Lecture 7: ANCOVA, short introduction to Linear Algebra

BIO144 Data Analysis in Biology

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Overview

- ANCOVA (*ANalysis of COVAriance*)
- Introduction to linear algebra

Course material covered today

Becherman & Petchey

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

Stahel

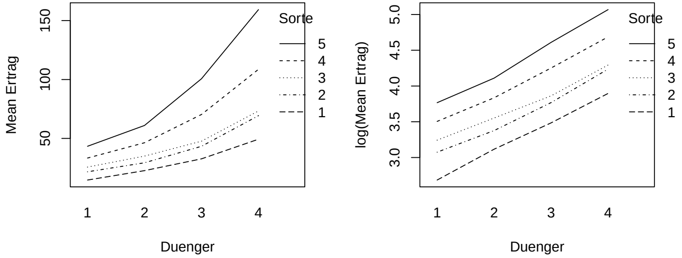
Recap of ANOVA

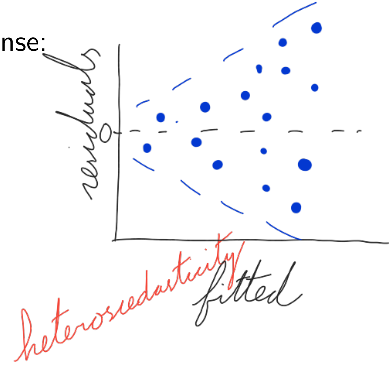
- ANOVA is a method to test whether the means of two or more groups differ
- Post-hoc tests and contrasts, including correction for p-values, to understand the differences between the groups
- Two-way ANOVA for factorial designs, interactions
- ANOVA: 'linear regression with categorical predictor(s)'
  - One categorical predictor = one-way ANOVA
  - Two categorical predictors= two-way ANOVA
  - *etc*.

Recap of two-way ANOVA example

The influence of four levels of fertilizer (DUENGER) on the yield (ERTRAG) of 5 crop species (SORTE) was investigated. For each DUENGER × ERTRAG combination, 3 measurements were made.

Interaction plot with ERTRAG and log(ERTRAG) as response:





Remember: We used log(ERTRAG), because residual plots were not ok otherwise.

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

intercept

```
## 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
```

4 levels − 1

5 levels − 1

59

+ 1 → intercept

60

read "bottom-up": if interaction is significant, don't interpret main effects

Questions:

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

↳ interaction can be dropped from model

```
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
##
## Residual standard error: 0.06755 on 40 degrees of freedom
```

interaction

read "bottom up"

Analysis of Covariance

ANCOVA:

- An extension of ANOVA
- A method to test whether the means of two or more groups differ, controlling for the effect of one (or more) continuous covariate(s)
- Makes an additional assumption about the "homogeneity of regression slopes"
  - No interaction between the categorical and (any of the) continuous covariate(s)
  - If there is an interaction, comparing group means becomes uninformative (the model may still be biologically interesting though!)
- A **linear model** (just like regression and ANOVA)

Given a categorical covariate x_i and a continuous covariate z_i, the ANCOVA equation is:

intercept

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

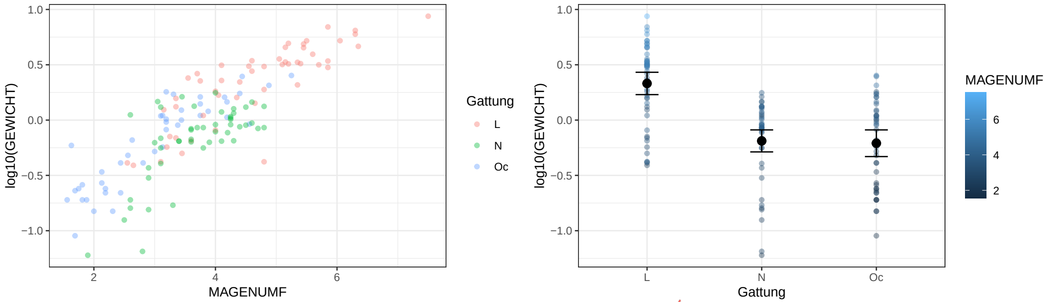
where $x_i^{(k)}$ is the kth dummy variable ($x_i^{(k)}$=1 if ith observation belongs to category k, 0 otherwise).

