# TMA4267 - Linear statistical models

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## Introduction

This is a brief summary of the course TMA4267 about linear statistical models. It includes the main content from the lecture held by ... recorded in, where some examples etc... are excluded.

The purpose of the notes is to give a good overview of the syllabus. I intend to add summaries of the lectures as I review them. I hope to include insights from projects / exercises where it is appropriate.

progress

• First reading	✓ Lecture 1-2	☐ Lecture 13-14
✓ Lecture 1-22	☐ Lecture 3-4	☐ Lecture 15-16
☐ Lecture 23	☐ Lecture 5-6	☐ Lecture 17-18
☐ Lecture 24	✓ Lecture 7-8	☐ Lecture 19-20
$\Box$ Lecture 25	☐ Lecture 9-10	☐ Lecture 21-22
• Gjennomgang	☐ Lecture 11-12	☐ Lecture 23
Exams		
□ May 2023	□ May 2017	□ May 2014
□ June 2019	☐ June 2016	□ August 2014
□ May 2018	□ May 2015	
Topics		
1		
Multivariate distributions an	d expectations (HS 4.1-4.2).	
Multivariate moments (HS $4$	.2 using HS 2.1-2.4).	
Transformations (HS 4.3, 4.4	)	
PCA (HS 11.1-11.3).		
Charactestic functions (HS 4	.2).	
2		
Multivariate normal distribu	tion (HS 4.4, 5.1).	
Estimation in the multivaria	te normal distribution (HS 3.3, 4	4.5).
Quadratic forms and idempo	tent matrices (FKLM Appendix	B, Th. B2, B8).

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3
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Multiple linear regression: model, parameter estimation (FKLM 3.1, 3.2).

Properties of estimators, fitted values, residuals (FKLM 3.2).

Inference about coefficients (FKLM 3.3).

Multiple linear regression: t-test about coefficients, ANOVA decomposition, coefficient of determination, F-test (FKLM 3.2, 3.3).

General F-test for regression coefficients (FKLM 3.2, 3.3, 3.5).

transformation of data (FKLM 3.2, 3.3, 3.4, 3.5).

#### 4

Model analysis and model selection (FKLM 3.4).

Multiple hypothesis testing (HBL).

Examples.

#### 5

ANOVA (HS 8.1.1).

Design of experiment (DOE): two-level factorial design (T).

### Keywords to know

### 1 Multivariate Distribution and its Generalisations

#### Lecture 1

random vector - vector with RV's as components

random matrix

cumulative distribution function (CDF)

$$F(x) = \mathbb{P}\left[\boldsymbol{X} \leq \boldsymbol{x}\right] = \mathbb{P}\left[X_1 \leq x_1, \dots, X_n \leq x_n\right]$$

absolutely continuous if there exists density function f such that:

$$F(\boldsymbol{x}) = \int_{-\infty}^{x_p} \cdots \int_{-\infty}^{x_1} f(u_1, \dots, u_p) du_1 \dots du_p$$

Then

$$\mathbb{P}\left[oldsymbol{X}\in D
ight] = \int_D f(oldsymbol{x}) doldsymbol{x} \quad orall D \subseteq \mathbb{R}^p$$

X is said to be discrete if it is consentraded on a countable (finite or infinite) set of points. Then integral becomes a sum. In the absolutely continuous case, we may write:

$$f(x) = f(x_1, \dots, x_p) = \frac{\partial^p F(x_1, \dots, x_p)}{\partial x_1 \dots \partial x_p}$$

#### Marginal distribution

Let  $X_A, X_B$  be two random vectors st  $X = (X_A, X_B)^T$  has cdf F. Then:

$$F_A(x_1,\ldots,x_k)=F(x_1,\ldots,x_k,\infty,\ldots,\infty)$$

In absolutely continuous case we find

$$f_A(x_1,\ldots,x_k) = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} f(x_1,\ldots,x_p) du_p \ldots du_{k+1}$$

#### Conditional distribution

$$f_{\boldsymbol{X}_B|\boldsymbol{X}_A=\boldsymbol{x}_A} = \frac{f(x_1,\ldots,x_p)}{f_A(x_1,\ldots,x_k)}$$

