Part II — Statistical Modelling

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Notes taken by Joseph Tedds using Dexter Chua's header and Gilles Castel's snippets.

Michaelmas 2019

Introduction to the statistical programming language R
Graphical summaries of data, e.g. histograms. Matrix computations. Writing simple functions. Simulation. [2]

Linear Models
Review of least squares and linear models. Characterisation of estimated coefficients, hypothesis tests and confidence regions. Prediction intervals. Model selection. BoxCox transformation. Leverages, residuals, qq-plots, multiple $\mathbb{R}^2$ and Cooks distances. [5]

Overview of basic inferential techniques
Asymptotic distribution of the maximum likelihood estimator. Approximate confidence regions. Wilks theorem. The delta method. Posterior distributions and credible intervals. [3]

Exponential dispersion families and generalised linear models (glm)
Exponential families and meanvariance relationship. Dispersion parameter and generalised linear models. Canonical link function. Iterative solution of likelihood equations. Regression for binomial data; use of logit and other link functions. Poisson regression models, and their surrogate use for multinomial data. Application to 2- and 3-way contingency tables. Hypothesis tests and model selection, including deviance and Akaikes Information Criterion. Residuals and model checking. [8]

Examples in R
Linear and generalised linear models. Interpretation of models, inference and model selection. [6]

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0 Introduction

This course is unusual in that 8 of the lectures are taken as practicals, with the following guidance.

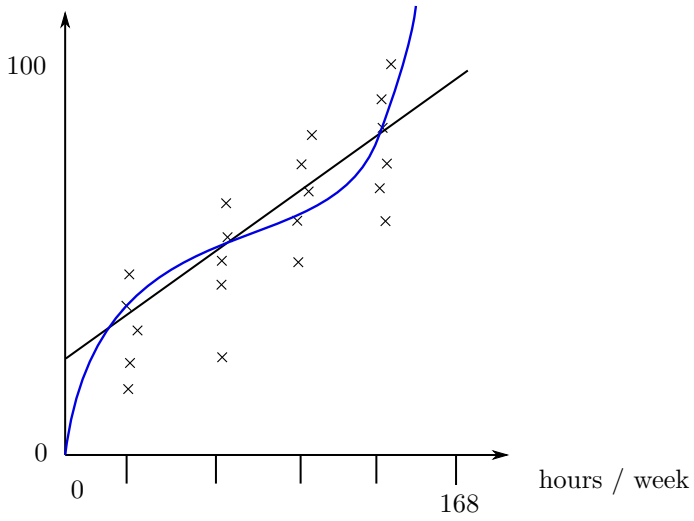
- Ideally use Linux, some things may not work on other operating systems
- Use R and R Studio

We study Data:

- $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n), i = 1, \ldots, n$, $n =$ sample size.
- $\mathbf{x}_i = (x_{i1}, \ldots, x_{ip})^T$ - predictors, covariates , independent or explanatory variables.
- y_i - targets, responses, dependent variables.

Objective: understand the functional relationship relating the y_i's to the $\mathbf{x}_i$'s to develop a regression function.

Example. $x_i =$ number of hours / week student i invests in on statistical modelling, $y_i =$ final grade of student i.



In the next section we model the Y's (note they are now upper-case) as random variables, as $Y_i = f(x_i, \theta) + \varepsilon_i$ independent.

- f is linear in θ
- $\varepsilon_i \approx$ errors / noise with potential causes as measurement errors or our limited understanding of the world.
- $\mathbb{E}[Y_i \mid X_i] = f(x_i, \theta) + \mathbb{E}[\varepsilon_i \mid x_i]$

In the sections thereafter, $\mathbb{E}[Y_i \mid x_i] = f_i(x_i, \theta)$, f_i is not necessarily linear in θ.

Warning. A word of caution, statistical models are not a perfect representation of the world, but they are useful approximations to make decisions.

1 Linear Models

1.1 Ordinary least squares (OLS)

Consider the linear regression model $Y = X\beta + \epsilon$,

$$Y = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix} \in \mathbb{R}^n, X = \begin{pmatrix} x_1^T \\ \vdots \\ x_n^T \end{pmatrix} \in \mathbb{R}^{n \times p}, \beta = \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_n \end{pmatrix} \in \mathbb{R}^p, \epsilon = \begin{pmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{pmatrix} \in \mathbb{R}^n.$$

where

(i) $\mathbb{E}[\epsilon_i] = 0$ - does not mean unbiased, but centred

(ii) $\operatorname{var} \epsilon_i = 0$ - homoskedastic

(iii) $\operatorname{cov}(\epsilon_i, \epsilon_j) = 0$ - uncorrelated = linear independence $\neq$ independence

Definition (Design matrix)**.** The design matrix X, unless otherwise stated : $p \leq n$, and $\mathbf{X}$ is full rank i.e. rank $X = p$.