Note 1: Again, for reasons of identifiability, we typically set $\beta_1 = 0$

Note 2: It is easy to add the interaction between x_i with z_i, but strictly speaking such a model would no longer be an ANCOVA

Once more: the earthworms

"Gewicht" of the worm was expressed as a function of "Magenumfang" and "Gattung"



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

compare species means, controlling for stomachsize

```r
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
## GattungOc   -0.0907298 0.12791000  -0.7093254 4.793107e-01
```

Important: The *p*-values for the estimates of `(Intercept)`, `GattungN` and `GattungOc` are not very meaningful (why?).

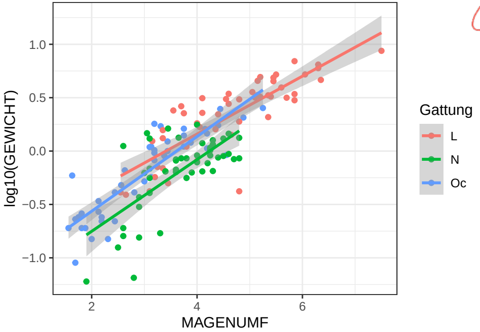
- multiple comparisons using same data:
  * species L vs species N
  * species L vs species Oc
- intercept = mean of species L when Magenumfang = 0

To understand if “Gattung” has an effect, **we need to carry out an** F-test $\rightarrow$ 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
```

To check whether the assumption of *homogeneity of regression slopes* holds, we need to make sure the **interaction** between `MAGENUMF` and `Gattung` is not significant:



↳ slopes are similar

↓

seems reasonable, but let's formally test!

→ We fit a new model, and again use the F-test:

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

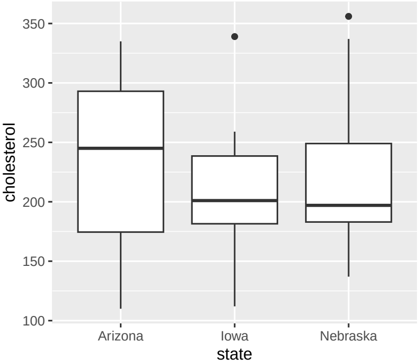
```
## Analysis of Variance Table
##
## Response: log(GEWICHT)
##                   Df  Sum Sq Mean Sq  F value    Pr(>F)
## MAGENUMF           1 104.866 104.866 414.4743 < 2.2e-16 ***
## Gattung            2   7.177   3.589  14.1835 2.521e-06 ***
## MAGENUMF:Gattung   2   0.917   0.458   1.8112    0.1673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

→ $p = 0.167$, the interaction is probably not relevant → ANCOVA makes sense

A new example: cholesterol levels

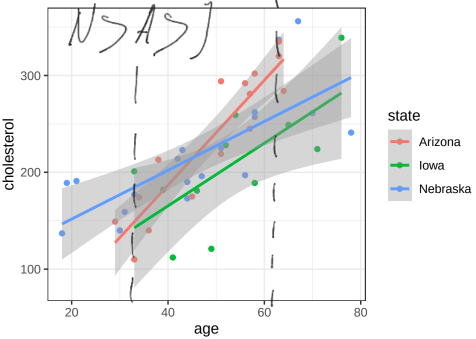
Example: Cholesterol levels [mg/ml] of 45 women from three US states were measured.

Question: Do these levels differ between the states, controlling for the age (years) of each subject?



The scatter plot already gives us a clue here. A > N > I

→ which mean is larger than which other mean, depends on the age at which you do the comparison



→ The slopes look somewhat different, so we include `state`, `age` and the interaction between the two into our model.