#### Independence

Say  $X_A, X_B$  are independent if

$$F(x_1,\ldots,x_p)=F_A(x_1,\ldots,x_k)F_B(x_{k+1},\ldots,x_p)\quad\forall x_1,\ldots x_p.$$

In the continuous case we have independence iff  $f = f_A \cdot f_B$ . In this case  $f(\boldsymbol{x}_B | \boldsymbol{x}_A) = f_B(\boldsymbol{x}_B)$ . Similar definition for independence when  $\boldsymbol{X}$  has N components and not just 2.

#### Multivariate expectations and moments

expectation defined as

$$\mathbb{E}\left[\boldsymbol{X}\right] = \left(\mathbb{E}\left[X_1\right], \dots, \mathbb{E}\left[X_p\right]\right)^T$$

#### Lecture 2

We can show  $\mathbb{E}[a\mathbf{X} + b\mathbf{Y}] = a\mathbb{E}[\mathbf{X}] + b\mathbb{E}[\mathbf{Y}]$ 

For (shape compatible) matrices A, B we have  $\mathbb{E}[AXB] = A\mathbb{E}[X]B$ 

Let X, Y be random matrices whose product is defined. Then  $\mathbb{E}[XY] = \mathbb{E}[X]\mathbb{E}[Y]$ .

#### Covariance matrix

Let  $\boldsymbol{X} = (X_1, \dots, X_p)^T$  and  $\mathbb{E}[\boldsymbol{X}] =: \boldsymbol{\mu} = (\mu_1, \dots, \mu_p)$ . We then define:

$$\operatorname{Var}\left[\boldsymbol{X}\right] = \operatorname{Cov}\left[\boldsymbol{X}\right] = \boldsymbol{\Sigma} = \begin{pmatrix} \sigma_{X_1X_1} & \dots & \sigma_{X_1X_p} \\ \vdots & \ddots & \vdots \\ \sigma_{X_pX_1} & \dots & \sigma_{X_pX_p} \end{pmatrix} = \mathbb{E}\left[(\boldsymbol{X} - \boldsymbol{\mu})(\boldsymbol{X} - \boldsymbol{\mu})^T\right]$$

This natrix is symmetric. We can also show:

$$\mathbf{\Sigma} = \mathbb{E}\left[\mathbf{X}\mathbf{X}^T\right] - \boldsymbol{\mu}\boldsymbol{\mu}^T.$$

The correlation matrix (with ones on the diagonal) is given by

$$\boldsymbol{\rho} = \begin{pmatrix} \rho_{X_1 X_1} & \dots & \rho_{X_1 X_p} \\ \vdots & \ddots & \vdots \\ \rho_{X_p X_1} & \dots & \rho_{X_p X_p} \end{pmatrix}, \quad \rho_{X_i X_j} = \frac{\sigma_{X_i X_j}}{\sqrt{\sigma_{X_i}} \sqrt{\sigma_{X_j}}}$$

For two random vectors X, Y we define their correlation matrix by

$$\boldsymbol{\Sigma}_{\boldsymbol{X}\boldsymbol{Y}} = \operatorname{Cov}\left[\boldsymbol{X},\boldsymbol{Y}\right] = \mathbb{E}\left[(\boldsymbol{X} - \boldsymbol{\mu}_{\boldsymbol{X}})(\boldsymbol{Y} - \boldsymbol{\mu}_{\boldsymbol{Y}})^T\right] = (\operatorname{Cov}\left[X_i,X_j\right])_{\substack{i=1,\dots,p\\j=1,\dots,q}}$$

#### 1.0.1 Matrix algebra

symmetric if  $\mathbf{A}^T = \mathbf{A}$ 

orthogonal if  $\mathbf{A}\mathbf{A}^T = \mathbf{A}^T\mathbf{A} = \mathbf{I}$ 

eigenvalue and eigenvector ... solution of  $\det(\boldsymbol{A}-\lambda\boldsymbol{I})$ 

also have  $\det A = \prod_{i=1}^p \lambda_i$ .

