Advanced dataanalysis and statistical modelling, Week 3

General Linear Models - part I

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Today

- The general linear model - intro
- The multivariate normal distribution
- Deviance
- Likelihood, score function and information matrix
- Estimation
- Fitted values
- Residuals
- Partitioning of variation
- Likelihood ratio tests
- The coefficient of determination

Overview

The general linear model - intro

- We will use the term *classical* GLM for the General linear model to distinguish it from GLM which is used for the Generalized linear model.
- The classical GLM leads to a unique way of describing the variations of experiments with a *continuous* variable.
- The classical GLM's include
  - Regression analysis
  - Analysis of variance - ANOVA
  - Analysis of covariance - ANCOVA
- The residuals are assumed to follow a multivariate normal distribution in the classical GLM.

The general linear model - intro

- Classical GLM's are naturally studied in the framework of the multivariate normal distribution.
- We will consider the set of n observations as a sample from a n-dimensional normal distribution.
- Under the normal distribution model, maximum-likelihood estimation of mean value parameters may be interpreted geometrically as *projection* on an appropriate subspace.
- The likelihood-ratio test statistics for model reduction may be expressed in terms of *norms* of these projections.

General Linear Model

- A general linear model is:

$$\boldsymbol{Y} \sim N_n(\boldsymbol{X}\boldsymbol{\beta}, \sigma^2 \boldsymbol{I})$$

Example (Two-way ANOVA):

	B_1	B_2	B_3
A_1	y_{11}	y_{12}	y_{13}
A_2	y_{21}	y_{22}	y_{23}

Two way ANOVA (the model):

$$y_{ij} = \mu + \alpha_i + \beta_j + \varepsilon_{ij}, \quad \varepsilon_{ij} \sim \text{ i.i.d. } N(0, \sigma^2), \quad i = 1, 2, \quad j = 1, 2, 3.$$

An expanded view of this model is:

$$\begin{array}{llllllll}
y_{11} = \mu & + \alpha_1 & & + \beta_1 & & & & + \varepsilon_{11} \\
y_{21} = \mu & & + \alpha_2 & + \beta_1 & & & & + \varepsilon_{21} \\
y_{12} = \mu & + \alpha_1 & & & + \beta_2 & & & + \varepsilon_{12} \\
y_{22} = \mu & & + \alpha_2 & & + \beta_2 & & & + \varepsilon_{22} \\
y_{13} = \mu & + \alpha_1 & & & & + \beta_3 & & + \varepsilon_{13} \\
y_{23} = \mu & & + \alpha_2 & & & + \beta_3 & & + \varepsilon_{23}
\end{array}$$

The exact same in matrix notation (though not identifiable):

$$\underbrace{\begin{pmatrix} y_{11} \\ y_{21} \\ y_{12} \\ y_{22} \\ y_{13} \\ y_{23} \end{pmatrix}}_{\mathbf{y}} = \underbrace{\begin{pmatrix} 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 1 \end{pmatrix}}_{\mathbf{X}} \underbrace{\begin{pmatrix} \mu \\ \alpha_1 \\ \alpha_2 \\ \beta_1 \\ \beta_2 \\ \beta_3 \end{pmatrix}}_{\boldsymbol{\beta}} + \underbrace{\begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{21} \\ \varepsilon_{12} \\ \varepsilon_{22} \\ \varepsilon_{13} \\ \varepsilon_{23} \end{pmatrix}}_{\boldsymbol{\varepsilon}}$$

The default in R would be

$$\underbrace{\begin{pmatrix} y_{11} \\ y_{21} \\ y_{12} \\ y_{22} \\ y_{13} \\ y_{23} \end{pmatrix}}_{\mathbf{y}} = \underbrace{\begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 \end{pmatrix}}_{\mathbf{X}} \underbrace{\begin{pmatrix} \mu \\ \alpha_2 \\ \beta_2 \\ \beta_3 \end{pmatrix}}_{\boldsymbol{\beta}} + \underbrace{\begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{21} \\ \varepsilon_{12} \\ \varepsilon_{22} \\ \varepsilon_{13} \\ \varepsilon_{23} \end{pmatrix}}_{\boldsymbol{\varepsilon}}$$

- $\mathbf{y}$ is the vector of all observations
- $\mathbf{X}$ is known as the *design matrix*
- $\boldsymbol{\beta}$ is the vector of parameters
- ε is a vector of independent $N(0, \sigma^2)$ "measurement noise"
  - The vector ε is said to follow a *multivariate normal distribution*
  - Mean vector $\mathbf{0}$
  - Covariance matrix $\sigma^2\mathbf{I}$
  - Written as: $\varepsilon \sim N(\mathbf{0}, \sigma^2\mathbf{I})$
- $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \varepsilon$ specifies the model, and everything can be calculated from $\mathbf{y}$ and $\mathbf{X}$.

Construction of the design matrix

In a general linear model (with both factors and covariates), it is surprisingly easy to construct the design matrix $\mathbf{X}$.

- For each factor: Add one column for each level, with ones in the rows where the corresponding observation is from that level, and zeros otherwise.
- For each covariate: Add one column with the measurements of the covariate.
- Remove linear dependencies (if necessary)

Example: linear regression:

$$y_i = \alpha + \beta \cdot x_i + \varepsilon$$

In matrix notation:

$$\mathbf{y} = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ . & . \\ . & . \\ 1 & x_n \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} + \boldsymbol{\varepsilon}$$

Overview

The multivariate normal distribution

Let $\boldsymbol{Y} = (Y_1, Y_2, \ldots, Y_n)^T$ be a random vector with $Y_1, Y_2, \ldots, Y_n$ independent identically distributed (iid) $\mathrm{N}(0, 1)$ random variables.

Note that $\mathrm{E}[\boldsymbol{Y}] = \boldsymbol{0}$ and the variance-covariance matrix $\mathrm{Var}[\boldsymbol{Y}] = \boldsymbol{I}$.

Definition (Multivariate normal distribution)

$\boldsymbol{Z}$ has an k-dimensional multivariate normal distribution if $\boldsymbol{Z}$ has the same distribution as $\boldsymbol{AY} + \boldsymbol{b}$ for some n, some $k \times n$ matrix $\boldsymbol{A}$, and some k vector $\boldsymbol{b}$. We indicate the multivariate normal distribution by writing $\boldsymbol{Z} \sim \mathrm{N}(\boldsymbol{b}, \boldsymbol{AA}^T)$.

Since $\boldsymbol{A}$ and $\boldsymbol{b}$ are fixed, we have $\mathrm{E}[\boldsymbol{Z}] = \boldsymbol{b}$ and $\mathrm{Var}[\boldsymbol{Z}] = \boldsymbol{AA}^T$.

The multivariate normal distribution

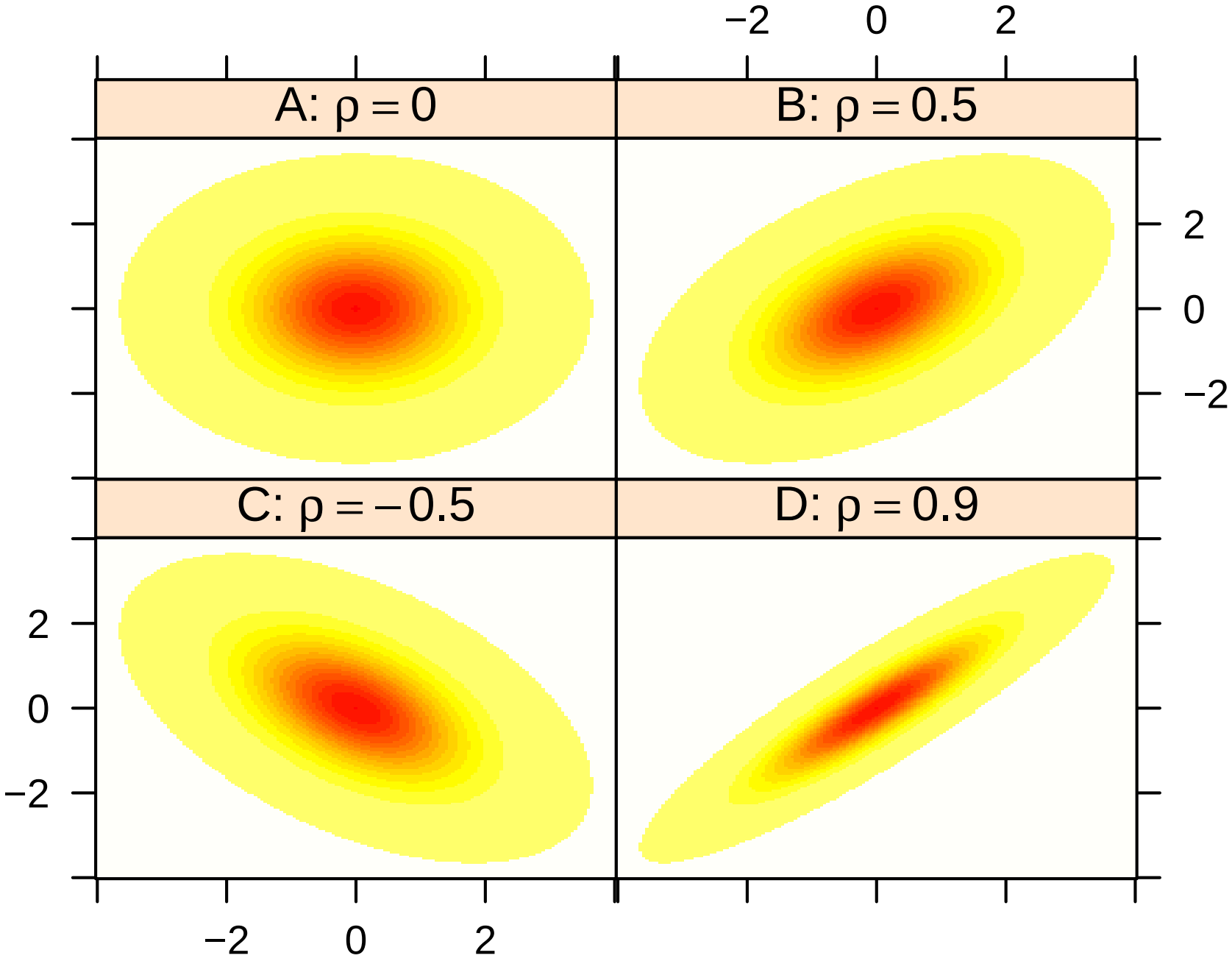
Let us assume that the variance-covariance matrix is known apart from a constant factor, σ^2, i.e. $\mathrm{Var}[\boldsymbol{Z}] = \sigma^2\boldsymbol{\Sigma}$.