→ no "homogeneity of regression slopes"

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
```

comparing means is not informative, it depends on the age

What does this mean?

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

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

mean cholesterol in Alaska at age = 0

bottom-up

```
##                       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
```

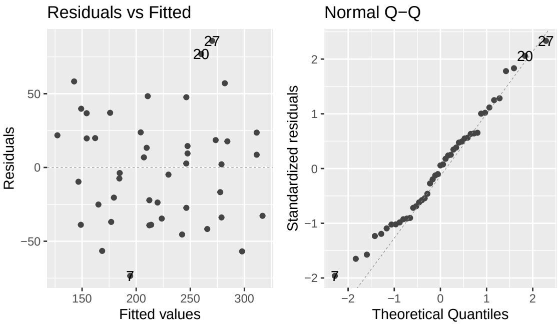
slope in Alaska

difference in slope with Alaska : 5.41 + -2.18

" " 5.41 + -2.90

Note: The strength of the association between `cholesterol` and age is less pronounced in Iowa and Nebraska than in Arizona → no ANCOVA!

As always, some model checking is necessary:



$\rightarrow$ This seems ok.

An introduction to linear algebra

Who remembers linear algebra, perhaps from high school?

Overview

- Some basics about
  - vectors
  - matrices
  - matrix algebra
  - matrix multiplication
- Why is linear algebra useful?
- What does it have to do with data analysis and statistics?
- Linear models in matrix notation.

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 as a vector: → columns in spreadsheet!

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

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

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

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

$$\tilde{X} = \begin{array}{c} \begin{matrix} \text{Intercept} & \text{Var 1} & \text{Var 2} \end{matrix} \\ \begin{pmatrix} 1 & x_1^{(1)} & x_1^{(2)} \\ 1 & x_2^{(1)} & x_2^{(2)} \\ \ldots & \ldots & \ldots \\ 1 & x_n^{(1)} & x_n^{(2)} \end{pmatrix} \end{array} .$$

"X tilde"

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:

Parameters

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

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 statistical 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:

n rows   m columns

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

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

Square matrix: $n = m$. Example:

$= 3$

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

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

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

The diagonal of a square matrix is given by $(a_{11}, a_{22}, \ldots, a_{nn})$. 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 $A^\top$:

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

Examples (note the "flip" in dimensions with non-square matrices):

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

$$\underset{[2 \times 4]\text{ Matrix}}{A = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \end{pmatrix}} \quad \Rightarrow \quad \underset{[4 \times 2]}{A^\top} = \begin{pmatrix} 1 & 5 \\ 2 & 6 \\ 3 & 7 \\ 4 & 8 \end{pmatrix}$$

- 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:

$\underline{n} \times \underline{1}$ Matrix

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

Transposing a vector leads to a *row vector*:

$1 \times n$ Matrix

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

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 dimensions.
- 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:

$$\underbrace{\begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix}}_{[2 \times 3]} + \underbrace{\begin{pmatrix} 3 & 6 \\ 2 & 5 \\ 1 & 4 \end{pmatrix}}_{[3, 2]} = \quad ?!$$

Multiplication by a scalar

$[1 \times 1]$ Matrix

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

Examples:

$$[2,3] \qquad [2,3]$$

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

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

Matrix multiplication

The multiplication of two matrices A and B is only defined if
number of columns in A = number of rows in B.

It is easiest to explain matrix multiplication with an example:

$$\begin{pmatrix} 2 & 1 \\ -1 & 0 \\ 3 & 1 \end{pmatrix} \cdot \begin{pmatrix} 3 & 1 \\ 4 & -2 \end{pmatrix} = \begin{pmatrix} 2\cdot 3 + 1\cdot 4 & 2\cdot 1 + 1\cdot -2 \\ -1\cdot 3 + 0\cdot 4 & -1\cdot 1 + 0\cdot -2 \\ 3\cdot 3 + 1\cdot 4 & 3\cdot 1 + 1\cdot -2 \end{pmatrix}$$