Jordan decomposition of symmetric matrix

$$A = \Gamma \Lambda \Gamma^T$$
,  $\Gamma = TODO$ :

Quadtraic form: let  $\boldsymbol{A}$  symmetric,  $\boldsymbol{x}$  a  $(p \times 1)$  vector:

$$Q(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} = \sum_{i=1}^p \sum_{j=1}^p x_i A_{ij} x_j$$

Theorem 1. Transforming  $\mathbf{y} = \mathbf{\Gamma}^T \mathbf{x}$  we obtain  $Q(\mathbf{x}) = \sum_{i=1}^p \lambda_i y_i^2$ 

A matrix is said to be *positive definite* if Q(x) > 0 for all  $x \neq 0$  and positive semi definite if  $\geq$ . We write A > 0 and  $A \geq 0$  respectively.

**Theorem 2.** The symmetric matrix A is positive definite iff  $\lambda_i > 0$  for all i.

From this we obtain two more usefull results. \* If A>0 the inverse exists and the determinant is >0

\* If A > 0 there exists a unique positive definite square root with decomposition:

$$A^{1/2} = \mathbf{\Gamma} \mathbf{\Lambda}^{1/2} \mathbf{\Gamma}^T.$$

- \*  $\Sigma \ge 0$
- \*  $\Sigma_{XY} = \Sigma_{YX}^T$
- \* If  $m{X} \sim (m{\mu_X}, m{\Sigma_{XX}}), m{Y} \sim (m{\mu_Y}, m{\Sigma_{YY}})$  then  $m{Z} = (m{X}, m{Y})^T$  has

$$oldsymbol{\Sigma_{ZZ}} = egin{pmatrix} \Sigma_{XX} & \Sigma_{XY} \ \Sigma YX & \Sigma_{YY} \end{pmatrix}$$

- \* Independence of  $\boldsymbol{X},\boldsymbol{Y}$  implies  $\operatorname{Cov}\left[\boldsymbol{X},\boldsymbol{Y}\right]=\boldsymbol{0}.$  (NB: the converse not true)
- \*  $\operatorname{Var}\left[\boldsymbol{A}\boldsymbol{X} + \boldsymbol{b}\right] = \boldsymbol{A}\operatorname{Var}\left[\boldsymbol{X}\right]\boldsymbol{A}^{T}$
- \*  $\operatorname{Cov}\left[\boldsymbol{X} + \boldsymbol{Y}, \boldsymbol{Z}\right] = \operatorname{Cov}\left[\boldsymbol{X}, \boldsymbol{Z}\right] + \operatorname{Cov}\left[\boldsymbol{Y}, \boldsymbol{Z}\right]$
- \*  $\operatorname{Var}\left[\boldsymbol{X}+\boldsymbol{Y}\right] = \operatorname{Var}\left[\boldsymbol{X}\right] + \operatorname{Cov}\left[\boldsymbol{X},\boldsymbol{Y}\right] + \operatorname{Cov}\left[\boldsymbol{Y},\boldsymbol{Z}\right] + \operatorname{Var}\left[\boldsymbol{Y}\right]$
- \*  $\operatorname{Cov}[AX, BY] = A\operatorname{Cov}[X, Y]B^T$

#### Lecture 3

Transformations

Lecture J

Mahalanolis transformation

[Recall univariate,  $x \sim (\mu, \sigma^2)$ 

Put 
$$y = \frac{x-\mu}{\sigma} \rightsquigarrow y \sim (0,1)$$

Now, for the multivariate cause:

$$x = (x_1, \dots, x_p)^{\top}, \quad x \sim (\mu, \Sigma), \Sigma \text{ now -single}$$

