Regression Methods

Anthony Davison

http://stat.epfl.ch

1 The Linear Model slide 2

1.1 Introduction slide 3

Dictionary

- **Regression**: (statistics) a measure of the relation between the mean value of
  - one variable (e.g., output), denoted y (the **response variable**) and
  - corresponding values of other variables (e.g., time and cost), denoted x (**explanatory variables**).
- The explanatory variables are also called **covariates** or **features** (ML).
- We avoid the terms **dependent variable** (Y) and **independent variable** (x) used in older books.

- Questions we try and answer:
  - (**description/explanation**) how does y depend on x? How much of the variation of y is due to x? Do I need all of x to explain the variation in y?
  - (**prediction**) what will y be if $x = x_+$?
  - (**causation**) if I change x, what will happen to y?
- The causation question presupposes that we can change (some of) x, which is not always true.

Linear model

- Simplest explanation of y in terms of x is **linear model**:

$$y = g(x) = x_1\beta_1 + \cdots + x_p\beta_p = x^{\mathrm{T}}\beta,$$

where

$$y \in \mathbb{R}, \quad x^{\mathrm{T}} = (x_1, \ldots, x_p) \in \mathbb{R}^p, \quad \beta^{\mathrm{T}} = (\beta_1, \ldots, \beta_p) \in \mathbb{R}^p.$$

- The data consist of n **instances/examples/cases** (x_j, y_j) for $j = 1, \ldots, n$, so

$$y_{n\times 1} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}, \quad X_{n\times p} = \begin{pmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \vdots & \\ x_{n1} & \cdots & x_{np} \end{pmatrix}, \quad \beta_{p\times 1} = \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_p \end{pmatrix}$$

and we write

$$y = X\beta.$$

- **Key point**: linearity refers to linearity in β, not in terms of elements of X, which might be polynomials, or basis functions, or ...
- Sometimes we can transform to a linear model. For example, the multiplicative expression $y = \gamma x_1^{\beta_1} x_2^{\beta_2}$ becomes

$$\log y = \log\gamma + \beta_1 \log x_1 + \beta_2 \log x_2.$$

Notation

- ☐ Vectors are column vectors
- ☐ We write $X_{n\times p}$ to give the dimensions of a matrix or vector
- ☐ a^{T} (row vector) is the transpose of a (column vector)
- ☐ $j \in \{1, \ldots, n\}$ (or sometimes i) indexes the rows of y (cases/examples)
- ☐ x_j^{T} is the jth row of X
- ☐ $r, s, t, \ldots \in \{1, \ldots, p\}$ indexes the columns of X (covariates/features)
- ☐ Roman letters (y, X, z, ...) denote observed quantities, and may be the realisations of random variables
- ☐ Greek letters ($\beta, \gamma, \theta, \sigma, \ldots$) denote unknown (often vector) parameters of models
- ☐ $\widehat{\beta}$ denotes an estimate of β
- ☐ α denotes the level of significance tests and confidence intervals
- ☐ If Q is scalar (or a row vector) and β is a vector, then $\partial Q/\partial\beta$ denotes the vector (or matrix) the same shape as β with elements $\partial Q/\partial\beta_r$.
- ☐ If Q is scalar and β, γ are vectors, then $\partial^2 Q/\partial\beta\partial\gamma^{\mathrm{T}}$ denotes the matrix with (r, s) element $\partial^2 Q/\partial\beta_r\partial\gamma_s$.
- ☐ $u \perp v$ means that the vectors u and v are orthogonal (i.e., $u^{\mathrm{T}}v = 0$); ditto for matrices.
- ☐ $Y \perp\!\!\!\perp Z$ means that the random variables Y and Z are independent.

Useful matrix decompositions

- ☐ **Singular value decomposition (SVD)**: any real matrix X can be written in the form

$$X_{n\times p} = U_{n\times n} D_{n\times p} V^{\mathrm{T}}_{p\times p}$$

  where
  - $U = (u_1, \ldots, u_n)$ and $V = (v_1, \ldots, v_p)$ are orthogonal (i.e., $U^{\mathrm{T}}U = UU^{\mathrm{T}} = I_n$, $V^{\mathrm{T}}V = VV^{\mathrm{T}} = I_p$) and D is $n \times p$ rectangular diagonal with real diagonal entries (**singular values**) $d_1 \geq \cdots \geq d_m \geq 0$, where $m = \min(n, p)$,
  - if one or more $d_j = 0$, then X is singular, and
  - the u_j and v_r respectively span the column and row spaces of X.
- ☐ The SVD implies that the ranks of X, $X^{\mathrm{T}}X$ and XX^{T} are equal and at most m.
- ☐ **Spectral theorem**: any real symmetric matrix H can be written as

$$H_{n\times n} = U_{n\times n} D_{n\times n} U^{\mathrm{T}}_{n\times n},$$

  where
  - $D = \mathrm{diag}(d_1, \ldots, d_n)$ contains the eigenvalues of H;
  - U is an orthogonal matrix whose columns are the corresponding eigenvectors; and
  - if H is positive semi-definite then $d_1 \geq \cdots \geq d_n \geq 0$.

Least squares fit

- Assume that
$$y = X\beta$$
and find the 'best fit' by choosing β to minimise the (squared) Euclidean distance between y and $X\beta$, i.e., the sum of squares
$$\|y - X\beta\|^2 = (y - X\beta)^{\mathrm{T}}(y - X\beta) = \sum_{j=1}^{n}(y_j - x_j^{\mathrm{T}}\beta)^2.$$
- In vector space terms, $y \in \mathbb{R}^n$ and $X\beta \in \mathrm{span}(X) \subset \mathbb{R}^n$.
- The 'best fit' vector $\widehat{y}$ is the vector in $\mathrm{span}(X)$ closest to y; Pythagoras' theorem (sketch) gives $\widehat{y} \perp (y - \widehat{y})$ (but see below).
- We call $\widehat{y} \in \mathbb{R}^n$ the **fitted value(s)** and $e = y - \widehat{y} \in \mathbb{R}^n$ the **residual (vector)**.

Lemma 1 *When X has rank p and $n \geq p$ then $\widehat{y} = X\widehat{\beta} = Hy$, where*
$$\widehat{\beta} = (X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}y, \quad H = X(X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}.$$
The 'hat matrix' H has rank p, is symmetric and idempotent, and satisfies $HX = X$: it gives the orthogonal projection of $\mathbb{R}^n$ onto $\mathrm{span}(X)$.

Note to Lemma 1

- If X has rank p, so too does the $p \times p$ matrix $X^{\mathrm{T}}X$, which is therefore invertible.
- The sum of squares
$$Q = (y - X\beta)^{\mathrm{T}}(y - X\beta) = y^{\mathrm{T}}y - \beta^{\mathrm{T}}X^{\mathrm{T}}y - y^{\mathrm{T}}X\beta + \beta^{\mathrm{T}}X^{\mathrm{T}}X\beta = y^{\mathrm{T}}y - 2y^{\mathrm{T}}X\beta + \beta^{\mathrm{T}}X^{\mathrm{T}}X\beta$$
has first and second derivatives (respectively a $p \times 1$ vector and $p \times p$ matrix)
$$\frac{\partial Q}{\partial \beta} = -2X^{\mathrm{T}}y + 2X^{\mathrm{T}}X\beta, \quad \frac{\partial^2 Q}{\partial \beta \partial \beta^{\mathrm{T}}} = 2X^{\mathrm{T}}X$$
with respect to β. Setting $\partial Q/\partial\beta = 0$ implies that $(X^{\mathrm{T}}X)\beta = X^{\mathrm{T}}y$, and as $X^{\mathrm{T}}X$ is invertible we can write
$$\widehat{\beta} = (X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}y, \quad \widehat{y} = X\widehat{\beta} = X(X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}y = Hy,$$
say. The matrix $X^{\mathrm{T}}X$ is positive definite, so $(y - X\beta)^{\mathrm{T}}(y - X\beta)$ is minimised at $\widehat{\beta}$.
- The $n \times n$ 'hat matrix' H (which 'puts a hat' on y) satisfies $H^{\mathrm{T}} = H$, $H^2 = H$, so it is symmetric and idempotent, i.e., its eigenvalues equal 0 or 1, and their multiplicities must be $n - p$ and p, as its rank is p. H is the matrix that projects $\mathbb{R}^n$ orthogonally onto the span of the columns of X, $\mathrm{span}(X)$.
- The inner product between $\widehat{y}$ and $y - \widehat{y}$ equals zero, because $\widehat{y} = Hy$, $y - \widehat{y} = (I - H)y$, and $\widehat{y}^{\mathrm{T}}(y - \widehat{y}) = y^{\mathrm{T}}H^{\mathrm{T}}(I - H)y = y^{\mathrm{T}}(H - H)y = 0$. Hence $\widehat{y}$ and $y - \widehat{y}$ are orthogonal.
- Clearly $HX = X(X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}X = X$, so $H(X\beta) = X\beta$ for any $\beta \in \mathbb{R}^p$, i.e., a vector in $\mathrm{span}(X)$ is left unchanged by multiplication by H.

Analysis of variance I

Lemma 2 *Let $X_{n\times p} = (X_0, X_1, \ldots, X_R)$ have rank p, where $p \le n$, and let H_r denote the projection matrices formed using $(X_0, \ldots, X_r)$, for $r = 0, \ldots, R$; hence $H_R = H$. Define $P_r = H_r - H_{r-1}$ for $r = 1, \ldots, R$ and $P_{R+1} = I - H$. Then (i) $H_r H_s = H_r$ whenever $r \le s$, (ii) $H_0 P_r = 0$ for any r, and (iii) the matrices P_r are symmetric and idempotent, with $P_r P_s = 0$ when $r \ne s$.*

- In the setup of Lemma 2 suppose we fit the models with projection matrices $H_0, \ldots, H_R = H$ and corresponding fitted values $\widehat{y}_r = H_r y$. Then

$$\begin{aligned} y &= \widehat{y}_0 + (\widehat{y}_1 - \widehat{y}_0) + \cdots + (\widehat{y}_R - \widehat{y}_{R-1}) + (y - \widehat{y}_R) \\ &= H_0 y + (H_1 - H_0)y + \cdots + (H_R - H_{R-1})y + (I - H)y \\ &= H_0 y + P_1 y + \cdots + P_R y + P_{R+1} y, \end{aligned}$$

  and Lemma 2 implies that the terms on the RHS are orthogonal, i.e.,

$$(H_0 y)^{\mathrm{T}}(P_r y) = 0, \quad (P_s y)^{\mathrm{T}}(P_r y) = 0, \quad r \ne s.$$

- Hence Pythagoras' theorem gives the **analysis of variance (ANOVA)** decomposition

$$\|y\|^2 = \|\widehat{y}_0\|^2 + \sum_{r=1}^{R} \|\widehat{y}_r - \widehat{y}_{r-1}\|^2 + \|y - \widehat{y}\|^2.$$

Note to Lemma 2

- (i) Let $\mathcal{V}_0 \subset \cdots \subset \mathcal{V}_R$ denote the linear spaces onto which $\mathbb{R}^n$ is projected by $H_0, \ldots, H_R = H$, and suppose that $r \le s$. Now $H_r y \in \mathcal{V}_r$ for any $y \in \mathbb{R}^n$, so as $\mathcal{V}_r \subset \mathcal{V}_s$, $H_r y \in \mathcal{V}_s$. Hence $H_s H_r y = H_r y$ for any $y \in \mathbb{R}^n$, so $H_s H_r = H_r$. This implies that

$$H_s H_r = H_r = H_r^{\mathrm{T}} = (H_s H_r)^{\mathrm{T}} = H_r^{\mathrm{T}} H_s^{\mathrm{T}} = H_r H_s, \quad s \ge r.$$

- (ii) For $r = 1, \ldots, R$, (i) yields $H_0 P_r = H_0 H_r - H_0 H_{r-1} = H_0 - H_0 = 0$, and $H_0 P_{R+1} = H_0(I - H_R) = 0$.
- (iii) The matrices $P_1, \ldots, P_R$ are symmetric because

$$P_r^{\mathrm{T}} = (H_r - H_{r-1})^{\mathrm{T}} = H_r^{\mathrm{T}} - H_{r-1}^{\mathrm{T}} = H_r - H_{r-1} = P_r,$$

  and idempotent because (i) gives

$$\begin{aligned} P_r^2 &= (H_r - H_{r-1})(H_r - H_{r-1}) \\ &= H_r^2 - H_r H_{r-1} - H_{r-1} H_r + H_{r-1}^2 \\ &= H_r - H_{r-1} - H_{r-1} + H_{r-1} \\ &= H_r - H_{r-1} = P_r. \end{aligned}$$

  Moreover if $r < s \le R$, then

$$\begin{aligned} P_r P_s &= (H_r - H_{r-1})(H_s - H_{s-1}) \\ &= H_r H_s - H_r H_{s-1} - H_s H_{r-1} + H_{r-1} H_{s-1} \\ &= H_r - H_r - H_{r-1} + H_{r-1} \\ &= 0. \end{aligned}$$

  The corresponding results for P_{R+1} are equally easy to check.

Analysis of variance II

- Usually $X_0 = 1_n$; then $\widehat{y}_0 = 1_n(1_n^{\mathrm{T}}1_n)^{-1}1_n^{\mathrm{T}}y = \overline{y}1_n$ and

$$\|y\|^2 - \|\widehat{y}_0\|^2 = \sum_{j=1}^{n} y_j^2 - \sum_{j=1}^{n} \overline{y}^2 = \sum_{j=1}^{n} (y_j - \overline{y})^2,$$

  equals n times the empirical variance of $y_1, \ldots, y_n$. Hence

$$\sum_{j=1}^{n} (y_j - \overline{y})^2 = \|y\|^2 - \|\widehat{y}_0\|^2 = \sum_{r=1}^{R} \|\widehat{y}_r - \widehat{y}_{r-1}\|^2 + \|y - \widehat{y}\|^2$$

  decomposes ('analyses') the variability of y around its average $\overline{y}$ into
  - the contributions $\|\widehat{y}_r - \widehat{y}_{r-1}\|^2$ due to adding the columns of X_r to $X_0, \ldots, X_{r-1}$,
  - the **residual sum of squares** $\|y - \widehat{y}\|^2$ left after fitting $X = (X_0, \ldots, X_R)$.
- Large $\|\widehat{y}_r - \widehat{y}_{r-1}\|^2$ implies that X_r explains a lot of the variation of y even after allowing for that explained by $X_0, \ldots, X_{r-1}$.
- The
  - **degrees of freedom** of a fit is the rank ν_r of the corresponding H_r, and the
  - **residual degrees of freedom** is $n - \nu_R = n - p$.

Terms

- A constant column $X_0 = 1_n$ is almost always present in the design matrix, so

$$X\beta = \begin{pmatrix} 1_n & X_1 & \cdots & X_R \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_R \end{pmatrix} = 1_n\beta_0 + X_1\beta_1 + \cdots + X_R\beta_R,$$

  where the matrices $X_1, \ldots, X_R$, the **terms**, are successively included.
- The baseline model with only 1_n has fitted value and residual vector

$$\widehat{y}_0 = \overline{y}1_n, \quad y - \widehat{y}_0 = y - \overline{y}1_n.$$

- Starting from the baseline we ask which terms lead to large reductions in the residual sum of squares, i.e., best explain the variation of y.
- The successive residual degrees of freedom, i.e., the ranks of the matrices $I - H_r$, are

$$n - 1 = n - \nu_0 \geq n - \nu_1 \geq \cdots \geq n - \nu_R.$$

- When the columns of X_{r+1} depend linearly on those of $1_n, X_1, \ldots, X_r$, we have $\nu_{r+1} = \nu_r$, so inclusion of X_{r+1} does not change the fitted value or improve the fit.

Model formulae

☐ A mean vector such as $1_n\beta_0 + X_1\beta_1 + X_2\beta_2$ is often written as the right-hand side of

$$\texttt{y} \sim \texttt{X1} + \texttt{X2}$$

where

- the columns of 1s is (silently) included first by default,
- `X1` and `X2` represent the vector subspaces of $\mathbb{R}^n$ generated by the corresponding terms, and
- $+$ represents addition of vector subspaces.

☐ Software generally drops any column of a design matrix that is linearly dependent on previous columns, and this affects which elements of β can be estimated and the meaning of estimates corresponding to later columns.

☐ Carefully choosing the order of terms in a model can give easily interpreted estimates of the parameters of interest — for example, if X_2 is full-rank and a column of 1s lies in $\mathrm{span}(X_1) + \mathrm{span}(X_2)$ then

$$\texttt{y} \sim \texttt{X1} + \texttt{X2}, \qquad \texttt{y} \sim \texttt{X2} + \texttt{X1} - \texttt{1},$$

span the same linear space but the second estimates the parameters of β_2 (unadjusted for the mean) and the parameters of β_1, adjusted for the presence of X_2.

ANOVA

Terms	Residual df	Residual SS	Term added	Reduction in residual df	Reduction in SS	Mean square
1_n	$n - \nu_0 = n - 1$	SS_0				
$1_n, X_1$	$n - \nu_1$	SS_1	X_1	$\nu_1 - \nu_0$	$\mathrm{SS}_0 - \mathrm{SS}_1$	$\frac{\mathrm{SS}_0 - \mathrm{SS}_1}{\nu_1 - \nu_0}$
$1_n, X_1, X_2$	$n - \nu_2$	SS_2	X_2	$\nu_2 - \nu_1$	$\mathrm{SS}_1 - \mathrm{SS}_2$	$\frac{\mathrm{SS}_1 - \mathrm{SS}_2}{\nu_2 - \nu_1}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$1_n, X_1, \ldots, X_R$	$n - \nu_R = n - p$	SS_R	X_R	$\nu_R - \nu_{R-1}$	$\mathrm{SS}_{R-1} - \mathrm{SS}_R$	$\frac{\mathrm{SS}_{R-1} - \mathrm{SS}_R}{\nu_R - \nu_{R-1}}$

☐ The sum of squares when including terms $1_n, X_1, \ldots, X_r$ is

$$\mathrm{SS}_r = \|y - \widehat{y}_r\|^2.$$

☐ The 'mean square' for term X_r,

$$\mathrm{MS}_r = \frac{\mathrm{SS}_{r-1} - \mathrm{SS}_r}{\nu_r - \nu_{r-1}}$$

is the average reduction in SS_r per degree of freedom when X_r is added to the model.

☐ Usually show only the RHS of the table and the bottom line of its LHS (next slide).

ANOVA table

Term added	df	Reduction in SS	Mean square
X_1	$\nu_1 - \nu_0$	$\mathrm{SS}_0 - \mathrm{SS}_1$	$\mathrm{MS}_1 = (\mathrm{SS}_0 - \mathrm{SS}_1)/(\nu_1 - \nu_0)$
X_2	$\nu_2 - \nu_1$	$\mathrm{SS}_1 - \mathrm{SS}_2$	$\mathrm{MS}_2 = (\mathrm{SS}_1 - \mathrm{SS}_2)/(\nu_2 - \nu_1)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
X_R	$\nu_R - \nu_{R-1}$	$\mathrm{SS}_{R-1} - \mathrm{SS}_R$	$\mathrm{MS}_R = (\mathrm{SS}_{R-1} - \mathrm{SS}_R)/(\nu_R - \nu_{R-1})$
Residual	$n - \nu_R$	SS_R	$\mathrm{MS}_{\mathrm{Res}} = \mathrm{SS}_R/(n - \nu_R)$

- Used to screen which terms give the largest reductions, comparing MS_r with the residual mean square $\mathrm{MS}_{\mathrm{Res}}$.
- Judge 'significance' of reductions relative to residual using F-tests (later).
- Problem: the order of adding terms matters, so there is no unique reduction in general.