$$= \begin{pmatrix} 10 & 0 \\ -3 & -1 \\ 13 & 1 \end{pmatrix}$$

▸ Matrix multiplication app

In general:

An $n \times m$ Matrix multiplied by an $m \times p$ Matrix= an $n \times p$ Matrix

Matrix multiplication rules I

Matrix multiplication does not follow the same rules as scalar multiplication!!

!

- The commutative property does not hold:
  - It is possible that $A \cdot B$ can be calculated, whereas $B \cdot A$ is not defined (see example on previous slide).

    ↳ wrong dimensions
  - In general, $A \cdot B \neq B \cdot A$, even if both are defined.
- It can happen that $A \cdot B = 0$ (a "zero matrix"), although both $A \neq 0$ and $B \neq 0$.
- The associative property holds: $A \cdot (B \cdot C) = (A \cdot B) \cdot C$.
- The distributive property holds:

$$
\begin{aligned}
A \cdot (B + C) &= (A \cdot B) + (A \cdot C) \\
(A + B) \cdot C &= A \cdot C + B \cdot C
\end{aligned}
$$

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:

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

column vector [n × 1] · row vector (1 × m) = [n × m]

If a and b have the same length:

[1 × 3] · [3 × 1] = [1 × 1]

$$a^\top \cdot b = \boxed{\sum_i a_i b_i} = \text{scalar}$$

$(1, 2, 3) \cdot \begin{pmatrix} 4 \\ 5 \\ 6 \end{pmatrix} = (1 \times 4) + (2 \times 5) + (3 \times 6) = 32$ scalar

Short exercise

$[n \times m] \cdot [m \times p] = [n \times p]$

Given vectors a and b and matrix C:

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

! not defined !

Calculate, if defined

- $a^\top \cdot b$ $\quad [1 \times 4] \cdot [2 \times 1]$
- $a \cdot b^\top$ $\quad [4 \times 1] \cdot [1 \times 2] \rightarrow \begin{pmatrix} 1 \\ -2 \\ 3 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} -2 & 4 \end{pmatrix} = \begin{pmatrix} -2 & 4 \\ 4 & -8 \\ -6 & 12 \\ 0 & 0 \end{pmatrix}$
- $C \cdot a$ $\rightarrow$ not defined!
- $C \cdot b$ $\rightarrow \begin{pmatrix} -2 \\ 10 \end{pmatrix}$

The length of a vector

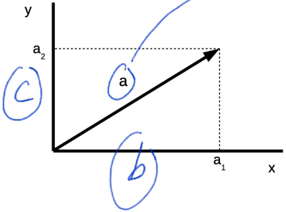
The length of a vector $a^\top = (a_1, a_2, \ldots, a_n)$ is defined as $||a||$ with

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

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

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

"$a^2 = b^2 + c^2$"



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:

$$\underbrace{A \cdot I} = \underbrace{A} \; .$$

Inverse matrix

Given a square 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: $A = B^{-1} \quad \Leftrightarrow \quad B = A^{-1}$

- 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 the example from slide 21/22: We said that a linear regression model can be written compactly using matrix multiplication:

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

Let's illustrate with a model with two predictor variabless $x^{(1)}$ and $x^{(2)}$:

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

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

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

Does this look complicated?

Let's have a look in R. . .

It does to me, but a little practice helps!!

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

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

Let's 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
## [4,]   23
## [5,]   22
```

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`:

```
r.lm <- lm(t.Y ~ x1 + x2)
summary(r.lm)$coef
```

```
##              Estimate Std. Error   t value    Pr(>|t|)
## (Intercept) 10.069826  0.5556231  18.12348 0.003030672
## x1           5.157981  0.1866953  27.62780 0.001307540
## x2          -1.896970  0.1577864 -12.02239 0.006847617
```

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 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 sometims does unreasonable things:

```
A + a
```

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

What happened here??

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 square 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?