

# Lecture 7: ANCOVA, short introduction to Linear Algebra

## BIO144 Data Analysis in Biology

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# Overview

- ▶ ANCOVA
- ▶ Introduction to linear Algebra

Note: ANCOVA = ANalysi of COVAriance (Kovarianzanalyse)

## Course material covered today

- ▶ "Getting Started with R" chapter 6.3
- ▶ "Lineare regression" chapters 3.A (p. 43-45) and 3.4, 3.5 (p. 39-42)

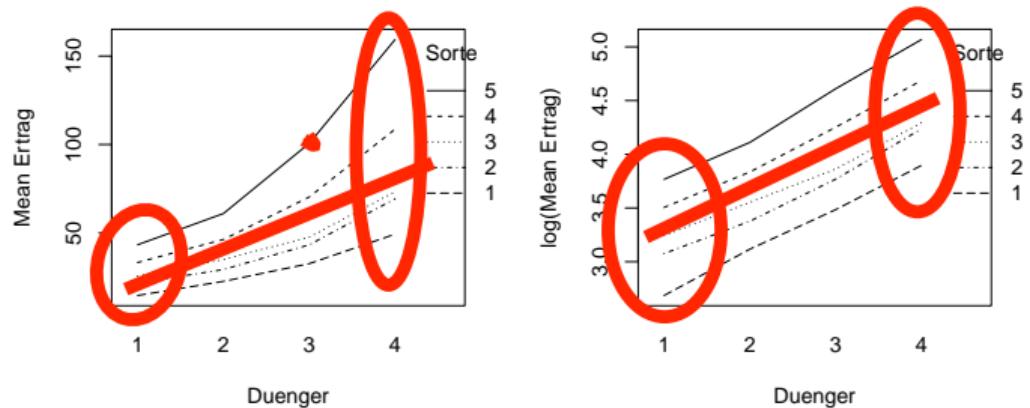
## Recap of ANOVA

- ▶ ANOVA is a method to test if the means of **two or more groups** are different.
- ▶ Post-hoc tests and contrasts, including correction for  $p$ -values, to understand the differences between the groups.
- ▶ Two-way ANOVA for factorial designs, interactions.
- ▶ ANOVA is a special case of linear regression with categorical covariates.

## Recap of two-way ANOVA example

Remember: Influence of four levels of fertilizer (DUENGER) on the yield (ERTRAG) on 5 species (SORTE) of crops was investigated. For each DUENGER  $\times$  ERTRAG combination, 3 repeats were taken.

Interaction plot with ERTRAG and  $\log(\text{ERTRAG})$  as response:



Remember: We used  $\log(\text{ERTRAG})$ , because the residual plots were otherwise not ok.

```
r.duenger2 <- lm(log(ERTRAG) ~ DUENGER*SORTE,d.duenger)
anova(r.duenger2)
```

```
## Analysis of Variance Table
##
## Response: log(ERTRAG)
##           Df  Sum Sq Mean Sq F value Pr(>F)
## DUENGER      3 11.6917 3.8972 854.0505 <2e-16 ***
## SORTE        4  8.5202 2.1300 466.7851 <2e-16 ***
## DUENGER:SORTE 12  0.0929 0.0077   1.6958 0.1045
## Residuals    40  0.1825 0.0046
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

## Questions:

- ▶ Number of parameters?
- ▶ Degrees of freedom (60 data points)?
- ▶ Interpretation?