Coefficient of determination

- **Coefficient of determination** R^2 measures reduction in variance of y as

$$R^2 = \frac{\|\widehat{y} - \overline{y}1_n\|^2}{\|y - \overline{y}1_n\|^2} = \frac{\{(H - H_0)y)\}^{\mathrm{T}}(H - H_0)y}{\{(I - H_0)y)\}^{\mathrm{T}}(I - H_0)y} = \frac{y^{\mathrm{T}}(H - H_0)y}{y^{\mathrm{T}}(I - H_0)y},$$

  where H_0 and H are the hat matrices for regression on 1_n and X, and $1_n \in \mathrm{span}(X)$.
- $R^2 \in [0, 1]$ is the squared empirical correlation between y and $\widehat{y}$, so $R^2 \approx 1$ implies that most of the variation in y is explained by $\widehat{y}$.
- There is a geometric interpretation, as the terms on the right of

$$(I_n - H_0)y = (I_n - H)y + (H - H_0)y$$

  are orthogonal (check this).
- Adding columns to X must increase R^2, unlike the **adjusted** R^2,

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

- If $1_n \notin \mathrm{span}(X)$, use

$$R^2_0 = \frac{\widehat{y}^{\mathrm{T}}\widehat{y}}{y^{\mathrm{T}}y}, \quad R^2_{0,a} = R^2_0 + (1 - R^2_0)\frac{n}{n-p}.$$

Comments

- ☐ We have supposed that $X_{n\times p}$ has rank p:
  - if X is rank-deficient, then a least squares algorithm usually drops columns that lie in the span of preceding ones, but care is needed to construct X so that the resulting $\widehat{\beta}$ is easy to interpret;
  - if X is nearly rank-deficient, then regularisation may be needed. More later ...
- ☐ Everything so far as purely numerical:
  - least squares estimation is a numerical technique for using X to approximate y;
  - $\widehat{y} = X\widehat{\beta}$ is the resulting approximation, which lies in $\mathrm{span}(X)$;
  - $\widehat{\beta}$ gives the coefficients of the columns of X for the best approximation;
  - the coefficient of determination R^2 measures how much of the overall variation of y was explained by X; and
  - the ANOVA decomposition summarises how much of the variation in y is explained by different subsets of columns of X (terms).
- ☐ For statistics we need to add some distributional assumptions ... shortly ...
- ☐ First some reminders ...

1.2 Inference

Reminder: Moment-generating function

Definition 3 *The* **moment-generating function (MGF)** *of a random vector* $Y_{n\times 1}$ *is*

$$M_Y(t) = \mathrm{E}(e^{t^{\mathrm{T}}Y}) = \mathrm{E}(e^{\sum_{j=1}^n t_j Y_j}), \quad t \in \mathcal{T} = \{t \in \mathbb{R}^n : M_Y(t) < \infty\},$$

and the **cumulant-generating function** *of* Y *is* $K_Y(t) = \log M_Y(t)$, $t \in \mathcal{T}$.

Then

- ☐ $0 \in \mathcal{T}$, so $M_Y(0) = 1$ and $K_Y(0) = 0$;
- ☐ if $\mathcal{T}$ contains an open set, then

$$\mu = \mathrm{E}(Y) = K'_Y(0) = \left.\frac{\partial K_Y(t)}{\partial t}\right|_{t=0}, \quad \Omega = \mathrm{var}(Y) = \left.\frac{\partial^2 K_Y(t)}{\partial t \partial t^{\mathrm{T}}}\right|_{t=0};$$

- ☐ if $\mathcal{A}, \mathcal{B}$ are disjoint subsets of $\{1, \ldots, n\}$ and $Y_{\mathcal{A}}$ denotes the sub-vector of Y containing $\{Y_j : j \in \mathcal{A}\}$, etc., then $Y_{\mathcal{A}} \perp\!\!\!\perp Y_{\mathcal{B}}$ if and only if

$$M_Y(t) = \mathrm{E}(e^{t_{\mathcal{A}}^{\mathrm{T}} Y_{\mathcal{A}} + t_{\mathcal{B}}^{\mathrm{T}} Y_{\mathcal{B}}}) = M_{Y_{\mathcal{A}}}(t_{\mathcal{A}}) M_{Y_{\mathcal{B}}}(t_{\mathcal{B}}), \quad t \in \mathcal{T};$$

- ☐ the MGF of $Y_{\mathcal{A}}$ equals $M_Y(t)$ evaluated with $t_{\mathcal{B}} = 0$;
- ☐ if we recognise an MGF, then we know the probability distribution that gave it.

Reminder: Multivariate normal distribution

A random variable $Y_{n\times 1}$ with real components has the **multivariate normal distribution,** $Y \sim \mathcal{N}_n(\mu, \Omega)$, if $a^{\mathrm{T}}Y \sim \mathcal{N}(a^{\mathrm{T}}\mu, a^{\mathrm{T}}\Omega a)$ for every constant vector $a_{n\times 1}$, and then

(a) Ω is symmetric semi-positive definite with real components and

$$\mathrm{E}(Y) = \mu_{n\times 1}, \quad \mathrm{var}(Y) = \Omega_{n\times n}, \quad M_Y(t) = \exp(t^{\mathrm{T}}\mu + \tfrac{1}{2}t^{\mathrm{T}}\Omega t), \quad t \in \mathbb{R}^n,$$

where we call μ the **mean vector** and Ω the **(co)variance matrix** of X;

(b) for any constants $a_{m\times 1}$ and $B_{m\times n}$, $a + BY \sim \mathcal{N}_m\left(a + B\mu, B\Omega B^{\mathrm{T}}\right)$;

(c) if $Y^{\mathrm{T}} = (Y_1^{\mathrm{T}}, Y_2^{\mathrm{T}})$, where Y_1 is $m \times 1$, and μ and Ω are partitioned correspondingly, then the marginal and conditional distributions of Y_1 are also multivariate normal:

$$Y_1 \sim \mathcal{N}_m(\mu_1, \Omega_{11}), \quad Y_1 \mid Y_2 = y_2 \sim \mathcal{N}_m\left\{\mu_1 + \Omega_{12}\Omega_{22}^{-1}(y_2 - \mu_2), \Omega_{11} - \Omega_{12}\Omega_{22}^{-1}\Omega_{21}\right\};$$

(d) $Y_1 \perp\!\!\!\perp Y_2$ iff $\Omega_{12} = 0$, and $a + BY \perp\!\!\!\perp c + DY$ iff $B\Omega D^{\mathrm{T}} = 0$;

(e) if $Y_1, \ldots, Y_n \overset{\text{iid}}{\sim} \mathcal{N}(\mu, \sigma^2)$, then $Y_{n\times 1} \sim \mathcal{N}_n(\mu 1_n, \sigma^2 I_n)$; and finally,

(f) Y has a density on $\mathbb{R}^n$ iff Ω is positive definite (i.e., has rank n), and then

$$f(y; \mu, \Omega) = \frac{1}{(2\pi)^{n/2}|\Omega|^{1/2}} \exp\left\{-\tfrac{1}{2}(y-\mu)^{\mathrm{T}}\Omega^{-1}(y-\mu)\right\}, \quad y \in \mathbb{R}^n. \tag{1}$$

Note: Multivariate normal distribution

(a) Let e_j denote the n-vector with 1 in the jth place and zeros everywhere else.

☐ Then $Y_j = e_j^{\mathrm{T}} Y \sim N(\mu_j, \omega_{jj})$, giving the mean and variance of Y_j.

☐ Now $\mathrm{var}(Y_j + Y_k) = \mathrm{var}(Y_j) + \mathrm{var}(Y_k) + 2\mathrm{cov}(Y_j, Y_k)$, and

$$Y_j + Y_k = (e_j + e_k)^{\mathrm{T}} Y \sim \mathcal{N}(\mu_j + \mu_k, \omega_{jj} + \omega_{kk} + 2\omega_{jk}),$$

which implies that $\mathrm{cov}(Y_j, Y_k) = \omega_{jk} = \omega_{kj}$. This gives the mean and covariance matrix of Y.

☐ Since $u^{\mathrm{T}} Y \sim \mathcal{N}(u^{\mathrm{T}}\mu, u^{\mathrm{T}}\Omega u)$, its MGF is $M_{u^{\mathrm{T}}Y}(t) = \mathrm{E}(e^{tu^{\mathrm{T}}Y}) = \exp(tu^{\mathrm{T}}\mu + \frac{1}{2}t^2 u^{\mathrm{T}}\Omega u)$. The MGF of Y is $M_Y(u) = \mathrm{E}(e^{u^{\mathrm{T}}Y}) = M_{u^{\mathrm{T}}Y}(1) = \exp(u^{\mathrm{T}}\mu + \frac{1}{2}u^{\mathrm{T}}\Omega u)$, for any $u \in \mathbb{R}^p$, as stated.

(b) The MGF of $a + BY$ equals

$$\begin{aligned}
\mathrm{E}\left[\exp\{t^{\mathrm{T}}(a + BY)\}\right] &= \mathrm{E}\left[\exp\{t^{\mathrm{T}}a + (B^{\mathrm{T}}t)^{\mathrm{T}}Y)\}\right] \\
&= e^{t^{\mathrm{T}}a} M_Y(B^{\mathrm{T}}t) \\
&= \exp\{t^{\mathrm{T}}a + (B^{\mathrm{T}}t)^{\mathrm{T}}\mu + \tfrac{1}{2}(B^{\mathrm{T}}t)^{\mathrm{T}}\Omega(B^{\mathrm{T}}t)\} \\
&= \exp\left\{t^{\mathrm{T}}(a + B\mu) + \tfrac{1}{2}t^{\mathrm{T}}(B\Omega B^{\mathrm{T}})t\right\},
\end{aligned}$$

which is the MGF of the $\mathcal{N}_m(a + B\mu, B\Omega B^{\mathrm{T}})$ distribution. Hence linear combinations of normal variables are themselves normal.

(c) Write $Y^{\mathrm{T}} = (Y_1^{\mathrm{T}}, Y_2^{\mathrm{T}})$ and partition μ and Ω conformally. Then

$$M_Y(t) = \exp\left\{t_1^{\mathrm{T}}\mu_1 + t_2^{\mathrm{T}}\mu_2 + \tfrac{1}{2}\left(t_1^{\mathrm{T}}\Omega_{11}t_1 + 2t_1^{\mathrm{T}}\Omega_{12}t_2 + t_2^{\mathrm{T}}\Omega_{22}t_2\right)\right\}$$

and by setting $t_2 = 0$ and $t_1 = 0$ we see that $M_{Y_1}(t_1) = \exp\left(t_1^{\mathrm{T}}\mu_1 + \frac{1}{2}t_1^{\mathrm{T}}\Omega_{11}t_1\right)$ and $M_{Y_2}(t_2) = \exp\left(t_2^{\mathrm{T}}\mu_2 + \frac{1}{2}t_2^{\mathrm{T}}\Omega_{22}t_2\right)$. Hence the marginal distribution of Y_1 is $\mathcal{N}_m(\mu_1, \Omega_{11})$.
For the conditional distribution, note that $W = Y_1 - \Omega_{12}\Omega_{22}^{-1}Y_2$ is a linear combination of Y and

$$\mathrm{E}(W) = \mu_1 - \Omega_{12}\Omega_{22}^{-1}\mu_2, \quad \mathrm{var}(W) = \Omega_{11} - \Omega_{12}\Omega_{22}^{-1}\Omega_{21}, \quad \mathrm{cov}(W, Y_2) = \Omega_{12} - \Omega_{12}\Omega_{22}^{-1}\Omega_{22} = 0.$$

Hence $W \perp\!\!\!\perp Y_2$. As $Y_1 = W + \Omega_{12}\Omega_{22}^{-1}Y_2$ and conditioning on Y_2 does not change the distribution of W,

$$\mathrm{E}(Y_1 \mid Y_2 = y_2) = \mathrm{E}(W) + \Omega_{12}\Omega_{22}^{-1}y_2, \quad \mathrm{var}(Y_1 \mid Y_2 = y_2) = \mathrm{var}(W + \Omega_{12}\Omega_{22}^{-1}y_2) = \mathrm{var}(W).$$

Putting the pieces together gives the stated conditional distribution.

(d) The joint MGF given in (c) factorises iff the variables are independent, and on inspecting it we see that

$$M_Y(t) = M_{Y_1}(t_1)M_{Y_2}(t_2) \quad \Longleftrightarrow \quad \Omega_{12} = 0.$$

The variance matrix of

$$\begin{pmatrix} a \\ c \end{pmatrix} + \begin{pmatrix} B \\ D \end{pmatrix} Y$$

is

$$\begin{pmatrix} B\Omega B^{\mathrm{T}} & B\Omega D^{\mathrm{T}} \\ D\Omega B^{\mathrm{T}} & D\Omega D^{\mathrm{T}} \end{pmatrix},$$

so $a + BY \perp\!\!\!\perp c + DY$ iff $B\Omega D^{\mathrm{T}} = 0$.

Note: Multivariate normal distribution II

(e) Each Y_j has mean μ and variance σ^2, and since they are independent, $\mathrm{cov}(Y_j, Y_k) = 0$ for $j \neq k$. If $u \in \mathbb{R}^n$, then $u^{\mathrm{T}}Y$ is a linear combination of normal variables, with mean $\sum_{j=1}^n u_j\mu = u^{\mathrm{T}}\mu 1_n$ and variance $\sum_{j=1}^n u_j^2\sigma^2 = u^{\mathrm{T}}\sigma^2 I_n u$, so $Y \sim \mathcal{N}_n(\mu 1_n, \sigma^2 I_n)$, as required.

(f) Since Ω is symmetric and positive semi-definite, the spectral theorem tells us that we may write $\Omega = ADA^{\mathrm{T}}$, where $D = \mathrm{diag}(d_1, \ldots, d_n)$ contains the (real) eigenvalues of Ω, with $d_1 \geq \cdots \geq d_n \geq 0$, and A is a $n \times n$ orthogonal matrix, i.e., $A^{\mathrm{T}}A = AA^{\mathrm{T}} = I_n$ and $|A| = 1$. The columns $A_1, \ldots, A_n$ of A are the eigenvectors corresponding to the respective eigenvalues,

$$\Omega = ADA^{\mathrm{T}} = \sum_{j=1}^n d_j a_j a_j^{\mathrm{T}},$$

with $|\Omega| = |ADA^{\mathrm{T}}| = |A| \times |D| \times |A^{\mathrm{T}}| = |D|$ and $\Omega^{-1} = AD^{-1}A^{\mathrm{T}}$ if the inverse exists.

☐ Now let $Z_1, \ldots, Z_n \overset{\text{iid}}{\sim} \mathcal{N}(0,1)$ $Z = (Z_1, \ldots, Z_n)^{\mathrm{T}}$, and $u \in \mathbb{R}^n$, set and consider

$$u^{\mathrm{T}}(\mu + AD^{1/2}Z) = u^{\mathrm{T}}\mu + \sum_{j=1}^n Z_j u^{\mathrm{T}} a_j d_j^{1/2}.$$

This is a linear combination of normal variables, so it has a normal distribution, with mean $u^{\mathrm{T}}\mu$ and variance

$$\mathrm{var}\left(u^{\mathrm{T}}\mu + \sum_{j=1}^n Z_j u^{\mathrm{T}} a_j d_j^{1/2}\right) = \sum_{j=1}^n d_j (u^{\mathrm{T}}a_j)^2 \mathrm{var}(Z_j) = u^{\mathrm{T}}\left(\sum_{j=1}^n d_j a_j a_j^{\mathrm{T}}\right) u = u^{\mathrm{T}}\Omega u,$$

so we can write $X = \mu + AD^{1/2}Z \sim N_n(\mu, \Omega)$.

☐ If Ω has rank n, then $d_n > 0$. The change of variables $z \mapsto x = \mu + AD^{1/2}z$ has Jacobian

$$\left|\frac{\partial x}{\partial z}\right| = |AD^{1/2}| = |A||D|^{1/2} = 1 \times |D|^{1/2} = |\Omega|^{1/2} > 0.$$

Moreover $z = D^{-1/2}A^{\mathrm{T}}(x - \mu)$, and therefore $z^{\mathrm{T}}z = (x-\mu)^{\mathrm{T}}\Omega^{-1}(x-\mu)$. Hence using the joint density of Z, $f_Z(z) = (2\pi)^{-n/2}\exp(-\sum_{j=1}^n z_j^2/2)$,

$$f_X(x) = f_Z(z)|_{z=D^{-1/2}A^{\mathrm{T}}(x-\mu)} \left|\frac{\partial z}{\partial x}\right| = (2\pi)^{-n/2} \exp\left(-\frac{z^{\mathrm{T}}z}{2}\right)\Bigg|_{z=D^{-1/2}A^{\mathrm{T}}(x-\mu)} |\Omega|^{-1/2},$$

which reduces to (1). If $d_n = 0$, then the Jacobian is zero, so the transformation $z \mapsto x$ is singular and X does not have a density on $\mathbb{R}^n$.

☐ Now suppose that $d_m > d_{m+1} = 0$, so just m eigenvalues of Ω are positive. Then

$$X = \mu + \sum_{j=1}^m Z_j a_j d_j^{1/2} \in \mathcal{S} = \mu + \mathrm{span}(a_1, \ldots, a_m),$$

where $\mathcal{S}$ is a hyperplane of dimension m passing through μ and generated by the vectors $a_1, \ldots, a_m$. In this case the previous argument shows that X has an m-dimensional Gaussian density on $\mathcal{S}$, but places no probability elsewhere.

Reminder: χ^2 distribution

Definition 4 *If* $Y_j \overset{\text{ind}}{\sim} \mathcal{N}(\mu_j, \sigma^2)$, *then* $W = Y_1^2 + \cdots + Y_\nu^2$ *has the* **non-central chi-square distribution with** ν **degrees of freedom (df) and non-centrality parameter** $\delta^2 = (\mu_1^2 + \cdots + \mu_\nu^2)/\sigma^2$; *we write* $W \sim \sigma^2 \chi^2_\nu(\delta^2)$. *Then*

$$M_W(t) = \exp\left(\frac{t\sigma^2\delta^2}{1-2t\sigma^2}\right)(1-2\sigma^2 t)^{-\nu/2}, \quad t < 1/(2\sigma^2).$$

If $\delta^2 = 0$ *and* $\sigma^2 = 1$ *then* W *has the (central)* **chi-square distribution with** ν **df**, *we write* $W \sim \chi^2_\nu$, *its MGF is* $M_W(t) = (1-2t)^{-\nu/2}$, *and its* p*-quantile is* $c_\nu(p)$.

Chi-square variables satisfy

- ☐ $\mathrm{E}(W) = \sigma^2(\nu + \delta^2)$, $\mathrm{var}(W) = 2\sigma^4(\nu + 2\delta^2)$;
- ☐ if $W_1 \sim \chi^2_{\nu_1} \perp\!\!\!\perp W_2 \sim \chi^2_{\nu_2}$, then $W_1 + W_2 \sim \chi^2_{\nu_1+\nu_2}$;
- ☐ $W \sim \chi^2_\nu$ implies that W has the gamma density

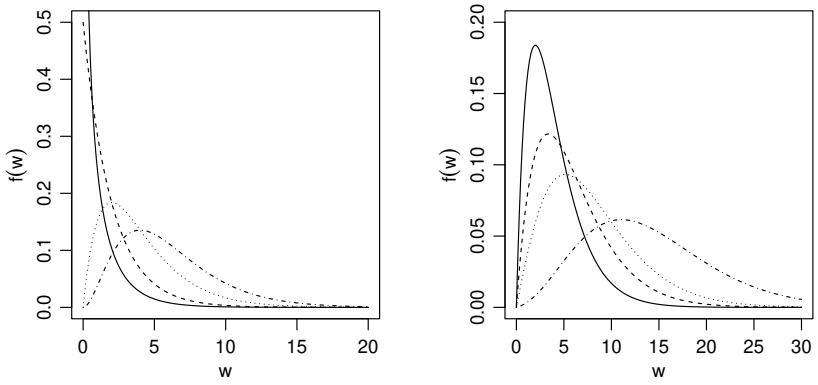
$$f(w) = \frac{\beta^\alpha w^{\alpha-1}}{\Gamma(\alpha)} e^{-\beta w}, \quad w > 0, \quad \alpha, \beta > 0,$$

with $\alpha = \nu/2$ and $\beta = 1/2$.

Reminder: χ^2_ν densities

Left: central densities with $\nu = 1, 2, 4, 6$ (solid, large dashes, small dashes, dot-dash).

Right: non-central densities with $\nu = 4$ and $\delta = 0, 2, 4, 10$ (solid, large dashes, small dashes, dot-dash).



