$$\mathbf{A} = \begin{pmatrix} a_{11} & \dots & a_{1m} \\ \vdots & \ddots & \vdots \\ a_{n1} & \dots & a_{nm} \end{pmatrix} = \begin{pmatrix} | & & | \\ \mathbf{a}_1 & \dots & \mathbf{a}_m \\ | & & | \end{pmatrix} \in \mathbb{R}^{n \times m}$$

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Matrices

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Matrices

- Multiplication of a vector $\mathbf{x} \in \mathbb{R}^m$ by a matrix $\mathbf{A} \in \mathbb{R}^{n \times m}$

$$\mathbf{A}\mathbf{x} = \mathbf{b} \in \mathbb{R}^n$$

$$b_i = \sum_{j=1}^{m} a_{ij} x_j$$

- Multiplication of two matrices $\mathbf{A} \in \mathbb{R}^{n_1 \times m}$ and $\mathbf{B} \in \mathbb{R}^{m \times n_2}$

$$\mathbf{A}\mathbf{B} = \mathbf{C} \in \mathbb{R}^{n_1 \times n_2}$$

$$c_{ij} = \sum_{k=1}^{m} a_{ik} b_{kj}$$

Matrices

- Inverse of a matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$

$$\mathbf{A}\mathbf{A}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$$

Whenever you can avoid calculating the inverse of a matrix AVOID IT! E.g. solving the linear equation system $\mathbf{A}\mathbf{x} = \mathbf{b}$ for $\mathbf{x}$ is much better than working with the inverse: $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$

Norm

- Norm: function $\|\cdot\| : \mathbb{R}^d \to \mathbb{R}_0^+$
- Properties ($x, y \in \mathbb{R}^d$ and $\lambda \in \mathbb{R}$)
    - $\|x\| = 0 \implies x = 0$
    - $\|\lambda x\| = |\lambda| \cdot \|x\|$
    - $\|x + y\| \leq \|x\| + \|y\|$
- p-Norm ($p \geq 1$)

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- 1-Norm: $\|x\|_1 = \sum_{i=1}^{d} |x_i|$.
- Euclidean norm (2-norm): $\|x\|_2 = \sqrt{\sum_{i=1}^{d} x_i^2}$.
- Maximum norm ($p \to \infty$): $\|x\|_\infty = \max_i |x_i|$.

Probability Theory Recap

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  - Expressing information
- Generic tool to express uncertainty, information, and coupling

(Discrete) Random Variables

- Intuitively: probability of *random variable* X taking on value x
- *Example*
  - A dice roll (X) can result in $\{1, \ldots, 6\}$
  - What is the probability of $X = x$ for $x \in \{1, \ldots, 6\}$

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- A bit more formally
  - Domain of X: $\mathrm{dom}(X)$ (or *sample space* Ω)
    - Set of possible values of a random variable
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    - Set of possible values of a random variable
    - Mutually exclusive: only one will happen
    - Collectively exhaustive: at least one will happen
  - Space of events $\mathcal{F} = \{E : E \subset \Omega\}$ and $A, B, \emptyset, \Omega \in \mathcal{F}$
    - For event $E \in \mathcal{F}$, $P(E) = \sum_{x \in E} P(X = x)$
    - $P(A) \in [0, 1]$
    - $P(\Omega) = 1$ (sure event)
    - $P(\emptyset) = 0$ (impossible event)
    - If $A \cap B = \emptyset$ then $P(A \cup B) = P(A) + P(B)$

(Discrete) Random Variables

- Notation
  - Random variable X (capital letter)
  - Value $x \in \text{dom}(X)$ is taken by X (lower case letter)
  - $P(X = x) \in \mathbb{R}$: $x \in \text{dom}(X) \rightarrow$ probability in $[0, 1]$
  - For event $E \subset \Omega$
    - $P(E)$: probability of X taking a value $x \in E$
    - $P(E) = \sum_{x \in E} P(X = x)$