The density for the k-dimensional random vector $\boldsymbol{Z}$ with mean $\boldsymbol{\mu}$ and covariance $\sigma^2\boldsymbol{\Sigma}$ is:

$$f_{\boldsymbol{Z}}(\boldsymbol{z}) = \frac{1}{(2\pi)^{k/2}\sigma^k\sqrt{\det\boldsymbol{\Sigma}}}\exp\left[-\frac{1}{2\sigma^2}(\boldsymbol{z}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{z}-\boldsymbol{\mu})\right]$$

where $\boldsymbol{\Sigma}$ is seen to be (a) symmetric and (b) positive semi-definite.

We write $\boldsymbol{Z} \sim \mathrm{N}_k(\boldsymbol{\mu}, \sigma^2\boldsymbol{\Sigma})$.


A: ρ = 0
B: ρ = 0.5
C: ρ = −0.5
D: ρ = 0.9
−2
0
2

The normal density as a statistical model

Consider now the n observations $\boldsymbol{Y} = (Y_1, Y_2, \ldots, Y_n)^T$, and assume that a statistical model is

$$\boldsymbol{Y} \sim \mathrm{N}_n(\boldsymbol{\mu}, \sigma^2\boldsymbol{\Sigma}) \text{ for } \boldsymbol{y} \in \mathbb{R}^n$$

The variance-covariance matrix for the observations is called the *dispersion matrix*, denoted $\mathrm{D}[\boldsymbol{Y}]$, i.e. the dispersion matrix for $\boldsymbol{Y}$ is

$$\mathrm{D}[\boldsymbol{Y}] = \sigma^2\boldsymbol{\Sigma}$$

Inner product and norm

Definition (Inner product and norm)

The bilinear form

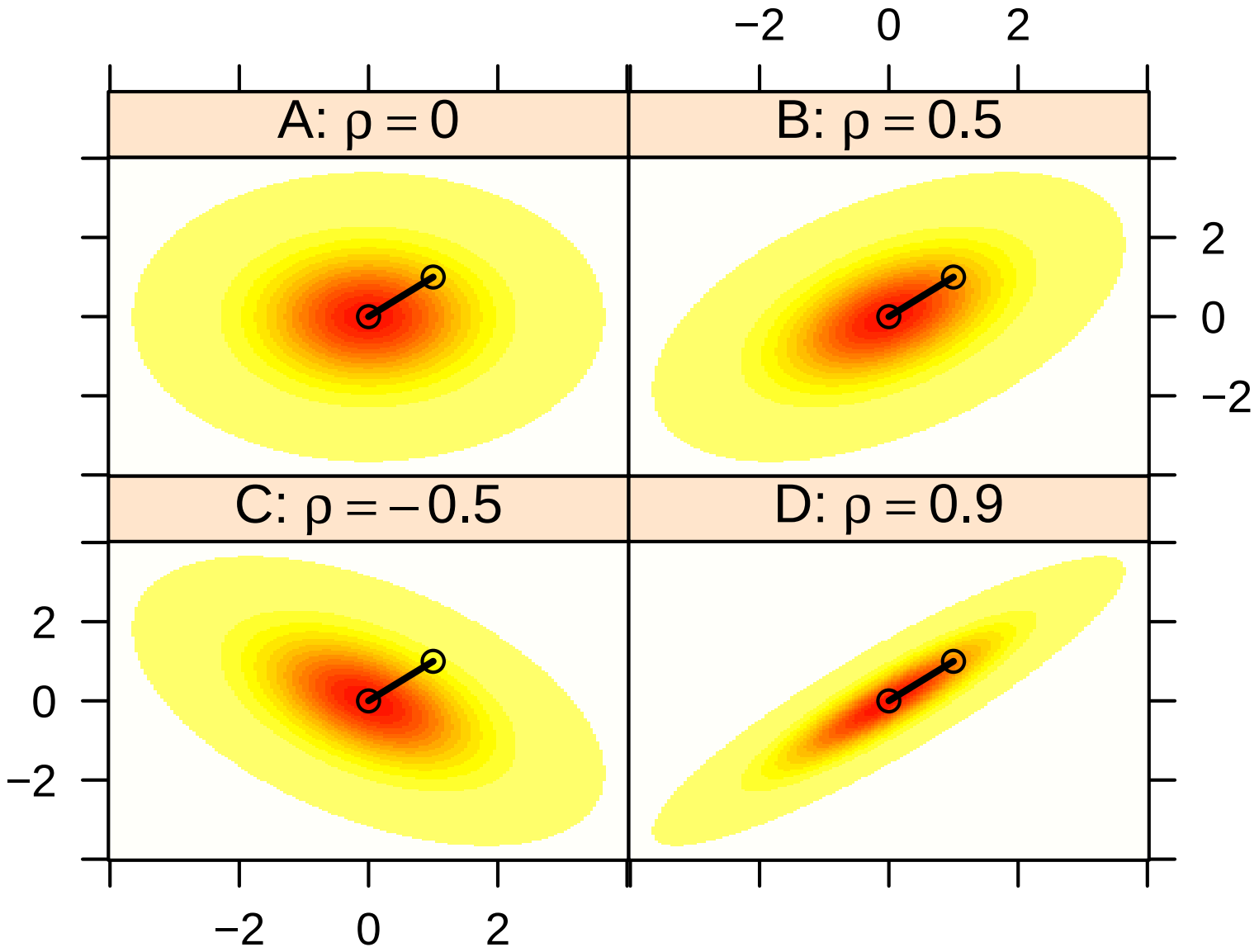
$$\delta_\Sigma(\boldsymbol{y}_1, \boldsymbol{y}_2) = \boldsymbol{y}_1^T \boldsymbol{\Sigma}^{-1} \boldsymbol{y}_2$$

defines an *inner product* in $\mathbb{R}^n$. Corresponding to this inner product we can define *orthogonality*, which is obtained when the inner product is zero.

A *norm* is defined by

$$||\boldsymbol{y}||_\Sigma = \sqrt{\delta_\Sigma(\boldsymbol{y}, \boldsymbol{y})}.$$

Order the vectors according to length (norm)



Deviance for normal distributed variables

Definition (Deviance for normal distributed variables)

Let us introduce the notation

$$\mathrm{D}(\boldsymbol{y};\boldsymbol{\mu}) = \delta_{\Sigma}(\boldsymbol{y}-\boldsymbol{\mu},\boldsymbol{y}-\boldsymbol{\mu}) = (\boldsymbol{y}-\boldsymbol{\mu})^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{y}-\boldsymbol{\mu})$$

to denote the quadratic norm of the vector $(\boldsymbol{y}-\boldsymbol{\mu})$ corresponding to the inner product defined by $\boldsymbol{\Sigma}^{-1}$.

For a normal distribution with $\boldsymbol{\Sigma} = \boldsymbol{I}$, the deviance is just the Residual Sum of Squares (RSS).