Note, $\theta = \beta$ in the introduction. If we want intercept,

$$X = \begin{pmatrix} 1 & x_1^T \\ \vdots & \vdots \\ 1 & x_n^T \end{pmatrix}, \theta = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \in \mathbb{R}^{p+1}$$

.
If we want higher order terms e.g. quadratic

$$X = \begin{pmatrix} 1 & x_1^T & x_{11}^2 & \cdots & x_{1p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n^T & x_{n1}^2 & \cdots & x_{np}^2 \end{pmatrix}, \theta = \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} \in \mathbb{R}^{2p+1}.$$

Remember, linear means linear in θ

Definition (Least squares)**.** The *least squares estimator*, $\hat{\beta}$ is defined as

$$\hat{\beta} = \underset{\mathbf{b} \in \mathbb{R}^n}{\operatorname{argmin}} \|Y - X\mathbf{b}\|^2.$$

On the example sheet, we will show that $\hat{\beta} = (X^T X^{-1}) X^T Y$

The fitted values are given by

$$\hat{Y} = X\hat{\beta} = \overbrace{X(X^T X^{-1}) X^T}^{P} Y = PY.$$

We call P the 'hat' matrix and it is an orthogonal projection onto the column space of X.

1.2 Orthogonal projection

Let $V \subseteq \mathbb{R}^n$ be linear. Its orthogonal complement is

$$V^\perp = \{\omega \in \mathbb{R}^n : \omega^T \cdot \mathbf{v} = 0 \ \forall \ \mathbf{v} \in V\}.$$

Fact. (i) $\mathbb{R} \cong V \oplus V^\perp$, so $\forall\ \mathbf{u} \in \mathbb{R}^n\ \exists\ \mathbf{v} \in V, \omega \in V^\perp$ such that $\mathbf{u} = \mathbf{v} + \mathbf{w}$

(ii) $(V^\perp)^\perp = V$

Definition (Orthogonal projection)**.** $\pi \in \mathbb{R}^{n\times n}$ is an *orthogonal projection* onto V if $\pi\mathbf{u} = \mathbf{v}$ whenever $\mathbf{u} = \mathbf{v} + \mathbf{w}, \mathbf{v} \in V, \mathbf{w} \in V^\perp$. π is an orthogonal projection if it is an orthogonal projection onto its column space.

Let π be an orthogonal projection onto V, properties

(i) The column space /range / image/ span of π is V (immediate from the fact above and the definition) so rank $\pi = \dim V$.

(ii) $I - \pi$ is an orthogonal projection onto $V^\perp$. Let $\mathbf{u} = \mathbf{v} + \mathbf{w}, \mathbf{v} \in V, \mathbf{w} \in v^\perp$,

$$(I - \pi)\mathbf{u} = \mathbf{0} + \mathbf{w}.$$

(iii) π is idempotent ($\pi^2 = \pi$) and π is symmetric ($\pi^T = \pi$). The former is by definition, the latter

$$\forall\ \mathbf{u}_1, \mathbf{u}_2 \in \mathbb{R}^n, (\pi\mathbf{u}_1)^T(I - \pi)\mathbf{u}_2 = \begin{cases} 0 \\ \mathbf{u}_1^T((\pi^T - \pi^T\pi)\mathbf{u}_2 \end{cases}.$$

$$\pi^T = \pi^T\pi \iff \pi i = \pi^T\pi = \pi^T.$$

In fact $\pi^2 = \pi = \pi^T$ is an alternative definition for an orthogonal projection. Let $\mathbf{v} \in$ span π.

$$\exists\ \mathbf{u} \in \mathbb{R}^n \pi\mathbf{u} = \mathbf{v} \implies \pi\mathbf{v} = \pi^2\mathbf{u} = \pi\mathbf{u} = \mathbf{v}.$$

Let $\mathbf{v} \in (\text{span } \pi)^\perp$,

$$\pi\mathbf{v} = \pi^T\mathbf{v} = 0.$$

(iv) Orthogonal bases of V and $V^\perp$ are eigenvectors π with eigenvalues 1 or 0. Thus, $\pi = \mathbf{u}D\mathbf{u}^T, \mathbf{u}$ orthonormal ($\mathbf{u}^T\mathbf{u} = \mathbf{u}\mathbf{u}^T = I$), D is diagonal matrix with 1's and 0's

1.3 Analysis of OLS

Recall

$$\hat{\beta} = \arg\min_{\mathbf{b}\in\mathbb{R}^p} \|Y - X\mathbf{b}\|^2 = \left(X^TX\right)^{-1} X^TY.$$

and $\hat{Y} = X\hat{\beta} = PY$

$$PX\mathbf{b} = X(X^TX)^{-1}X^TX\mathbf{b} = X\mathbf{b}.$$

If $w \in (\text{span } \pi)^\perp$

$$Pw = X\left(X^TX\right)^{-1}\underbrace{X^T\mathbf{w}}_{\mathbf{0}} = \mathbf{0}.$$

P is an orthogonal projection onto span X, $\hat{Y}$ is a projection of Y onto span X.