Would tine  $y = \varphi(x)$  sit.  $y \sim (0, I)$ 

This is:

$$y = \Sigma^{-1/2}(x - \mu)$$

Where  $\Sigma^{-1/2} = (\Sigma^{1/2})^{-1}$  and  $\Sigma^{1/2}$  the unique pos-des square toot of  $\Sigma$ . Fys-sth arse:

$$\Sigma = \operatorname{diaq}\left(\sigma_1^2, \dots \sigma^2\right)$$

sine iid...tres, envier sh to do

 $\cdot \frac{1}{\sigma}$ 

[proof that it works:

$$E(y) = E\left(\Sigma^{-1/2}(x-\mu)\right) = \Sigma^{-1/2}(E(x)-\mu) = 0$$

$$\operatorname{Var}(y) = \operatorname{Var}\left(\Sigma^{-1/2}(x-\mu)\right) = \operatorname{Var}\left(\Sigma^{-1/2}x\right)$$

$$= \Sigma^{-1/2}\operatorname{Var}(x)\left(\Sigma^{-1/2}\right)^{\top} = \operatorname{sm}$$

$$\Sigma^{-1/2}$$

$$= \underbrace{\Sigma^{-1/2} \Sigma^{1/2}}_{I} \underbrace{\Sigma^{1/2} \Sigma^{-1/2}}_{I} = I$$

Principal components analysis (HS 11.1-11.J)

Observe realisations of a random vector

$$x = (x_1, \dots, x_p)^{\top}, \quad x \sim (\mu, \Sigma)$$

Aim: reduction of dimensionality

Remove some components and heep comports with Lave in formation — Large variance

Forest transform 
$$x \to y = Ax + b_2y = \begin{pmatrix} y_1 \\ \vdots \\ y_p \end{pmatrix}$$
 so that:

$$(1) E(y) = 0$$

(2)  $Cov(y_i, y_j) = 0, \quad i \neq j$ 

i.e. Var(y) is diagonal

(3)  $\operatorname{Var}(y_1) \ge \operatorname{Var}(y_2) \ge \cdots \ge \operatorname{Ver}(y_r)$ 

We have (Jordan decomposition)

#### Lecture 4

#### Lecture 5

### 2 The Multivariate Normal Distribution

#### Lecture 7

#### 2.1 Estimation of the multivariate normal distribution

#### 2.1.1 Univariate case

From the univariate case we recall that if  $X_1, \ldots, X_n \sim N(\mu, \sigma^2)$  are independent, then the MLE estimators are:

$$\widehat{\mu} = \bar{X} = \frac{1}{n} \sum_{i=1}^{n} X_i$$

$$\sigma^{2} = \frac{1}{n} \sum_{i=1}^{n} (X_{i} - \bar{X})^{2}$$

But since we found that  $\mathbb{E}\left[\sigma^2\right] = \frac{n-1}{n}\sigma^2$  is biased, we use instead the estimator

$$S^{2} = \frac{1}{n-1} \sum_{i=1}^{n} (X_{i} - \bar{X})^{2}.$$

We further proved that

- 1.  $\bar{X} \sim N(\mu, \sigma^2/n)$
- 2.  $\frac{(n-1)S^2}{\sigma^2} \sim \chi_{n-1}^2$
- 3.  $\bar{X}, S^2$  are independent (for the normal distribution)
- 4.  $\sqrt{n} \frac{\bar{X} \mu}{S} \sim t_{n-1}$  (student t distribution)

Our next goal is to obtain the result for the multivariate case.

#### 2.1.2 Multivatiate case

In this case, we have p-variate independent random vectors  $X_1, ..., X_n \sim N(\mu, \Sigma)$  where we denote  $X_i = (X_{i1}, ..., X_{ip})^T$ . These make up the columns of the  $(n \times p)$  data matrix or feature matrix

 $\boldsymbol{X}$  given as:

$$\boldsymbol{X} = \begin{pmatrix} X_{11} & \cdots & X_{1p} \\ \vdots & \ddots & \vdots \\ X_{n1} & \cdots & X_{np} \end{pmatrix}^{\text{samples}} = \begin{pmatrix} \boldsymbol{X}_1^T \\ \vdots \\ \boldsymbol{X}_n^T \end{pmatrix} = (\boldsymbol{X}_1 \cdots \boldsymbol{X}_n)^T.$$
for types  $\rightarrow$ 