Deviance for normal distributed variables

Using this notation the normal density is expressed as a density defined on any finite dimensional vector space equipped with the inner product, δ_Σ:

$$f(\boldsymbol{y};\boldsymbol{\mu},\sigma^2) = \frac{1}{(\sqrt{2\pi})^n \sigma^n \sqrt{\det(\boldsymbol{\Sigma})}} \exp\left[-\frac{1}{2\sigma^2} \mathrm{D}(\boldsymbol{y};\boldsymbol{\mu})\right].$$

Overview

The likelihood and log-likelihood function

- The likelihood function is:

$$L(\boldsymbol{\mu}, \sigma^2; \boldsymbol{y}) = \frac{1}{(\sqrt{2\pi})^n \sigma^n \sqrt{\det(\boldsymbol{\Sigma})}} \exp\left[-\frac{1}{2\sigma^2} \mathrm{D}(\boldsymbol{y}; \boldsymbol{\mu})\right]$$

- The log-likelihood function is (apart from an additive constant):

$$\begin{aligned}\ell(\boldsymbol{\mu}, \sigma^2; \boldsymbol{y}) &= -(n/2)\log(\sigma^2) - \frac{1}{2\sigma^2}\,(\boldsymbol{y}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\boldsymbol{y}-\boldsymbol{\mu}) \\ &= -(n/2)\log(\sigma^2) - \frac{1}{2\sigma^2}\,\mathrm{D}(\boldsymbol{y}; \boldsymbol{\mu}).\end{aligned}$$

The score function, observed - and expected information for μ

- The score function wrt. $\boldsymbol{\mu}$ is

$$\frac{\partial}{\partial \boldsymbol{\mu}} \ell(\boldsymbol{\mu}, \sigma^2; \boldsymbol{y}) = \frac{1}{\sigma^2} \left[\boldsymbol{\Sigma}^{-1} \boldsymbol{y} - \boldsymbol{\Sigma}^{-1} \boldsymbol{\mu} \right] = \frac{1}{\sigma^2} \boldsymbol{\Sigma}^{-1} (\boldsymbol{y} - \boldsymbol{\mu})$$

- The observed information (wrt. $\boldsymbol{\mu}$) is

$$\boldsymbol{j}(\boldsymbol{\mu}; \boldsymbol{y}) = \frac{1}{\sigma^2} \boldsymbol{\Sigma}^{-1}.$$

- It is seen that the observed information does not depend on the observations $\boldsymbol{y}$. Hence the expected information is

$$\boldsymbol{i}(\boldsymbol{\mu}) = \frac{1}{\sigma^2} \boldsymbol{\Sigma}^{-1}.$$

The general linear model

In the case of a normal density the observation Y_i is most often written as

$$Y_i = \mu_i + \epsilon_i$$

which for all n observations $(Y_1, Y_2, \ldots, Y_n)$ can be written on the matrix form

$$\boldsymbol{Y} = \boldsymbol{\mu} + \boldsymbol{\epsilon}$$

where

$$\boldsymbol{Y} \sim \mathrm{N}_n(\boldsymbol{\mu}, \sigma^2 \boldsymbol{\Sigma}) \ \text{ for } \ \boldsymbol{y} \in \mathbb{R}^n$$

In many applications we will asume that $\boldsymbol{\Sigma} = \boldsymbol{I}$.

General Linear Models

- In the *linear model* it is assumed that $\boldsymbol{\mu}$ belongs to a linear (or affine) subspace Ω_0 of $\mathbb{R}^n$.
- The *full model* is a model with $\Omega_{full} = \mathbb{R}^n$ and hence each observation fits the model perfectly, i.e. $\widehat{\boldsymbol{\mu}} = \boldsymbol{y}$.
- The most restricted model is the *null model* with $\Omega_{null} = \mathbb{R}$. It only describes the variations of the observations by a common mean value for all observations.
- In practice, one often starts with formulating a rather comprehensive model with $\Omega = \mathbb{R}^k$, where $k < n$. We will call such a model a *sufficient model*.

The General Linear Model

Definition (The general linear model)

Assume that $Y_1, Y_2, \ldots, Y_n$ is normally distributed as described before. A *general linear model* for $Y_1, Y_2, \ldots, Y_n$ is a model where an affine hypothesis is formulated for $\boldsymbol{\mu}$. The hypothesis is of the form

$$\mathcal{H}_0 : \boldsymbol{\mu} - \boldsymbol{\mu}_0 \in \Omega_0,$$

where Ω_0 is a linear subspace of $\mathbb{R}^n$ of dimension k, and where $\boldsymbol{\mu}_0$ denotes a vector of *known offset values*.

Definition (Dimension of general linear model)

The dimension of the subspace Ω_0 for the linear model is the *dimension of the model*.

The design matrix

Definition (Design matrix for classical GLM)

Assume that the linear subspace $\Omega_0 = \text{span}\{x_1, \ldots, x_k\}$, i.e. the subspace is spanned by k vectors ($k < n$).
Consider a general linear model where the hypothesis can be written as

$$\mathcal{H}_0 : \boldsymbol{\mu} - \boldsymbol{\mu}_0 = \boldsymbol{X}\boldsymbol{\beta} \text{ with } \boldsymbol{\beta} \in \mathbb{R}^k,$$

where $\boldsymbol{X}$ has full rank. The $n \times k$ matrix $\boldsymbol{X}$ of known deterministic coefficients is called the *design matrix*.
The i^{th} row of the design matrix is given by the *model vector*

$$\boldsymbol{x}_i^T = \begin{pmatrix} x_{i1} \\ x_{i2} \\ \vdots \\ x_{ik} \end{pmatrix}^T,$$

for the i^{th} observation.

Overview

Estimation of mean value parameters

Under the hypothesis

$$\mathcal{H}_0 : \boldsymbol{\mu} \in \Omega_0 \ ,$$

the maximum likelihood estimate for the set $\boldsymbol{\mu}$ is found as the orthogonal projection (with respect to δ_Σ), $p_0(\boldsymbol{y})$ of $\boldsymbol{y}$ onto the linear subspace Ω_0.

Theorem (ML estimates of mean value parameters)

For hypothesis of the form

$$\mathcal{H}_0 : \boldsymbol{\mu}(\boldsymbol{\beta}) = \boldsymbol{X}\boldsymbol{\beta}$$

the maximum likelihood estimated for $\boldsymbol{\beta}$ is found as a solution to the normal equation

$$\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{y} = \boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X}\widehat{\boldsymbol{\beta}}.$$

If $\boldsymbol{X}$ has full rank, the solution is uniquely given by

$$\widehat{\boldsymbol{\beta}} = (\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{y}$$

Properties of the ML estimator

Theorem (Properties of the ML estimator)

For the ML estimator we have

$$\widehat{\boldsymbol{\beta}} \sim \mathrm{N}_k(\boldsymbol{\beta}, \sigma^2 \, (\boldsymbol{X}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{X})^{-1})$$

Unknown $\boldsymbol{\Sigma}$

Notice that it has been assumed that $\boldsymbol{\Sigma}$ is known. If $\boldsymbol{\Sigma}$ is unknown different possiblities exist

- The relaxation algorithm described in Madsen (2008) [a].
- Likelihood based method, either direct or by restricted maximum likelihood (eg. `gls` in the the `nlme` package of R)

[a] Madsen, H. (2008) Time Series Analysis. Chapman, Hall

Expectaion and variance of MLE

The ML estimate of $\boldsymbol{\beta}$ is central

$$\begin{aligned} E[\hat{\boldsymbol{\beta}}] =& E[(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{Y}] \\ =& (\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}E[\boldsymbol{X}\boldsymbol{\beta}+\boldsymbol{\epsilon}] \\ =& (\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X}\boldsymbol{\beta} = \boldsymbol{\beta} \end{aligned}$$

with variance

$$\begin{aligned} V[\hat{\boldsymbol{\beta}}] =& V[(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{Y}] \\ =& (\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}V[\boldsymbol{X}\boldsymbol{\beta}+\boldsymbol{\epsilon}]\boldsymbol{\Sigma}^{-1}\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1} \\ =& \sigma^2(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{\Sigma}\boldsymbol{\Sigma}^{-1}\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1} \\ =& \sigma^2(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1} \end{aligned}$$

Fitted values

Fitted – or predicted – values

The *fitted* values $\widehat{\boldsymbol{\mu}} = \boldsymbol{X}\widehat{\boldsymbol{\beta}}$ is found as the projection of $\boldsymbol{y}$ (denoted $p_0(\boldsymbol{y})$) on to the subspace Ω_0 spanned by $\boldsymbol{X}$, and $\widehat{\boldsymbol{\beta}}$ denotes the local coordinates for the projection.

Definition (Projection matrix)

A matrix $\boldsymbol{H}$ is a *projection matrix* if and only if
(a) $\boldsymbol{H}^T = \boldsymbol{H}$ and
(b) $\boldsymbol{H}^2 = \boldsymbol{H}$, i.e. the matrix is *idempotent*.