Reminder: Student t distribution

Definition 5 *If $Z \sim \mathcal{N}(0,1) \perp\!\!\!\perp W \sim \chi^2_\nu$, then $T = Z/(W/\nu)^{1/2}$ has the* **Student t distribution with ν df**, *$T \sim t_\nu$, and we write $t_\nu(p)$ for the corresponding p-quantile. The density function of T is*

$$f_T(t) = \frac{\Gamma\{(\nu+1)/2\}}{\sqrt{\nu\pi}\Gamma(\nu/2)} \frac{1}{(1+t^2/\nu)^{(\nu+1)/2}}, \quad -\infty < t < \infty, \ \nu = 1, 2, \ldots.$$

Properties:

- the mean and variance exist only for $\nu \geq 2$ and $\nu \geq 3$ respectively, and then

$$\mathrm{E}(T) = 0, \quad \mathrm{var}(T) = \frac{\nu}{\nu - 2};$$

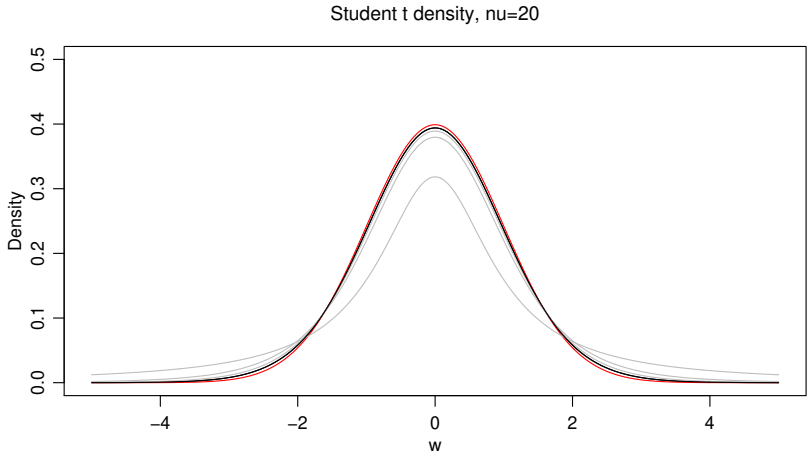
- with $\nu = 1$ we have the **Cauchy density**,

$$\frac{1}{\pi(1+t^2)}, \quad -\infty < t < \infty,$$

  and then T has no moments;
- as $\nu \to \infty$, the limiting distribution of T is $\mathcal{N}(0,1)$; usually the approximation is 'good enough' for $\nu > 25$ (say).

Reminder: Student t densities

Student t density functions with $\nu = 1, 5, 10, 20$ (black, $\nu = 20$), and the standard normal density (red):



Reminder: F distribution

Definition 6 *If* $W_1, W_2 \overset{\text{ind}}{\sim} \chi^2_{\nu_1}, \chi^2_{\nu_2}$, *then*

$$F = \frac{W_1/\nu_1}{W_2/\nu_2}$$

has the F **distribution with** ν_1 **and** ν_2 **df**: *we write* $F \sim F_{\nu_1,\nu_2}$.
The density function is

$$f_F(u) = \frac{\Gamma\left(\frac{1}{2}\nu_1 + \frac{1}{2}\nu_2\right) \nu_1^{\nu_1/2} \nu_2^{\nu_2/2}}{\Gamma\left(\frac{1}{2}\nu_1\right)\Gamma\left(\frac{1}{2}\nu_2\right)} \frac{u^{\frac{1}{2}\nu_1 - 1}}{(\nu_2 + \nu_1 u)^{(\nu_1+\nu_2)/2}}, \quad u > 0,\ \nu_1, \nu_2 = 1, 2, \ldots,$$

and the p*-quantile is written* $F_{\nu_1,\nu_2}(p)$.

Reminder: Computation

- ☐ Quantiles of the $\mathcal{N}(\mu, \sigma^2)$, χ^2_ν, t_ν, F_{ν_1,ν_2} distributions can be found in tables, or in environments such as `R` (see `http://www.r-project.org/`), where they can also be simulated.
- ☐ Examples:

```
R : Copyright 2005, The R Foundation for Statistical Computing
Version 2.2.1  (2005-12-20 r36812)
...
> qnorm(0.025)    # this is a comment; access normal quantiles
[1] -1.959964     # the [1] means this is the first  element of a vector
> ?qnorm          # help on use of function qnorm()
> qchisq(0.025,df=3)  # chi-squared quantiles, nu=3
[1] 0.2157953
> qt(0.025,df=3)     # t quantiles, nu=3
[1] -3.182446
> qf(0.025,df1=3,df2=4)  # F quantiles, nu1=3, nu2=4
[1] 0.06622087
```


Statistical models

- ☐ Least squares fitting gives a deterministic description of the variation in some numbers y in terms of other numbers X.
- ☐ A **statistical model** is a description of data y in terms of a collection of probability distributions on the sample space for y.
- ☐ We distinguish
  - **primary** aspects of a model, which specify what questions we aim to answer, from
  - **secondary** aspects, which complete the model, indicate what analysis might be suitable, and determine the precision of conclusions.
- ☐ Often the primary aspects are embodied in one or more **parameters** of the model.
- ☐ (Almost) all models are **tentative**, and we must check that they are reasonable.

Second-order and normal assumptions

- Two distributional assumptions are in general use for the linear model:
  - **second-order assumptions**,

$$y \sim (X\beta, \sigma^2 V), \quad \text{i.e.,} \quad \mathrm{E}(y) = X\beta, \quad \mathrm{var}(y) = \sigma^2 V_{n\times n};$$

  - **normal assumptions**,

$$y \sim \mathcal{N}_n(X\beta, \sigma^2 V),$$

    i.e., y has a multivariate normal distribution with mean vector $X\beta$ and positive definite (co)variance matrix $\sigma^2 V$.
- X is called the **design matrix**: more later.
- V is assumed known. Unless stated otherwise we set $V = I_n$, so the y_j are uncorrelated; if normal they are therefore independent.
- If $V \neq I_n$, then we can perform **weighted least squares (WLS)** estimation, minimising

$$\|y - X\beta\|_V^2 = (y - X\beta)^T W (y - X\beta),$$

  where $W = V^{-1}$ is the **weight matrix**.
- Above the **linearity** is (usually) primary, whereas the **distributional assumption**, use of weights, ..., are (usually) secondary.

Consequences of second-order assumptions

Lemma 7 *Under the second-order assumptions, $\widehat{\beta}$ is an unbiased estimator of β,*

$$\mathrm{E}(\widehat{\beta}) = \beta, \quad \mathrm{var}(\widehat{\beta}) = \sigma^2 (X^{\mathrm{T}} X)^{-1}.$$

and $S^2 = (n-p)^{-1}\|y - \widehat{y}\|^2$ is an unbiased estimator of σ^2.

Theorem 8 (Gauss–Markov) *The least squares estimator $\widehat{\beta}$ has the smallest variance among all estimators $\tilde{\beta} = A_{p\times n} y$; it is the* **best linear unbiased estimator (BLUE)** *of β.*

- Obviously these results hold under the (stronger) normal assumptions.
- The Gauss–Markov theorem only concerns linear estimators. Nonlinear estimators of β might have smaller variance than $\sigma^2 (X^{\mathrm{T}} X)^{-1}$ (and in fact the optimal maximum likelihood estimators of β for non-normal models will be nonlinear in y).

Note to Lemma 7

- ☐ Recall that expectation is linear, and that $\mathrm{var}(A_{p\times n}y) = A\mathrm{var}(y)A^{\mathrm{T}}$.
- ☐ Set $A_{p\times n} = (X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}$ and note that

$$\begin{aligned}\mathrm{E}(\widehat{\beta}) &= \mathrm{E}(Ay) = A\mathrm{E}(y) = (X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}X\beta = \beta,\\ \mathrm{var}(\widehat{\beta}) &= A\mathrm{var}(y)A^{\mathrm{T}} = (X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}I_n\sigma^2\{(X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}\}^{\mathrm{T}} = \sigma^2(X^{\mathrm{T}}X)^{-1}.\end{aligned}$$

- ☐ Recall that $\mathrm{E}(yy^{\mathrm{T}}) = \mathrm{var}(y) + \mathrm{E}(y)\mathrm{E}(y)^{\mathrm{T}} = \sigma^2 I_n + X\beta\beta^{\mathrm{T}}X^{\mathrm{T}}$, and note that

$$\|y-\widehat{y}\|^2 = (y-\widehat{y})^{\mathrm{T}}(y-\widehat{y}) = y^{\mathrm{T}}(I_n-H)^{\mathrm{T}}(I_n-H)y = y^{\mathrm{T}}(I_n-H)y = \mathrm{tr}\{(I_n-H)yy^{\mathrm{T}}\}.$$

Hence $\mathrm{E}(\|y-\widehat{y}\|^2)$ equals

$$\mathrm{E}[\mathrm{tr}\{(I_n-H)yy^{\mathrm{T}}\}] = \mathrm{tr}\{(I_n-H)\mathrm{E}(yy^{\mathrm{T}})\} = \mathrm{tr}\{(I_n-H)(\sigma^2 I_n + X\beta\beta^{\mathrm{T}}X^{\mathrm{T}})\} = \sigma^2\mathrm{tr}(I_n-H),$$

because $(I_n-H)X = 0$. Moreover $\mathrm{tr}(I_n) = n$ and

$$\mathrm{tr}(H) = \mathrm{tr}\{X(X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}\} = \mathrm{tr}\{(X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}X\} = \mathrm{tr}(I_p) = p,$$

so $\mathrm{E}(S^2) = \sigma^2$, because

$$\mathrm{E}(\|y-\widehat{y}\|^2) = \sigma^2\mathrm{tr}(I_n-H) = \sigma^2(n-p).$$

Note to Theorem 8

- ☐ Let $\tilde{\beta}$ denote any unbiased estimator of β that is linear in y. Then a $p\times n$ matrix A exists such that $\tilde{\beta} = Ay$, and unbiasedness implies that $\mathrm{E}(\tilde{\beta}) = AX\beta = \beta$ for any parameter vector β; this entails $AX = I_p$. Now

$$\begin{aligned}\mathrm{var}(\tilde{\beta}) - \mathrm{var}(\widehat{\beta}) &= A\sigma^2 I_n A^{\mathrm{T}} - \sigma^2(X^{\mathrm{T}}X)^{-1}\\ &= \sigma^2\left\{AA^{\mathrm{T}} - AX(X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}A^{\mathrm{T}}\right\}\\ &= \sigma^2 A(I_n-H)A^{\mathrm{T}}\\ &= \sigma^2 A(I_n-H)(I_n-H)^{\mathrm{T}}A^{\mathrm{T}}\end{aligned}$$

and this $p\times p$ matrix is positive semidefinite. Thus $\widehat{\beta}$ has smallest variance in finite samples among all linear unbiased estimators of β.

- ☐ This is a finite-sample result that holds for all n and X (of rank p, with $n \geq p$).

Second-order assumptions and large samples

☐ We can write $y_j = x_j^{\mathrm{T}}\beta + \sigma\varepsilon_j$, where $\varepsilon_j \overset{\text{ind}}{\sim} (0,1)$, so

$$\widehat{\beta} = (X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}y = \sum_{j=1}^{n}(X^{\mathrm{T}}X)^{-1}x_j y_j = \beta + \sigma n^{-1}\sum_{j=1}^{n} a_j\varepsilon_j,$$

say, where $a_1, \ldots, a_n$ are $p \times 1$ vectors. We have $\mathrm{E}(\widehat{\beta}) = \beta$ and $\mathrm{var}(\widehat{\beta}) = (X^{\mathrm{T}}X)^{-1}$, but is $\widehat{\beta}$ approximately normal for large n?

☐ The a_j, or equivalently X, must be such that no single y_j can dominate in $n^{-1}\sum a_j\varepsilon_j$.

Theorem 9 (no proof) *Let $\{X_n\}$ be a sequence of $n \times p$ design matrices each of rank p, let $h_{11}^n, \ldots, h_{nn}^n$ be the diagonal elements of the hat matrices $X_n(X_n^{\mathrm{T}}X_n)^{-1}X_n^{\mathrm{T}}$ and let $y_n \sim (X_n\beta, \sigma^2 I_n)$ for each n. If*

$$\lim_{n\to\infty}\max_{j=1,\ldots,n} h_{jj} = 0,$$

then the corresponding sequence of least squares estimators $\widehat{\beta}_n$ satisfies

$$(X_n^{\mathrm{T}}X_n)^{1/2}(\widehat{\beta}_n - \beta) \xrightarrow{D} \mathcal{N}_p(0, \sigma^2 I_p), \quad n \to \infty,$$

i.e., if H has a 'well-behaved' diagonal, then $\widehat{\beta} \dot{\sim} \mathcal{N}_p\{\beta, \sigma^2(X^{\mathrm{T}}X)^{-1}\}$ in large samples.

Normal-theory linear model

The following results allow exact inferences for β and σ^2, and in analysis of variance.

Theorem 10 *Under the normal-theory linear model,*

$$\widehat{\beta} \sim \mathcal{N}_p\{\beta, \sigma^2(X^{\mathrm{T}}X)^{-1}\} \quad \perp\!\!\!\perp \quad \frac{(n-p)S^2}{\sigma^2} \sim \chi^2_{n-p}.$$

Lemma 11 *If $y \sim \mathcal{N}_n(\mu, \sigma^2 I_n)$ and H is symmetric and idempotent with rank p, then $y^{\mathrm{T}}Hy \sim \sigma^2\chi_p^2(\delta^2)$, where $\sigma^2\delta^2 = \mu^{\mathrm{T}}H\mu$.*

Theorem 12 *If $y \sim \mathcal{N}_n(\mu, \sigma^2 I_n)$ and a linear model is fitted whose design matrix X is structured as in Lemma 2, then the sums of squares in the ANOVA decomposition*

$$\sum_{j=1}^{n}(y_j - \overline{y})^2 = \sum_{r=1}^{R}\|\widehat{y}_r - \widehat{y}_{r-1}\|^2 + \|y - \widehat{y}\|^2 = \sum_{r=1}^{R+1}\|P_r y\|^2$$

are independent and $\|P_r y\|^2 \sim \sigma^2\chi^2_{\nu_{r-1}-\nu_r}(\delta_r^2/\sigma^2)$, where $\sigma^2\delta_r^2 = \mu^{\mathrm{T}}P_r\mu$. If X_r does not explain any variation in μ after allowing for $X_0, \ldots, X_{r-1}$, then $P_r\mu = 0$, so $\delta_r^2 = 0$.

Theorem 12 implies that the sums of squares for terms that explain variation in y will tend to be larger than sums of squares for other terms, which can be used to estimate σ^2.

Note to Theorem 10

- ☐ The first part is easy, because $\widehat{\beta}$ is a linear combination of normal variables so it is normal, and its mean and variance matrix were given by Lemma 7.
- ☐ Likewise the residual $e = y - \widehat{y} = (I - H)y$ is a linear combination of y with mean 0_n and variance $(I - H)\sigma^2$, so $e \sim \mathcal{N}_n\{0_p, (I - H)\sigma^2\}$.
- ☐ As $\mathrm{cov}(\widehat{\beta}, e)$ equals

  $$\mathrm{cov}\{(X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}y, (I - H)y\} = (X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}\mathrm{cov}(y)(I - H)^{\mathrm{T}} = \sigma^2(X^{\mathrm{T}}X)^{-1}\{(I - H)X\}^{\mathrm{T}} = 0,$$

  we see that $\widehat{\beta}$ is independent of (any function of) e, and therefore in particular of

  $$(n - p)S^2/\sigma^2 = \|y - \widehat{y}\|^2/\sigma^2 = e^{\mathrm{T}}e/\sigma^2.$$

- ☐ The eigenvalues of H are p 1's and $n - p$ 0's, so those of $I - H$ are $n - p$ 1's and p 0's. The spectral decomposition implies that there exists an $n \times n$ orthogonal matrix U such that $I - H = UDU^{\mathrm{T}}$, where $D = \mathrm{diag}(1, \ldots, 1, 0, \ldots, 0)$ and $UU^{\mathrm{T}} = U^{\mathrm{T}}U = I_n$. Thus $Z = U^{\mathrm{T}}e/\sigma$ has mean vector 0_n and variance matrix

  $$\mathrm{var}(Z) = U^{\mathrm{T}}\mathrm{var}(e)U/\sigma^2 = U^{\mathrm{T}}(I - H)\sigma^2U/\sigma^2 = U^{\mathrm{T}}UDU^{\mathrm{T}}U = D,$$

  i.e. the $Z_1, \ldots, Z_n$ are independent normal variables, $n - p$ of them have variance 1 and p of them have variance 0 and therefore equal 0 with probability one. Hence, as required,

  $$(n - p)S^2/\sigma^2 = e^{\mathrm{T}}e/\sigma^2 = (UZ)^{\mathrm{T}}(UZ) = Z^{\mathrm{T}}U^{\mathrm{T}}UZ = \sum_{j=1}^{n-p} Z_j^2 \sim \chi^2_{n-p}.$$

Note to Lemma 11

The spectral decomposition of H is UDU^{T}, where D is diagonal with p 1's and $n - p$ 0's, and $Z = U^{\mathrm{T}}y \sim \mathcal{N}_n(U^{\mathrm{T}}\mu, \sigma^2 I_n)$; note that the Z_j are independent. Now

$$y^{\mathrm{T}}Hy = (U^{\mathrm{T}}y)^{\mathrm{T}}D(U^{\mathrm{T}}y) = \sum_{j=1}^{n} d_j Z_j^2 = \sum_{j:d_j=1} Z_j^2,$$

which has a (possibly non-central) χ^2 distribution with $p = \mathrm{tr}(H)$ degrees of freedom, scale parameter σ^2 and

$$\sigma^2\delta^2 = \sum_{j:d_j=1} \mathrm{E}(Z_j)^2 = \sum_{j=1}^{n} d_j \mathrm{E}(Z_j)^2 = (U^{\mathrm{T}}\mu)^{\mathrm{T}}D(U^{\mathrm{T}}\mu) = \mu^{\mathrm{T}}H\mu.$$

Note to Theorem 12

- As $P_r P_s = 0$ for $r \neq s$, we have $\mathrm{cov}(P_r y, P_s y) = P_r \mathrm{var}(y) P_s^{\mathrm{T}} = \sigma^2 P_r P_s = 0$, i.e., $P_r y$ and $P_s y$ are independent. Hence the terms in the ANOVA decomposition are independent.
- P_r is a symmetric idempotent matrix, so Lemma 11 gives

$$\|P_r y\|^2 \sim \sigma^2 \chi^2_\nu(\delta_r^2/\sigma^2), \quad \delta_r^2 = \mu^{\mathrm{T}} P_r \mu,$$

  where $\nu = \mathrm{rank}(P_r)$. These ranks are $\nu_{r-1} - \nu_r$ for $r = 1, \ldots, R$, and $\nu_{R+1} = n - p$ for $P_{R+1} = I_n - H$.
- If X_r does not explain any variation in μ after allowing for $X_0, \ldots, X_{r-1}$, then $H_r \mu = H_{r-1}\mu \in \mathcal{V}_{r-1}$, i.e., $P_r \mu = 0$, and thus $\delta_r^2 = 0$.

Inference on β

- Theorem 10 implies that for any constant $c_{p\times 1}$, $c^{\mathrm{T}}\widehat{\beta} \sim \mathcal{N}\{c^{\mathrm{T}}\beta, \sigma^2 c^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}c\}$, so

$$Z = \frac{c^{\mathrm{T}}\widehat{\beta} - c^{\mathrm{T}}\beta}{\sigma\sqrt{c^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}c}} \sim \mathcal{N}(0,1) \quad \perp\!\!\!\perp \quad (n-p)S^2/\sigma^2 = W \sim \chi^2_{n-p},$$

  and thus

$$\frac{c^{\mathrm{T}}\widehat{\beta}_r - c^{\mathrm{T}}\beta_r}{S\sqrt{c^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}c}} = \frac{Z}{\sqrt{W/(n-p)}} \sim t_{n-p}.$$

- Let v_{rs} denote the (r,s) element of $(X^{\mathrm{T}}X)^{-1}$, so v_{rr} denotes its rth diagonal element.
- Different choices of c allow inferences on the elements of β.
- For example, if $c^{\mathrm{T}} = (c_1, \ldots, c_p)$, $c_r = 1$ and $c_s = 0$ for $s \neq r$, then $c^{\mathrm{T}}\beta = \beta_r$, and we
  - test the hypothesis that $\beta_r = \beta_r^0$ by comparing $(\widehat{\beta}_r - \beta_r^0)/(S v_{rr}^{1/2})$ to the t_{n-p} distribution, and
  - a $(1-\alpha)$ confidence interval for β_r has limits

$$\widehat{\beta}_r \pm S v_{rr}^{1/2} t_{n-p}(1-\alpha/2), \quad 0 < \alpha < 1.$$

- Likewise we can compare β_r and β_s by setting $c_r = 1$, $c_s = -1$ and all other $c_t = 0$.

Prediction

- Inference for the value of a further random variable Y_+ with known $p \times 1$ covariate vector x_+ and satisfying the linear model, so $Y_+ \sim \mathcal{N}(x_+^{\mathrm{T}}\beta, \sigma^2)$ independent of the other variables, is performed by noting that $Y_+ \perp\!\!\!\perp \widehat{\beta}, S^2$ and

$$Y_+ - x_+^{\mathrm{T}}\widehat{\beta} \sim \mathcal{N}\left[0, \sigma^2\{1 + x_+^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}x_+\}\right],$$

  so

$$\frac{Y_+ - x_+^{\mathrm{T}}\widehat{\beta}}{S\{1 + x_+^{\mathrm{T}}(X^{\mathrm{T}}X)^{-1}x_+\}^{1/2}} \sim t_{n-p},$$

  which leads to prediction intervals for Y_+ once $\widehat{\beta}$ and S have been observed.
- Although we expect inferences for β and σ^2 to hold as approximations under second-order assumptions, this is not the case for inference on Y_+. (Why not?)