```
summary(r.duenger2)
```

```
##  
## Call:  
## lm(formula = log(ERTRAG) ~ DUENGER * SORTE, data = d.duenger)  
##  
## Residuals:  
##      Min       1Q   Median     3Q    Max  
## -0.120968 -0.045595  0.008984  0.049072  0.102175  
##  
## Coefficients:  
##             Estimate Std. Error t value Pr(>|t|)  
## (Intercept) 2.68505   0.03900 68.846 < 2e-16 ***  
## DUENGER2    0.43165   0.05516  7.826 1.36e-09 ***  
## DUENGER3    0.79997   0.05516 14.504 < 2e-16 ***  
## DUENGER4    1.21152   0.05516 21.966 < 2e-16 ***  
## SORTE2      0.38979   0.05516  7.067 1.51e-08 ***  
## SORTE3      0.55799   0.05516 10.117 1.38e-12 ***  
## SORTE4      0.82018   0.05516 14.870 < 2e-16 ***  
## SORTE5      1.08169   0.05516 19.612 < 2e-16 ***  
## DUENGER2:SORTE2 -0.12949  0.07800 -1.660  0.105  
## DUENGER3:SORTE2 -0.10613  0.07800 -1.361  0.181  
## DUENGER4:SORTE2 -0.04924  0.07800 -0.631  0.531  
## DUENGER2:SORTE3 -0.12180  0.07800 -1.562  0.126  
## DUENGER3:SORTE3 -0.18034  0.07800 -2.312  0.026 *  
## DUENGER4:SORTE3 -0.16061  0.07800 -2.059  0.046 *  
## DUENGER2:SORTE4 -0.10138  0.07800 -1.300  0.201  
## DUENGER3:SORTE4 -0.05311  0.07800 -0.681  0.500  
## DUENGER4:SORTE4 -0.02954  0.07800 -0.379  0.707  
## DUENGER2:SORTE5 -0.08779  0.07800 -1.125  0.267  
## DUENGER3:SORTE5  0.04370  0.07800  0.560  0.578  
## DUENGER4:SORTE5  0.09014  0.07800  1.156  0.255  
## ---  
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ',' 1
```

# Analysis of Covariance (ANCOVA)

An ANCOVA is an analysis of variance (ANOVA), **including** also at least one **continuous covariate**.

ANCOVA unifies several concepts that we approached in this course so far:

- ▶ Linear regression
- ▶ Categorical covariates
- ▶ Interactions (of continuous and categorical covariates)
- ▶ Analysis of Variance (ANOVA)

As such, it is a **special case of the linear regression model**.

Given a categorical covariate  $x_i$  and a continuous covariate  $z_i$ . Then the ANCOVA equation (without interactions) is given as

$$y_i = \beta_0 + \beta_1 x_i^{(1)} + \dots + \beta_k x_i^{(k)} + \beta_z z_i + \epsilon_i ,$$

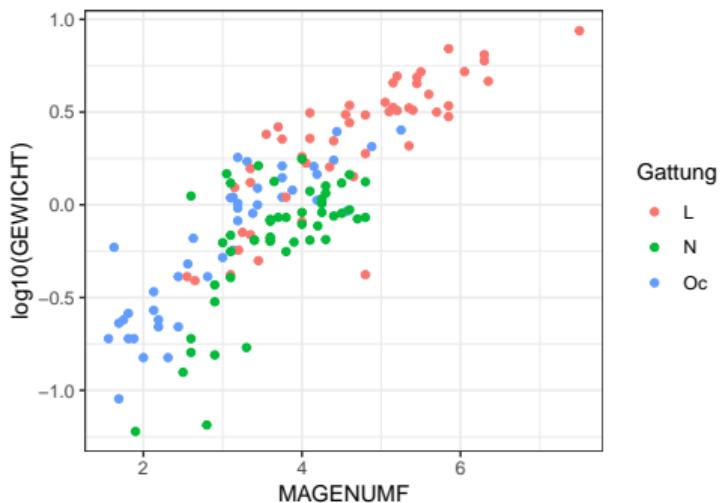
where  $x_i^{(k)}$  is the  $k$ th dummy variable ( $x_i^{(k)}=1$  if  $i$ th observation belongs to category  $k$ , 0 otherwise).

**Note 1:** It is straightforward to add an interaction of  $x_i$  with  $z_i$ .

**Note 2:** Again, for identifiability reason, we typically set  $\beta_1 = 0$ .

## Once more: the earthworms

“Magenumfang” was used to predict “Gewicht” of the worm, including as covariate also the worm species.



Categorical and continuous covariates were used to predict a continuous outcome → ANCOVA.