We want to estimate  $\mu$ ,  $\Sigma$ . Again we denote:

$$\widehat{\boldsymbol{\mu}} = \bar{\boldsymbol{X}} = \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{X}_{i} = \frac{1}{n} \boldsymbol{X}^{T} \mathbf{1}$$

$$\boldsymbol{S}^{2} = \frac{1}{n} \sum_{i=1}^{n} (\boldsymbol{X}_{i} - \bar{\boldsymbol{X}})^{T} (\boldsymbol{X}_{i} - \bar{\boldsymbol{X}}) = \frac{1}{n} \boldsymbol{X}^{T} \left( \boldsymbol{I} - \frac{1}{n} \mathbf{1} \mathbf{1}^{T} \right) \boldsymbol{X}.$$

The matrix  $C = I - \frac{1}{n} \mathbf{1} \mathbf{1}^T$  is called the *centering matrix* because its action is to remove the mean of a vector:

$$oldsymbol{C}oldsymbol{y} = egin{pmatrix} 1 - rac{1}{n} & \cdots & rac{1}{n} \ dots & \ddots & dots \ rac{1}{n} & \cdots & 1 - rac{1}{n} \end{pmatrix} egin{pmatrix} y_1 \ dots \ y_n \end{pmatrix} = egin{pmatrix} y_1 - ar{y} \ dots \ y_n - ar{y} \end{pmatrix}.$$

We note that

- 1. C is symmetric
- 2.  $\boldsymbol{C}$  is idempotent

For the estimators, we may prove:

Proposition 1.  $\bar{X} \sim N(\mu, \frac{1}{n}\Sigma)$ 

*Proof.* By characteristic function.

Proposition 2.  $\mathbb{E}[S] = \frac{n-1}{n}\Sigma$ .

Hence we obtain an unbiased estimator as

$$S = \frac{1}{n-1} \sum_{i=1}^{n} (\boldsymbol{X}_i - \bar{\boldsymbol{X}}) (\boldsymbol{X}_i - \bar{\boldsymbol{X}})^T.$$

#### Lecture 8

#### 2.1.3 Quadratic forms

Let  $\mathbf{X} = (X_1, \dots, X_p)^T$  be a  $(p \times 1)$  random vector and  $\mathbf{A} = (a_i j) \in \mathbb{R}^{p \times p}$  a matrix. This gives a quadratic form:

$$\boldsymbol{X}^T \boldsymbol{A} \boldsymbol{X} = \sum_{i,j} X_i a_{ij} X_j.$$

Theorem 3. (Trace formula)  $\mathbb{E}\left[\boldsymbol{X}^{T}\boldsymbol{A}\boldsymbol{X}\right] = \operatorname{tr}(\boldsymbol{A}\boldsymbol{\Sigma}) + \boldsymbol{\mu}^{T}\boldsymbol{A}\boldsymbol{\mu}$ 

*Proof.* Using that  $Cov[X_i, X_j] = \mathbb{E}[X_i X_j] - \mathbb{E}[X_i] \mathbb{E}[X_j]$  we obtain the result:

$$\mathbb{E}\left[\boldsymbol{X}^{T}\boldsymbol{A}\boldsymbol{X}\right] = \sum_{ij} a_{ij}\mathbb{E}\left[X_{i}X_{j}\right] = \sum_{ij} a_{ij}(\Sigma_{ij} - \mu_{i}\mu_{j})$$
$$= \sum_{ij} a_{ij}\Sigma_{ij} - \sum_{ij} a_{ij}\mu_{i}\mu_{j} = \operatorname{tr}(\boldsymbol{A}\boldsymbol{\Sigma}) - \boldsymbol{\mu}^{T}\boldsymbol{A}\boldsymbol{\mu}.$$

#### 2.1.4 Idempotent matrices

Recall that the (square) matrix A is said to be idempotent of AA = A. We have the following:

Proposition 3. Let A be idempotent.

- 1. I A is also idempotent.
- 2. A(I A) = (I A)A = 0.
- 3. The only non-singular idenpotent matrix is I.
- 4. All eigenvalues of idempotent matrices are 0 or 1.

*Proof.* We have:

1. 
$$(I - A)^2 = I^2 - AI - IA + A^2 = 0.$$

- 2. Obvious
- 3. Later
- 4.  $\lambda x = Ax = AAx = \lambda^2 x$ .