1.3 Analysis of Variance slide 33

Analysis of variance

☐ We previously saw that

$$\sum_{j=1}^{n}(y_j-\overline{y})^2=\|y\|^2-\|\widehat{y}_0\|^2=\sum_{r=1}^{R}\|\widehat{y}_r-\widehat{y}_{r-1}\|^2+\|y-\widehat{y}\|^2$$

decomposes ('analyses') the variability of y around its average $\overline{y}$ into

- the contributions $\|\widehat{y}_r-\widehat{y}_{r-1}\|^2$ due to adding the columns of X_r to $X_0,\ldots,X_{r-1}$,
- the **residual sum of squares** $\|y-\widehat{y}\|^2$ left after fitting $X=(X_0,\ldots,X_R)$.

☐ Large $\|\widehat{y}_r-\widehat{y}_{r-1}\|^2$ implies that X_r explains a lot of the variation of y even after allowing for that explained by $X_0,\ldots,X_{r-1}$.

☐ Theorem 12 implies that under the normal assumptions, and if $\mathrm{E}(y)=\mu$ lies in the column space of X, the sums of squares on the RHS above are independent and satisfy

$$\|\widehat{y}_r-\widehat{y}_{r-1}\|^2=\|P_r y\|^2\sim\sigma^2\chi^2_{\nu_{r-1}-\nu_r}(\delta_r^2/\sigma^2)\quad\perp\!\!\!\perp\quad\|y-\widehat{y}\|^2\sim\sigma^2\chi^2_{n-p}.$$

Hence if $\delta_r^2=0$, i.e., $\mu\in\mathrm{span}(X_0,\ldots,X_{r-1})$, then

$$\frac{\|\widehat{y}_r-\widehat{y}_{r-1}\|^2/(\nu_{r-1}-\nu_r)}{\|y-\widehat{y}\|^2/(n-p)}\sim F_{\nu_{r-1}-\nu_r,n-p}.$$

ANOVA table

Term added	df	Reduction in SS	Mean square
X_1	$n-1-\nu_1$	$\mathrm{SS}_0-\mathrm{SS}_1$	$\mathrm{MS}_1=(\mathrm{SS}_0-\mathrm{SS}_1)/(n-1-\nu_1)$
X_2	$\nu_1-\nu_2$	$\mathrm{SS}_1-\mathrm{SS}_2$	$\mathrm{MS}_2=(\mathrm{SS}_1-\mathrm{SS}_2)/(\nu_1-\nu_2)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
X_R	$\nu_{R-1}-\nu_R$	$\mathrm{SS}_{R-1}-\mathrm{SS}_R$	$\mathrm{MS}_R=(\mathrm{SS}_{R-1}-\mathrm{SS}_R)/(\nu_{R-1}-\nu_R)$
Residual	$\nu_R=n-p$	SS_R	$\mathrm{MS}_{\mathrm{Res}}=\mathrm{SS}_R/\nu_R$

☐ If $\mu\in\mathrm{span}(X)$ then the residual mean square $\mathrm{MS}_{\mathrm{Res}}$ gives an estimate of σ^2.

☐ We test for an effect of term X_r by noting that

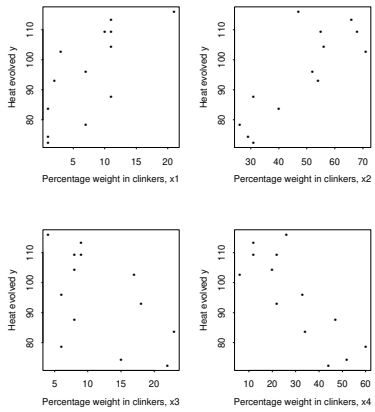
- if X_r explains no more than $(X_0,\ldots,X_{r-1})$, then

$$F_r=\frac{\mathrm{MS}_r}{\mathrm{MS}_{\mathrm{Res}}}\sim F_{\nu_{r-1}-\nu_r,\nu_R},$$

- if X_r does have additional explanatory power, then the distribution of MS_r is shifted to the right, and we expect F_r to be large relative to its null distribution.

Example: Cement data

Percentage weights in clinkers of 4 four constitutents of cement $(x_1, \ldots, x_4)$ and heat evolved y in calories, in $n = 13$ samples.



Example: Cement data

```
> cement
   x1 x2 x3 x4     y
1   7 26  6 60  78.5
2   1 29 15 52  74.3
3  11 56  8 20 104.3
4  11 31  8 47  87.6
5   7 52  6 33  95.9
6  11 55  9 22 109.2
7   3 71 17  6 102.7
8   1 31 22 44  72.5
9   2 54 18 22  93.1
10 21 47  4 26 115.9
11  1 40 23 34  83.8
12 11 66  9 12 113.3
13 10 68  8 12 109.4
```

Example: Cement data

- Reductions in overall sum of squares when terms entered in the order given.
- Clearly x_1 and x_2 should be included, maybe not the others.

Term	df	Reduction in sum of squares	Mean square	F
x_1	1	1450.1	1450.1	242.5
x_2	1	1207.8	1207.8	202.0
x_3	1	9.79	9.79	1.64
x_4	1	0.25	0.25	0.04
Residual	8	47.86	5.98	

Example: Cement data

- What if we change the order of the terms?

Term	df	Reduction in sum of squares	Mean square	F
x_4	1	1831.9	1831.9	306.2
x_3	1	708.1	708.1	118.4
x_2	1	101.9	101.9	17.04
x_1	1	26.0	26.0	4.34
Residual	8	47.86	5.98	

- Should x_1 and x_2 be included or not?

Orthogonality

- In general, the ANOVA and ANOVA table depend on the order of inclusion of terms.
- Its interpretation is unclear if X_r is significant when included early, but not when it is included late. Is the term important or not?
- In a model with orthogonal terms,

$$X\beta = 1_n\beta_0 + X_1\beta_1 + X_2\beta_2, \quad X_r^{\mathrm{T}}X_s = X_r^{\mathrm{T}}1_n = 0, \quad r \neq s.$$

we obtain

$$\begin{pmatrix} \widehat{\beta}_0 \\ \widehat{\beta}_1 \\ \widehat{\beta}_2 \end{pmatrix} = \begin{pmatrix} 1^{\mathrm{T}}1 & 0 & 0 \\ 0 & X_1^{\mathrm{T}}X_1 & 0 \\ 0 & 0 & X_2^{\mathrm{T}}X_2 \end{pmatrix}^{-1} \begin{pmatrix} 1 & X_1 & X_2 \end{pmatrix}^{\mathrm{T}} y$$

so since $\widehat{y} = X\widehat{\beta}$, we have

$$y^{\mathrm{T}}y - \widehat{y}^{\mathrm{T}}\widehat{y} = y^{\mathrm{T}}y - n\overline{y}^2 - \widehat{\beta}_1^{\mathrm{T}}X_1^{\mathrm{T}}X_1\widehat{\beta}_1 - \widehat{\beta}_2^{\mathrm{T}}X_2^{\mathrm{T}}X_2\widehat{\beta}_2,$$

and the residual sums of squares for the sub-models $1_n\beta_0$, $1_n\beta_0 + X_1\beta_1$, $1_n\beta_0 + X_2\beta_2$ are

$$y^{\mathrm{T}}y - n\overline{y}^2, \quad y^{\mathrm{T}}y - n\overline{y}^2 - \widehat{\beta}_1^{\mathrm{T}}X_1^{\mathrm{T}}X_1\widehat{\beta}_1, \quad y^{\mathrm{T}}y - n\overline{y}^2 - \widehat{\beta}_2^{\mathrm{T}}X_2^{\mathrm{T}}X_2\widehat{\beta}_2,$$

so the reductions do not depend on the order of inclusion. Hooray!

Balance

- Balanced design matrices induce orthogonality after fitting 1_n (or a more complex design X_0).
- Gram–Schmidt orthogonalisation with respect to early terms makes later terms mutually orthogonal, leading to a clear interpretation of the ANOVA for the later terms.
- If we write $H_0 = X_0(X_0^{\mathrm{T}}X_0)^{-1}X_0^{\mathrm{T}}$ and let

$$Z_r = P_0X_r = (I_n - H_0)X_r, \quad r = 1, 2,$$

denote the versions of X_1 and X_2 after adjusting for X_0, then

$$\begin{aligned} X_0\beta_0 + X_1\beta_1 + X_2\beta_2 &= (X_0\beta_0 + H_0X_1\beta_1 + H_0X_2\beta_2) + P_0X_1\beta_1 + P_0X_2\beta_2 \\ &= Z_0\gamma_0 + Z_1\beta_1 + Z_2\beta_2, \end{aligned}$$

say, and $Z_1^{\mathrm{T}}Z_0 = Z_2^{\mathrm{T}}Z_0 = 0$, because $P_0X_0 = P_0H_0 = 0$.
- If the design satisfies $Z_1^{\mathrm{T}}Z_2 = 0$, then the order of inclusion of X_1, X_2 is irrelevant, provided X_0 is already present in the fit.

Example 13 (3×2 layout) *Observations and their means written as*

$$\begin{array}{cc} y_{11} & y_{12} \\ y_{21} & y_{22}, \\ y_{31} & y_{32} \end{array} \qquad \begin{array}{cc} \mu + \alpha_1 + \delta_1 & \mu + \alpha_2 + \delta_1 \\ \mu + \alpha_1 + \delta_2 & \mu + \alpha_2 + \delta_2. \\ \mu + \alpha_1 + \delta_3 & \mu + \alpha_2 + \delta_3 \end{array}$$

Note to Example 13

☐ In terms of the parameter vector $(\mu, \alpha_1, \alpha_2, \delta_1, \delta_2, \delta_3)^{\mathrm{T}}$, the design matrix is

$$X^*_{6\times 6} = \begin{pmatrix} 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 1 \end{pmatrix}, \quad \text{with responses} \quad y = \begin{pmatrix} y_{11} \\ y_{12} \\ y_{21} \\ y_{22} \\ y_{31} \\ y_{32} \end{pmatrix},$$

with $X_0 \equiv 1_6$ the first column of X^*, columns 2–3 the term X^*_1 for columns, and columns 4–6 the term X^*_2 for rows.

☐ This model has six parameters, but they cannot all be estimated, because X_0 lies in the column spaces of X^*_1 and X^*_2, and it is easy to check that X^* has rank 4. The usual way to deal with this is to set $\alpha_1 = \delta_1 = 0$, corresponding to dropping columns 2 and 4 of X^*, giving the so-called *corner-point parametrization* in which the means are

$$\begin{array}{cc} y_{11} & y_{12} \\ y_{21} & y_{22}, \\ y_{31} & y_{32} \end{array} \qquad \begin{array}{cc} \mu & \mu + \alpha_2 \\ \mu + \delta_2 & \mu + \alpha_2 + \delta_2, \\ \mu + \delta_3 & \mu + \alpha_2 + \delta_3 \end{array}$$

i.e.,

- the 'grand mean' μ corresponds to the mean of observations with the first level of every factor,
- α_2 corresponds to the mean difference between column 2 and column 1,
- δ_2 corresponds to the mean difference between row 2 and row 1, and
- δ_3 corresponds to the mean difference between row 3 and row 1.

This is the default in R. More rarely we might set $\sum_c \alpha_c = \sum_r \delta_r = 0$.

☐ Even after these columns are dropped to give

$$X = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 \end{pmatrix},$$

the terms X_1 for columns and X_2 for rows are not orthogonal, and they are not orthogonal to 1_n. On the other hand Z_1 and Z_2 in the corresponding centred matrix,

$$\begin{pmatrix} 1 & -\frac{1}{2} & -\frac{1}{3} & -\frac{1}{3} \\ 1 & \frac{1}{2} & -\frac{1}{3} & -\frac{1}{3} \\ 1 & -\frac{1}{2} & \frac{2}{3} & -\frac{1}{3} \\ 1 & \frac{1}{2} & \frac{2}{3} & -\frac{1}{3} \\ 1 & -\frac{1}{2} & -\frac{1}{3} & \frac{2}{3} \\ 1 & \frac{1}{2} & -\frac{1}{3} & \frac{2}{3} \end{pmatrix}$$

are orthogonal to the constant by construction and to each other because the design is balanced: δ_2 and δ_3 each occur equally often with α_2 and without α_2. This balance implies that if μ is fitted first, the reductions in sums of squares due to X_1 and X_2, or equivalently Z_1 and Z_2, are unique.

1.4 Diagnostics

Assumptions and model checking

- How heavily do our conclusions depend on our assumptions?
- In any given context,
  - **primary** aspects relate to the questions our analysis will address,
  - **secondary** aspects relate to how we go about finding answers to them.
- Concerns about primary aspects suggest that we should start again.
- Concerns about secondary aspects suggest that we modify the analysis.
- **Regression diagnostics** check that a fitted model is adequate:
  - Does y depend linearly on the columns of X?
  - Does y depend systematically on variables omitted from X?
  - Are the variances constant?
  - Are the responses uncorrelated/independent?
  - Are there outliers or otherwise unusual data?
  - Are the responses normally distributed?
- Usually these involve plots, sometimes tests — **beware over-interpretation**!
- Key question: 'how would the failure I see/suspect change my conclusions?'

Residuals

- The **raw residuals**

$$e = y - \widehat{y} = y - X\widehat{\beta} = (I_n - H)y$$

  have $\mathrm{E}(e) = 0$, $\mathrm{var}(e) = \sigma^2(I_n - H)$ if model correct, so

$$\mathrm{var}(e_j) = \sigma^2(1 - h_{jj}) \quad \mathrm{cov}(e_j, e_k) = -\sigma^2 h_{jk},\ j \neq k.$$

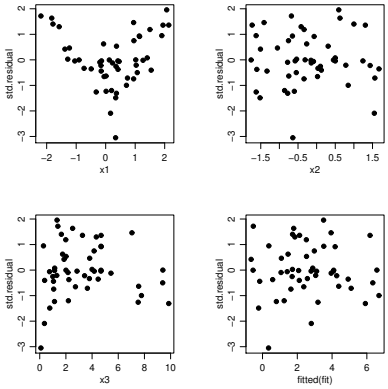
- To (roughly) equalise the variances we define **standardized residuals**

$$r_j = \frac{e_j}{s(1-h_{jj})^{1/2}} = \frac{y_j - x_j^{\mathrm{T}}\widehat{\beta}}{s(1-h_{jj})^{1/2}}, \quad j = 1, \ldots, n,$$

  with s replacing σ. Then $\mathrm{E}(r_j) = 0$ and $\mathrm{var}(r_j) \doteq 1$.
- Although $e^{\mathrm{T}}\widehat{y} = \mathrm{cov}(e, \widehat{y}) = 0$ (check!), this only implies no linear relation between e and $\widehat{y}$.
- We check
  - linearity by plotting r_j against the covariates (those in X and those not in X);
  - constant variance by plotting r_j (or $|r_j|$) against fitted values $\widehat{y}_j$;
  - independence by ACF of residuals (if data time-ordered);
  - for outliers, which are visible as unusual residuals; and
  - normality using a normal QQ-plot of r_j.

Checking linearity

☐ Plot r against each covariate, included or not in the model, and against $\widehat{y}$, which is uncorrelated with e (as $\widehat{y}^{\mathrm{T}}e = 0$):

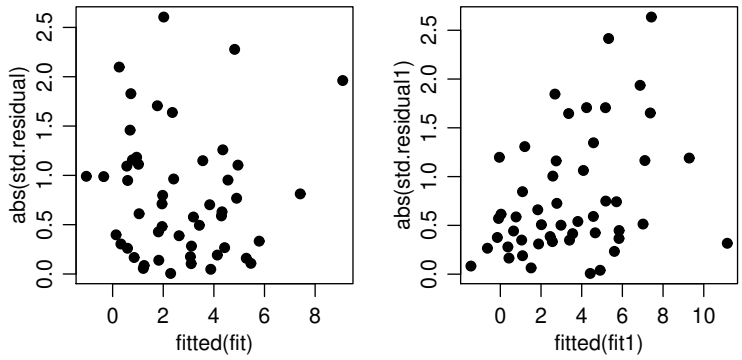


Checking the variance

☐ Does $\mathrm{var}(y)$ depend on $\mathrm{E}(y)$?

☐ Variance function shows how $\mathrm{var}(y)$ depends on $\mu = \mathrm{E}(y)$. For normal linear model should have $\mathrm{var}(y) = \sigma^2$, so variance is constant function of μ

☐ Plot r or $|r|$ against $\widehat{y}$:



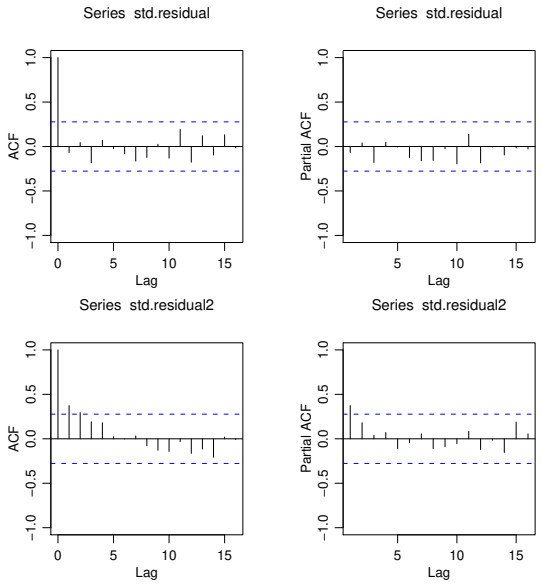
Checking independence

- ☐ Dependence can greatly increase uncertainty of final conclusions.
- ☐ Substantive knowledge is helpful in suggesting whether it might be present:
  - were the data gathered in temporal/spatial/. . . order?
  - were the data sampled/gathered in groups (e.g., spatial, several observations on different individuals, . . .)?
  - was randomisation used? If so, how?
- ☐ If observations are time-ordered, try using correlogram (ACF) and partial correlogram (PACF) to estimate serial correlations and partial correlations

$$\mathrm{corr}(r_j, r_{j+t}), \quad \mathrm{corr}(r_j, r_{j+t} \mid r_{j+1}, \ldots, r_{j+t-1}), \quad t = 1, \ldots$$

- ☐ On next page, top panels show uncorrelated residuals, lower ones show evidence of correlation, suggesting use of a time series model.

Checking independence



Checking for outliers and normality

- ☐ Normal Q-Q plot for $Y_1, \ldots, Y_n \overset{\text{iid}}{\sim} \mathcal{N}(\mu, \sigma^2)$ graphs ordered values

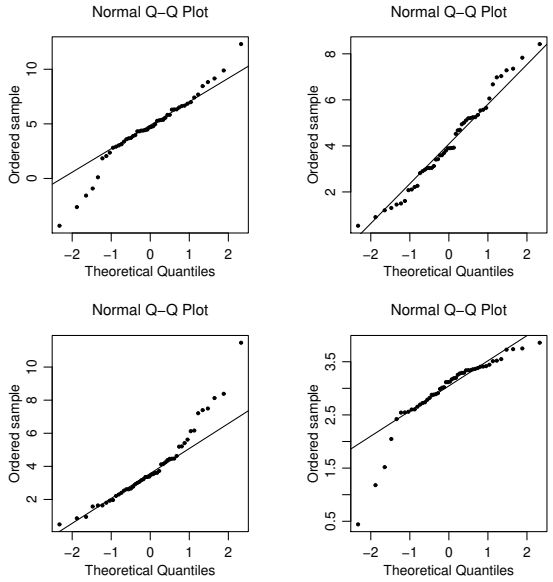
$$Y_{(1)} \leq Y_{(2)} \leq \cdots \leq Y_{(n)}$$

  against (approximate) expected normal order statistics

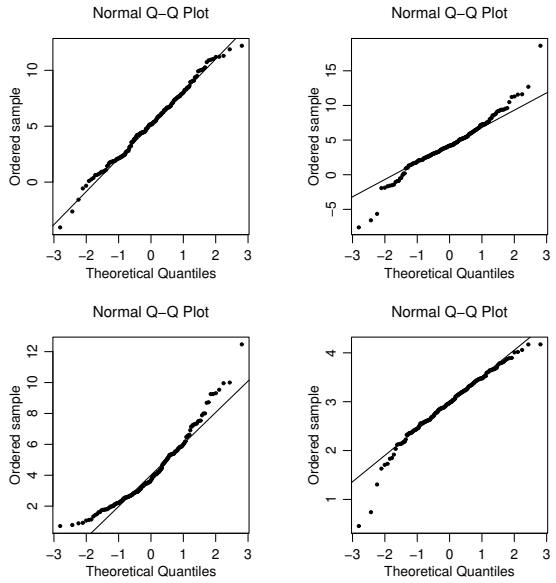
$$\Phi^{-1}\{1/(n+1)\}, \Phi^{-1}\{2/(n+1)\}, \ldots, \Phi^{-1}\{n/(n+1)\}.$$

- ☐ Normality — roughly straight line, slope σ, intercept μ.
- ☐ Outliers, skewness, heavy tails (easily) seen.
- ☐ Beware over-interpretation of such plots when n is small — often useful to add simulation envelope.
- ☐ Apply to standardized residuals r_j from regression model.