```
r.lm <- lm(log(GEWICHT) ~ MAGENUMF + Gattung,d.wurm)
summary(r.lm)$coef
```

```
##             Estimate Std. Error     t value   Pr(>|t|) 
## (Intercept) -2.5355459  0.22147279 -11.4485663 8.617670e-22
## MAGENUMF      0.7118725  0.04528843  15.7186392 1.232126e-32
## GattungN     -0.5151344  0.11009219  -4.6791186 6.760621e-06
## Gattung0c    -0.0907298  0.12791000  -0.7093254 4.793107e-01
```

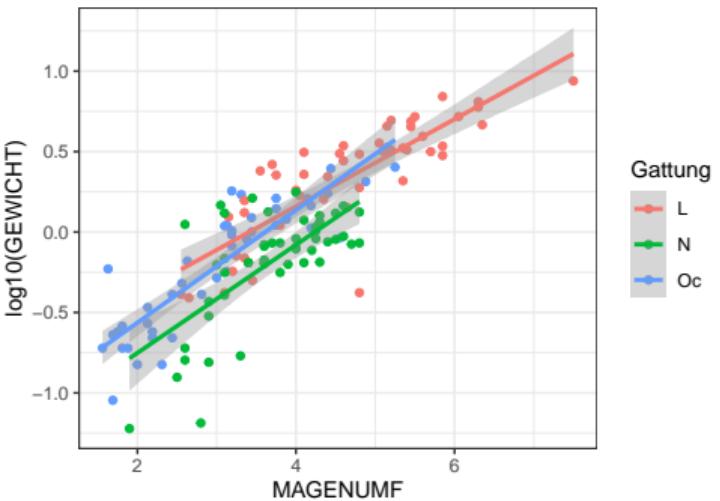
**Important:** The  $p$ -values for the entries GattungN and Gattung0c are not very meaningful (why?).

To understand if “Gattung” has an effect, **we need to carry out an F-test** → ANOVA table:

```
anova(r.lm)

## Analysis of Variance Table
##
## Response: log(GEWICHT)
##           Df  Sum Sq Mean Sq F value    Pr(>F)    
## MAGENUMF    1 104.866 104.866  409.69 < 2.2e-16 ***
## Gattung     2   7.177   3.589   14.02 2.842e-06 ***
## Residuals 139  35.579   0.256
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

We also included an **interaction term** between MAGENUMF and Gattung to allow for different slopes:



→ We again need the **F-test** to check whether the respective interaction term is needed:

```
r.lm2<- lm(log(GEWICHT) ~ MAGENUMF * Gattung,d.wurm)
anova(r.lm2)
```

```
## Analysis of Variance Table
##
## Response: log(GEWICHT)
##                               Df  Sum Sq Mean Sq F value    Pr(>F)
## MAGENUMF                  1 104.866 104.866 414.4743 < 2.2e-16 ***
## Gattung                   2   7.177   3.589  14.1835 2.521e-06 ***
## MAGENUMF:Gattung          2   0.917   0.458   1.8112   0.1673
## Residuals                 137  34.662   0.253
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

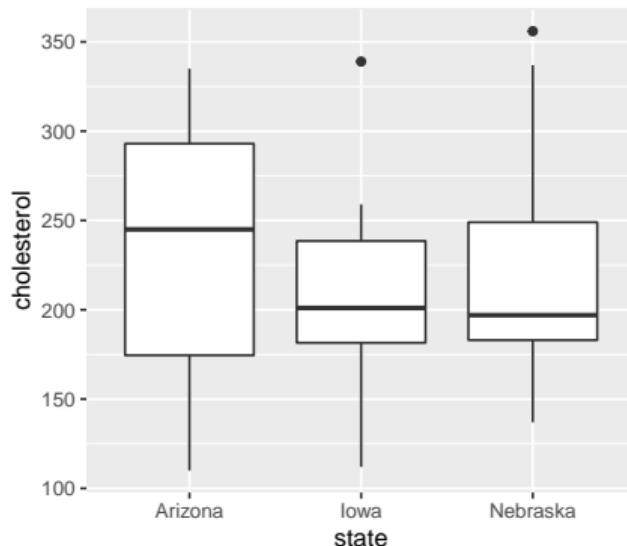
→  $p = 0.167$ , thus interaction is probably not relevant.

## A new example: cholesterol levels

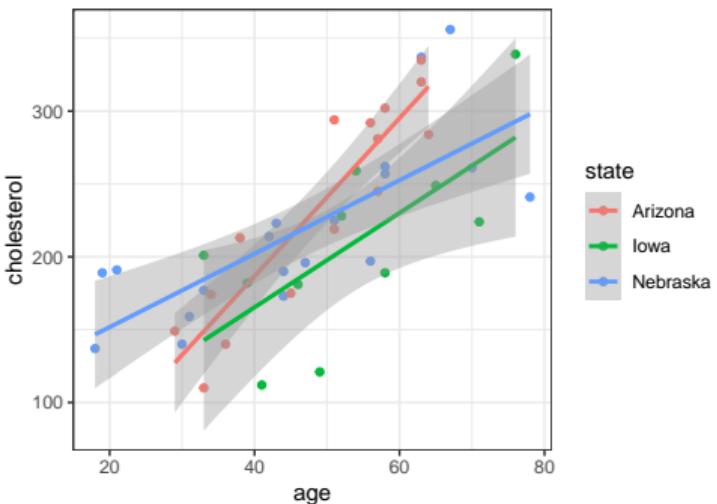
**Example:** Cholesterol levels [mg/ml] for 45 women from three US states (Iowa, Nebraska, Arizona), were measured.

**Question:** Do these levels differ between the states?

Age (years) may be a relevant covariate.



The scatter plot gives an idea about the model that might be useful here:



→ We include state, age and the interaction of the two.

Doing the analysis:

