Part II — Statistical Modelling

Based on lectures by A. J. Coca

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

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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]

Contents

0 Introduction

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

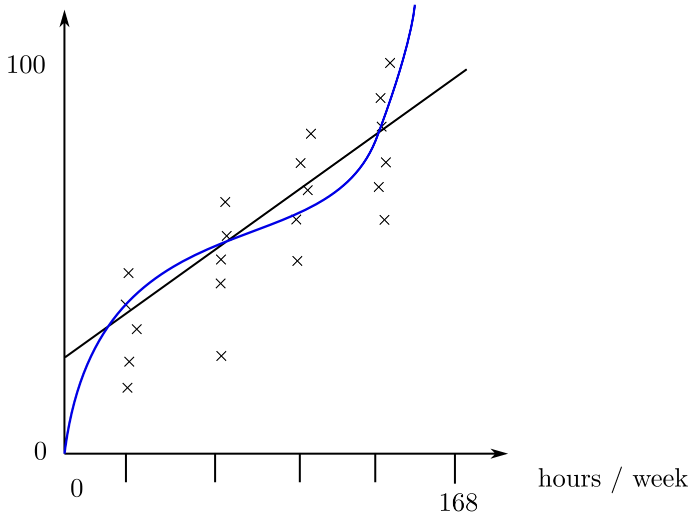
- Ideally use Linux, some things may not work on other operating systems
- Use R and R Studio

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 $V_{-k}^\perp \subseteqq V^\perp$

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

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

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

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

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

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

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

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

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

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

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

.

□

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

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

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 ,

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

.

□

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

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

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

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

2 Exponential families and generalised linear models

3 Specific regression problems