The hat matrix

- Consider the model

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}; \quad \boldsymbol{\epsilon} \sim N(\boldsymbol{0}, \sigma^2 \boldsymbol{I})$$

1: The matrix

$$\boldsymbol{H} = \boldsymbol{X}[\boldsymbol{X}^T\boldsymbol{X}]^{-1}\boldsymbol{X}^T$$

is a projection matrix.

- The projection matrix provides the predicted values $\widehat{\boldsymbol{\mu}}$, since

$$\widehat{\boldsymbol{\mu}} = p_0(\boldsymbol{y}) = \boldsymbol{X}\widehat{\boldsymbol{\beta}} = \boldsymbol{H}\boldsymbol{y}$$

- Furthermore
  2: $\boldsymbol{I} - \boldsymbol{H}$ is also a projection matrix
  3: $Tr(\boldsymbol{H}) = p$,
  4: $Tr(\boldsymbol{I} - \boldsymbol{H}) = n - p$

Projections - PROOFs

PROOF:

1: $$\begin{aligned}\boldsymbol{H}^2 &= \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T \\ &= \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T = \boldsymbol{H}\end{aligned}$$
$$\begin{aligned}\boldsymbol{H}^T &= (\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T)^T = ((\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T)^T\boldsymbol{X}^T \\ &= \boldsymbol{X}((\boldsymbol{X}^T\boldsymbol{X})^{-1})^T\boldsymbol{X}^T = \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T = \boldsymbol{H}\end{aligned}$$

2: $$(\boldsymbol{I}-\boldsymbol{H})^2 = \boldsymbol{I}+\boldsymbol{H}^2-\boldsymbol{I}\boldsymbol{H}-\boldsymbol{H}\boldsymbol{I} = \boldsymbol{I}-\boldsymbol{H}$$
$$(\boldsymbol{I}-\boldsymbol{H})^T = \boldsymbol{I}^T-\boldsymbol{H}^T = \boldsymbol{I}-\boldsymbol{H}$$

3[1]: $$\begin{aligned}Tr(\boldsymbol{H}) &= Tr(\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T) \\ &= Tr((\boldsymbol{X}^T\boldsymbol{X})^{-1}(\boldsymbol{X}^T\boldsymbol{X})) = Tr(\boldsymbol{I}_p) = p\end{aligned}$$

4: $$Tr(\boldsymbol{I}-\boldsymbol{H}) = Tr(\boldsymbol{I}) - Tr(\boldsymbol{H}) = n-p$$

[1] We use the relation $Tr(ABC) = Tr(BCA) = Tr(CAB)$

The hat matrix

- It follows that the predicted values are normally distributed with

$$\mathrm{D}[\mathbf{X}\widehat{\boldsymbol{\beta}}] = \sigma^2 \boldsymbol{X}[\boldsymbol{X}^T\boldsymbol{X}]^{-1}\boldsymbol{X}^T = \sigma^2\boldsymbol{H}$$

- The matrix $\boldsymbol{H}$ is often termed the *hat matrix* since it transforms the observations $\boldsymbol{y}$ to their predicted values symbolized by a "hat" on the μ's.
- The observed *residuals* are

$$\boldsymbol{r} = \boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}} = (\boldsymbol{I} - \boldsymbol{H})\boldsymbol{y}$$

- The distribution of the residuals is also normal with

$$D[\boldsymbol{r}(\boldsymbol{Y})] = \sigma^2(\boldsymbol{I} - \boldsymbol{H})$$

Residuals

Orthogonality

The maximum likelihood estimate for $\boldsymbol{\beta}$ is found as the value of $\boldsymbol{\beta}$ which minimizes the *distance* $||\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}||$.

The normal equations show that (still assuming $\boldsymbol{\Sigma} = \boldsymbol{I}$)

$$\begin{aligned}\delta(\boldsymbol{y} - \hat{\boldsymbol{y}}, \hat{\boldsymbol{y}}) =& (\boldsymbol{y} - \hat{\boldsymbol{y}})^T \hat{\boldsymbol{y}} \\ =& \boldsymbol{y}^T (\boldsymbol{I} - \boldsymbol{H})^T \boldsymbol{H} \boldsymbol{y} \\ =& \boldsymbol{y}^T (\boldsymbol{H} - \boldsymbol{H}) \boldsymbol{y} = 0\end{aligned}$$

i.e. the *residuals* are orthogonal (with respect to $\boldsymbol{\Sigma}^{-1}$) to the subspace Ω_0.

The residuals are thus orthogonal to the fitted – or predicted – values.

Residuals

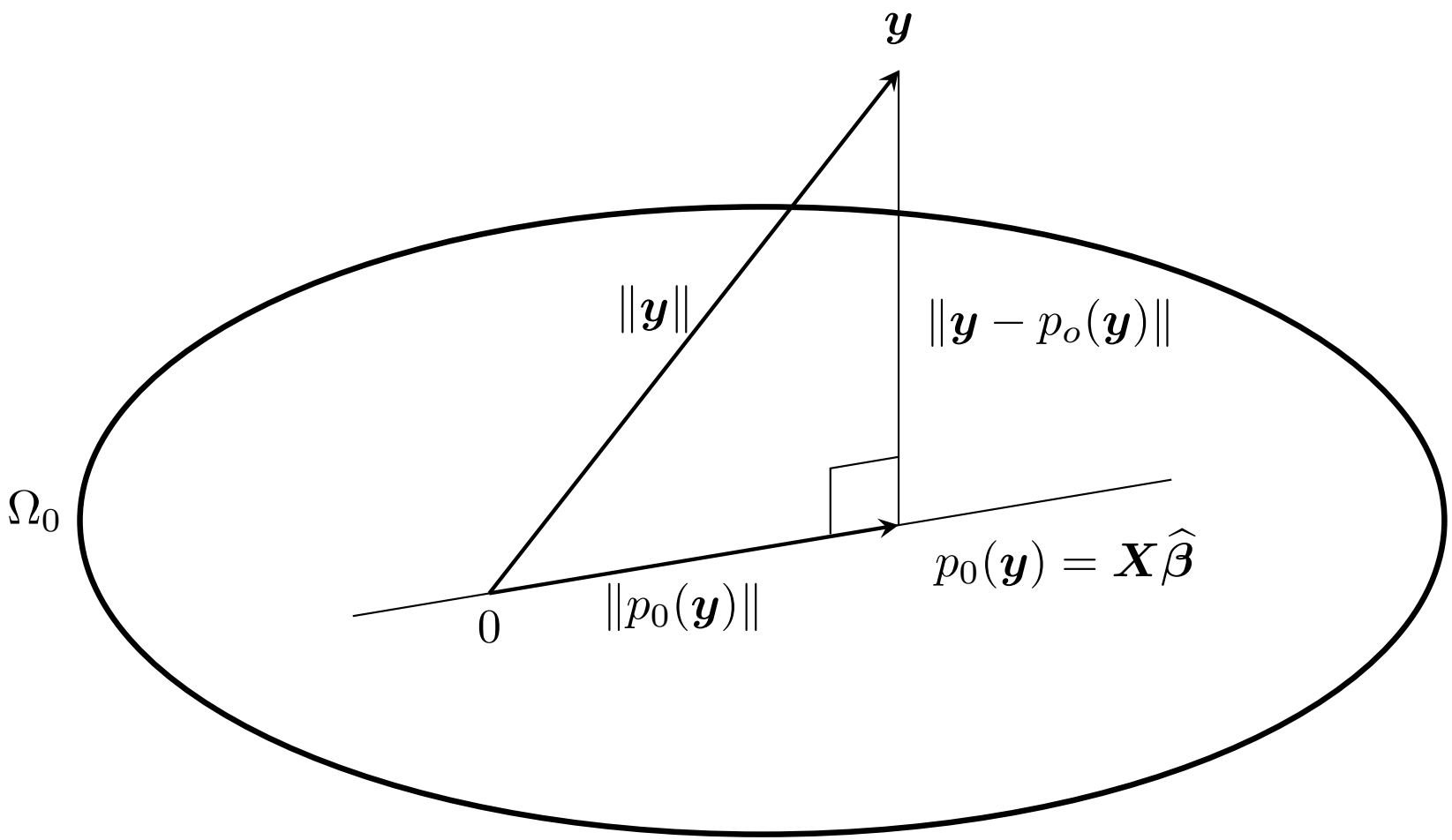


Figure: Orthogonality between the residual $(\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}})$ and the vector $\boldsymbol{X}\widehat{\boldsymbol{\beta}}$.

Residuals

- The residuals $\boldsymbol{r} = (\boldsymbol{I} - \boldsymbol{H})\boldsymbol{Y}$ are normally distributed with

$$\mathrm{D}[\boldsymbol{r}] = \sigma^2(\boldsymbol{I} - \boldsymbol{H})$$

- The individual residuals do not have the same variance.
- The residuals are thus belonging to a subspace of dimension $n - k$, which is orthogonal to Ω_0.
- It may be shown that the distribution of the residuals $\boldsymbol{r}$ is independent of the fitted values $\boldsymbol{X}\widehat{\boldsymbol{\beta}}$ (follows from orthogonality and normality).