Before our next important result, we recall from linear algebra that:

1. Let  $\mathbf{A} \in \mathbb{R}^{p \times p}$  have eigenvalues  $\lambda_1, \dots, \lambda_p$ . Then:

$$\operatorname{tr}(\boldsymbol{A}) = \sum \lambda_i, \quad \det(\boldsymbol{A}) = \prod \lambda_i.$$

2. The matrix  $\mathbf{A} \in \mathbb{R}^{p \times p}$  of rank r has spectral decomposition:

$$\boldsymbol{A} = \boldsymbol{P} \boldsymbol{\Lambda} \boldsymbol{P}^T$$

where P is the matrix with eigenvalues as columns and  $\Lambda$  the diagonal matrix of eigenvalues. Note that  $P \in \mathbb{R}^{p \times r}$ ,  $\Lambda \in \mathbb{R}^{r \times r}$ . TODO: something about orthonormal

Note that for  $\boldsymbol{A}$  symmetric and idempotent, we have  $\boldsymbol{\Lambda} = \boldsymbol{I}_r$  in point 2 and rank $(\boldsymbol{A}) = \operatorname{tr}(\boldsymbol{A}) = r$  due to point 1.

The following theorem will be used extensively in the sequel.

**Theorem 4.**  $Z \sim N(0, I_p)$  and let R, S be symmetric and idempotent of rank r, s respectively. Suppose also RS = 0. Then

1.  $\mathbf{Z}^T \mathbf{R} \mathbf{Z} \sim \chi_r^2$ 

- 2.  $\mathbf{Z}^T \mathbf{R} \mathbf{Z}$  and  $\mathbf{Z}^T \mathbf{S} \mathbf{Z}$  are independent
- 3.  $\frac{\mathbf{Z}^T \mathbf{R} \mathbf{Z}/r}{\mathbf{Z}^T \mathbf{S} \mathbf{Z}/s} \sim F_{r,s}$ .

*Proof.* We have: TODO:

1.

2.

3. By definition.

## 3 Multiple Linear Regression

We assume that we have  $i=1,\ldots,n$  observations of a response variable  $Y_i$  depending on k explanatory variables  $x_{ij}$  through a linear model:

$$Y_i = \beta_0 + \beta_1 x_{i1} + \dots + \beta_k x_{ik} + \varepsilon_i.$$

It can be written on matrix form as:

$$\begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix} = \begin{pmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nk} \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{pmatrix} + \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{pmatrix}.$$

$$\mathbf{Y}$$

The matrix X is reffered to as the design matrix. The  $\varepsilon$ 's are errors and the  $\beta$ 's the parameters.

#### Lecture 9

Assumptions

- 1.  $\boldsymbol{X}$  is of cull column rank
- 2.  $E\varepsilon = \mathbf{0}$
- 3. Homostochastic:  $Var[(]\varepsilon_i) = 0 \quad \forall i$ .
- 4. If X is random, then 2 and 3 are conditioned on X.
- 5. Normality of errors:  $\boldsymbol{\varepsilon} \sim N(0, \sigma^2 I_n)$ .

... obtain least squares estimators  $\widehat{\boldsymbol{\beta}}, \widehat{\boldsymbol{\sigma}}^2$  of  $\boldsymbol{\beta}, \boldsymbol{\sigma}^2$ 

Residuals ...

#### Parameter estimation

Two approaches: LSE and MLE ...

$$\widehat{oldsymbol{eta}} = rg\min_{oldsymbol{eta} \in \mathbb{R}^{k+1}} \sum_{i=1}^n (Y_i - oldsymbol{x}_i^T oldsymbol{eta})^2$$

... deducing that LSE and MLE give the same result ...

...

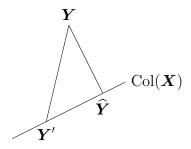
Hat matrix

ghjfiodeifgoerjfkdworw9u0gryhj

Du fulgte ikke med nei

#### Lecture 10

#### Lecture 11



#### Lecture 12

questions about independence. Detour into sigma algebras etc ...