The reverse is true: if π is an orthogonal projection onto V, then

$$\pi\mathbf{u} = \arg\min_{\mathbf{v}\in V}\|\mathbf{u}-\mathbf{v}\|^2 \ \forall\ \mathbf{u}\in\mathbb{R}^n.$$

$\hat{\beta}$ is the vector of coefficients of the closest vector in span X to Y as a linear combination of the columns of X Alternative representation of OLS:
Let $X_j = (X_{\cdot j}), X_{-j}$ is X without X_j, $P_{-j} = X_{-j}\left(X_{-j}^T X_{-j}\right)^{-1} X_{-j}^T$

Proposition. Let $X_j^\perp = (I - P_{-j})X_j$. Then

$$\hat{\beta}_j = \frac{\left(X_j^\perp\right)^T Y}{\|X_j^\perp\|^2}.$$

Proof.

$$\begin{aligned}
\left(X_j^\perp\right)^T Y &= X_j^T(I-P_{-j})Y \\
&= X_j^T(I-P_{-j})(PY+(I-P)Y) \\
&= X_j^T(I-P_{-j})PY + X_j^T \underbrace{X_j^T(I-P_{-j})(I-P)Y}_{X_j^T(I-P)Y=0} \\
&= X_j^T(I-P_{-j})PY
\end{aligned}$$

With the reduction of the second term coming from $V_{-k}^\perp \subseteqq V^\perp$

$$\begin{aligned}
\left(X_j^\perp\right)^T &= X_j^T(I-P_{-j})X \\
&= X_j^T \begin{pmatrix} 0 & \cdots & 0 & \underset{j^{\text{th}}\text{ element}}{(I-P_{-j})} & 0\cdots & 0 \end{pmatrix} \\
&= \begin{pmatrix} 0 & \cdots & 0 & X_j^T(I-P_{-j})^2X_j & 0 & \cdots & 0 \end{pmatrix} \\
&= \begin{pmatrix} 0 & \cdots & 0 & \|X_j^\perp\|^2 & 0 & \cdots & 0 \end{pmatrix}
\end{aligned}$$

Hence

$$\left(X_j^\perp\right)^T Y = \left(X_j^\perp\right)^T X\hat{\beta} = \begin{pmatrix} 0 & \cdots & 0 & \|X_j^\perp\|^2\beta_j & 0 & \cdots & 0 \end{pmatrix}.$$

□

Recall if $\mathbf{z}_i \in \mathbb{R}^{n_i}, i = 1, 2$

$$\operatorname{cov}(\mathbf{z}_1,\mathbf{z}_2) = \mathbb{E}\left[(\mathbf{z}_1 - \mathbb{E}[\mathbf{z}_1])(\mathbf{z}_2 - \mathbb{E}[\mathbf{z}_2]\right].$$

$$(\operatorname{cov}(\mathbf{z}_1,\mathbf{z}_2))_{ij} = \frac{\operatorname{cov}(\mathbf{z}_1,\mathbf{z}_2)_{ij}}{\sqrt{(\operatorname{var}\mathbf{z}_1)_{ii}(\operatorname{var}\mathbf{z}_2)_{jj}}}.$$

$$\forall\ \mathbf{a}_i\in\mathbb{R}^{n_i},\quad \operatorname{cov}(\mathbf{z}_1+\mathbf{a}_1,\mathbf{z}_2+\mathbf{a}_2) = \operatorname{cov}(\mathbf{z}_1,\mathbf{z}_2).$$

and if $A\in\mathbb{R}^{d\times n}, b\in\mathbb{R}^d$

$$\mathbb{E}[\mathbf{b}+A\mathbf{z}_1] = \mathbf{b} + A\mathbb{E}[\mathbf{z}_1].$$

Then,

$$\begin{aligned}\operatorname{var}\hat{\beta}_j &= \frac{1}{\|X_j^{\perp}\|^4}\operatorname{var}\left(X_j^{\perp}\right)^T Y \\ &= \frac{1}{\|X_j^{\perp}\|^4}\operatorname{var}(X_j^{\perp})^T\varepsilon \\ &= \frac{1}{\|X_J^{\perp}\|^4}\left(X_j^{\perp}\right)^T \operatorname{var}\varepsilon\ X_j^{\perp} \\ &= \frac{\sigma^2}{\|X_j^{\perp}\|^2}\end{aligned}$$

.

Now, $\hat{\beta} \in \mathbb{R}^p$, $\hat{\beta}$ is unbiased. Indeed

$$\mathbb{E}_\beta\left[\hat{\beta}\right] = \mathbb{E}\left[(X^TX)^{-1}X^T(X\beta+\epsilon)\right] = \beta.$$

.

$$\begin{aligned}\operatorname{var}(\hat{\beta}) &= \operatorname{var}((X^TX)^{-1}XY) \\ &= \operatorname{var}((X^TX)^{-1}X^T\epsilon) \\ &= (X^TX)^{-1}X^T\underbrace{\operatorname{var}\epsilon}_{\sigma^2 I}X(X^TX)^{-1} \\ &= \sigma^2(X^TX)^{-1}\end{aligned}$$

.

This is optimal in the following sense.