Checking normality, $n = 50$



Checking normality, $n = 200$



Leverage and influence

- ☐ Does **case** (x_j, y_j) strongly influence the fitted model (picture)?
- ☐ As

$$\mathrm{var}(y_j - \widehat{y}_j) = \mathrm{var}(y_j - x_j^{\mathrm{T}}\beta) = \sigma^2(1 - h_{jj}),$$

  having **leverage** $h_{jj} \doteq 1$ implies that $\widehat{y}_j \approx y_j$ — need one parameter to fit this case.
- ☐ As $\mathrm{tr}(H) = \sum_{j=1}^{n} h_{jj} = p$, the average h_{jj} is p/n. If $h_{jj} > 2p/n$, then jth case should be checked (rule of thumb), e.g. by refitting without (x_j, y_j).
- ☐ Let $\widehat{y}_{-j}$ be fitted values for (all) data when (x_j, y_j) is dropped and use **Cook's distance**

$$C_j = \frac{1}{ps^2}(\widehat{y} - \widehat{y}_{-j})^{\mathrm{T}}(\widehat{y} - \widehat{y}_{-j}) = \cdots = \frac{r_j^2 h_{jj}}{p(1 - h_{jj})}$$

  to measure the difference between $\widehat{y}$ and $\widehat{y}_{-j}$.
- ☐ Large C_j implies large r_j and/or large h_{jj}.
- ☐ Cases with $C_j > 8/(n - 2p)$ worth a closer look (rule of thumb).
- ☐ High leverage and/or influence need not be bad, just need to be aware of it.
- ☐ These ideas are not very useful in large samples, since the plots become uninformative.

Response transformation

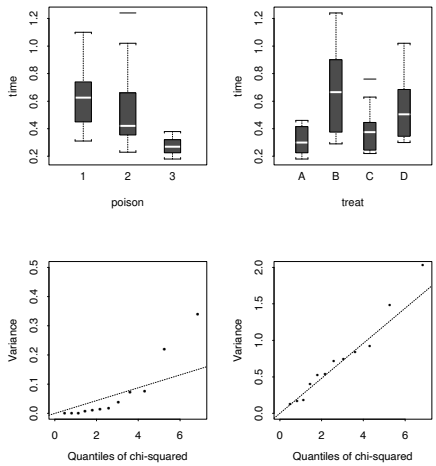
- ☐ Linear model for y may be better applied for some transformation $g(y)$, especially if some y are much larger than others, or the variance is non-constant.
- ☐ Survival times y_{ptj} in 10-hour units of animals in a 3×4 factorial experiment with four replicates, with (below) average (standard deviation) for the poison $\times$ treatment combinations:
  - generally see higher SD and mean together,
  - times must be positive, so linear model inappropriate?

Treatment	Poison 1	Poison 2	Poison 3
A	0.31, 0.45, 0.46, 0.43	0.36, 0.29, 0.40, 0.23	0.22, 0.21, 0.18, 0.23
B	0.82, 1.10, 0.88, 0.72	0.92, 0.61, 0.49, 1.24	0.30, 0.37, 0.38, 0.29
C	0.43, 0.45, 0.63, 0.76	0.44, 0.35, 0.31, 0.40	0.23, 0.25, 0.24, 0.22
D	0.45, 0.71, 0.66, 0.62	0.56, 1.02, 0.71, 0.38	0.30, 0.36, 0.31, 0.33

Treatment	Poison 1	Poison 2	Poison 3	Average
A	0.41 (0.07)	0.32 (0.08)	0.21 (0.02)	0.31
B	0.88 (0.16)	0.82 (0.34)	0.34 (0.05)	0.68
C	0.57 (0.16)	0.38 (0.06)	0.24 (0.01)	0.39
D	0.61 (0.11)	0.67 (0.27)	0.33 (0.03)	0.53
Average	0.62	0.55	0.28	0.48

Example: Poison data

Upper panels: dependence of responses on the factor levels. Lower left: χ^2_3 probability plots of the $3s^2_{pt}$, where s^2_{pt} is the sample variance of y_{ptj}. Lower right: same for y^{-1}_{ptj}.



Box–Cox transformation

- For $y > 0$, the **Box–Cox transformation**

$$y^{(\lambda)} = \begin{cases} \frac{y^\lambda - 1}{\lambda}, & \lambda \neq 0, \\ \log y, & \lambda = 0, \end{cases}$$

  includes the inverse ($\lambda = -1$), log ($\lambda = 0$), cube and square roots ($\lambda = \frac{1}{3}, \frac{1}{2}$), original scale ($\lambda = 1$) and square ($\lambda = 2$); sometimes map $y \mapsto y + c > 0$.

- Suppose normal linear model

$$y^{(\lambda)} \sim \mathcal{N}_n(X\beta, \sigma^2 I_n)$$

  applies for some β, σ and λ to be determined. Here X contains 1_n, so use of $y^{(\lambda)}$ just changes intercept and rescales β and σ.

- Use profile log likelihood for λ to choose 'best' transformation (usually from list above to aid interpretation).

- Interpretation of β depends on λ, so usually we ignore the fact that λ was estimated, unless we are not interested in β (e.g., when performing 'automatic' prediction).

Example: Poison data

- Fits of two-way layout model, with interaction:

$$y_{tpj}^{(\lambda)} \sim \mathcal{N}(\mu + \alpha_t + \beta_p + \gamma_{tp}, \sigma^2), \quad t = 1,2,3,4,\ p = 1,2,3,\ j = 1,2,3,4.$$

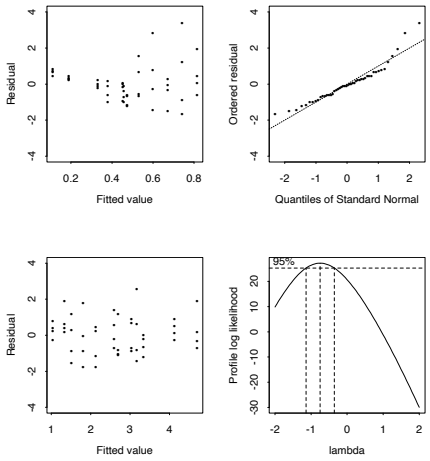
- Analyses of variance with responses y and y^{-1}. For MS and F read 'Mean square' and 'F statistic'.

- The terms explain appreciably more of the variation of y^{-1}, suggesting that this is a preferable choice of response.

Term	df	Response y			Response y^{-1}		
		SS	MS	F	SS	MS	F
Poisons	2	1.033	0.517	23.22	34.88	17.44	72.63
Treatments	3	0.921	0.307	13.81	20.41	6.80	28.34
Treatments × Poisons	6	0.250	0.042	1.87	1.57	0.26	1.09
Residual	36	0.801	0.022		8.64	0.24	

Example: Poison data

Top: residuals for model without interactions γ_{tp}; clearly problematic.
Lower right: profile log likelihood for Box–Cox λ, showing 95% confidence interval.
Lower left: residuals for the two-way layout model (no interactions) for $1/y$.



Summary on model-checking

- ☐ Recall the distinction between primary and secondary assumptions. Use of the standard linear model when the secondary assumptions fail leads to inefficient estimation and over-confident uncertainty assessment, but is not usually disastrous per se.
- ☐ When they fail ...
  - **Linearity** (primary): add terms (e.g., x^2) to the model, transform the covariate (e.g., to $\log x$), or question the basic setup;
  - **Constant variance** (secondary): use a response transformation (below), weighted least squares, or question primary aspects. Non-constant variance affects uncertainty assessment, but not estimation;
  - **Lack of correlation (independence)** (secondary): use a correlated error model (e.g., time series or random effects). Dependence affects uncertainty assessment, but not estimation;
  - **normality** (secondary): often does not matter, because the CLT applies to the estimators. It does matter for prediction, which is affected by the distribution of individual responses;
- ☐ Checking leverage and influence may be useful in small and moderate samples, but rarely in large samples. In any case, automatic dropping of outlying and/or influential cases is dangerous!

1.5 Model Building

Goals

- ☐ What to do faced with a set of data?
- ☐ Two main aims:
  - **understand** (science) — maybe have prior idea/hypotheses on how response depends on explanatory variables. Interpretation is key.
  - **predict/control** (technology) — don't really care how y depends on X. Interpretation not critical (though this describes only prediction in the narrowest of senses).
- ☐ There is no reason that a single model will do both, or even that there must be a single 'best' model:
  - maybe two models with different interpretations both fit about equally well, and then future work might aim to choose between them;
  - prediction with a mixture of models might be better than using a single model.

Meta-algorithm

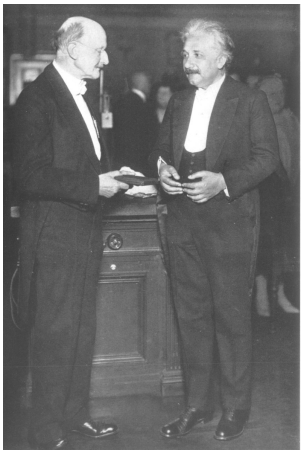
- ☐ **Collect** data intended to answer question of interest;
- ☐ **examine** data (graphs, look for outliers, problems with sampling scheme);
- ☐ **choose/construct** response variable (transformations? independence?);
- ☐ **consider** what models are coherent with context of problem (limiting properties, units, similar problems/datasets, covariates that must be included, ...);
- ☐ **iterate**:
  - fit models, compare quality of fits;
  - check interpretations of $\widehat{\beta}, \widehat{\sigma}^2$ and
  - check fit (diagnostics, outliers, ...)

  until satisfied; finally
- ☐ give **conclusions**—careful interpretation of best model(s) in terms of original problem, consider deficiencies, and explain what extra data might overcome them.

Initial examination of data

- ☐ Plot y against covariates, look for outliers, non-constant variance, nonlinearity, etc.
- ☐ Plot covariates against each other, look for dependence.
- ☐ Try to understand covariates (e.g., dimensions), are transformations needed?
- ☐ May need to reduce dimension of X by **regularisation** — many ways to do this (later).

Albert Einstein (1879–1955)



'Everything should be made as simple as possible, *but no simpler*.'

William of Occam (?1285–1347/9)

Occam's razor: *Pluralitas non est ponenda sine necessitate*: entities should not be multiplied beyond necessity.

Automatic variable selection

- Assume linear model $\mathrm{E}(y) = X\beta$
- 2^p possible subsets of columns of X, plus transformations, ...
- Example: $p = 17$ gives 131072 possible subsets of variables
- Fast algorithms (e.g., branch and bound, `leaps` in `R`) exist visit them all or just subsets (e.g., stepwise), but we need criteria for comparing models.
- Many proposals for model comparison
  - cross-validation,
  - information criteria (AIC, $\mathrm{AIC_c}$, BIC, NIC, TIC, ...)
  - Mallow's C_p,
  - ...
- Most involve minimising estimated prediction error for future data *like those observed*!

Prediction error

- True model $y \sim (\mu, \sigma^2 I_n)$, we assume (perhaps incorrectly) that $\mu = X\beta$, fit $X_{n\times p}$ and obtain fitted value
$$X\widehat{\beta} = Hy \sim (H\mu, \sigma^2 H).$$
- Terminology
  - the **true model** has $\mu = X\beta$ and all $\beta_r \neq 0$;
  - a **correct model** has $\mu = X\beta$ but some $\beta_r = 0$;
  - a **wrong** model has $\mu \notin \mathrm{span}(X)$;

  so $(I_n - H)\mu = 0$ if the model is true or correct, and $(I_n - H)\mu \neq 0$ if it is wrong.
- The **prediction error** for an independent dataset y_+ with mean vector μ is
$$\Delta = n^{-1}\mathrm{E}\left\{(y_+ - X\widehat{\beta})^{\mathrm{T}}(y_+ - X\widehat{\beta})\right\} = \begin{cases} n^{-1}\mu^{\mathrm{T}}(I-H)\mu + (1+p/n)\sigma^2, & \text{wrong,} \\ (1+q/n)\sigma^2, & \text{true,} \\ (1+p/n)\sigma^2, & \text{correct,} \end{cases}$$
  where $\mathrm{E}(\cdot)$ is over both y_+ and y and $p \geq q = \#\{\beta_r : \beta_r \neq 0\}$ when $\mu \in \mathrm{span}(X)$.
- In principle we should write $\Delta \equiv \Delta(X)$.

Note: Computation of Δ

Let $y \sim (\mu, \sigma^2 I)$ and fit $X\beta$, obtaining fitted value

$$X\widehat{\beta} = Hy \sim (H\mu, \sigma^2 H),$$

where $H\mu = \mu$, i.e., $(I - H)\mu = 0$ if $\mu \in \text{span}(X)$, but otherwise $(I - H)\mu \neq 0$.
We have a new data set $y_+ \sim (\mu, \sigma^2 I)$, and we compute the average error in predicting y_+ using $X\widehat{\beta}$, i.e.,

$$\Delta = n^{-1}\text{E}\left\{(y_+ - X\widehat{\beta})^{\text{T}}(y_+ - X\widehat{\beta})\right\}.$$

Let $e_+ = y_+ - X\widehat{\beta}$ and note that as the trace of a scalar is the scalar and trace is a linear operator,

$$\text{E}(e_+^{\text{T}} e_+) = \text{E}\{\text{tr}(e_+^{\text{T}} e_+)\} = \text{E}\{\text{tr}(e_+ e_+^{\text{T}})\} = \text{tr}\{\text{E}(e_+ e_+^{\text{T}})\} = \text{tr}\{\text{var}(e_+) + \text{E}(e_+)\text{E}(e_+)^{\text{T}})\}.$$

Now as y_+ and y are independent and $\text{var}(X\widehat{\beta}) = \sigma^2 H$, we have

$$y_+ - X\widehat{\beta} \sim (\mu - H\mu, \sigma^2 I + \sigma^2 H),$$

so the computation above gives

$$\text{E}\left\{(y_+ - X\widehat{\beta})^{\text{T}}(y_+ - X\widehat{\beta})\right\} = \text{tr}\{\sigma^2(I + H) + (I - H)\mu\mu^{\text{T}}(I - H)\} = \sigma^2(n + p) + \mu^{\text{T}}(I - H)\mu,$$

because $\text{tr}(I + H) = n + p$ and $I - H$ is symmetric and idempotent, giving

$$\Delta = \begin{cases} n^{-1}\mu^{\text{T}}(I - H)\mu + (1 + p/n)\sigma^2, & \text{wrong model,} \\ (1 + q/n)\sigma^2, & \text{true model,} \\ (1 + p/n)\sigma^2, & \text{correct model.} \end{cases}$$

Bias/variance trade-off

- ☐ Minimising Δ involves balancing the
  - **bias** $n^{-1}\mu^{\text{T}}(I - H)\mu$, which is reduced by including useful terms in X, and
  - **variance** $(1 + p/n)\sigma^2$, which is increased by including useless terms in X.
- ☐ We would like to minimise Δ, but it depends on the unknown μ and σ.
- ☐ The **cross-validation** estimator of Δ splits the data into X', y' and X^*, y^*, then
  - for each possible subset $\mathcal{S}$ of columns of X^*:
    - ▷ compute $\widehat{\beta}^*_{\mathcal{S}}$ by regressing y^* on $X^*_{\mathcal{S}}$;
    - ▷ use $\widehat{\beta}^*_{\mathcal{S}}$ to estimate the prediction error for $\mathcal{S}$ by

$$\widehat{\Delta}_{\mathcal{S}} = (n')^{-1}(y' - X'_{\mathcal{S}}\widehat{\beta}^*_{\mathcal{S}})^{\text{T}}(y' - X'_{\mathcal{S}}\widehat{\beta}^*_{\mathcal{S}});$$

  - finally choose the set of columns $\mathcal{S}$ for which $\widehat{\Delta}_{\mathcal{S}}$ is minimised.
- ☐ This estimator depends on the split, and since $X' \neq X^*$ in general, $\widehat{\Delta}_{\mathcal{S}}$ does not estimate $\Delta_{\mathcal{S}}$, so it would be preferable to use the entire dataset ...

Leave-one-out cross-validation

- Simplest way to use entire dataset is **leave-one-out cross-validation (CV)**, minimising

$$n\widehat{\Delta}_{\mathrm{CV}} = \mathrm{CV} = \sum_{j=1}^{n}(y_j - x_j^{\mathrm{T}}\widehat{\beta}_{-j})^2,$$

  where $\widehat{\beta}_{-j}$ is estimate computed without (x_j, y_j).
- This seems to require n fits, but the lemma below implies that with one fit we have

$$\mathrm{CV} = \sum_{j=1}^{n}\frac{(y_j - x_j^{\mathrm{T}}\widehat{\beta})^2}{(1-h_{jj})^2}.$$

Lemma 14 *For a fit $\widehat{y} = Hy$ where H has jth diagonal element h_{jj} and $\widehat{y}_{j,-j}$ is the fitted value for y_j obtained when (x_j, y_j) is dropped,*

$$y_j - \widehat{y}_{j,-j} = \frac{y_j - \widehat{y}_j}{1-h_{jj}},$$

and therefore

$$\sum_{j=1}^{n}(y_j - \widehat{y}_{j,-j})^2 = \sum_{j=1}^{n}\frac{(y_j - \widehat{y}_j)^2}{(1-h_{jj})^2}.$$

Note to Lemma 14

- Consider any linear fit $\widehat{y} = Hy$, and note that $\widehat{y}_j = \sum_{i=1}^{n} h_{ji}y_i$.
- Now suppose we leave out (x_j, y_j) and compute the corresponding (penalized) estimate

$$\widehat{\beta}_{-j} = \mathrm{argmin}_{\beta} \quad \sum_{i\neq j}(y_i - x_i^{\mathrm{T}}\beta)^2 + \lambda p(\beta),$$

  and fitted value $y_j^* = \widehat{y}_{j,-j} = x_j^{\mathrm{T}}\widehat{\beta}_{-j}$ corresponding to x_j.
- Inserting (x_j, y_j^*) back into the dataset used to compute $\widehat{\beta}_{-j}$ changes nothing, because $(y^* - x_j^{\mathrm{T}}\widehat{\beta}_{-j})^2 = 0$ and $p(\beta)$ does not depend on the data. For this new dataset,

$$y_j^* = \sum_{i\neq j} h_{ji}y_i + h_{jj}y_j^* = \sum_{i=1}^{n} h_{ji}y_i + h_{jj}(y_j^* - y_j) = \widehat{y}_j + h_{jj}(y_j^* - y_j)$$

  so

$$y_j - y_j^* = y_j - \widehat{y}_j + h_{jj}(y_j - y_j^*),$$

  leading to

$$y_j - y_j^* = y_j - \widehat{y}_{j,-j} = \frac{y_j - \widehat{y}_j}{1-h_{jj}},$$

  and thus to the given formula.

Generalized cross-validation

- Leave-one-out CV can be unstable if some of the h_{jj} are large.
- **Generalised cross-validation (GCV)** replaces all the h_{jj} by their average $\mathrm{tr}(H)/n = p/n$, giving

$$\mathrm{GCV} = \sum_{j=1}^{n} \frac{(y_j - x_j^{\mathrm{T}}\widehat{\beta})^2}{(1-p/n)^2},$$

  and hence

$$\mathrm{E}(\mathrm{GCV}) = \mu^{\mathrm{T}}(I-H)\mu/(1-p/n)^2 + n\sigma^2/(1-p/n) \approx n\Delta.$$

- Often choose the model that minimises GCV or CV.
- Note that these only require the second-order assumptions.