```
r.lm <- lm(cholesterol ~ age*state,data=d.chol)
anova(r.lm)
```

```
## Analysis of Variance Table
##
## Response: cholesterol
##           Df Sum Sq Mean Sq F value    Pr(>F)
## age        1 96524  96524 61.8961 1.424e-09 ***
## state      2 11474   5737  3.6789  0.03438 *
## age:state  2 12665   6332  4.0606  0.02501 *
## Residuals 39 60819    1559
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Interpretation?

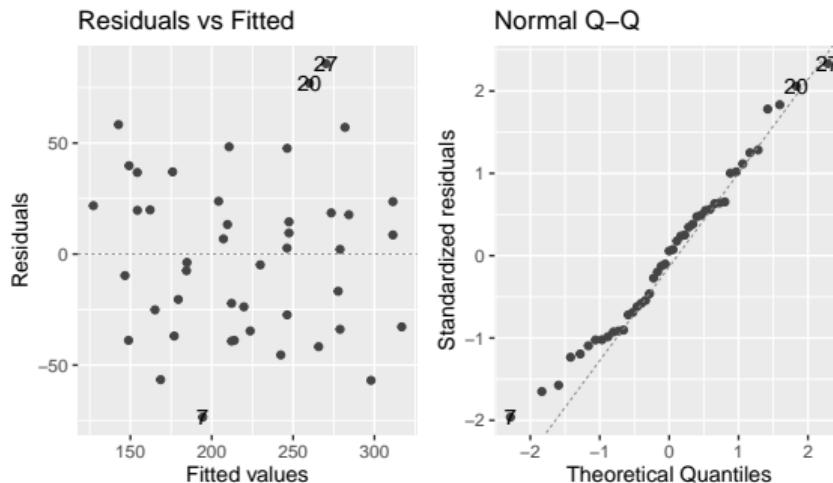
Compare the results from the previous slide to the estimated coefficients:

```
r.lm <- lm(cholesterol ~ age*state, data=d.chol)
summary(r.lm)$coef
```

	Estimate	Std. Error	t value	Pr(> t )
## (Intercept)	-29.895169	43.7353712	-0.6835467	4.983027e-01
## age	5.416908	0.8679635	6.2409400	2.396876e-07
## stateIowa	65.706383	66.7677031	0.9841043	3.311303e-01
## stateNebraska	131.192935	50.8573164	2.5796276	1.377434e-02
## age:stateIowa	-2.178763	1.2672928	-1.7192264	9.350204e-02
## age:stateNebraska	-2.896470	1.0166558	-2.8490174	6.967607e-03

**Note:** The  $p$ -values for the age coefficient is not the same as in the ANOVA table.  
**Reason:** `anova()` tests the models against one another in the **order** specified.

As always, some model checking is necessary:



→ This seems ok.

# An introduction to linear Algebra

Who has some knowledge of linear Algebra?

## Overview

- ▶ The basics about
  - ▶ vectors
  - ▶ matrices
  - ▶ matrix algebra
  - ▶ matrix multiplication
- ▶ Why is linear Algebra useful?
- ▶ What does it have to do with data analysis and statistics?
- ▶ Regression equations in matrix notation.

$$\begin{bmatrix} 1, 2, 5, \dots \\ 3, 5, 2, \dots \end{bmatrix}$$

## Motivation

Why are vectors, matrices and their algebraic rules useful?