Theorem (Gauss-Markov)**.** $\hat{\beta}$ is BLUE (Best Linear Unbiased Estimator) i.e. $\forall\ \tilde{\beta}$ linear (in Y) and unbiased estimator

$$\operatorname{var}\tilde{\beta} - \operatorname{var}\hat{\beta} \text{ is positive semidefinite.}$$

Proof. Let $\tilde{\beta} = CY = \hat{\beta} + \underbrace{(C-(X^TX)^{-1}X^T)}_{D}Y$. Note $\mathbb{E}_\beta\left[\tilde{\beta}\right] = \beta\ \forall\ \beta \in \mathbb{R}^p$, so

$$0 = DX\beta \implies DX = 0$$

as this is true $\forall\ \beta$. Then,

$$\operatorname{var}\tilde{\beta} = \operatorname{var}\hat{\beta} + \operatorname{var}DY + 2\operatorname{cov}(\hat{\beta}, DY).$$

$$\operatorname{var}DY = \operatorname{var}D\epsilon = \sigma^2 DD^T,$$

which is positive semi-definite by definition.

.

$$\begin{aligned}\operatorname{cov}(\hat{\beta}, DY) &= \operatorname{cov}((X^TX)^{-1}X^T\epsilon, D\epsilon) \\ &= (X^TX)^{-1}\underbrace{X^TD^t}_{=0}\sigma^2\end{aligned}$$

.

□

Consequently, if x^* is a new observation

Exercise.

$$\mathbb{E}\left[((x^*)^T\hat{\beta} - (x^*)^T\beta)^2\right] \leq \mathbb{E}\left[\left((x^*)^T\tilde{\beta} - (x^*)^T\beta\right)^2\right] \ \forall\ \tilde{\beta} \text{ LUE}.$$

We can also measure the quality of a regression procedure $\tilde{\beta}$ by its mean-squared prediction error:

$$\text{MSPE}(\tilde{\beta}) = \frac{1}{n}\mathbb{E}\left[\|X\tilde{\beta} - X\beta\|^2\right].$$

Proposition.

$$\text{MSPE}(\hat{\beta}) = \sigma^2\frac{p}{n}.$$

Proof. First note that

$$X\hat{\beta} = PY = X\beta + P\epsilon.$$

$$\|X\hat{\beta} - X\beta\|^2 = \|P\epsilon\|^2 = \epsilon^T P\epsilon^T = \text{Tr}(\epsilon^T P\epsilon) = \text{Tr}(P\epsilon^T\epsilon).$$

$$\begin{aligned}\mathbb{E}\left[\text{LHS}\right] &= \text{Tr}(P\mathbb{E}\left[\epsilon^T\epsilon\right] \\ &= \sigma^2\text{Tr}P \\ &= \sigma^2 p\end{aligned}$$

.

□

Lastly, $\hat{\epsilon} = Y - \hat{Y} = (I-P)Y$ is the vector of residuals. This satisfies

$$\begin{aligned}\text{cov}(\hat{\epsilon}, \hat{Y}) &= \text{cov}((I-P)\epsilon, P\epsilon) \\ &= \sigma^2 X(X^TX)^{-1}\underbrace{X^T(I-P)^T}_{=0} = 0\end{aligned}$$

.

So $\hat{\epsilon}$ and $\hat{Y}$ are uncorrelated.

1.4 Normal Errors

1.4.1 Multivariate normal and related distributions

Definition (Multivariate normal)**.** $Z \in \mathbb{R}^d$ is *multivariate normal* if $\forall\ t \in \mathbb{R}^d, t^TZ$ is univariate normal. Thus $\forall\ m \in \mathbb{R}^{k, A\in\mathbb{R}^{k\times d}}, m + AZ$ is (multivariate) normal.

Fact. Normal distributions are uniquely characterised by their mean and variance. So write

$$Z \sim N_d(\mu, \Sigma).$$

if $\mathbb{E}\left[Z\right] = \mu, \text{var}\, Z = \Sigma$

$$\implies m + Az \sim N_k(m + A\mu, A\epsilon A^T).$$

If Σ is invertible , Z has density

$$f(z;\mu,\Sigma) = \frac{1}{\sqrt{(2\pi)^n |\det\Sigma|}} \exp\left(-\frac{1}{2}(z-\mu)\Sigma^{-1}(z-\mu)\right) \ \forall\ z \in \mathbb{R}^d.$$

Proposition. Let Z_1, Z_2 be jointly normal (i.e. (Z_1, Z_2) is multivariate normal).

$$\operatorname{cov}(Z_1, Z_2) = 0 \iff Z_1, Z_2 \text{ are independent } (Z_1 \perp Z_2).$$

Proof. The backward direction is immediate.
In the other direction, let $Z_1' \overset{d}{Z_1}, Z_2' \overset{d}{=} Z_2$. Note

$$\mathbb{E}\left[(Z_1', Z_2')\right] = \left(\mathbb{E}\left[Z_1'\right], \mathbb{E}\left[Z_2'\right]\right) = \mathbb{E}\left[(Z_1, Z_2\right].$$

$$\operatorname{var}(Z_1', Z_2') = \begin{pmatrix} \operatorname{var} Z_1' & \operatorname{cov}(Z_1', Z_2') \\ \operatorname{cov}(Z_1', Z_2') & \operatorname{var} Z_2' \end{pmatrix} = \begin{pmatrix} \operatorname{var} Z_1 & 0 \\ 0 & \operatorname{var} Z_2 \end{pmatrix} = \operatorname{var}(Z_1, Z_2).$$

Also, (Z_1', Z_2') is normal because sums of independent normals is normal. Thus the conclusion follows by the fact above. □