Generalization

The results above apply to the model

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}; \quad \boldsymbol{\epsilon} \sim N(\boldsymbol{0}, \sigma^2 \boldsymbol{I})$$

In order to generalise to the model

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}; \quad \boldsymbol{\epsilon} \sim N(\boldsymbol{0}, \sigma^2 \boldsymbol{\Sigma})$$

Consider the "square root" $(\boldsymbol{T})$ of $\boldsymbol{\Sigma} = \boldsymbol{T}\boldsymbol{T}^T$, and rewrite the model

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{T}\boldsymbol{e}; \quad \boldsymbol{e} \sim N(\boldsymbol{0}, \sigma^2 \boldsymbol{I})$$

to $(\boldsymbol{Z} = \boldsymbol{T}^{-1}\boldsymbol{Y})$

$$\boldsymbol{Z} = \boldsymbol{T}^{-1}\boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{e}; \quad \boldsymbol{e} \sim N(\boldsymbol{0}, \sigma^2 \boldsymbol{I})$$

then the results apply to $\boldsymbol{Z}$ and back transformation will give the results in the original domain.

Example[2]

Two items A and B are wheigted on a balance, first seperately then together, giving the observations y_1, y_2, y_3, and the model

$$\begin{aligned} Y_1 &= \beta_A + \epsilon_1 \\ Y_2 &= \beta_B + \epsilon_2 \\ Y_3 &= \beta_A + \beta_B + \epsilon_3 \end{aligned}$$

with $\epsilon_i \sim N(0, \sigma^2)$.

[2] from Bingham and Fry (2010)

Example

Or in matrix notation

$$\begin{aligned}\boldsymbol{Y} &= \begin{bmatrix}1 & 0\\ 0 & 1\\ 1 & 1\end{bmatrix}\begin{bmatrix}\beta_A\\ \beta_B\end{bmatrix} + \epsilon\\ &= \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}\end{aligned}$$

with $\boldsymbol{\epsilon} \sim N(\boldsymbol{0}, \sigma^2\boldsymbol{I})$. Hence

$$\begin{aligned}\hat{\boldsymbol{\beta}} &= (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}\\ &= \frac{1}{3}\begin{bmatrix}2 & -1 & 1\\ -1 & 2 & 1\end{bmatrix}\boldsymbol{y}\end{aligned}$$

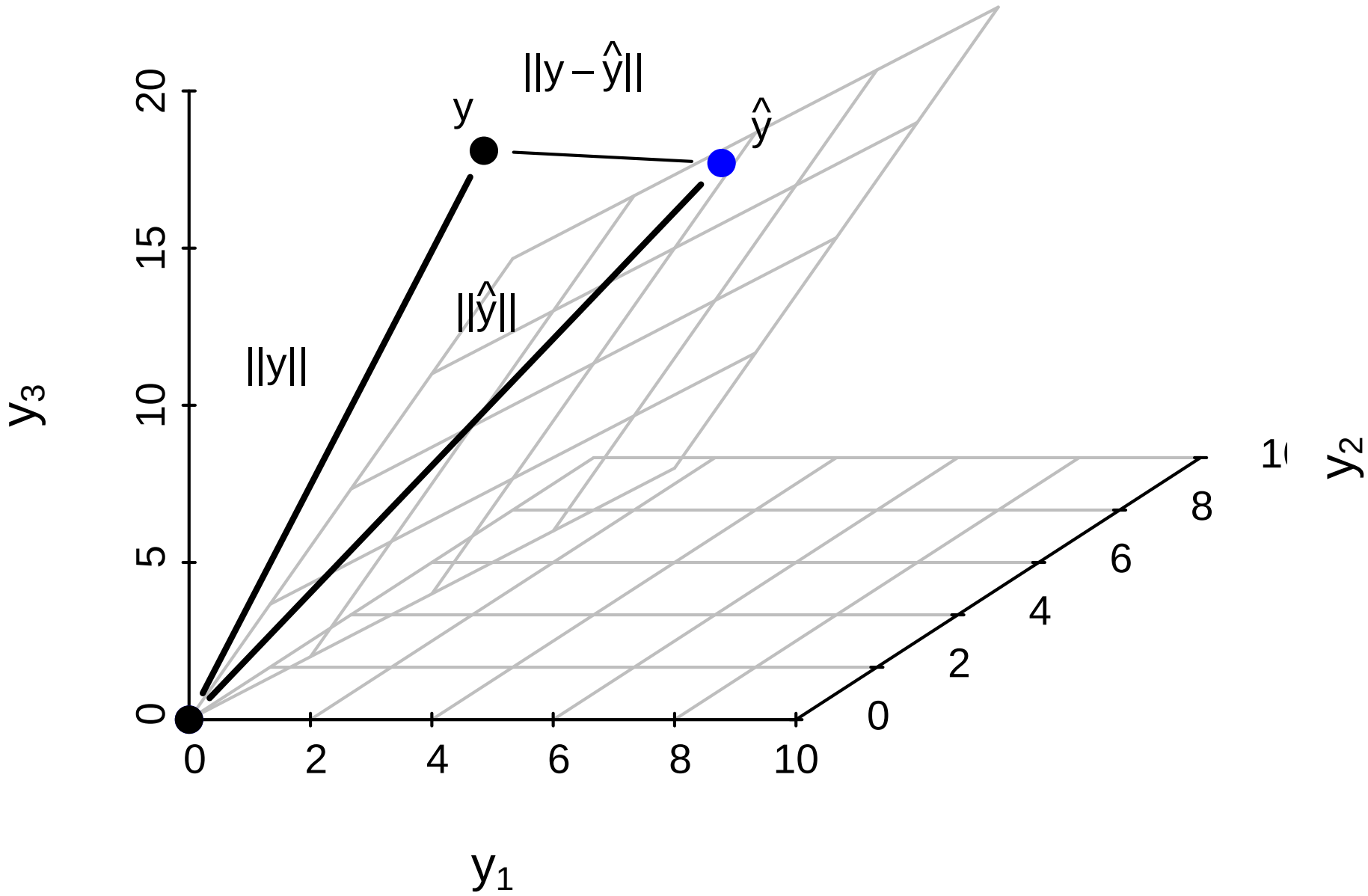
Example

And

$$\begin{aligned}\hat{\boldsymbol{y}} =& \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y} \\ =& \frac{1}{3}\begin{bmatrix} 2 & -1 & 1 \\ -1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}\boldsymbol{y} \\ =& \boldsymbol{H}\boldsymbol{y}\end{aligned}$$

The projection H defines a 2-dimensional surface in $\mathbb{R}^3$.

Exercise: Formulate a model $y_i = x_{1,i}\beta_1 + x_{2,i}\beta_2$ such that the test $\beta_A = \beta_B$ is equivalent to testing $\beta_2 = 0$


$\|y - \hat{y}\|$
y
$\hat{y}$
$\|\hat{y}\|$
$\|y\|$
y_3
y_1
y_2
0
5
10
15
20
0
2
4
6
8
10
0
2
4
6
8

Overview

Cochran's theorem

Theorem (Cochran's theorem)

Suppose that $\boldsymbol{Y} \sim N_n(\boldsymbol{0}, \boldsymbol{I}_n)$ *(i.e. standard multivariate Gaussian random variable)*

$$\boldsymbol{Y}^T\boldsymbol{Y} = \boldsymbol{Y}^T\boldsymbol{H}_1\boldsymbol{Y} + \boldsymbol{Y}^T\boldsymbol{H}_2\boldsymbol{Y} + \cdots + \boldsymbol{Y}^T\boldsymbol{H}_k\boldsymbol{Y}$$

where $\boldsymbol{H}_i$ *is a symmetric* $n \times n$ *matrix with rank* n_i, $i = 1, 2, \ldots, k$.
Then any one of the following conditions implies the other two:

i. *The ranks of the* $\boldsymbol{H}_i$ *adds to* n, *i.e.* $\sum_{i=1}^k n_i = n$
ii. *Each quadratic form* $\boldsymbol{Y}^T\boldsymbol{H}_i\boldsymbol{Y} \sim \chi^2_{n_i}$ *(thus the* H_i *are positive semidefinite)*
iii. *All the quadratic forms* $\boldsymbol{Y}^T\boldsymbol{H}_i\boldsymbol{Y}$ *are independent (necessary and sufficient condition).*

Partitioning of variation

Partitioning of the variation

$$
\begin{aligned}
\mathrm{D}(\boldsymbol{y}; \boldsymbol{X}\boldsymbol{\beta}) &= \mathrm{D}(\boldsymbol{y}; \boldsymbol{X}\widehat{\boldsymbol{\beta}}) + \mathrm{D}(\boldsymbol{X}\widehat{\boldsymbol{\beta}}; \boldsymbol{X}\boldsymbol{\beta}) \\
&= (\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}}) + \\
&\quad (\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta})^T \boldsymbol{X}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{X} (\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}) \\
&\geq (\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}})
\end{aligned}
$$