Note: Properties of GCV

We have $(1-p/n)^2\mathrm{GCV} = e^{\mathrm{T}}e$ where $e = y - X\widehat{\beta} = (I-H)y \sim ((I-H)\mu, (I-H)\sigma^2)$, and

$$\mathrm{E}\left(e^{\mathrm{T}}e\right) = \mathrm{E}\left\{\mathrm{tr}\left(ee^{\mathrm{T}}\right)\right\} = \mathrm{tr}\left\{\mathrm{E}(e)\mathrm{E}(e)^{\mathrm{T}} + \mathrm{var}(e)\right\} = \mu^{\mathrm{T}}(I-H)\mu + \sigma^2\mathrm{tr}(I-H).$$

Now note that $\mathrm{tr}(I-H) = n-p$ and divide by $(1-p/n)^2$ to give (almost) the required result, for which we need also $(1-p/n)^{-1} \approx 1 + p/n$, for $p \ll n$.

Akaike information criterion

- The above arguments apply only to least squares estimators. More generally, we could aim to minimise the **Kullback–Leibler discrepancy**

$$D(f_\theta, g) = \int \log\left\{\frac{g(y)}{f(y;\theta)}\right\} g(y)\,\mathrm{d}y \geq 0,$$

  between **candidate model** $f_\theta \equiv f(y;\theta)$ and true model g, based on $Y_1, \ldots, Y_n \overset{\mathrm{iid}}{\sim} g$.
- Suppose that θ_g minimises $D(f_\theta, g)$ within the family of candidate models, and is estimated by the MLE $\widehat{\theta}$, with log likelihood $\widehat{\ell}$.
- We suppose there is an independent sample $Y_1^+, \ldots, Y_n^+ \overset{\mathrm{iid}}{\sim} g$ and aim to estimate

$$\mathrm{E}_g\left(\mathrm{E}_g^+\left[\sum_{j=1}^{n} \log\left\{\frac{g(Y_j^+)}{f(Y_j^+;\widehat{\theta})}\right\}\right]\right) = n\mathrm{E}_g\left\{D(f_{\widehat{\theta}}, g)\right\}; \tag{2}$$

  the outer expectation is over the distribution of $\widehat{\theta}$, which is independent of Y^+.
- After tedious expansions we end up trying to minimise the **Akaike information criterion**

$$\mathrm{AIC} = -2\widehat{\ell} + 2p \qquad (\equiv n\log\mathrm{RSS} + 2p \text{ in linear model}).$$

Note: Derivation of AIC

- Taylor series expansion shows that $\log f(y;\widehat{\theta})$ approximately equals

$$\log f(y;\theta_g) + (\widehat{\theta}-\theta_g)^{\mathrm{T}}\frac{\partial \log f(y;\theta_g)}{\partial\theta} + \tfrac{1}{2}(\widehat{\theta}-\theta_g)^{\mathrm{T}}\frac{\partial^2 \log f(y;\theta_g)}{\partial\theta\partial\theta^{\mathrm{T}}}(\widehat{\theta}-\theta_g),$$

  and as θ_g minimizes $D(f_\theta, g)$,

$$\int \frac{\partial \log f(y;\theta_g)}{\partial\theta} g(y)\,dy = 0.$$

  Hence taking expectation over $Y_1^+,\ldots,Y_n^+$, we get

$$nD(f_{\widehat{\theta}}, g) = n\int \log\left\{\frac{g(y)}{f(y;\widehat{\theta})}\right\} g(y)\,dy \doteq nD(f_{\theta_g}, g) + \tfrac{1}{2}\mathrm{tr}\left\{(\widehat{\theta}-\theta_g)(\widehat{\theta}-\theta_g)^{\mathrm{T}} I_g(\theta_g)\right\},$$

  where we have used the fact that the trace of a scalar is itself.

- Expectation over the distribution of $\widehat{\theta}$ gives its variance matrix, $I_g(\theta_g)^{-1}K(\theta_g)I_g(\theta_g)^{-1}$, and hence

$$n\mathrm{E}_g\left\{D(f_{\widehat{\theta}}, g)\right\} \doteq nD(f_{\theta_g}, g) + \tfrac{1}{2}\mathrm{tr}\left\{I_g(\theta_g)^{-1}K(\theta_g)\right\}, \tag{3}$$

  where the second term penalizes the dimension p of θ. The first term here is $O(n)$ but the second is $O(p)$. When $f_{\theta_g} = g$, $I_g(\theta_g) = K(\theta_g)$ so $\mathrm{tr}\left\{I_g(\theta_g)^{-1}K(\theta_g)\right\} = p$.

- To build an estimator, note that $\int \log g(y)\, g(y)\,dy$ is constant and can be ignored. Now $\ell(\widehat{\theta}) = \ell(\theta_g) + \{\ell(\widehat{\theta}) - \ell(\theta_g)\}$, so

$$\begin{aligned}\mathrm{E}_g\left\{-\ell(\widehat{\theta})\right\} &= -\mathrm{E}_g\left\{\ell(\theta_g) + \tfrac{1}{2}W(\theta_g)\right\}\\ &\doteq nD(f_{\theta_g}, g) - \tfrac{1}{2}\mathrm{tr}\left\{I(\theta_g)^{-1}K(\theta_g)\right\} - n\int \log g(y)\, g(y)\,dy,\end{aligned}$$

  where we have used the fact that under the wrong model, the likelihood ratio statistic $W(\theta_g)$ has mean approximately $\mathrm{tr}\left\{I(\theta_g)^{-1}K(\theta_g)\right\}$. Hence $-\ell(\widehat{\theta})$ tends to underestimate $nD(f_{\theta_g}, g) - n\int \log g(y)\, g(y)\,dy$. On reflection this is obvious, because $\ell(\widehat{\theta}) \geq \ell(\theta_g)$ by definition of $\widehat{\theta}$. As p increases, so will the extent of overestimation.

- An estimator is $-\ell(\widehat{\theta}) + c$, where c estimates $\mathrm{tr}\left\{I(\theta_g)^{-1}K(\theta_g)\right\}$. Two possible choices of c are p and $\mathrm{tr}(\widehat{I}^{-1}\widehat{K})$, and these lead to

$$\mathrm{AIC} = 2\{-\ell(\widehat{\theta}) + p\}, \quad \mathrm{NIC} = 2\{-\ell(\widehat{\theta}) + \mathrm{tr}(\widehat{J}^{-1}\widehat{K})\}; \tag{4}$$

  another possibility is $\mathrm{BIC} = -2\ell(\widehat{\theta}) + p\log n$.

- The model is chosen to minimize AIC, say, with the factor 2 putting differences of AIC on the same scale as likelihood ratio statistics. Such criteria are used far beyond random samples, and even in cases where the theory above doesn't work.

- In particular, the maximised log-likelihood for a normal-theory linear model with residual sum of squares RSS can be shown to be

$$-\frac{n}{2}\log(2\pi\widehat{\sigma}) - \frac{n}{2} \equiv -\frac{n}{2}\log \mathrm{RSS} + \text{constants},$$

  which leads to the formula given on the slide.

Other model selection criteria

- **'Corrected' AIC** for (normal-theory) regression problems:

$$\mathrm{AIC_c} \equiv n \log \widehat{\sigma}^2 + n \frac{1 + p/n}{1 - (p+2)/n}.$$

- **Bayes' information criterion**

$$\mathrm{BIC} = -2\widehat{\ell} + p \log n.$$

- **Mallows C_p**:

$$C_p = \frac{SS_p}{s^2} + 2p - n,$$

where SS_p is RSS for fitted model and s^2 estimates σ^2.

- When the true model is a candidate and $n \to \infty$,
  - AIC is **inconsistent** — it will not choose the true model with probability one, but tends to pick a more complex model;
  - $\mathrm{AIC_c}$ is also inconsistent but gives better results in finite samples;
  - BIC is **consistent** — it chooses the true model with probability $\to 1$.

  These results suppose that the models are fixed, but in practice we also have $p \to \infty$ when $n \to \infty$, because we fit ever more complex models when we have more data.

Simulation experiment

Number of times models were selected using various model selection criteria in 50 repetitions using simulated normal data for each of 20 design matrices. The true model has $p = 3$.

n		Number of covariates						
		1	2	3	4	5	6	7
10	C_p		131	504	91	63	83	128
	BIC		72	373	97	83	109	266
	AIC		52	329	97	91	125	306
	$\mathrm{AIC_c}$	15	398	565	18	4		
20	C_p		4	673	121	88	61	53
	BIC		6	781	104	52	30	27
	AIC		2	577	144	104	76	97
	$\mathrm{AIC_c}$		8	859	94	30	8	1
40	C_p			712	107	73	66	42
	BIC			904	56	20	15	5
	AIC			673	114	90	69	54
	$\mathrm{AIC_c}$			786	105	52	41	16

Stepwise methods

- In principle we might wish to fit all 2^p possible choices of covariates, but in practice this is possible only for 'modest' p, using **leaps** or similar methods (or approximations).
- When p is too large for exhaustive searches, we instead consider subsets of the models, using the methods below (or variants).
- **Forward selection**: starting from the model with a constant only,
  1. add each remaining term separately to the current model;
  2. if none of these terms improves the fit, stop; otherwise
  3. update the current model to include the most useful new term; go to 1
- **Backward elimination**: starting from the model with all terms,
  1. if all terms are 'useful', stop; otherwise
  2. update current model by dropping the 'least useful' term; go to 1
- **Stepwise**: starting from an arbitrary model,
  1. consider three options—add a term, delete a term, swap a term in the model for one not in the model;
  2. if model unchanged, stop; otherwise go to 1
- 'Useful' means 'reduces the AIC' (but in the past meant 'is significant using an F test').

Stepwise methods: Comments

- Original formulation of stepwise used F tests (or even arbitrary numbers!) to assess significance, but this finds spurious models.
- Systematic search minimising AIC or similar over all possible models is preferable, but is often infeasible.
- Compare AICs for different models at each step—i.e., use AIC (or AIC_c) as objective function.
- Important not to fixate on a specific model, or assume that there is a single 'best' model, but to consider any models whose AIC is within (say) 2 of the minimum — especially if the interpretations of competing models differ.

Example: Nuclear power stations

```
> nuclear
     cost  date t1 t2  cap pr ne ct bw cum.n pt
1  460.05 68.58 14 46  687  0  1  0  0    14  0
2  452.99 67.33 10 73 1065  0  0  1  0     1  0
3  443.22 67.33 10 85 1065  1  0  1  0     1  0
4  652.32 68.00 11 67 1065  0  1  1  0    12  0
5  642.23 68.00 11 78 1065  1  1  1  0    12  0
6  345.39 67.92 13 51  514  0  1  1  0     3  0
7  272.37 68.17 12 50  822  0  0  0  0     5  0
8  317.21 68.42 14 59  457  0  0  0  0     1  0
9  457.12 68.42 15 55  822  1  0  0  0     5  0
10 690.19 68.33 12 71  792  0  1  1  1     2  0
...
32 270.71 67.83  7 80  886  1  0  0  1    11  1
```


Example: Nuclear power stations

	Full model		Backward		Forward	
	Est (SE)	t	Est (SE)	t	Est (SE)	t
Constant	-14.24 (4.229)	-3.37	-13.26 (3.140)	-4.22	-7.627 (2.875)	-2.66
date	0.209 (0.065)	3.21	0.212 (0.043)	4.91	0.136 (0.040)	3.38
log(T1)	0.092 (0.244)	0.38				
log(T2)	0.290 (0.273)	1.05				
log(cap)	0.694 (0.136)	5.10	0.723 (0.119)	6.09	0.671 (0.141)	4.75
PR	-0.092 (0.077)	-1.20				
NE	0.258 (0.077)	3.35	0.249 (0.074)	3.36		
CT	0.120 (0.066)	1.82	0.140 (0.060)	2.32		
BW	0.033 (0.101)	0.33				
log(N)	-0.080 (0.046)	-1.74	-0.088 (0.042)	-2.11		
PT	-0.224 (0.123)	-1.83	-0.226 (0.114)	-1.99	-0.490 (0.103)	-4.77
s (df)	0.164 (21)		0.159 (25)		0.195 (28)	

M-estimation

- The least squares estimates are linear in y and therefore very sensitive to outliers.
- When $y_i \mapsto y_i + c$,

$$\widehat{\beta} = \sum_{j=1}^{n} (X^{\mathrm{T}}X)^{-1} x_j y_j \mapsto \sum_{j=1}^{n} (X^{\mathrm{T}}X)^{-1} x_j y_j + (X^{\mathrm{T}}X)^{-1} x_i c = \widehat{\beta} + (X^{\mathrm{T}}X)^{-1} x_i c,$$

  which could be arbitrarily far from $\widehat{\beta}$.
- Try and fix this by replacing

$$\min_{\beta} \sum_{j=1}^{n} (y_j - x_j^{\mathrm{T}}\beta)^2 \qquad \text{by} \qquad \min_{\beta} \sum_{j=1}^{n} \rho\left\{(y_j - x_j^{\mathrm{T}}\beta)/\sigma\right\},$$

  for function $\rho(\cdot)$ that will give a more robust **M**(aximum likelihood-like)-**estimator**, or equivalently solving the $p \times 1$ system of **estimating equations**

$$\frac{1}{\sigma} \sum_{j=1}^{n} x_j \rho'\left\{(y_j - x_j^{\mathrm{T}}\beta)/\sigma\right\} = X^{\mathrm{T}}\rho' = 0$$

  say, where $\rho'_{n\times 1}$ has jth element $\mathrm{d}\rho(u)/\mathrm{d}u$ for $u = (y_j - x_j^{\mathrm{T}}\beta)/\sigma$.

Choice of ρ

- Choose $\rho(u)$ to have desirable properties, e.g., to downweight outliers:

$$\begin{aligned}
\rho(u) &= u^2/2 \quad \text{(normal errors)},\\
\rho(u) &= |u| \quad \text{(Laplace errors)},\\
\rho(u) &= \nu \log(1 + u^2/\nu)/2 \quad (t_\nu \text{ errors}),\\
\rho(u) &= \begin{cases} u^2/2, & |u| < c,\\ c(2|u| - c)/2, & \text{otherwise,} \end{cases} \quad \text{(Huber function).}
\end{aligned}$$

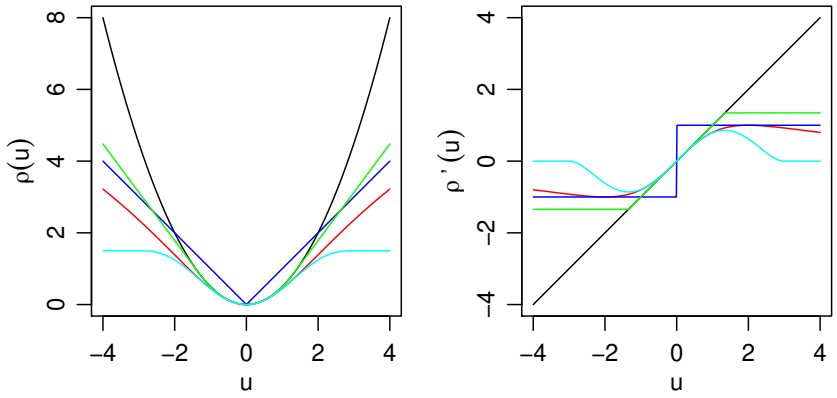
- The function $\rho'(u)$ is also called the **influence function** of the estimator, as its value determines what influence an observation at u has on the estimator:
  - Huber $\rho'(u)$ is bounded,
  - t_ν function is bounded and **redescending**, as $\lim_{u\to\pm\infty} \rho'(u) = 0$;
  - Tukey's **biweight**

$$\rho'(u) = u\left\{1 - (u/c)^2\right\}^2 I(|u| < c),$$

    which gives $\rho'(u) = 0$ when $|u| > c$, is also redescending, giving no weight to observations outside $\pm c$.

ρ and ρ'

Functions ρ and ρ' for least squares (black), t_5 (red), Laplace (blue), Huber (green) and biweight (cyan) estimators.



Estimation

- We need to solve

$$X^{\mathrm{T}}\rho' = 0,$$

where ρ' has $j\mathrm{th}$ element

$$\sigma^{-1}\rho'\{(y_j - x_j^{\mathrm{T}}\beta)/\sigma\} \propto \frac{\rho'\{(y_j - x_j^{\mathrm{T}}\beta)/\sigma\}}{y_j - x_j^{\mathrm{T}}\beta} \times (y_j - x_j^{\mathrm{T}}\beta) = w_j(\beta,\sigma)(y_j - x_j^{\mathrm{T}}\beta),$$

say, so we write the estimating equation as

$$X^{\mathrm{T}}W(y - X\beta) = 0,$$

with $W = \mathrm{diag}\{w_1(\beta,\sigma), \ldots, w_n(\beta,\sigma)\}$.

- We use **iterative weighted least squares**: choose some initial $\tilde{\beta}$ and σ, then iterate to convergence the steps
  - compute W using the current $\tilde{\beta}$,
  - compute the weighted least squares estimate,

$$\tilde{\beta} = (X^{\mathrm{T}}WX)^{-1}X^{\mathrm{T}}Wy.$$

- Estimate σ using median absolute deviation of residuals $y_j - x_j^{\mathrm{T}}\tilde{\beta}$ at each iteration, or similar robust scale estimate.

M-estimator variance

- Estimator $\tilde{\beta}$ is solution to $p \times 1$ system of equations

$$g(y;\beta) = X^{\mathrm{T}}\rho' = 0.$$

- Can show that if the estimating function g is **unbiased**, i.e.

$$\mathrm{E}\left\{g(Y;\beta);\beta\right\} = 0, \quad \text{for any } \beta,$$

then under mild regularity conditions

$$\tilde{\beta} \mathrel{\dot{\sim}} \mathcal{N}_p\left(\beta, \mathrm{E}\left\{-\frac{\partial g(Y;\beta)}{\partial \beta^{\mathrm{T}}}\right\}^{-1} \mathrm{var}\left\{g(Y;\beta)\right\} \mathrm{E}\left\{-\frac{\partial g(Y;\beta)}{\partial \beta^{\mathrm{T}}}\right\}^{-1}\right).$$

This is another **sandwich** variance matrix, with

$$\mathrm{E}\left\{-\frac{\partial g(Y;\beta)}{\partial \beta^{\mathrm{T}}}\right\} = X^{\mathrm{T}}W_1X, \quad \mathrm{var}\left\{g(Y;\beta)\right\} = X^{\mathrm{T}}W_2X,$$

so if $W_1 = A(\sigma)I_n$, $W_2 = \sigma^2 B(\sigma)I_n$, then

$$\mathrm{var}(\tilde{\beta}) \doteq \sigma^2(X^{\mathrm{T}}X)^{-1} \times B(\sigma)/A(\sigma)^2.$$

Note: Sandwich matrix I

☐ The $p \times 1$ estimating function is

$$g(y;\beta) = \sum_{j=1}^{n} x_j \rho'\left(\frac{y_j - x_j^{\mathrm{T}}\beta}{\sigma}\right),$$

and unbiasedness implies that if the individual densities are $\sigma^{-1} f\{(y_j - x_j^{\mathrm{T}}\beta)/\sigma\}$, then

$$0 = \mathrm{E}\left\{g(y;\beta)\right\} = \sum_{j=1}^{n} x_j \int \rho'\left(\frac{y_j - x_j^{\mathrm{T}}\beta}{\sigma}\right)\sigma^{-1} f\left(\frac{y_j - x_j^{\mathrm{T}}\beta}{\sigma}\right)\mathrm{d}y_j = X^{\mathrm{T}} a_{n\times 1},$$

say, where a_j is the jth integral above, and setting $u = (y_j - x_j^{\mathrm{T}}\beta)/\sigma$ shows that all the a_j equal

$$\int \rho'(u)\, f(u)\,\mathrm{d}u = 0; \tag{5}$$

this is true by symmetry if the error distribution and ρ' are symmetric around the origin. Now

$$\frac{\partial g(y;\beta)}{\partial \beta^{\mathrm{T}}} = -\frac{1}{\sigma}\sum_{j=1}^{n} x_j x_j^{\mathrm{T}} \rho''\left(\frac{y_j - x_j^{\mathrm{T}}\beta}{\sigma}\right),$$

whose expectation is (using the same transformation)

$$\begin{aligned}
\mathrm{E}\left\{\frac{\partial g(y;\beta)}{\partial \beta^{\mathrm{T}}}\right\} &= -\frac{1}{\sigma}\sum_{j=1}^{n} x_j x_j^{\mathrm{T}} \mathrm{E}\left\{\rho''\left(\frac{Y_j - x_j^{\mathrm{T}}\beta}{\sigma}\right)\right\} \\
&= -\frac{1}{\sigma}\sum_{j=1}^{n} x_j x_j^{\mathrm{T}} \int \rho''(u) f(u)\,\mathrm{d}u = -\frac{1}{\sigma} X^{\mathrm{T}} X A(\sigma),
\end{aligned}$$

say.