Definition (χ^2 distribution)**.** $X \sim \chi^2_k$ (on k degrees of freedom), if

$$X \overset{d}{=} \sum_{j=1}^{k} Z_j^2, \quad Z_j \overset{\text{iid}}{\sim} N(0,1).$$

Proposition. Let $\pi \in \mathbb{R}^{n\times n}$ be an orthogonal projection with rank k and $\epsilon \sim N_n(0, \sigma^2 I)$. Then

$$\|\pi\epsilon\|^2 \sim \sigma^2 \chi^2_k.$$

Proof. Recall that $\pi = UDU^T$ and noting that $U^T\epsilon \sim N_n(0, \sigma^2 I)$. Then ,

$$\begin{aligned} \|\pi\epsilon\|^2 &= \epsilon^T UDU^T UDU^T \epsilon \\ &= \|Du^T\epsilon\|^2 \\ &\overset{d}{=} \|D\epsilon\|^2 \\ &= \sum_{j:D_{jj}=1} \epsilon_j^2 \\ &\overset{d}{=} \sigma^2 \sum_{j:D_{jj}=1} Z_j^2 \end{aligned}$$

.

□

Definition (t-student distribution)**.** $T \sim t_k$ (on k degrees of freedom) if

$$T \overset{d}{=} \frac{Z}{\sqrt{X/k}}, Z \sim N(0,1), X \sim X_k^2 \text{ independent.}$$

Definition (F distribution)**.** $F \sim F_{k,l}$ (on k, l degrees of freedom) if

$$F \overset{d}{=} \frac{X_1/k}{X_2/l}, X_1 \sim \chi^2_k, X_2 \sim \chi^2_l \text{ independent.}$$

1.4.2 Maximum likelihood estimation

Let $Y \in \mathbb{R}^n$ has density $f(\cdot, \theta), \theta \in \Theta \subseteq \mathbb{R}^p$ unknown (Θ paraneter space unknown). If data y is a realisation of Y, the likelihood function is

$$L(\theta) = f(y : \theta), \theta \in \Theta.$$

Then

$$\hat{\theta}_{\text{MLE}} = \arg\min_{\theta \in \Theta} L(\theta).$$

It is usually easier to work with the log-likelihood $\ell(\theta) = \log L(\theta)$. Many times we define them up to constants

Example. The t-statistic is given by

$$\frac{\hat{\beta} - \beta}{\sqrt{\text{var}(\hat{\beta})}}.$$

In the second practical we look at

$$\frac{\hat{\beta}_j}{\sqrt{\tilde{\sigma}^2 (X^T X)^{-1}_{jj}}} \sim t_{n-p}.$$

Where

$$\tilde{\sigma^2} = \frac{n}{n-p}\hat{\sigma}^2 = \frac{n}{n-p}\frac{1}{n}\|Y - X\hat{\beta}\|^2 = \frac{1}{n-p}\|(I-P)Y\|^2$$

and $\hat{\sigma}^2$ is the MLE for σ^2.

Assume that $\varepsilon_i \overset{\text{iid}}{\sim} N(0, \sigma^2)$ or $\varepsilon \sim N_n(0, \sigma^2)$. Then

$$Y = X\beta + \varepsilon \sim N_n(X\beta, \sigma^2 I)$$

and the likelihood is

$$L(\beta, \sigma^2) = \frac{1}{\sqrt{(2\pi)^n \sigma^{2n}}} \exp\left(\frac{1}{2\sigma^2}(\mathbf{y} - X\beta)^T(\mathbf{y} - X\beta)\right), \beta \in \mathbb{R}^p, \sigma^2 > 0.$$

Thus the log-likelihood (up to constants) is

$$\ell(\beta, \sigma^2) = -\frac{n}{2}\log\sigma^2 - \frac{1}{2}\sum_{i=1}^{n}\left(y_i - Xi^T\beta\right)^2.$$

It follows that

$$\hat{\beta}_{\text{MLE}} = \hat{\beta} = (X^T X)^{-1} X^T Y$$

and

$$\sigma^2_{\text{MLE}} = \frac{1}{n}\|Y - X\hat{\beta}\|^2 = \frac{1}{n}\|(I-P)Y\|^2.$$

Both estimators are intuitive under our model assumptions without $\varepsilon \sim N_n(0, \sigma^2 I)$ necessarily. However, the distributional assumptions on ε induce distributions on the estimators, which will allow us to perform inference.

1.4.3 Inference for the normal linear model

Distributions of $\hat{\beta}_{\text{MLE}}$ and $\hat{\sigma^2}_{\text{MLE}}$:
Note

$$\hat{\beta}_{\text{MLE}} = \beta + (X^T X)^{-1} X^T \varepsilon \sim N_p(\beta, \sigma^2 (X^T X)^{-1})$$

also

$$\hat{\sigma^2}_{MLE} = \frac{1}{n} \|(I - P)\varepsilon\|^2 \sim \frac{\sigma^2}{n} \chi^2_{n-p}.$$