Partitioning of variation

χ^2-distribution of individual contributions

Under $\mathcal{H}_0$ it follows from the normal distribution of $\boldsymbol{Y}$ that

$$\mathrm{D}(\boldsymbol{y}; \boldsymbol{X}\boldsymbol{\beta}) = (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}) \sim \sigma^2 \chi^2_n$$

Furthermore, it follows from the normal distribution of $\boldsymbol{r}$ and of $\widehat{\boldsymbol{\beta}}$ that

$$\mathrm{D}(\boldsymbol{y}; \boldsymbol{X}\widehat{\boldsymbol{\beta}}) = (\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}}) \sim \sigma^2 \chi^2_{n-k}$$
$$\mathrm{D}(\boldsymbol{X}\widehat{\boldsymbol{\beta}}; \boldsymbol{X}\boldsymbol{\beta}) = (\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta})^T \boldsymbol{X}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{X} (\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}) \sim \sigma^2 \chi^2_k$$

moreover, the independence of $\boldsymbol{r}$ and $\boldsymbol{X}\widehat{\boldsymbol{\beta}}$ implies that $\mathrm{D}(\boldsymbol{y}; \boldsymbol{X}\widehat{\boldsymbol{\beta}})$ and $\mathrm{D}(\boldsymbol{X}\widehat{\boldsymbol{\beta}}; \boldsymbol{X}\boldsymbol{\beta})$ are independent.
Thus, the $\sigma^2\chi^2_n$-distribution on the left side is partitioned into two independent χ^2 distributed variables with $n-k$ and k degrees of freedom, respectively.

Estimation of the residual variance σ^2

Theorem (Estimation of the variance)

Under the hypothesis

$$\mathcal{H}_0 : \boldsymbol{\mu}(\boldsymbol{\beta}) = \boldsymbol{X}\boldsymbol{\beta}$$

the maximum marginal likelihood estimator for the variance σ^2 is

$$\widehat{\sigma}^2 = \frac{\mathrm{D}(\boldsymbol{y}; \boldsymbol{X}\widehat{\boldsymbol{\beta}})}{n-k} = \frac{(\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{y} - \boldsymbol{X}\widehat{\boldsymbol{\beta}})}{n-k}$$

Under the hypothesis, $\widehat{\sigma}^2 \sim \sigma^2 \chi^2_f / f$ with $f = n - k$.

Likelihood ratio tests

- In the classical GLM case the exact distribution of the likelihood ratio test statistic may be derived.
- Consider the following model for the data $\boldsymbol{Y} \sim \mathrm{N}_n(\boldsymbol{\mu}, \sigma^2\boldsymbol{\Sigma})$.
- Let us assume that we have the sufficient model

$$\mathcal{H}_1 : \boldsymbol{\mu} \in \Omega_1 \subset \mathbb{R}^n$$

  with $\dim(\Omega_1) = m_1$.
- Now we want to test whether the model may be reduced to a model where μ is restricted to some subspace of Ω_1, and hence we introduce $\Omega_0 \subset \Omega_1$ as a linear (affine) subspace with $\dim(\Omega_0) = m_0$.

Model reduction

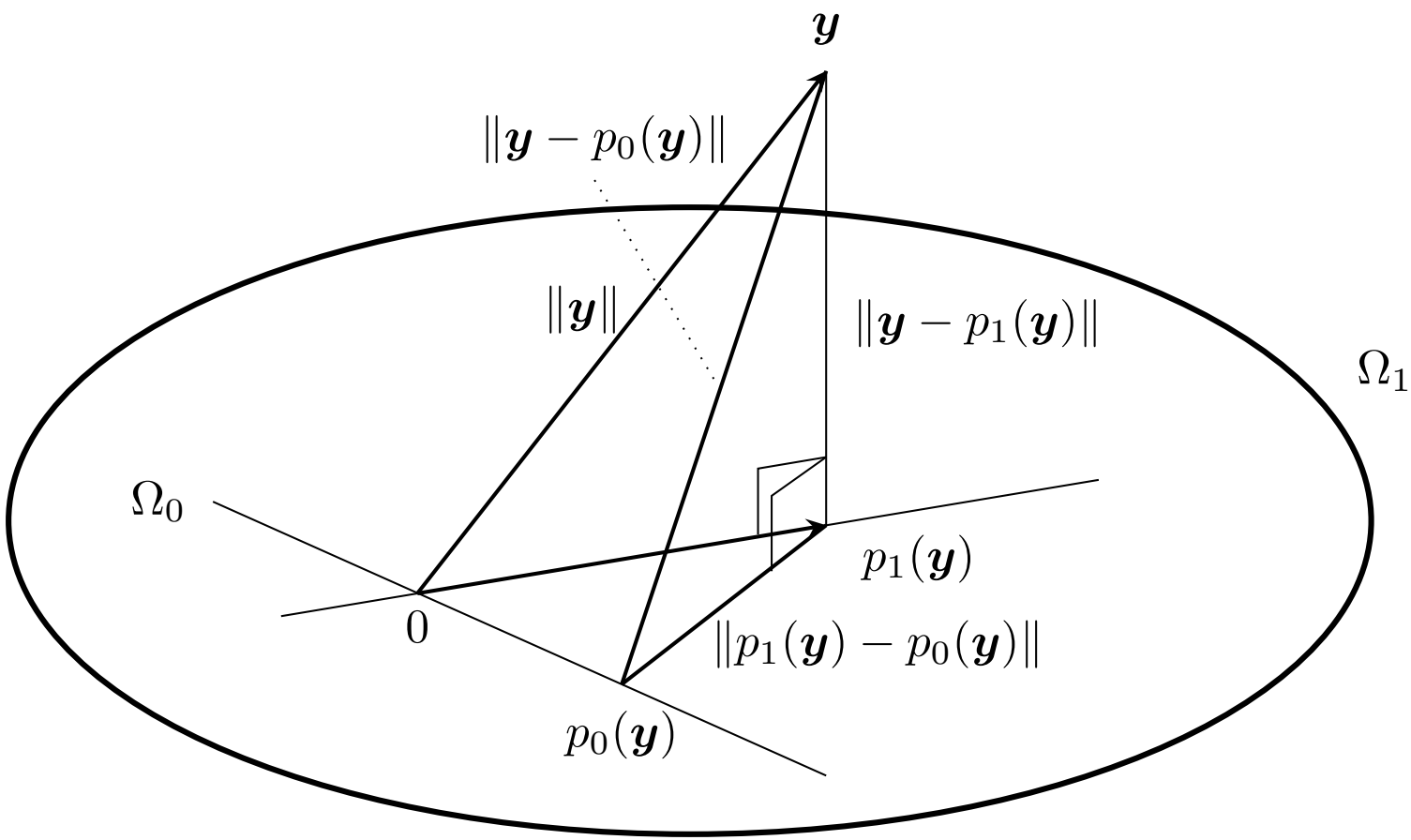
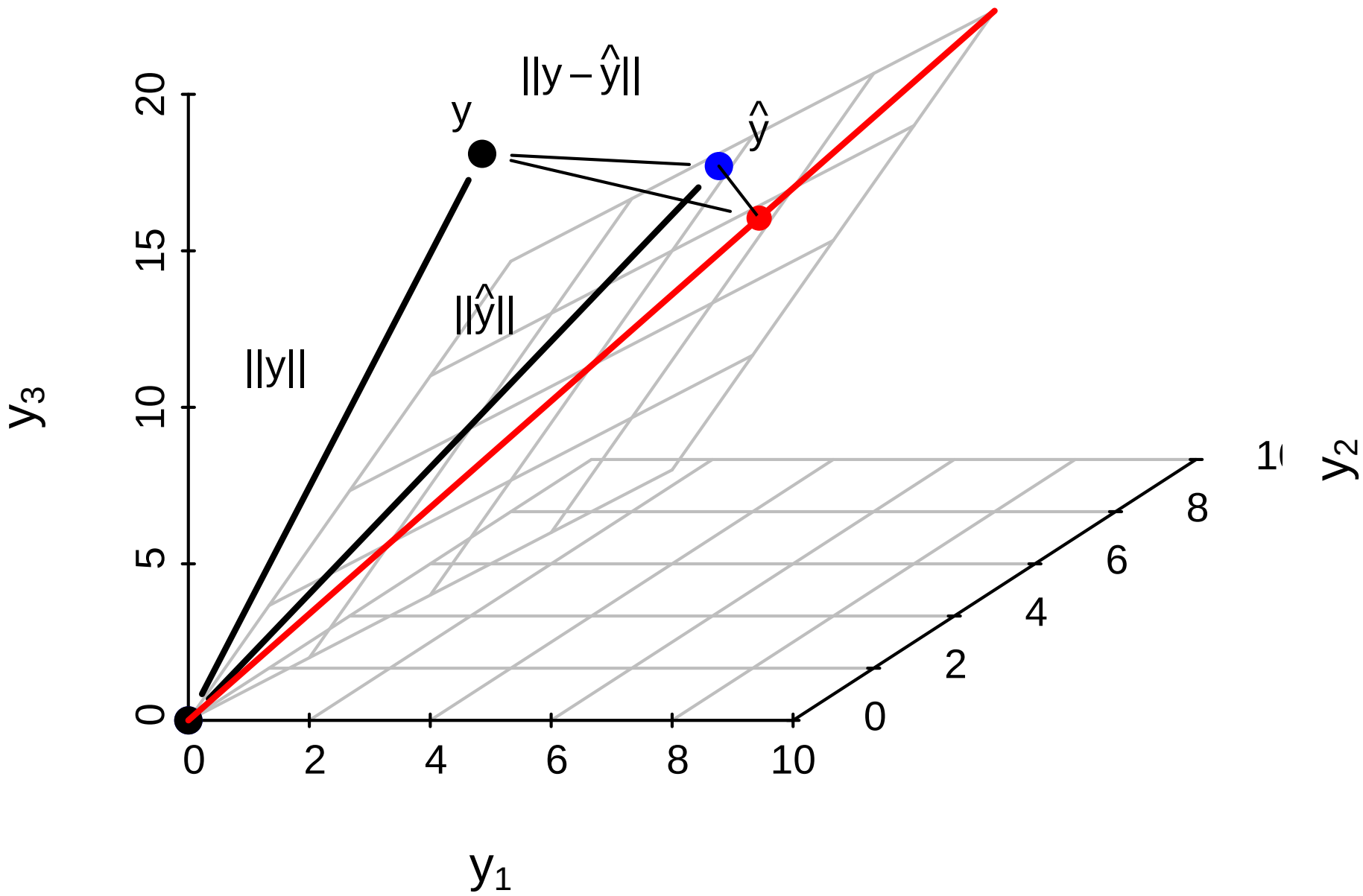