- ▶ **Example 1:** The observations for a covariate  $x$  or the response  $y$  for all individuals  $1 \leq i \leq n$  can be stored in a vector (vectors and matrices are always given in **bold** letters):

$$x = \begin{pmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{pmatrix}, \quad y = \begin{pmatrix} y_1 \\ y_2 \\ \dots \\ y_n \end{pmatrix}.$$

- ▶ **Example 2:** Covariance matrices for multiple variables. Say we have  $x^{(1)}$  and  $x^{(2)}$ . The **covariance matrix** is then given as

$$\begin{pmatrix} \text{Var}(x^{(1)}) & \text{Cov}(x^{(1)}, x^{(2)}) \\ \text{Cov}(x^{(1)}, x^{(2)}) & \text{Var}(x^{(2)}) \end{pmatrix}.$$

- **Example 3:** The **data** (e.g. of some regression model) can be stored in a **matrix**:

$$\tilde{X} = \begin{pmatrix} 1 & x_1^{(1)} & x_1^{(2)} \\ 1 & x_2^{(1)} & x_2^{(2)} \\ \dots & \dots & \dots \\ 1 & x_n^{(1)} & x_n^{(2)} \end{pmatrix}.$$

This is the so-called **design matrix** with a vector of 1's in the first column.

- **Example 4:** A linear regression model can be written compactly using **matrix multiplication**:

$$y = \tilde{X} \cdot \tilde{\beta} + e,$$

with  $\tilde{\beta}$  the vector of regression coefficients and  $e$  the vector of errors

Why do we discuss this topic in our course?

- ▶ Useful for **compact notation**.
- ▶ Enables you to **understand many statistical texts** (books, research articles) that remain inaccessible otherwise.
- ▶ Useful for **efficient coding**, e.g. in R, which helps to increase speed and to reduce error rates.
- ▶ More advanced concepts often rely on linear algebra, e.g. **principal component analysis** (PCA) or **random effects** models.
- ▶ Is part of a **general education** (Allgemeinbildung) ;-)

# Matrices

An  $n \times m$  Matrix is given as

$$A = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1m} \\ a_{21} & a_{22} & \dots & a_{2m} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nm} \end{pmatrix},$$

with rows  $1 = 1, \dots, n$  and columns  $j = 1, \dots, m$ .

**Quadratic matrix:**  $n = m$ . Example:

$$\begin{pmatrix} 1 & 2 & 3 \\ 4 & 3 & 2 \\ 6 & 1 & 9 \end{pmatrix}$$

**Symmetric matrix:**  $a_{ij} = a_{ji}$ . Example:

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 4 \\ 3 & 4 & 5 \end{pmatrix}.$$

**The diagonal of a quadratic matrix** is given by  $(a_{11}, a_{22}, \dots, a_{nn})$ . Example: the diagonal of the above matrix is given as

$$(a_{11}, a_{22}, a_{33}) = (1, 3, 5).$$

**Diagonal matrix:** A matrix that has entries  $\neq 0$  only on the diagonal. Example:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 5 \end{pmatrix}.$$

**Transposing a matrix:** Given a matrix  $A$ . Exchange the rows by the columns and vice versa. This leads to the **transposed matrix**  $A^\top$ :

$$A = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1m} \\ a_{21} & a_{22} & \dots & a_{2m} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nm} \end{pmatrix} \Rightarrow A^\top = \begin{pmatrix} a_{11} & a_{21} & \dots & a_{n1} \\ a_{12} & a_{22} & \dots & a_{n2} \\ \vdots & \vdots & & \vdots \\ a_{1m} & a_{2m} & \dots & a_{nm} \end{pmatrix}.$$

Examples (note also the change of dimensions):

$$A = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \\ 13 & 14 & 15 & 16 \end{pmatrix} \Rightarrow A^\top = \begin{pmatrix} 1 & 5 & 9 & 13 \\ 2 & 6 & 10 & 14 \\ 3 & 7 & 11 & 15 \\ 4 & 8 & 12 & 16 \end{pmatrix}$$

$$A = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \end{pmatrix} \xrightarrow{\text{2}} A^\top = \begin{pmatrix} 1 & 5 \\ 2 & 6 \\ 3 & 7 \\ 4 & 8 \end{pmatrix} \xrightarrow{\text{4}}$$

- ▶ Transposing a matrix **twice** leads to the original matrix:

$$(A^\top)^\top = A .$$

- ▶ When a matrix is **symmetric**, then

$$A^\top = A .$$

This is true in particular for diagonal matrices.