In particular, $\mathbb{E}\left[\hat{\sigma^2}_{\text{MLE}}\right] = \frac{\sigma^2}{n}(n-p) \implies \hat{\sigma^2}_{\text{MLE}}$ is biased (but asymptotically unbiased). So let

$$\tilde{\sigma^2} = \frac{n}{n-p} \hat{\sigma^2}_{\text{MLE}} = \frac{1}{n-p} \|(I - P)Y\|^2 \sim \frac{\sigma^2}{n-p} \chi^2_{n-p}.$$

What can we say about their joint distribution? Recall that PY and $(I-P)Y$ are uncorrelated;

$$\begin{pmatrix} PY \\ (I-P)Y \end{pmatrix} = \begin{pmatrix} P \\ I - P \end{pmatrix} Y$$

is a linear transformation of Y (normal). Then we know by our earlier work that $PY \perp (I-P)Y$. Note $\hat{\beta} = (X^T X)^{-1} X^T PY \implies \hat{\beta} \perp \tilde{\sigma^2}$.
Inference for β :
Note that

$$\frac{\hat{\beta} - \beta}{\sqrt{\tilde{\sigma^2}}} = \frac{N_p(0, (X^T X)^{-1})}{\sqrt{\chi^2_{n-p}/(n-p)}},$$

with the numerator and denominator independent. This is a *pivot* i.e. id does not depend on the unknown parameters (β, σ^2) and hence can be used for inference.

Example.

$$C_j(\alpha) := \{b \in \mathbb{R} : \left| \frac{\hat{\beta}_j - b}{\sqrt{\tilde{\sigma^2}(X^T X)^{-1}_{jj}}} \right| \leq t_{n-p}(\frac{\alpha}{2})\} \quad j = 1. \ldots, p,$$

where if $T \sim t_{n-p}$, then

$$\mathbb{P}\left(-t_{n-p}(\frac{\alpha}{2}) \leq T \leq T_{n-p}(\frac{\alpha}{2})\right) = 1 - \alpha.$$

Since

$$\frac{\hat{\beta}_j - \beta}{\sqrt{\tilde{\sigma^2}(X^T X)^{-1}_{jj}}} \sim t_{n-p},$$

then $\mathbb{P}_{\beta,\sigma^2}(\beta_j \in C_j(\alpha)) = 1 - \alpha$. So $C_j(\alpha)$ is a $(1-\alpha)$-confidence interval for β_j. Note,

$$\prod_{j=1}^{p} C_j(\alpha)$$

is not a $(1-\alpha)$-confidence interval cuboid for β (too small). Though

$$\prod_{j=1}^{p} C_j(\frac{\alpha}{p})$$

has a confidence / coverage of $\geq 1-\alpha$. However, the latter is too large / conservative generally.

A smaller (and exact) alternative. Consider

$$\|X(\hat{\beta}-\beta\|^2 = \|P\varepsilon\|^2 \sim \sigma^2\chi^2_p$$

independent of $\tilde{\sigma^2}$. Let

$$C(\alpha) = \{\mathbf{b} \in R^p : \frac{\|X(\hat{\beta}-\beta\|^2}{\tilde{\sigma^2}} \leq F_{p,n-p}(\alpha)\}.$$

If $F \sim F_{p,n-p}$, then $\mathbb{P}(F \leq F_{p,n-p}(\alpha)) = 1-\alpha$. Then $\mathbb{P}_{\beta,\sigma^2}(\beta \in C(\alpha)) = 1-\alpha$. Note, the same arguments allows us to construct hypotheses tests.

Example. We can test $H_0 : \beta_j = \beta_{j,0}$ v.s. $H_1 : \beta_j \neq \beta_{j,0}$ with

$$\phi_j = 1\{\beta_{j,0} \notin C_j(\alpha)\}.$$

We can also test $H_0 : \beta = \beta_0$ v.s. $\beta \neq \beta_0$ with

$$\phi = 1\{\beta_0 \notin C(\alpha)\}.$$

Prediction Intervals:
Let $\mathbf{x}^*$ be a new observation. Note

$$\mathbf{x}^{*T}(\hat{\beta}-\beta) = \mathbf{x}^{*T}(X^TX)^{-1}X^T \sim N\left(0, \mathbf{x}^{*T}(X^TX)^{-1}\mathbf{x}^*\right),$$

and

$$\frac{\mathbf{x}^{*T}(\hat{\beta}-\beta)}{\sqrt{\tilde{\sigma^2}\mathbf{x}^{*T}(X^TX)^{-1}\mathbf{x}^*}} \sim t_{n-p}$$

can be used to perform inference for the regression function at $\mathbf{x}^*$ i.e. $x^{*T}\beta$. Let $Y^* = x^*\beta + \varepsilon^*, \varepsilon \sim N(0,\sigma^2)$ is independent of ε. We can also construct a $(1-\alpha)$-prediction interval for Y^* i.e. a random interval I depending only on Y such that $\mathbb{P}(Y^* \in I) = 1-\alpha$. Indeed,

$$Y^* - X^{*T}\hat{\beta} = \varepsilon^* + x^{*T}(\beta-\hat{\beta}) \sim N(0, \sigma^2(1+x^{*T}(X^TX)^{-1}X^*)).$$

So we can use the pivot

$$\frac{Y^* - X^{*T}\beta}{\sqrt{\tilde{\sigma}^2(1+x^{*T}(X^TX)^{-1}x^*)}} \sim t_{n-p}.$$

Note that the confidence intervals for Y^* will be larger than those for $x^{*T}\beta$ because of the additional variability / uncertainty coming from ϵ^*.