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Example Two binary RV: Cavity (X) and Toothache (Y)

$P(X, Y)$	$Y = T$	$Y = F$
$X = T$	0.04	0.06
$X = F$	0.01	0.89

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We write: $P(X = F, Y = T) = 0.01$

Joint Probability Distributions – Definitions

Marginal probability of X given $P(X, Y)$

$$P(X) = \sum_Y P(X, Y)$$

$P(X, Y)$	$Y = T$	$Y = F$	$P(X)$
$X = T$	0.15	0.20	0.35
$X = F$	0.05	0.60	0.65
$P(Y)$	0.20	0.80	

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	$P(X\|Y = T)$	$P(X\|Y = F)$
$X = T$	0.75	0.25
$X = F$	0.25	0.75

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Extends for more than two variables (vector of variables)

$$X = (X_1, \ldots, X_n)$$
$$P(X_1, \ldots, X_{n-1}, X_n)$$
$$P(X_n | X_1, \ldots, X_{n-1})$$

Joint Probability Distributions – Properties

- Product rule

$$P(X, Y) = P(X|Y)\ P(Y) = P(Y|X)\ P(X)$$

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- Bayes rule

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Joint Probability Distributions

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- Graphical models
  - Descriptions of joint probability distributions
- Correlations, interdependence, and coupling
  - Expressed in terms of joint probability distributions

Bayes Rule

- Thomas Bayes (1702–1761)
- Trivial implication of marginal and conditional probability
- Important: interpretation and use

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$$P(\text{cause}|\text{effect}) = \frac{P(\text{effect}|\text{cause})}{P(\text{effect})}\, P(\text{cause})$$

Bayesian Inference – Example (by @xamat)

- Bad COVID antibody test kit
  - 95% sensitivity and specificity
  - 5% chance of being wrong (both sides)
    - 1 - sensitivity|specificity
- Population with COVID antibodies: 5%

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- $P(\text{ab}|\text{pos}) = \frac{0.95 \cdot 0.05}{0.95 \cdot 0.05 + 0.05 \cdot 0.95} = 0.5$ (!)

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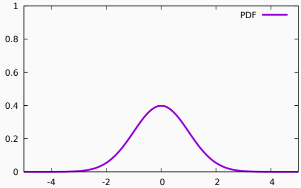
$$P(X \in (a, b)) = \int_a^b f(x)dx$$



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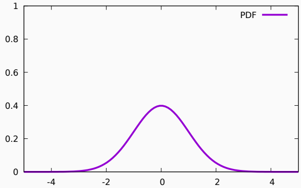

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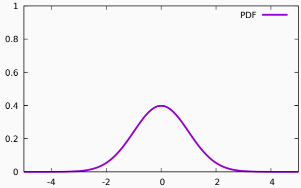
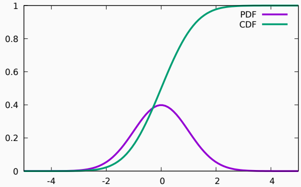
- Cumulative distribution function (CDF) $F(x) = P(X \leq x)$

$$F(x) = \int_{-\infty}^{x} f(t)dt$$





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- Inference problem: compute $P(Y|E)$
- Issue: size of table $P(Y_{1:k}, E_{1:m}, H_{1:n})$ is d^{k+m+n}
  - d: number of possible values for each variable
  - If all binary variables: 2^{k+m+n}
  - Remember those $H_{1:n}$?