# Vectors

A vector is nothing else than  $n$  numbers written in a column:

$$b = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

**Transposing** a vector leads to a *row vector*:

$$\begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}^\top = \begin{pmatrix} b_1 & b_2 & \dots & b_n \end{pmatrix}$$

**Note:** By definition (by default), a vector is always a column vector.

## Addition and subtraction

- ▶ Adding and subtracting matrices and vectors is only possible when the objects have the **same dimension**.
- ▶ Examples: Elementwise addition (or subtraction)

$$\begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix} + \begin{pmatrix} 3 & 2 & 1 \\ 6 & 5 & 4 \end{pmatrix} = \begin{pmatrix} 4 & 4 & 4 \\ 10 & 10 & 10 \end{pmatrix}$$

$$\begin{pmatrix} 1 \\ 4 \end{pmatrix} - \begin{pmatrix} 3 \\ 9 \end{pmatrix} = \begin{pmatrix} -2 \\ -5 \end{pmatrix}$$

- ▶ But this addition is **not defined**:

$$\begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix} + \begin{pmatrix} 3 & 6 \\ 2 & 5 \\ 1 & 4 \end{pmatrix} =$$

## Multiplication by a scalar

Multiplication with a “number” (scalar) is simple: Multiply each element in a vector or a matrix.

Examples:

$$3 \cdot \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix} = \begin{pmatrix} 3 & 6 & 9 \\ 12 & 15 & 18 \end{pmatrix}$$

$$-2 \cdot \begin{pmatrix} 1 \\ 4 \\ -2 \end{pmatrix} = \begin{pmatrix} -2 \\ -8 \\ 4 \end{pmatrix}$$

# Matrix multiplication

The multiplication of two matrices  $A$  and  $B$  is **defined if**

$$\text{number of columns in } A = \text{number of rows in } B.$$

It is easiest to explain matrix multiplication with an example:

$$\begin{aligned}
 \begin{pmatrix} 2 & 1 \\ -1 & 0 \\ 3 & 1 \end{pmatrix} \cdot \begin{pmatrix} 3 & 1 \\ 4 & -2 \end{pmatrix} &= \begin{pmatrix} 2 \cdot 3 + 1 \cdot 4 & 2 \cdot 1 + 1 \cdot (-2) \\ (-1) \cdot 3 + 0 \cdot 4 & (-1) \cdot 1 + 0 \cdot (-2) \\ 3 \cdot 3 + 1 \cdot 4 & 3 \cdot 1 + 1 \cdot (-2) \end{pmatrix} \\
 &= \begin{pmatrix} 10 & 0 \\ -3 & -1 \\ 13 & 1 \end{pmatrix}
 \end{aligned}$$

[► Matrix multiplication app](#)

\*      %\*%

# Matrix multiplication rules I

Attention: Matrix multiplication does **not** follow the same rules as scalar multiplication!!!

- ▶ It can happen that  $A \cdot B$  can be calculated, but  $B \cdot A$  is not defined (see example on previous slide).
- ▶ In general:  $A \cdot B \neq B \cdot A$ , even if both are defined.
- ▶ It can happen that  $A \cdot B = 0$  (0 matrix), although both  $A \neq 0$  and  $B \neq 0$ .
- ▶ The **Assoziativgesetz holds:**  $A \cdot (B \cdot C) = (A \cdot B) \cdot C$ .
- ▶ The **Distributivgesetz holds:**

$$A \cdot (B + C) = A \cdot B + A \cdot C$$

$$(A + B) \cdot C = A \cdot C + B \cdot C$$

## Matrix multiplication rules II

- ▶ Transposing inverts the order:  $(A \cdot B)^\top = B^\top \cdot A^\top$ .
- ▶ The product  $A \cdot A^\top$  is **always symmetric**.
- ▶ All these rules also hold for **vectors**, which can be interpreted as  $n \times 1$  matrices:

$$a \cdot b^\top = \begin{pmatrix} a_1 b_1 & a_1 b_2 & \dots & a_1 b_m \\ a_2 b_1 & a_2 b_2 & \dots & a_2 b_m \\ \vdots & \vdots & & \vdots \\ a_n b_1 & a_n b_2 & \dots & a_n b_m \end{pmatrix}$$