1.4.4 Testing significance of groups of variables

Let

$$X = (X_0.X_1), \beta = \begin{pmatrix}\beta_0\\ \beta_1\end{pmatrix}, X_0 \in \mathbb{R}^{n\times p_0}, X_1 \in \mathbb{R}^{n\times(p-p_0)}, \beta_0 \in \mathbb{R}^{p_0}, \beta_1 \in \mathbb{R}^{p-p_0}.$$

Without loss of generality, we wish to test $H_0 : \beta_1 = 0$ v.s. $H_1 : \beta_1 \neq 0$. We can construct a generalised likelihood ratio test : recall if Y has density $f(y, \theta), \theta \in \Theta$ unknown, the likelihood ratio test for $H_0 : \theta \in \Theta_0$ vs $H_1 : \theta \notin \Theta_0$, where $\Theta_0 \subseteq \Theta$ reject H_0 for large values of

$$\omega_{LR} := 2 \log \frac{\sup_{\theta' \in \Theta} L(\theta')}{\sup_{\theta' \in \Theta_0} L(\theta')} = 2(\sup_{\theta' \in \Theta} \ell(\theta') - \sup_{\theta' \in \Theta_0} \ell(\theta').$$

Notation. Write $\check{\beta}_0$ and $\check{\sigma}^2$ for the MLEs under the null i.e. $Y = X_0\beta_0 + \varepsilon$

$$\varepsilon \sim N_n(0, \sigma^2 I), \text{ so } \check{\beta}_0 = (X_0^T X_0)^{-1} X_0^T Y, \check{\sigma}^2 = \frac{1}{n}\|Y - X_0\check{\beta}_0\|^2.$$

Then

$$\omega_{LR} = 2(-\frac{n}{2}\log\hat{\sigma}^2 - \frac{1}{2\hat{\sigma}^2}\|Y - X\hat{\beta}^2\| + \frac{n}{2}\log\check{\sigma}^2 + \frac{1}{2\check{\sigma}^2}\|Y - X_0\check{\beta}_0\|^2 = n\log(\|(I-P_0)Y\|^2/\|(I-P)Y\|^2).$$

Note $I - P_0 = I - P + P - P_0$ and $PP_0 = P_0$

$$(I - P)(P - P_0) = 0 \implies \|(I - P_0)Y\|^2 = \|(I - P)Y\|^2 + \|(P - P_0)Y\|^2$$

and

$$\frac{\|(I - P_0)Y\|^2}{\|(I - P)Y\|^2} = 1 + \frac{\|(P - P_0)\varepsilon\|^2}{\|(I - P)\varepsilon\|^2}.$$

We claim that $P - P_0$ is an orthogonal projection. Indeed, $P - P_0$ is symmetric and by $P_0P = P_0^T P = (PP_0)^T = P_0^T = P_0$, so

$$(P - P_0)^2 = P - PP_0 - P_0P + P_0 = P - P_0.$$

Also note that if π is an orthogonal projection, then $\text{rank}\pi = \text{tr}\pi$ so,

$$\text{rank}(P - P_0) = \text{tr}(P - P_0) = \text{tr}P - \text{tr}P_0 = \text{rank}P - \text{rank}P_0 = p - p_0$$

and we conclude that $\|(P - P_0)\varepsilon\|^2 \sim \sigma^2\chi^2_{p-p_0}$. Note

$$\text{cov}((I - P)\varepsilon, (P - P_0)\varepsilon) = \sigma^2(I - P)(P - P_0) = 0$$

and

$$\begin{pmatrix} (I - P)\varepsilon \\ (P - P_0)\varepsilon \end{pmatrix}$$

is a linear transformation of ε (normal) so $(I - P)\varepsilon \perp (P - P_0)\varepsilon$. So we take the test

$$\phi = 1\{\frac{\|(P - P_0)Y\|^2/(p - p_0)}{\|(I - P)Y\|^2}/(n - p) \geq F_{p-p_0,n-p}(\alpha)\}.$$

This test has a significance level of α.

1.4.5 Model checking

The validity of our inferential conclusions depends on our assumptions about the distribution of ε being correct. If any of them fail we have the following remarks:

Remark. (i) $\mathbb{E}[\varepsilon_i] = 0$. If not, the coefficients in the linear model should be interpreted with care ($Y = X\beta + \mu + (\varepsilon - \mu)$), $\tilde{\sigma}^2$ is inflated, F-tests will have the correct size (example sheet) but they may lose power.

(ii) $\operatorname{var}\varepsilon_i = \sigma^2$. If not, $\hat{\beta}$ is not as efficient as it could be, and confidence sets and hypothesis test levels may not be correct. If the variance are known up to a multiplicative constant, then do weighted least squares (ex sheet).

(iii) $\operatorname{cov}(\varepsilon_i, \varepsilon_j) = 0 \ \forall \ i, j$. This usually occurs with temporal / spatial data, confidence sets and levels may be wrong.

(iv) ε is normal. If the first assumptions hold, then the inferential procedures hold asymptotically thanks to the central limit theorem.