Figure: Model reduction. The partitioning of the deviance corresponding to a test of the hypothesis $\mathcal{H}_0 : \mu \in \Omega_0$ under the assumption of $\mathcal{H}_1 : \mu \in \Omega_1$.


||y − ŷ||
y
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y3
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y2
0
5
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15
20
0
2
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10
0
2
4
6
8

Test for model reduction

Theorem (A test for model reduction)

The likelihood ratio test statistic for testing

$$\mathcal{H}_0 : \boldsymbol{\mu} \in \Omega_0 \quad \text{against the alternative} \quad \mathcal{H}_1 : \boldsymbol{\mu} \in \Omega_1 \setminus \Omega_0$$

is a monotone function of

$$F(\boldsymbol{y}) = \frac{\mathrm{D}(p_1(\boldsymbol{y}); p_0(\boldsymbol{y}))/(m_1 - m_0)}{\mathrm{D}(\boldsymbol{y}; p_1(\boldsymbol{y}))/(n - m_1)}$$

where $p_1(\boldsymbol{y})$ and $p_0(\boldsymbol{y})$ denote the projection of $\boldsymbol{y}$ on Ω_1 and Ω_0, respectively. Under $\mathcal{H}_0$ we have

$$F \sim F(m_1 - m_0, n - m_1)$$

i.e. large values of F reflects a conflict between the data and $\mathcal{H}_0$, and hence lead to rejection of $\mathcal{H}_0$. The p-value of the test is found as $p = P[F(m_1 - m_0, n - m_1) \geq F_{obs}]$, where F_{obs} is the observed value of F given the data.

Test for model reduction

- The partitioning of the variation is presented in a Deviance table (or an *ANalysis Of VAriance table*, ANOVA).
- The table reflects the partitioning in the test for *model reduction*.
- The deviance between the variation of the model from the hypothesis is measured using the deviance of the observations from the model as a reference.
- Under $\mathcal{H}_0$ they are both χ^2 distributed, orthogonal and thus independent.
- This means that the ratio is F distributed.
- If the test quantity is large this shows evidence against the model reduction tested using $\mathcal{H}_0$.

Deviance table

Source	f	Deviance	Test statistic, F
Model versus hypothesis	$m_1 - m_0$	$\|\|p_1(\boldsymbol{y}) - p_0(\boldsymbol{y})\|\|^2$	$\frac{\|\|p_1(\boldsymbol{y}) - p_0(\boldsymbol{y})\|\|^2/(m_1 - m_0)}{\|\|\boldsymbol{y} - p_1(\boldsymbol{y})\|\|^2/(n - m_1)}$
Residual under model	$n - m_1$	$\|\|\boldsymbol{y} - p_1(\boldsymbol{y})\|\|^2$	
Residual under hypothesis	$n - m_0$	$\|\|\boldsymbol{y} - p_0(\boldsymbol{y})\|\|^2$	

Table: Deviance table corresponding to a test for model reduction as specified by $\mathcal{H}_0$. For $\Sigma = \boldsymbol{I}$ this corresponds to an analysis of variance table, and then 'Deviance' is equal to the 'Sum of Squared deviations (SS)'

Test for model reduction

The test is a conditional test

It should be noted that the test has been derived as a *conditional test*. It is a test for the hypothesis $\mathcal{H}_0 : \boldsymbol{\mu} \in \Omega_0$ under the assumption that $\mathcal{H}_1 : \boldsymbol{\mu} \in \Omega_1$ is true. The test does in no way assess whether $\mathcal{H}_1$ is in agreement with the data. On the contrary in the test the residual variation under $\mathcal{H}_1$ is used to estimate σ^2, i.e. to assess $\mathrm{D}(\boldsymbol{y}; p_1(\boldsymbol{y}))$.

The test does not depend on the particular parametrization of the hypotheses

Note that the test does only depend on the two sub-spaces Ω_1 and Ω_0, but not on how the subspaces have been parametrized (the particular choice of basis, i.e. the design matrix). Therefore it is sometimes said that the test is *coordinate free*.

Initial test for model 'sufficiency'

- In practice, one often starts with formulating a rather comprehensive model, a *sufficient model*, and then tests whether the model may be reduced to the *null model* with $\Omega_{null} = \mathbb{R}$, i.e. $\dim \Omega_{null} = 1$.
- The hypotheses are

$$\mathcal{H}_{null} : \boldsymbol{\mu} \in \mathbb{R}$$

$$\mathcal{H}_1 : \boldsymbol{\mu} \in \Omega_1 \setminus \mathbb{R}.$$

  where $\dim \Omega_1 = k$.

- The hypothesis is a hypothesis of "Total homogeneity", namely that all observations are satisfactorily represented by their common mean.

Deviance table

Source	f	Deviance	Test statistic, F
Model $\mathcal{H}_{null}$	$k-1$	$\|\|p_1(\boldsymbol{y}) - p_{null}(\boldsymbol{y})\|\|^2$	$\frac{\|\|p_1(\boldsymbol{y}) - p_{null}(\boldsymbol{y})\|\|^2/(k-1)}{\|\|\boldsymbol{y} - p_1(\boldsymbol{y})\|\|^2/(n-k)}$
Residual under $\mathcal{H}_1$	$n-k$	$\|\|\boldsymbol{y} - p_1(\boldsymbol{y})\|\|^2$	
Total	$n-1$	$\|\|\boldsymbol{y} - p_{null}(\boldsymbol{y})\|\|^2$	

Table: Deviance table corresponding to the test for model reduction to the null model.

Under $\mathcal{H}_{null}$, $F \sim F(k-1, n-k)$, and hence large values of F would indicate rejection of the hypothesis $\mathcal{H}_{null}$. The p-value of the test is $p = P[F(k-1, n-k) \geq F_{obs}]$.

Overview

Coefficient of determination, R^2

- The *coefficient of determination*, R^2, is defined as

$$R^2 = \frac{\mathrm{D}(p_1(\boldsymbol{y}); p_{null}(\boldsymbol{y}))}{\mathrm{D}(\boldsymbol{y}; p_{null}(\boldsymbol{y}))} = 1 - \frac{\mathrm{D}(\boldsymbol{y}; p_1(\boldsymbol{y}))}{\mathrm{D}(\boldsymbol{y}; p_{null}(\boldsymbol{y}))}, \quad 0 \leq R^2 \leq 1.$$

- Suppose you want to predict Y. If you do not know the x's, then the best prediction is $\overline{y}$. The variability corresponding to this prediction is expressed by the *total variation*.
- If the model is utilized for the prediction, then the prediction error is reduced to the *residual variation*.
- R^2 expresses the fraction of the total variation that is explained by the model.
- As more variables are added to the model, $\mathrm{D}(\boldsymbol{y}; p_1(\boldsymbol{y}))$ will decrease, and R^2 will increase.