**Theorem 5.** Suppose X, Y are independent random variables and that f, g are two measurable functions. Then f(X), g(Y) are also independent.

ANOVA - Analysis of variance

**Theorem 6.** (ANOVA decomposition) Assuming the necessarry assumptions,

$$\underbrace{\sum_{i=1}^{n} (Y_i - \bar{Y})}_{\text{SST}} = \underbrace{\sum_{i=1}^{n} (\hat{Y}_i - \bar{Y})}_{\text{SSR}} + \underbrace{\sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2}_{\text{SSE}}.$$

*Proof.* TODO: there aint space in the margin

The 3 sums are called *total sum of squares*, regression sum of squares and error sum of squares respectively. This decomposition motivates the following definition.

**Definition 1.** The part of the total variation due to the model is called the *coefficient of determination* or the *R2-score*:

$$R^2 = \frac{\text{SSR}}{\text{SST}} \stackrel{\text{thm}}{=} 1 - \frac{\text{SSE}}{\text{SST}}.$$

One may also prove another representation:

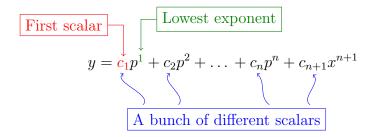
$$R^{2} = \frac{\left(\sum_{i=1}^{n} (Y_{i} - \bar{Y})(\widehat{Y}_{i} - \bar{Y})\right)^{2}}{\sum_{i=1}^{n} (Y_{i} - \bar{Y})^{2} \sum_{i=1}^{n} (\widehat{Y}_{i} - \bar{Y})}.$$

This is the square of the empirical correlation between  $Y, \hat{Y}$ .

#### Lecture 13

#### Fictional model

"Fictional model" using  $x_{ij}$  as response for some fixed feature j.



... TODO:

#### General F-test

#### TODO: important to have on yellow paper

We set up a much more general problem. Let  $A \in \mathbb{R}^{r \times p}$ , r < p, rank(A) = r,  $\mathbf{d} \in \mathbb{R}^d$ . We test the hypothesis:

$$H_0: A\boldsymbol{\beta} = \boldsymbol{d}, \qquad H_1: A\boldsymbol{\beta} \neq \boldsymbol{d}.$$

Some special cases of this general setup are.

1. r = 1, d = 0, A = (0, ..., 1, ..., 0) with 1 at index i, gives the test

$$H_0: \beta_i = 0, \qquad H_1: \beta_i \neq 0.$$

2.  $r = 1, d = 0, A = (0, \dots, 1, \dots, -1, \dots, 0)$  with 1 at index i and -1 at index j, gives the test

$$H_0: \beta_i = \beta_j, \qquad H_1: \beta_i \neq \beta_j.$$

3.  $r = k, d = \mathbf{0} \in \mathbb{R}^k, A = (\mathbf{0}, \operatorname{diag}(1)) \in \mathbb{R}^{k \times p}$ , gives the test

$$H_0: \beta_i = 0 \quad \forall i \in \{1, \dots, k\},$$
  $H_1: \beta_i \neq 0 \text{ for some } i \in \{1, \dots, k\}.$ 

### Lecture 14

Let  $\mathcal{B}$  be the space of  $\boldsymbol{\beta}$  satisfying  $H_0$ . The restricted problem is:

$$\widehat{\boldsymbol{\beta}}^R = \operatorname*{arg\,min}_{oldsymbol{eta} \in \mathcal{B}} (oldsymbol{Y} - oldsymbol{X} oldsymbol{eta})^T (oldsymbol{Y} - oldsymbol{X} oldsymbol{eta}).$$

Using lagrange multipliers and a bag of tricks, we obtain:

$$\widehat{\boldsymbol{\beta}}^R = \widehat{\boldsymbol{\beta}} - (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{A}^T (\boldsymbol{A} (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{A}^T)^{-1} (\boldsymbol{A} \widehat{\boldsymbol{\beta}} - \boldsymbol{d}).$$

Denoting  $\Delta = \widehat{\boldsymbol{\beta}} - \widehat{\boldsymbol{\beta}}^R$ , we find:

$$SSE^R = SSE + \Delta^T \boldsymbol{X}^T \boldsymbol{X} \Delta$$

... IMPORTANT: the concrete expressions for the F statistic...