☐ The components of these sums are independent, so

$$\mathrm{var}\left\{g(Y;\beta)\right\} = \mathrm{var}\left\{\sum_{j=1}^{n} x_j \rho'\left(\frac{Y_j - x_j^{\mathrm{T}}\beta}{\sigma}\right),\right\} = \sum_{j=1}^{n} x_j x_j^{\mathrm{T}} \mathrm{var}\left\{\rho'\left(\frac{Y_j - x_j^{\mathrm{T}}\beta}{\sigma}\right)\right\},$$

where the substitution $u = (y_j - x_j^{\mathrm{T}}\beta)/\sigma$ and (**??**) show that the variance term can be written as

$$\mathrm{var}\left\{\rho'\left(\frac{Y_j - x_j^{\mathrm{T}}\beta}{\sigma}\right)\right\} = \int \rho'(u)^2 f(u)\,\mathrm{d}u = B(\sigma).$$

☐ The sandwich variance formula is therefore

$$\left\{-\frac{1}{\sigma}X^{\mathrm{T}}XA(\sigma)\right\}^{-1} X^{\mathrm{T}}XB(\sigma)\left\{-\frac{1}{\sigma}X^{\mathrm{T}}XA(\sigma)\right\}^{-1} = (X^{\mathrm{T}}X)^{-1} \times \frac{\sigma^2 B(\sigma)}{A(\sigma)^2}.$$

The variance of the LSE is $\mathrm{var}(Y_j)(X^{\mathrm{T}}X)^{-1}$, so the asymptotic relative efficiency of the M-estimator based on ρ and the LSE is

$$\frac{\mathrm{var}(Y_j)}{\sigma^2} \times \frac{A(\sigma)^2}{B(\sigma)}.$$

Note: Sandwich matrix II

- As a check on this, note that for the normal distribution $\rho'(u) = u$, $f(u) = (2\pi)^{-1}e^{-u^2/2}$, so $A(\sigma) = B(\sigma) = 1$, which gives ARE of 1. If we take $\rho'(u) = \text{sign}(u)$ with the normal density, we have $B(\sigma) = 1$, $A(\sigma) = -2/(2\pi)^{1/2}$, so the sandwich variance formula gives $\sigma^2(X^{\mathrm{T}}X)^{-1}\pi/2$. So using the ρ-function corresponding to the Laplace distribution when the data are in fact normally distributed leads to an estimator which is $\pi/2 \approx 1.57$ times more variable than would be the case if the appropriate ρ-function were used.
- If we take the ρ-function $\rho'(u) = u$ corresponding to the normal density, and the errors are in fact Laplace, $g(u) = (1/2)e^{-|u|}$, we have

$$A(\sigma) = \int (-1) f(u)\,\mathrm{d}u = 1, \quad B(\sigma) = \int u^2 f(u)\,\mathrm{d}u = 2$$

  and the asymptotic relative efficiency is $1/2$.

Efficiency

- Efficiency of M-estimators of β relative to LSEs of β is

$$\frac{\text{var}(Y_j)}{\sigma^2} \times \frac{A(\sigma)^2}{B(\sigma)};$$

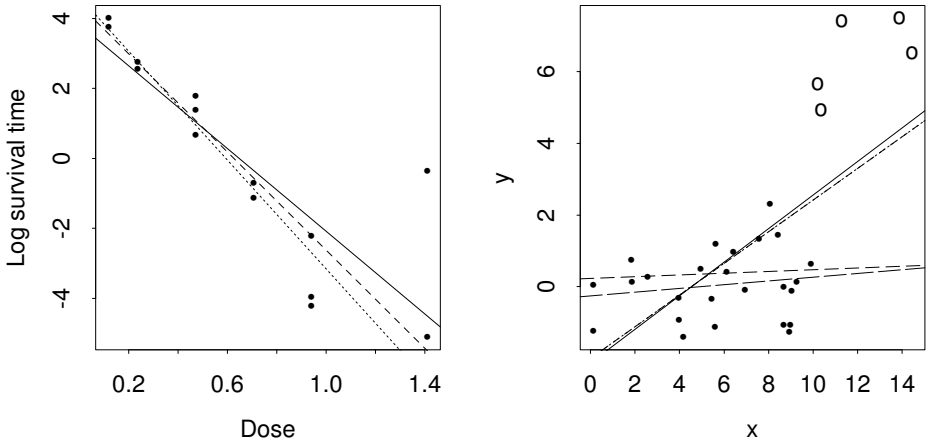
  for example, the Huber estimator is 95% efficient if $c = 1.345$.
- In practice need to balance robustness and efficiency, increasing the latter by increasing c.
- High numbers of outliers can wreck M-estimators.
- Highly robust **least trimmed squares** estimators obtained by minimising

$$\sum_{j=1}^{q} (y_j - x_j^{\mathrm{T}}\beta)^2_{(j)},$$

  where $q = \lfloor n/2 \rfloor + \lfloor (p+1)/2 \rfloor$.

Example: Survival data

Left: log survival proportions for rats given doses of radiation, with lines fitted by least squares with (solid) and without (dots) the outlier, and a Huber fit for the entire data (dashes). Right: simulated data with a batch of outliers (circles), and fits by least squares to all data (solid), least squares to good data only (large dash), Huber (dot-dash), biweight (dashes), and least trimmed squares (medium dash). The Huber and biweight fits are the same to plotting accuracy.



Simulation (right-hand panel on slide 85)

Table 1: Bias (standard deviation) of estimators of slope in sample of 25 good data and k outliers, estimated from 200 replications.

k	Least squares		M-estimation		Least trimmed
	No outliers	With outliers	Huber	Biweight	squares
1	0.00 (0.07)	0.17 (0.06)	0.07 (0.07)	0.01 (0.07)	-0.01 (0.13)
2	0.00 (0.07)	0.26 (0.06)	0.13 (0.07)	0.02 (0.09)	0.01 (0.14)
5	0.00 (0.07)	0.41 (0.05)	0.38 (0.06)	0.19 (0.19)	0.01 (0.14)
10	0.00 (0.06)	0.48 (0.04)	0.48 (0.04)	0.46 (0.12)	0.05 (0.20)

Good strategy is initial fit using least trimmed squares, then robust fit using this as starting point.

Quantile regression

- The Laplace distribution has

$$\rho(u) = |u| = uI(u \geq 0) - uI(u < 0),$$

and for continuous Y, the solution to $\mathrm{E}\{\rho'(Y - \theta)\} = 0$ is the median of Y. Hence

$$\operatorname{argmin} \sum_{j=1}^{n} \rho(y_j - x_j^{\mathrm{T}}\beta)$$

estimates the median of y as a linear function of $X\beta$.

- **Quantile regression** takes $\tau \in (0, 1)$ and uses the **check function**

$$\rho_\tau(u) = \tau uI(u \geq 0) - (1 - \tau)uI(u < 0);$$

then

$$\tilde{\beta}_\tau = \operatorname{argmin} \sum_{j=1}^{n} \rho_\tau(y_j - x_j^{\mathrm{T}}\beta)$$

estimates the τ quantile of y as a linear function of $X\beta$.

- For numerical purposes it may be better to round the cusp of ρ.
- Note that $\rho''_\tau(u) = 0$, so it's better to bootstrap to find $\mathrm{var}(\tilde{\beta}_\tau)$.

Expectile regression

- Quantile regression can be used to estimate value-at-risk in finance settings, but it has the drawback of just counting how many residuals are above/below the quantile.
- **Expectile regression** extends the LSE in the same way, taking

$$\rho_\tau(y - \theta) = \eta_\tau(y - \theta) - \eta_\tau(y), \quad \eta_\tau(u) = |I(u \leq 0) - \tau|u^2,$$

so $\tau = 1/2$ gives the LSE, while taking $\tau > 1/2$ leads to a more general form of LSE, with good properties for risk estimation in finance applications (coherent elicitable risk measure).

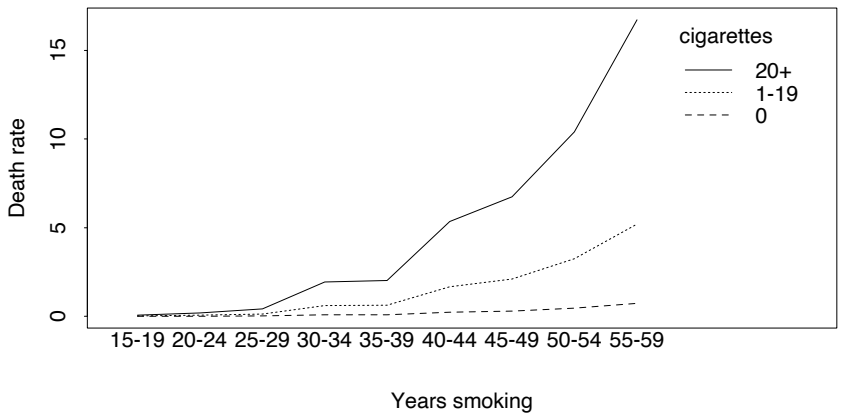
Smoking data

Table 2: Lung cancer deaths in British male physicians (Doll and Hill, 1952). The table gives man-years at risk T/number of cases y of lung cancer, cross-classified by years of smoking t, taken to be age minus 20 years, and number of cigarettes smoked per day, d.

Years of smoking t	Daily cigarette consumption d						
	Nonsmokers	1–9	10–14	15–19	20–24	25–34	35+
15–19	10366/1	3121	3577	4317	5683	3042	670
20–24	8162	2937	3286/1	4214	6385/1	4050/1	1166
25–29	5969	2288	2546/1	3185	5483/1	4290/4	1482
30–34	4496	2015	2219/2	2560/4	4687/6	4268/9	1580/4
35–39	3512	1648/1	1826	1893	3646/5	3529/9	1336/6
40–44	2201	1310/2	1386/1	1334/2	2411/12	2424/11	924/10
45–49	1421	927	988/2	849/2	1567/9	1409/10	556/7
50–54	1121	710/3	684/4	470/2	857/7	663/5	255/4
55–59	826/2	606	449/3	280/5	416/7	284/3	104/1

Smoking data

Lung cancer deaths in British male physicians. The figure shows the rate of deaths per 1000 man-years at risk, for each of three levels of daily cigarette consumption.



Smoking data

- Suppose number of deaths y has Poisson distribution, mean $T\lambda(d,t)$, where T is man-years at risk, d is number of cigarettes smoked daily and t is time smoking (years).
- Take
$$\lambda(d,t) = \beta_0 t^{\beta_1}\left(1+\beta_2 d^{\beta_3}\right):$$
  - background rate of lung cancer is $\beta_0 t^{\beta_1}$ for non-smoker,
  - additional risk due to smoking d cigarettes/day is $\beta_2 d^{\beta_3}$.
- With $x_j = (T_j, d_j, t_j)$, can write this as
$$\begin{aligned} y_j &\sim \text{Poiss}\{\mu(\beta; x_j)\}, \\ \mu(\beta; x) &= T\beta_0 t^{\beta_1}\left(1+\beta_2 d^{\beta_3}\right), \quad j = 1,\ldots,n: \end{aligned}$$
  a nonlinear model with Poisson-distributed response.

Comments

- Linear model $y \sim (X\beta, \sigma^2 I_n)$
  - applicable for continuous response $y \in \mathbb{R}$
  - assumes linear dependence of mean response $\text{E}(y)$ on covariates X
  - sometimes assumes y normal
- Lots of data not like this
- Need extensions for
  - nonlinear dependence on covariates
  - arbitrary response distribution (binomial, Poisson, exponential, ...)
  - dependent responses
  - variance non-constant (and related to mean?)
  - censoring, truncation, ...
  - ...

Simple fixes

- Just fit a linear model anyway
  - Might work as an approximation, but usually extrapolates really badly.
- Fit a linear model to transformed responses
  - E.g., take variance-stabilising transformation for y, such as $2\sqrt{y}$ when y is Poisson
  - Can be helpful, but usually the obvious transformation can't give linearity.
- Instead we attempt to fit the model using likelihood estimation.

Revision: Likelihood

Definition 15 *Let y be a data set, assumed to be the realisation of a random variable $Y \sim f(y;\theta)$, where the unknown parameter θ lies in the parameter space $\Omega_\theta \subset \mathbb{R}^p$. Then the* **likelihood** *(for θ based on y) and the corresponding* **log likelihood** *are*

$$L(\theta) = L(\theta; y) = f_Y(y;\theta), \quad \ell(\theta) = \log L(\theta), \quad \theta \in \Omega_\theta.$$

The **maximum likelihood estimate** *(MLE) $\widehat{\theta}$ satisfies $\ell(\widehat{\theta}) \geq \ell(\theta)$, for all $\theta \in \Omega_\theta$.*
Often $\widehat{\theta}$ is unique and in many cases it satisfies the **score (or likelihood) equation**

$$\frac{\partial \ell(\theta)}{\partial \theta} = 0,$$

which is interpreted as a vector equation of dimension $p \times 1$ if θ is a $p \times 1$ vector.
The **observed information** *and* **expected (Fisher) information** *are defined as*

$$J(\theta) = -\frac{\partial^2 \ell(\theta)}{\partial \theta \partial \theta^{\mathrm{T}}}, \quad I(\theta) = \mathrm{E}\left\{J(\theta)\right\};$$

these are $p \times p$ matrices if θ has dimension p.

Revision: Maximum likelihood estimator

- In large samples from a **regular model** in which the true parameter is $\theta^0_{p\times 1}$, the maximum likelihood estimator $\widehat{\theta}$ has an approximate normal distribution,

$$\widehat{\theta} \mathrel{\dot\sim} \mathcal{N}_p\left\{\theta^0, J(\widehat{\theta})^{-1}\right\},$$

  so we can compute an approximate $(1-2\alpha)$ confidence interval for the rth parameter θ^0_r as

$$\widehat{\theta}_r \pm z_\alpha v_{rr}^{1/2},$$

  where v_{rr} is the rth diagonal element of the matrix $J(\widehat{\theta})^{-1}$.

- This is easily implemented:
  - we code the negative log likelihood $-\ell(\theta)$ (and check the code carefully!);
  - we minimise $-\ell(\theta)$ numerically, ensuring that the minimisation routine returns $\widehat{\theta}$ and the Hessian matrix $J(\widehat{\theta}) = -\partial^2 \ell(\theta)/\partial\theta\partial\theta^{\mathrm{T}}|_{\theta=\widehat{\theta}}$
  - we compute $J(\widehat{\theta})^{-1}$, and use the square roots of its diagonal elements, $v_{11}^{1/2}, \ldots, v_{dd}^{1/2}$, as standard errors for the corresponding elements of $\widehat{\theta}$.

Revision: Regular model

We say that a statistical model $f(y;\theta)$ is **regular (for likelihood inference)** if

1. the true value θ^0 of θ is interior to the parameter space $\Omega_\theta \subset \mathbb{R}^p$;
2. the densities defined by any two different values of θ are distinct;
3. there is an open set $\mathcal{I} \subset \Omega_\theta$ containing θ^0 within which the first three derivatives of the log likelihood with respect to elements of θ exist almost surely, and

$$|\partial^3 \log f(Y_j;\theta)/\partial\theta_r\partial\theta_s\partial\theta_t| \leq g(Y_j)$$

   uniformly for $\theta \in \mathcal{I}$, where $0 < \mathrm{E}_0\{g(Y_j)\} = K < \infty$; and
4. for $\theta \in \mathcal{I}$ we can interchange differentation with respect to θ and integration, that is,

$$\frac{\partial}{\partial\theta}\int f(y;\theta)\,dy = \int \frac{\partial f(y;\theta)}{\partial\theta}\,dy, \quad \frac{\partial^2}{\partial\theta\partial\theta^{\mathrm{T}}}\int f(y;\theta)\,dy = \int \frac{\partial^2 f(y;\theta)}{\partial\theta\partial\theta^{\mathrm{T}}}\,dy.$$

The results are also true under weaker conditions, for non-identically distributed and dependent data.

Revision: Comments on regular models

Condition

1. is needed so that $\widehat{\theta}$ can lie 'on both sides' of θ^0 and hence can have a limiting normal distribution, once standardized—**fails**, for example, if θ has a discrete component (e.g. changepoint $\gamma \in \{1,\ldots,n\}$);
2. is needed to be able to identify the model on the basis of the data;
3. ensures the validity of Taylor series expansions of $\ell(\theta)$—not usually a problem;
4. ensures that the score statistic has a limiting normal distribution—can **fail** in some models — sometimes good news, leading to faster convergence than $n^{-1/2}$.

All the above assumes the postulated model is correct! — there is a literature on what happens when we fit the wrong model, or if the parameter dimension increases with n, or ... usually there are no generic results for such cases.

Revision: Likelihood ratio statistic

- ☐ Model $f_B(y)$ is **nested** within model $f_A(y)$ if A reduces to B on restricting some parameters:
  - for example, the model $Y_1, \ldots, Y_n \overset{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$ is nested within the model $Y_1, \ldots, Y_n \overset{\text{iid}}{\sim} \mathcal{N}(\mu, \sigma^2)$, because the first is obtained from the second by setting $\mu = 0$;
  - the maximised log likelihoods satisfy $\widehat{\ell}_A \geq \widehat{\ell}_B$, because the more comprehensive model A contains the simpler model B.
- ☐ The **likelihood ratio statistic** for comparing them is

$$W = 2(\widehat{\ell}_A - \widehat{\ell}_B).$$

- ☐ If the model is regular, the simpler model is true, and A has q more parameters than B, then

$$W \dot{\sim} \chi^2_q.$$

- ☐ This implicitly assumes that ML inference for model A is OK, so that the approximation $\widehat{\theta}_A \dot{\sim} \mathcal{N}\{\theta_A, J_A(\widehat{\theta}_A)^{-1}\}$ is adequate.

Revision: Profile log likelihood

- ☐ Consider a regular log likelihood $\ell(\psi, \lambda)$, where the **parameter of interest** ψ is variation independent of the **nuisance parameter** λ, i.e., $(\psi, \lambda) \in \Omega_\psi \times \Omega_\lambda$, and the overall MLE is $(\widehat{\psi}, \widehat{\lambda})$.
- ☐ For a confidence set for ψ, without reference to λ, we use the **profile log likelihood**

$$\ell_{\text{p}}(\psi) = \max_{\lambda \in \Omega_\lambda} \ell(\psi, \lambda) = \ell(\psi, \widehat{\lambda}_\psi),$$

  say, and, based on the limiting distribution of the likelihood ratio statistic, take as $(1 - 2\alpha)$ confidence region the set

$$\left\{ \psi \in \Omega_\psi : 2\{\ell(\widehat{\psi}, \widehat{\lambda}) - \ell(\psi, \widehat{\lambda}_\psi)\} \leq \chi^2_{\dim \psi}(1 - 2\alpha) \right\}.$$

- ☐ When ψ is scalar, this yields

$$\left\{ \psi \in \Omega_\psi : \ell(\psi, \widehat{\lambda}_\psi)\} \geq \ell(\widehat{\psi}, \widehat{\lambda}) - \tfrac{1}{2}\chi^2_1(1 - 2\alpha) \right\},$$

  and $\frac{1}{2}\chi^2_1(0.95) = 1.92$.
- ☐ Such intervals are generally better than the standard interval $\widehat{\psi} \pm z_\alpha \text{SE}$, particularly when the distribution of $\widehat{\psi}$ is asymmetric, but require more computation, since they involve many maximisations of ℓ.

Model setup

- ☐ Independent random variables $Y_1, \ldots, Y_n$, with observed values $y_1, \ldots, y_n$, and covariates $x_1, \ldots, x_n$.
- ☐ Suppose that probability density of Y_j is $f(y_j; \eta_j, \phi)$, where $\eta_j = \eta(\beta, x_j)$, and ϕ is common to all models.
- ☐ Log likelihood is

$$\ell(\beta, \phi) = \sum_{j=1}^{n} \ell_j(\beta, \phi) = \sum_{j=1}^{n} \log f\{y_j; \eta(\beta, x_j), \phi\}.$$

- ☐ More generally, just let $\ell_j(\beta, \phi)$ denote the log likelihood contribution from the jth observation.
- ☐ Suppose ϕ known (for now), suppress it, and estimate β.