Adjusted coefficient of determination, R^2_{adj}

- The *adjusted coefficient of determination* aims to correct that R^2 increases as more variables are added to the model.
- It is defined as:

$$R^2_{adj} = 1 - \frac{\mathrm{D}(\boldsymbol{y}; p_1(\boldsymbol{y}))/(n-k)}{\mathrm{D}(\boldsymbol{y}; p_{null}(\boldsymbol{y}))/(n-1)}.$$

- It charges a penalty for the number of variables in the model.
- As more variables are added to the model, $\mathrm{D}(\boldsymbol{y}; p_1(\boldsymbol{y}))$ decreases, but the corresponding degrees of freedom also decreases.
- The numerator in may increase if the reduction in the residual deviance caused by the additional variables does not compensate for the loss in the degrees of freedom.

Overview

Proof (and more) of th. 3.5

We consider the model

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}; \quad \boldsymbol{\epsilon} \sim N(\boldsymbol{0}, \sigma^2\boldsymbol{\Sigma}) \tag{1}$$

The estimate of $\boldsymbol{\beta}$ is

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{Y} \tag{2}$$

hence the expected value of $\boldsymbol{Y}$ can be written as

$$\hat{\boldsymbol{Y}} = \boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{Y} = \boldsymbol{H}_y\boldsymbol{Y} \tag{3}$$

If $\boldsymbol{\Sigma} = \boldsymbol{I}$ then $\boldsymbol{H}_y$ is a projection matrix and the proof can be based on properties of projection matrices. However in the general case $\boldsymbol{H}_y$ is not a projection matrix.

Recal that a matrix $\boldsymbol{H}$ is a projection matrix iff

$$\boldsymbol{H} = \boldsymbol{H}^T; \quad \boldsymbol{H}^2 = \boldsymbol{H} \tag{4}$$

Now

$$\begin{aligned}
\boldsymbol{H}_y^T =& (\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1})^T && (5)\\
=& ((\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1})^T\boldsymbol{X}^T && (6)\\
=& (\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1})^T(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T && (7)\\
=& \boldsymbol{\Sigma}^{-1}\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T \neq \boldsymbol{H}_y && (8)
\end{aligned}$$

Hence $\boldsymbol{H}_y$ is not a projection matrix.

Now consider the (non unique) "square root" ($\boldsymbol{T}$) of $\boldsymbol{\Sigma} = \boldsymbol{T}\boldsymbol{T}^T$ (since $\boldsymbol{\Sigma}$ is a variance covariance matrix this square root exist).

$$\boldsymbol{Y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{T}\boldsymbol{e}; \quad \boldsymbol{e} \sim N(\boldsymbol{0}, \sigma^2 \boldsymbol{I}) \tag{9}$$

Since $V(\boldsymbol{T}\boldsymbol{e}) = \sigma^2\boldsymbol{\Sigma}$ we have $\boldsymbol{T}\boldsymbol{e} \sim N(\boldsymbol{0}, \sigma^2\boldsymbol{\Sigma})$.
Now we can rewrite this as ($\boldsymbol{Z} = \boldsymbol{T}^{-1}\boldsymbol{Y}$)

$$\boldsymbol{Z} = \boldsymbol{T}^{-1}\boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{e}; \quad \boldsymbol{e} \sim N(\boldsymbol{0}, \sigma^2 \boldsymbol{I}) \tag{10}$$

The resulting estimate $\tilde{\boldsymbol{\beta}}$ is (we use the short hand notation $\boldsymbol{T}^{-T} = (\boldsymbol{T}^{-1})^T$)

$$\begin{aligned}
\tilde{\boldsymbol{\beta}} =& (\boldsymbol{X}^T\boldsymbol{T}^{-T}\boldsymbol{T}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{T}^{-T}\boldsymbol{Z} && (11)\\
=& (\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{T}^{-T}\boldsymbol{T}^{-1}\boldsymbol{Y} && (12)\\
=& (\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{Y} && (13)\\
=& \hat{\boldsymbol{\beta}} && (14)
\end{aligned}$$

The expected value of $\boldsymbol{Z}$ is

$$\hat{\boldsymbol{Z}} = \boldsymbol{T}^{-1}\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{T}^{-T}\boldsymbol{Z} \tag{15}$$

$$= \boldsymbol{H}_z\boldsymbol{Z} \tag{16}$$

The matrix $\boldsymbol{H}_z$ is a projection matrix

$$\boldsymbol{H}_z^T = (\boldsymbol{T}^{-1}\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{T}^{-T})^T \tag{17}$$

$$= (\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{T}^{-T})^T\boldsymbol{T}^{-T} \tag{18}$$

$$= \boldsymbol{T}^{-1}\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{T}^{-T} = \boldsymbol{H}_z \tag{19}$$

$$\boldsymbol{H}_z^2 = \boldsymbol{T}^{-1}\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{T}^{-T}\boldsymbol{T}^{-1}\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{T}^{-T} \tag{20}$$

$$= \boldsymbol{T}^{-1}\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{T}^{-T} \tag{21}$$

$$= \boldsymbol{T}^{-1}\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{T}^{-T} = \boldsymbol{H}_z \tag{22}$$

Hence $\boldsymbol{H}_z$ is a projection matrix.

Note that since $\boldsymbol{H}_z$ is a projection matrix then $\boldsymbol{I} - \boldsymbol{H}_z$ is also a projection matrix. The expected value of SSE_z is

$$E[SSE_z] = E[\boldsymbol{Z}^T(\boldsymbol{I} - \boldsymbol{H}_z)\boldsymbol{Z}] \tag{23}$$

Using prop. 3.22 of Bingham and Fry (2010), we can rewrite

$$\begin{aligned} E[SSE_z] =& Tr((\boldsymbol{I} - \boldsymbol{H}_z)V[\boldsymbol{Z}]) + E[\boldsymbol{Z}^T](\boldsymbol{I} - \boldsymbol{H}_z)E[\boldsymbol{Z}] && (24)\\ =& \sigma^2 Tr(\boldsymbol{I} - \boldsymbol{H}_z) + E[\boldsymbol{Z}^T](\boldsymbol{I} - \boldsymbol{H}_z)E[\boldsymbol{Z}] && (25) \end{aligned}$$

Take it piece by piece

$$\begin{aligned} E[\boldsymbol{Z}^T](\boldsymbol{I} - \boldsymbol{H}_z) =& \boldsymbol{\beta}^T \boldsymbol{X}^T \boldsymbol{T}^{-T}(\boldsymbol{I} - \boldsymbol{T}^{-1}\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{T}^{-T}) && (26)\\ =& \boldsymbol{\beta}^T(\boldsymbol{X}^T\boldsymbol{T}^{-T} - \boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{T}^{-T}) && (27)\\ =& \boldsymbol{\beta}^T\boldsymbol{0} = \boldsymbol{0} && (28) \end{aligned}$$

Hence

$$E[SSE_z] = \sigma^2(n - Tr(\boldsymbol{H}_z)) \tag{29}$$

The second piece

$$\begin{aligned} Tr(\boldsymbol{H}_z) =& Tr(\boldsymbol{T}^{-1}\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{T}^{-T}) && (30)\\ =& Tr(\boldsymbol{X}(\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{T}^{-T}\boldsymbol{T}^{-1}) && (31)\\ =& Tr((\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{\Sigma}^{-1}\boldsymbol{X}) && (32)\\ =& Tr(\boldsymbol{I}_p) = p && (33) \end{aligned}$$

With $\boldsymbol{X} \in \mathbb{R}^{n\times p}$. Hence

$$E[SSE_z] = \sigma^2(n-p) \quad (34)$$

Also

$$\begin{aligned} SSE_z =& (\boldsymbol{T}^{-1}\boldsymbol{Y} - \boldsymbol{T}^{-1}\boldsymbol{X}\hat{\boldsymbol{\beta}})^T(\boldsymbol{T}^{-1}\boldsymbol{Y} - \boldsymbol{T}^{-1}\boldsymbol{X}\hat{\boldsymbol{\beta}}) && (35)\\ =& (\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})^T\boldsymbol{T}^{-T}\boldsymbol{T}^{-1}(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}}) && (36)\\ =& (\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})^T\boldsymbol{\Sigma}^{-1}(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}}) && (37)\\ =& SSE_y && (38) \end{aligned}$$

Hence an unbiased estimator for σ^2 is

$$\hat{\sigma}^2 = \frac{SSE_z}{n-p} \tag{39}$$

$$= \frac{SSE_y}{n-p} \tag{40}$$

$$= \frac{(\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{Y} - \boldsymbol{X}\hat{\boldsymbol{\beta}})}{n-p} \tag{41}$$

Note also that the distribution ($\sigma^2 \chi^2_{n-p}$) of $\hat{\sigma}^2$ follows directly from SSE_z