If  $a$  and  $b$  have the **same length**:

$$a^\top \cdot b = \sum_i a_i b_i$$

## Short exercise

Given vectors  $a$  and  $b$  and matrix  $C$ :

$$b_T = (-2, 4)$$

$$a = \begin{pmatrix} 1 \\ -2 \\ 3 \\ 0 \end{pmatrix}, \quad b = \begin{pmatrix} -2 \\ 4 \end{pmatrix}, \quad C = \begin{pmatrix} 1 & 0 \\ -1 & 2 \end{pmatrix}$$

Calculate, if defined

- ▶  $a^T \cdot b$
- ▶  $a \cdot b^T$
- ▶  $C \cdot a$
- ▶  $C \cdot b$

$$4 \neq 2$$

$$\begin{bmatrix} -2 & 4 \\ 4 & -8 \\ = & = \end{bmatrix}$$

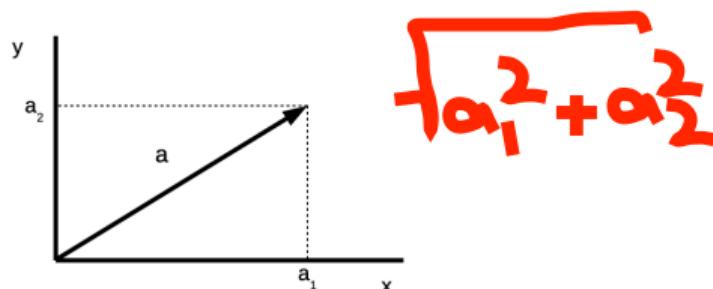
## The length of a vector

The **length of a vector**  $a^\top = (a_1, a_2, \dots, a_n)$  is defined as  $\|a\|$  with

$$\|a\|^2 = a^\top \cdot a = \sum_i a_i^2 .$$

This is basically the **Pythagoras** idea in 2, 3, ...  $n$  dimensions.

In 2 dimensions:  $\|a\| = \sqrt{a_1^2 + a_2^2}$ :



## Identity matrix (Einheitsmatrix)

The identity matrix (of dimension  $m$ ) is probably the simplest matrix that exists. It has 1's on the diagonal and 0's everywhere else:

$$I = \begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & 1 \end{pmatrix}$$

Multiplication with the identity matrix leaves a  $m \times n$  matrix  $A$  unchanged:

$$A \cdot I = A .$$

# Inverse matrix

Given a quadratic matrix  $A$  that fulfills

$$B \cdot A = I ,$$

then  $B$  is called the **inverse** of  $A$  (and vice versa). One then writes

$$B = A^{-1} .$$

Note:

- ▶ In that case it also holds that  $A \cdot B = I$ .
- ▶ Therefore:  $A = B^{-1} \Leftrightarrow B = A^{-1}$

- ▶ The inverse of  $A$  may **not exist**. If it exists,  $A$  is **regular**, otherwise **singular**.
- ▶  $(A^{-1})^{-1} = A$ .
- ▶ The inverse of a matrix product is given as

$$(A \cdot B)^{-1} = B^{-1} \cdot A^{-1} .$$

- ▶ It is

$$(A^\top)^{-1} = (A^{-1})^\top .$$

Therefore one may also write  $A^{-\top}$ .

## Linear regression in matrix notation

Linear regression with  $n$  data points can be understood as an **equation system with  $n$  equations**.

Remember example 4 from slide 21: We said that a linear regression model can be written compactly using **matrix multiplication**:

$$y = \tilde{X} \cdot \tilde{\beta} + e .$$

Task: Verify this now, using a model with two variables  $x^{(1)}$  and  $x^{(2)}$  and

$$y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}, \quad \tilde{X} = \begin{pmatrix} 1 & x_1^{(1)} & x_1^{(2)} \\ 1 & x_2^{(1)} & x_2^{(2)} \\ \dots & \dots & \dots \\ 1 & x_n^{(1)} & x_n^{(2)} \end{pmatrix}, \quad \tilde{\beta} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix}, \quad e = \begin{pmatrix} e_1 \\ e_2 \\ \vdots \\ e_n \end{pmatrix}.$$

It can be shown (see Stahel 3.4f,g) that **the least-squares estimates  $\hat{\beta}$**  can be calculated as

$$\hat{\beta} = (\tilde{X}^\top \tilde{X})^{-1} \cdot \tilde{X}^\top \cdot y$$

Does this look complicated?

Let's test this in R ....