We claim that the under  $H_0$ , we have

$$F = \frac{SSE^R - SSE/r}{SSE/(n-p)} \sim F_{r,n-p}.$$

*Proof.* what the

#### Lecture 15

 $\dots$  example  $\dots$ 

#### Transformations of data

Motivation: ...

box cox transformation

variance stabilising transformation

Suppose  $\mu = \varepsilon(Y_i)$  and that  $\text{Var}[(|Y_i)|]$  depends on  $\mu$ . ...

## 4 Model Analysis, Selection and Multiple Hypothesis Testing

#### Lecture 16

...

## Lecture 17

Suppose k covariates. Then  $2^k$  possible models from maximal:

$$Y_i = \beta_0 + \beta_1 x_{i1} + \dots + \beta_k x_{ik}.$$

to minimal:

$$Y_i = \beta_0$$
.

We want to arrive at a compromise between simplisity and goodness of fit.

1. Adjusted coefficient of determination:

$$R_{\text{adj}}^2 = 1 - \frac{\text{SSE}/(n-k-1)}{\text{SST}/(n-1)}$$

- 2.
- 3.
- 4.

example...

Multiple hypothesis testing motivation ...

#### Lecture 18

. . .

FWER = probability of at least one false positive finding

... two representations

The Bonferrony method

The Šidák method

...

example 2019

. . .

example 2020

## 5 ANOVA and Design of Experiment

#### Lecture 19

Example with three groups and their means ... rewrite to regression problem ...

### Analysis of varance (ANOVA)

p treatments, samples ...

#### Lecture 20

... cont ... + brief on two way ANOVA

#### Lecture 21

### 5.1 Two level factorial design

We suppose we have k main factors  $x_1, \ldots, x_k$  making up a model of the form:

$$Y = \beta_0 + \beta_1 x_1 + \dots + \beta_k x_k + \varepsilon, \quad \varepsilon \sim N(0, \sigma^2).$$

Further we suppose a feature matrix  $\boldsymbol{X}$  satisfying:

- 1. Each column has entries  $\pm 1$ .
- 2. The colomns are orthogonal, i.e.  $\mathbf{1}^{\mathbf{T}} x_{i} = \sum_{i=1}^{n} \mathbf{x}_{ij} = \mathbf{0}$  and  $x_{i} T x_{j} = n \delta_{ij}$ .

This in particular implies that we have  $X^TX = nI_n$ . Using results from regression analysis, this significantly simplifies our estimators:

TODO: expressions

**Definition 2.** The main effect of main factor j is defined as:

effect<sub>j</sub> = response at high level – response at low level =  $2\beta_j$ .

The estimated effect is naturally

$$\widehat{\text{effect}_j} = \text{estimated response at high level} - \text{estimated response at low level} = 2\widehat{\beta}_j$$
.

To go from this to a  $2^k$ -design, we take into account interactions of the factors modelled as products of main factors:

$$Y = \beta_0 + \beta_1 x_1 + \dots + \beta_k x_k + \beta_{1,2} x_1 x_2 + \dots + \beta_{k-1,k} x_{k-1} k_k + \dots + \beta_{1,2,\dots,k} x_1 \cdots x_k.$$

We extend the design matrix accordingly, and note that we still satisfy the assumptions.

TODO: example?

#### 5.1.1 Inference about effect

Need inference about  $\sigma^2$ ... cannot use estimator from multiple linear regression since for MLR we have  $\hat{\sigma}^2 = \frac{\text{SSE}}{n-p}$  and here n=p. We have to resort to one of two methods.

- 1. neglect some effects ... then these are normally dist ... use these as estimator ...
- 2. Lenth's method ...

#### Lecture 22

#### Resolution

resolution

#### Blocking

Vi tester en sitering [1].

# References

 $[1] \;\;$  test.  $test\ bok.$  Ed. by Trond. UiO, 2030.

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