Any violation of the above may be checked by looking at

$$\hat{\epsilon} = Y - X\hat{\beta} = (I - P)Y.$$

To check $\mathbb{E}[\varepsilon_i] = 0$ plot $\hat{\varepsilon}$ against $\hat{Y}$ (and sometimes v.s. the covariance), if the assumption holds we should expect to see no trends.
To check $\operatorname{var}\varepsilon_i$ (and $\operatorname{cov}(\varepsilon_i, \varepsilon_j)$) note that $\operatorname{var}\hat{\varepsilon} = \sigma^2(I - P)$ so define the studentised residuals

$$\hat{\eta}_i = \frac{\hat{\varepsilon}_i}{\tilde{\sigma}\sqrt{1 - P_i}},$$

where $P_i = P_{ii}$ is the leverage of the ith observation. Note if $\tilde{\sigma} \leftrightarrow \tilde{\sigma}_{-i}$ (thet corrected MLE when excluding (x_i, Y_i). Then $\hat{\eta}_i \sim t_{n-1-p}$. Note: if $\hat{\varepsilon}_i \neq 0$ a.s., $p_i \neq 1$. Also, assume $n \gg p \implies \tilde{\sigma} \approx \sigma$ with low deviation and $\operatorname{var}(\hat{\eta}_i) \approx 1$. Thus, plot $\sqrt{(\hat{\eta}_i)}$ vs $\hat{Y}$ ($|\cdot|$ avoids the 2-sidedness ; $\sqrt{\cdot}$ brings the studentised residuals closer to 1 if $\operatorname{var}(\hat{\eta}_i) \approx 1$). We expect a flat cloud of points around 1. Furthermore, under our model assumptions, $\hat{\eta}_i$ are approximately $\overset{\text{iid}}{\sim} N(0, 1)$. We check this with a Q-Q (Quantile-Quantile) plot.
Coefficients of determination Popular measure of goodness of fit of a model. It compares the residual sum of squares (RSS) of the model vs that of an intercept only model

$$R^2 = \frac{\|Y - \hat{Y}1_n\|^2 - \|(I - P)Y\|^2}{\|Y - \hat{Y}1_n\|^2}, 1_n = (1, 1, \ldots, 1)^T \in \mathbb{R}^n.$$

Note

$$R^2 = \frac{\operatorname{var}_n Y - \hat{\sigma}^2}{\operatorname{var}_n Y} \ \in [0, 1].$$

So R^2 is the proportion of the total variation of the data explained by the model. If we have a larger R^2 value, then we have a better fit, but it always grows whenever we add a new variable. The adjusted

$$\tilde{R}^2 = 1 - \frac{n - 1}{n - p}(1 - R^2).$$

Observation A few observations may not agree with our model assumptions i.e. outliers. So, we go back to the data, they could be very informative or we may have to exclude them.
Leverage $\hat{Y}_i = (PY)_i = \sum_{j=1}^n P_{ij}Y_j$ and $\text{var}(\hat{\varepsilon}_i) = \sigma^2(1-p_i), p_i = P_{ii}$ - the leverage of the ith observable . Thus p_i measures the contribution of Y_i to $\hat{Y}_i$. If $\pi \approx 1$, the model is forced to go through Y_i. It is possible that excluding such an observation does not change $\hat{\beta}$ much, but R^2 and F-tests with H_0 : intercept-only model may be highly affected therefore p_i is a measure of influence. Note $\sum_{i=1}^n p_i = \text{tr}(P) = p$ so our rule of thumb is that if $p_i > 3\frac{p}{n}$ then there is a concern that our ith observation is too influential.
Cook's Distance Defined as

$$D_i = \frac{\|X(\hat{\beta} - \hat{\beta}_{-i}\|^2/p}{\tilde{\sigma}^2},$$

where $\hat{\beta}_{-i}$ is the MLE when excluding (X_i, Y_i). Note

$$D_i = \frac{1}{p}\frac{P_i}{1-p_i}\hat{\eta}_i^2.$$

Recall that

$$\mathbb{P}\left(\frac{\|X(\hat{\beta}-\beta)\|^2/p}{\tilde{\sigma}^2} \leq F_{p,n-p}(\alpha)\right) = 1-\alpha.$$

So we get another rule of thumb, the ith observation's influence may be worrying if $D_i > F_{p,n-p}(0.5)$ i.e. removing (X_i, Y_i) pushes the MLE beyond a 50 confidence interval around $\hat{\beta}$.

2 Exponential families and generalised linear models

$$Y = \begin{pmatrix} Y_{11} \\ \vdots \\ Y_{1n_1} \\ Y_{21} \\ \vdots \\ Y_{2n_2} \\ \vdots \\ Y_{J1} \\ \vdots Y_{Jn_J} \end{pmatrix}, X = \begin{pmatrix} 1 & 0 & \cdots & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 1 & 0 & \cdots & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & 0 & \cdots & 0 \\ & & \vdots & & \\ 0 & \cdots & \cdots & 0 & 1 \\ \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & \cdots & \cdots & 0 & 1 \end{pmatrix} \beta = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_J \end{pmatrix}$$

3 Specific regression problems