## Doing linear algebra in R

Let us look at model  $y = \tilde{X} \cdot \tilde{\beta} + e$  with coefficients

$\beta_0 = 10, \beta_1 = 5, \beta_2 = -2$  and variables

$i$	$x_i^{(1)}$	$x_i^{(2)}$
1	0	4
2	1	1
3	2	0
4	3	1
5	4	4

Thus the model is given as

$$y_i = 10 + 5x_i^{(1)} - 2x_i^{(2)} + \epsilon_i, \text{ for } 1 \leq i \leq n.$$

Let us start by generating the “true” response, calculated as  $\tilde{X}\tilde{\beta}$

```
x1 <- c(0,1,2,3,4)
x2 <- c(4,1,0,1,4)
Xtilde <- matrix(c(rep(1,5),x1,x2),ncol=3)
Xtilde
```

```
##      [,1] [,2] [,3]
## [1,]     1     0     4
## [2,]     1     1     1
## [3,]     1     2     0
## [4,]     1     3     1
## [5,]     1     4     4
```

```
t.beta <- c(10,5,-2)
t.y <- Xtilde%*%t.beta
t.y
```

```
##      [,1]
## [1,]     2
## [2,]    13
## [3,]    20
```

Next, we generate the vector containing the  $\epsilon_i \sim N(0, \sigma^2)$  with  $\sigma^2 = 1$ :

```
t.e <- rnorm(5,0,1)
t.e
```

```
## [1] 0.7606833 -0.3257157 0.6830309 0.9070262 0.9342162
```

which we add to the “true”  $y = \tilde{X}\tilde{\beta}$  values, to obtain the “observed” values:

```
t.Y <- t.y + t.e
t.Y
```

```
## [,1]
## [1,] 2.760683
## [2,] 12.674284
## [3,] 20.683031
## [4,] 23.907026
## [5,] 22.934216
```

It is now possible to fit the model with lm:

ANOVA < lm(t.Y ~ x1 + x2)

Alternatively, we can use formula

$$\hat{\beta} = (\tilde{X}^\top \tilde{X})^{-1} \tilde{X}^\top y$$

to find the parameter estimates:

```
solve(t(Xtilde) %*% Xtilde) %*% t(Xtilde) %*% t.Y
```

```
##           [,1]
## [1,] 10.069826
## [2,]  5.157981
## [3,] -1.896970
```

- ▶ `solve()` calculates the **inverse** (here the inverse of  $\tilde{X}^\top \tilde{X}$ ).
- ▶ `t()` gives the **transposed** (here of  $\tilde{X}^\top$ ).

**Task:** Do this calculation by yourself and verify for each step that the dimensions of the matrices and the vector are indeed fitting, so that this expression is defined.

## Appendix

# Some R commands for matrix algebra

Reading vectors and a matrices into R:

```
a <- c(1,2,3)  
a
```

```
## [1] 1 2 3
```

```
A <- matrix(c(1,2,3,4,5,6),byrow=T,nrow=2)  
B <- matrix(c(6,5,4,3,2,1),byrow=T,nrow=2)  
A
```

```
##      [,1] [,2] [,3]  
## [1,]     1     2     3  
## [2,]     4     5     6
```

```
B
```

```
##      [,1] [,2] [,3]  
## [1,]     6     5     4  
## [2,]     3     2     1
```

Adding and subtracting:

A + B

```
##      [,1] [,2] [,3]
## [1,]    7    7    7
## [2,]    7    7    7
```

A - B

```
##      [,1] [,2] [,3]
## [1,]   -5   -3   -1
## [2,]    1    3    5
```

However, be careful, R sometimes does unreasonable things:

A + a

```
##      [,1] [,2] [,3]
## [1,]    2    5    5
## [2,]    6    6    9
```

## Matrix multiplication:

```
C <- A %*% t(B)  
C
```

```
##      [,1] [,2]  
## [1,]    28   10  
## [2,]    73   28
```

```
A%*%a
```

```
##      [,1]  
## [1,]    14  
## [2,]    32
```

Matrix inversion (possible for quadratic matrices only):

```
solve(C)
```

```
##      [,1]      [,2]  
## [1,]  0.5185185 -0.1851852  
## [2,] -1.3518519  0.5185185
```

```
C %*% solve(C)
```

```
##      [,1] [,2]  
## [1,]    1   0  
## [2,]    0   1
```

Why does `solve(A)` or `solve(B)` not work?