Cheat Sheet (1)

- Random variable X
  - Values $x \in \text{dom}(x) \rightarrow$ probabilities $P(X = x) \in [0, 1]$
- Probability distribution of X
  - Table (array) of probabilities for each value $x \in \text{dom}(X)$
  - Normalization: $\sum_X P(X) = 1$
- Joint distribution $P(X, Y)$
  - Table (matrix) of probabilities for each value $x, y \in \text{dom}(X) \times \text{dom}(Y)$
- Marginal $P(X) = \sum_Y P(X, Y)$
  - Summing along columns/rows (Y)
- Conditional $P(X|Y) = \frac{P(X,Y)}{P(Y)}$
  - Normalizing each column/row (Y)

Cheat Sheet (2)

- Properties

$$P(X, Y) = P(X|Y)\ P(Y) = P(Y|X)\ P(X)$$

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$$P(Y|X) = \frac{P(X|Y)}{P(X)} P(Y) \quad \left[\text{posterior} = \frac{\text{likelihood}}{\text{evidence}}\ \text{prior}\right]$$

- Inference: to compute

$$P(Y_{1:k}|E_{1:m}) = \frac{P(Y_{1:k}, E_{1:m})}{P(E_{1:m})} \propto \sum_{H_{1:n}} P(Y_{1:k}, E_{1:m}, H_{1:n})$$

Supervised Machine Learning Recap

Supervised Machine Learning

- Goal
    - Find $f : X \rightarrow Y$
    - Deterministic mapping: $y = f(x)$
    - Set of inputs: X
    - Set of target variables: Y (outputs)

Supervised Machine Learning

- Goal
  - Find $f : X \to Y$
  - Deterministic mapping: $y = f(x)$
  - Set of inputs: X
  - Set of target variables: Y (outputs)
- Relation between X and Y
  - Joint probability distribution: $P(X, Y)$
  - Generally unknown

Supervised Machine Learning (cont.)

- If $P(X, Y)$ was known

$$P(Y|X) = \frac{P(X, Y)}{P(X)}$$

Supervised Machine Learning (cont.)

- If $P(X, Y)$ was known

$$P(Y|X) = \frac{P(X, Y)}{P(X)}$$

$$P(y|x) = \frac{P(x, y)}{P(x)} = \frac{P(x, y)}{\sum_{y' \in Y} P(x, y')}$$

Supervised Machine Learning (cont.)

- If $P(X, Y)$ was known

$$P(Y|X) = \frac{P(X, Y)}{P(X)}$$

$$P(y|x) = \frac{P(x, y)}{P(x)} = \frac{P(x, y)}{\sum_{y' \in Y} P(x, y')}$$

$$f(x) = \text{argmax}_{y \in Y} P(y|x)$$

Supervised Machine Learning (cont.)

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- Learn a model for $P(Y|X)$ directly

Supervised Machine Learning (cont.)

- $P(X, Y)$: usually not necessary
- Learn a model for $P(Y|X)$ directly
- Or even
    - Learn deterministic $f : X \to Y$ instead of $P(Y|X)$
    - Find $f(x)$ that minimizes generalization error
        - Error for new and unseen $x \in X$

Generalization Error

Generalization error of $f(x)$ (theoretical risk) is the expected loss

$$R[f] = \int_{X \times Y} \ell(x, y, f) dP(X, Y)$$

where $\ell : X \times Y \times F \to \mathbb{R}_0^+$ is a *loss function*

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- BUT: joint probability $P(X, Y)$ is still unknown
- Therefore: $\inf_f R[f]$ cannot be computed directly
- Solution
    - Approximate $R[f]$ using an N-sample (training set)

      $$\mathcal{D} = \{(x_n, y_n)\}_{n=1 \ldots N} \in X \times Y$$

      drawn *independently and identically distributed* (iid) from $P(X, Y)$

Empirical Risk Minimization

Minimize the empirical risk on $\mathcal{D} = \{(x_n, y_n)\}_{n=1\ldots N}$

$$\hat{R}_{\mathcal{D}}[f] = \frac{1}{N}\sum_{n=1}^{N} \ell(x_n, y_n, f)$$

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- *Example* regression tasks on the squared loss

$$\ell(x, y, f) = (f(x) - y)^2$$

$$\hat{R}_{\mathcal{D}}[f] = \frac{1}{N} \sum_{n=1}^{N} (f(x_n) - y_n)^2$$