Example 16 (Normal regression model) *Express the normal regression model in the terms above.*

Note to Example 16

Here $Y_j \overset{\text{ind}}{\sim} \mathcal{N}(\mu_j, \sigma^2)$ with $\mu_j = \eta_j = \eta(x_j; \beta)$, so obviously

$$\eta_j = \eta(x_j; \beta), \quad \phi = \sigma^2, \quad \ell_j \equiv -\tfrac{1}{2}\{(y_j - \eta_j)^2/\phi + \log \phi\}.$$

Iterative weighted least squares (IWLS)

- ☐ General approach for estimation in regression models, based on Newton–Raphson iteration
- ☐ Assume that ϕ is fixed, and write

$$\ell(\beta) = \sum_{j=1}^{n} \ell_j\{\eta_j(\beta)\}.$$

- ☐ MLEs $\widehat{\beta}$ usually satisfy

$$\frac{\partial \ell(\widehat{\beta})}{\partial \beta_r} = 0, \qquad r = 1, \ldots, p,$$

or equivalently

$$\frac{\partial \ell(\widehat{\beta})}{\partial \beta} = \frac{\partial \eta^{\mathrm{T}}}{\partial \beta} \frac{\partial \ell}{\partial \eta} = \frac{\partial \eta^{\mathrm{T}}}{\partial \beta} u(\widehat{\beta}) = \sum_{j=1}^{n} \frac{\partial \eta_j}{\partial \beta} \frac{\partial \ell_j\{\eta_j(\beta)\}}{\partial \eta_j} = 0, \tag{6}$$

where $u(\beta)$ is $n \times 1$ vector with jth element $\partial \ell / \partial \eta_j$.

IWLS II

- Newton–Raphson update step:

$$\widehat{\beta} = (X^{\mathrm{T}} W X)^{-1} X^{\mathrm{T}} W z,$$

where

$$\begin{aligned} X_{n\times p} &= \partial\eta/\partial\beta^{\mathrm{T}}, \quad \text{(design matrix)} \\ W_{n\times n} &= \mathrm{diag}\{\mathrm{E}(-\partial^2\ell_j/\partial\eta_j^2)\}, \quad \text{(weights)} \\ z_{n\times 1} &= X\beta + W^{-1}u, \quad \text{(adjusted dependent variable)} \end{aligned}$$

- Thus to obtain MLEs $\widehat{\beta}$ we use the **IWLS algorithm**:
- take an initial $\widehat{\beta}$. Repeat
  - compute X, W, u, z;
  - compute new $\widehat{\beta}$ and replace the preceding value;

  until changes in $\ell(\widehat{\beta})$ (or, sometimes, $\widehat{\beta}$, or both) are lower than some tolerance.
- Sometimes a line search is added, if $\ell(\widehat{\beta}_{\mathrm{new}}) < \ell(\widehat{\beta}_{\mathrm{old}})$: i.e., we half the step length and try again.

Derivation of IWLS algorithm

- To find the maximum likelihood estimate $\widehat{\beta}$ starting from a trial value β, we make a Taylor series expansion in (3), to obtain

$$\frac{\partial \eta^{\mathrm{T}}(\beta)}{\partial \beta} u(\beta) + \left\{ \sum_{j=1}^{n} \frac{\partial \eta_j(\beta)}{\partial \beta} \frac{\partial^2 \ell_j(\beta)}{\partial \eta_j^2} \frac{\partial \eta_j(\beta)}{\partial \beta^{\mathrm{T}}} + \sum_{j=1}^{n} \frac{\partial^2 \eta_j(\beta)}{\partial \beta \partial \beta^{\mathrm{T}}} u_j(\beta) \right\} (\widehat{\beta} - \beta) \doteq 0. \tag{7}$$

  If we denote the $p \times p$ matrix in braces on the left by $-J(\beta)$, assumed invertible, we can rearrange (**??**) to obtain

$$\widehat{\beta} \doteq \beta + J(\beta)^{-1} \frac{\partial \eta^{\mathrm{T}}(\beta)}{\partial \beta} u(\beta). \tag{8}$$

  This suggests that maximum likelihood estimates may be obtained by starting from a particular β, using (**??**) to obtain $\widehat{\beta}$, then setting β equal to $\widehat{\beta}$, and iterating (**??**) until convergence. This is the Newton–Raphson algorithm applied to our particular setting. In practice it can be more convenient to replace $J(\beta)$ by its expected value

$$I(\beta) = \sum_{j=1}^{n} \frac{\partial \eta_j(\beta)}{\partial \beta} \mathrm{E}\left(-\frac{\partial^2 \ell_j}{\partial \eta_j^2} \right) \frac{\partial \eta_j(\beta)}{\partial \beta^{\mathrm{T}}};$$

  the other term vanishes because $\mathrm{E}\{u_j(\beta)\} = 0$. We write

$$I(\beta) = X(\beta)^{\mathrm{T}} W(\beta) X(\beta), \tag{9}$$

  where $X(\beta)$ is the $n \times p$ matrix $\partial \eta(\beta)/\partial \beta^{\mathrm{T}}$ and $W(\beta)$ is the $n \times n$ diagonal matrix whose jth diagonal element is $\mathrm{E}(-\partial^2 \ell_j / \partial \eta_j^2)$.

- If we replace $J(\beta)$ by $X(\beta)^{\mathrm{T}} W(\beta) X(\beta)$ and reorganize (**??**), we obtain

$$\widehat{\beta} = (X^{\mathrm{T}} W X)^{-1} X^{\mathrm{T}} W (X\beta + W^{-1} u) = (X^{\mathrm{T}} W X)^{-1} X^{\mathrm{T}} W z, \tag{10}$$

  say, where the dependence of the terms on the right on β has been suppressed. That is, starting from β, the updated estimate $\widehat{\beta}$ is obtained by weighted linear regression of the $n \times 1$ vector **adjusted dependent variable**

$$z = X(\beta)\beta + W(\beta)^{-1} u(\beta)$$

  on the columns of $X(\beta)$, using weight matrix $W(\beta)$. The maximum likelihood estimates are obtained by repeating this step until the log likelihood, the estimates, or more often both, are essentially unchanged. The variable z plays the role of the response or dependent variable in the weighted least squares step.

- Often the structure of a model simplifies the estimation of an unknown value of ϕ. It may be estimated by a separate step between iterations of $\widehat{\beta}$, by including it in the step (**??**), or from the profile log likelihood $\ell_{\mathrm{p}}(\phi)$.

Examples

Example 17 (Normal nonlinear model) *Give the components of the IWLS algorithm for the normal nonlinear model.*

Note to Example 17

- Here the mean of the jth observation is $\eta_j = \eta(x_j; \beta)$. The log likelihood contribution $\ell_j(\eta_j)$ is

$$\ell_j(\eta_j, \sigma^2) \equiv -\tfrac{1}{2}\left\{\log \sigma^2 + \frac{1}{\sigma^2}(y_j - \eta_j)^2\right\},$$

so

$$u_j(\eta_j) = \frac{\partial \ell_j}{\partial \eta_j} = \frac{1}{\sigma^2}(y_j - \eta_j), \qquad \frac{\partial^2 \ell_j}{\partial \eta_j^2} = -\frac{1}{\sigma^2};$$

the jth element on the diagonal of W is the constant σ^{-2}.
The jth row of the matrix $X = \partial\eta/\partial\beta^{\mathrm{T}}$ is $(\partial\eta_j/\partial\beta_0, \ldots, \partial\eta_j/\partial\beta_{p-1})$, and as η_j is nonlinear as a function of β, X depends on β.
After some simplification, we see that the new value for $\widehat{\beta}$ given by (**??**) is

$$\widehat{\beta} \doteq (X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}(X\beta + y - \eta), \tag{11}$$

where X and η are evaluated at the current β. Here $\eta \neq X\beta$ and (**??**) must be iterated.

- The log likelihood is a function of β only through the sum of squares, $\mathrm{SS}(\beta) = \sum_{j=1}^{n}\{y_j - \eta_j(\beta)\}^2$. The profile log likelihood for σ^2 is

$$\ell_{\mathrm{p}}(\sigma^2) = \max_{\beta} \ell(\beta, \sigma^2) \equiv -\tfrac{1}{2}\left\{n \log \sigma^2 + \mathrm{SS}(\widehat{\beta})/\sigma^2\right\},$$

so the maximum likelihood estimator of σ^2 is $\widehat{\sigma}^2 = \mathrm{SS}(\widehat{\beta})/n$. Although $S^2 = \mathrm{SS}(\widehat{\beta})/(n-p)$ is not unbiased when the model is nonlinear, it turns out to have smaller bias than $\widehat{\sigma}^2$, and is preferable in applications.

- In some cases the error variance depends on covariates, and we write the variance of the jth response as $\sigma_j^2 = \sigma^2(x_j, \gamma)$. Such models may be fitted by alternating iterative weighted least squares updates for β treating γ as fixed at a current value with those for γ with β fixed, convergence being attained when neither estimates nor log likelihood change materially.

Deviance

- Let $\widehat{\eta}_j = \eta_j(\widehat{\beta}, x_j)$, where $\widehat{\beta}$ is MLE of β, giving maximised log likelihood $\ell(\widehat{\beta})$ and $\widehat{\eta}^{\mathrm{T}} = (\widehat{\eta}_1, \ldots, \widehat{\eta}_n)$.
- Let $\tilde{\eta}_j$ be the value of η_j that maximises $\log f(y_j; \eta_j)$, and let $\tilde{\eta}^{\mathrm{T}} = (\tilde{\eta}_1, \ldots, \tilde{\eta}_n)$. This corresponds to the **saturated model**, with

$$\#\text{parameters in } \eta = \#\text{observations in } y,$$

which will give the largest likelihood possible.

- Define the **scaled deviance**:

$$D = 2\sum_{j=1}^{n}\{\log f(y_j; \tilde{\eta}_j) - \log f(y_j; \widehat{\eta}_j)\} \geq 0.$$

- Small D implies $\widehat{\eta} \approx \tilde{\eta}$, so model fits well.
- Large D implies poor fit — like $SS(\widehat{\beta})$ in linear model.

Differences of deviances

- Consider two models:
  - Model A: $\beta^{\mathrm{T}} = (\beta_1, \ldots, \beta_p) \in \mathbb{R}^p$ vary freely — MLEs $\widehat{\eta}^A = \eta(\widehat{\beta}^A)$;
  - Model B: $(\beta_1, \ldots, \beta_q) \in \mathbb{R}^q$ vary freely, but $\beta_{q+1}, \ldots, \beta_p$ are fixed — hence q free parameters, MLEs $\widehat{\eta}^B = \eta(\widehat{\beta}^B)$.
- Model B is **nested within** model A: B can be obtained by restricting A.
- Likelihood ratio statistic for comparing the models is

$$2(\widehat{\ell}_A - \widehat{\ell}_B) = 2\sum_{j=1}^{n} \left\{\log f(y_j; \widehat{\eta}_j^A) - \log f(y_j; \widehat{\eta}_j^B)\right\} = D_B - D_A,$$

  and this $\dot{\sim} \chi^2_{p-q}$ if the models are regular.
- If ϕ unknown, replace it by an estimate: same distributional approximations will apply.

Example 18 (Normal linear model) *Find the difference of deviances in the normal linear model.*

Note to Example 18

- Suppose that the y_j are normal with means η_j and known variance ϕ. Then

$$\log f(y_j; \eta_j, \phi) = -\tfrac{1}{2}\left\{\log(2\pi\phi) + (y_j - \eta_j)^2/\phi\right\}$$

  is maximized with respect to η_j when $\tilde{\eta}_j = y_j$, giving $\log f(y_j; \tilde{\eta}_j, \phi) = -\frac{1}{2}\log(2\pi\phi)$. Therefore the scaled deviance for a model with fitted means $\widehat{\eta}_j$ is

$$D = \phi^{-1}\sum_{j=1}^{n}(y_j - \widehat{\eta}_j)^2,$$

  which is just the residual sum of squares for the model, divided by ϕ. If $\eta_j = x_j^{\mathrm{T}}\beta$ is the correct normal linear model, the distribution of the residual sum of squares is $\phi\chi^2_{n-p}$, so values of D extreme relative to the χ^2_{n-p} distribution call the model into question.
- The difference between deviances for nested models A and B in which β has dimensions p and $q < p$,

$$D_B - D_A = \phi^{-1}\sum_{j=1}^{n}\left\{(y_j - \widehat{\eta}_j^B)^2 - (y_j - \widehat{\eta}_j^A)^2\right\} \quad \dot{\sim} \quad \chi^2_{p-q}$$

  when model B is correct. This distribution is exact for linear models.
- If ϕ is unknown, it is replaced by an estimate. The large-sample properties of deviance differences outlined above still apply, though in small samples it may be better to replace the approximating χ^2 distribution by an F distribution with denominator degrees of freedom equal to the degrees of freedom for estimation of ϕ.

2.2 Model Checking

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Model checking

- Two basic approaches:
  - overall tests either using generic statistic (e.g., chi-squared) or by **model expansion** (e.g., adding a term and testing for significance);
  - **regression diagnostics** for detecting a few possibly dodgy observations.
- Most widely used diagnostics in the linear model $y = X_{n\times p}\beta + \varepsilon$ are **residuals** $e_j = y_j - \widehat{y}_j$ and (much better) **standardized residuals**

$$r_j = \frac{y_j - \widehat{y}_j}{s(1-h_{jj})^{1/2}}, \quad j = 1, \ldots, n,$$

where the **leverage** h_{jj} is the jth diagonal element of the hat matrix $H = X(X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}$, and the **Cook statistic**

$$C_j = \frac{1}{ps^2}(\widehat{y} - \widehat{y}_{-j})^{\mathrm{T}}(\widehat{y} - \widehat{y}_{-j}) = \frac{r_j^2 h_{jj}}{p(1-h_{jj})},$$

which measures the effect of deleting the jth case (x_j, y_j) on the fitted model.

Diagnostics in general case

- Linear model ideas work as approximations (2nd order Taylor series, painful expansions).
- **Leverage** h_{jj} defined as jth diagonal element of

$$H = W^{1/2}X(X^{\mathrm{T}}WX)^{-1}X^{\mathrm{T}}W^{1/2},$$

depends in general on $\widehat{\beta}$, unlike in linear model.
- **Cook statistic** is change in deviance

$$C_j = 2p^{-1}\left\{\ell(\widehat{\beta}) - \ell(\widehat{\beta}_{-j})\right\} \doteq \frac{h_{jj}}{p(1-h_{jj})} r_{Pj}^2,$$

where $\widehat{\beta}_{-j}$ is MLE when jth case (x_j, y_j) is dropped, and r_{Pj} is **standardized Pearson residual** (see below).
- There are several types of residual (see next page).

Residuals in general case

- **Deviance residual**:
$$d_j = \text{sign}(\tilde{\eta}_j - \widehat{\eta}_j)[2\{\ell_j(\tilde{\eta}_j;\phi) - \ell_j(\widehat{\eta}_j;\phi)\}]^{1/2},$$
for which $\sum d_j^2 = D$ is deviance.
- **Pearson residual**: $u_j(\widehat{\beta})/\sqrt{w_j(\widehat{\beta})}$.
- Standardized versions
$$r_{Dj} = \frac{d_j}{(1-h_{jj})^{1/2}}, \quad r_{Pj} = \frac{u_j(\widehat{\beta})}{\{w_j(\widehat{\beta})(1-h_{jj})\}^{1/2}},$$
and (even better)
$$r_j^* = r_{Dj} + r_{Dj}^{-1}\log(r_{Pj}/r_{Dj}) \dot{\sim} N(0,1)$$
for many models.
- These all reduce to usual standardized residual for normal linear model.

Example

Example 19 (Gumbel linear model) *Give the components of the IWLS algorithm for fitting the linear model*
$$y_j = \beta_0 + \beta_1(x_j - \overline{x}) + \tau\varepsilon_j, \quad j = 1,\ldots,n,$$
with Gumbel errors having density function
$$f(y_j;\eta_j,\tau) = \tau^{-1}\exp\left\{-\frac{y_j-\eta_j}{\tau} - \exp\left(-\frac{y_j-\eta_j}{\tau}\right)\right\},$$
where $\tau > 0$ and $\eta_j = \beta_0 + \beta_1(x_j - \overline{x})$; this distribution is natural for maxima; note that τ^2 is not the variance.

Note to Example 19

- As the data are annual maxima, it is more appropriate to suppose that y_j has the Gumbel density

$$f(y_j;\eta_j,\tau)=\tau^{-1}\exp\left\{-\frac{y_j-\eta_j}{\tau}-\exp\left(-\frac{y_j-\eta_j}{\tau}\right)\right\}, \tag{12}$$

  where τ is a scale parameter and $\eta_j=\beta_0+\beta_1(x_j-\overline{x})$; here we have replaced the γs with βs for continuity with the general discussion above.

- In this case

$$\ell_j(\eta_j,\tau)=-\log\tau-\frac{y_j-\eta_j}{\tau}-\exp\left(-\frac{y_j-\eta_j}{\tau}\right), \tag{13}$$

  and it is straightforward to establish that

$$\frac{\partial\ell_j(\eta_j,\tau)}{\partial\eta_j}=\tau^{-1}\left\{1-\exp\left(-\frac{y_j-\eta_j}{\tau}\right)\right\},\quad \mathrm{E}\left\{-\frac{\partial^2\ell_j(\eta_j,\tau)}{\partial\eta_j^2}\right\}=\tau^{-2},$$

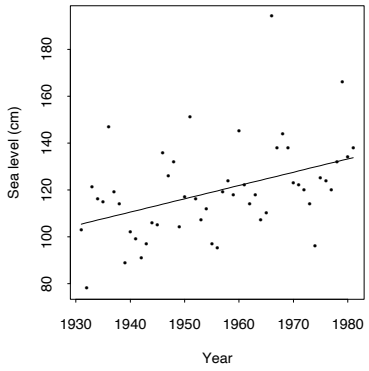
  that $\partial\eta/\partial\beta^{\mathrm{T}}=X$ is the $n\times 2$ matrix whose jth row is $(1,x_j-\overline{x})$, and $W=\tau^{-2}I_n$. Hence (**??**) becomes $\widehat{\beta}\doteq(X^{\mathrm{T}}X)^{-1}(X\beta+\tau^2u)$, where the jth element of u is $\tau^{-1}[1-\exp\{-(y_j-\eta_j)/\tau\}]$.

- Here it is simplest to fix τ, to obtain $\widehat{\beta}$ by iterating (**??**) for each fixed value of τ, and then to repeat this over a range of values of τ, giving the profile log likelihood $\ell_{\mathrm{p}}(\tau)$ and hence confidence intervals for τ. Confidence intervals for β_0 and β_1 are obtained from the information matrix.

- With starting value chosen to be the least squares estimates of β, and with $\tau=5$, 19 iterations of (**??**) were required to give estimates and a maximized log likelihood whose relative change was less than 10^{-6} between successive iterations. We then took $\tau=5.5,\ldots,40$, using $\widehat{\beta}$ from the preceding iteration as starting-value for the next; in most cases just three iterations were needed. The left panel of Figure 1 shows a close-up of $\ell_{\mathrm{p}}(\tau)$; its maximum is at $\widehat{\tau}=14.5$, and the 95% confidence interval for τ is $(11.9,18.1)$. The maximum likelihood estimates of β_0 and β_1 are 111.4 and 0.563, with standard errors 2.14 and 0.137; these compare with standard errors 2.61 and 0.177 for the least squares estimates. There is some gain in precision in using the more appropriate model.

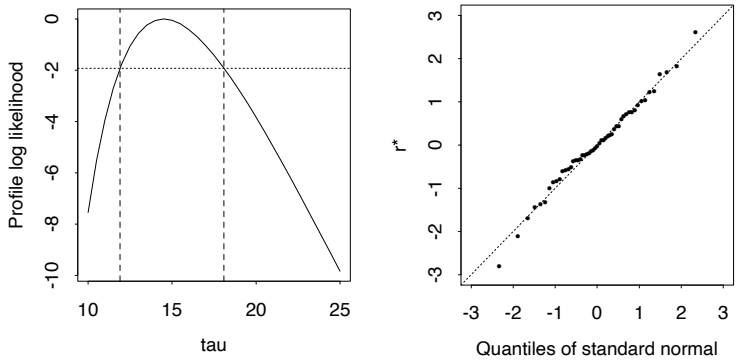
Venice data

Example 20 (Venice sea level data) *The figure below shows annual maximum sea levels in Venice, from 1931–1981. The very large value in 1966 is not an outlier. The fit of a Gumbel model to the data using IWLS gives MLEs (SEs)* $\widehat{\beta}_0 = 111.4\ (2.14)$ *(cm) and* $\widehat{\beta}_1 = 0.563\ (0.137)$ *(cm/year). The standard errors for LSEs are* 2.61, 0.177, *larger than for MLEs with Gumbel model — gain in precision through using appropriate model.*



Venice data

Figure 1: Gumbel analysis of Venice data. Left panel: profile log likelihood $\ell_p(\tau) = \max_\beta \ell(\beta, \tau)$, with 95% confidence interval $(11.9, 18.1)$ (cm) for τ. Right panel: normal probability plot of residuals r_j^*.



Summary

- For regression problems with independent responses y_j dependent on parameters β through parameter $\eta_j = \eta(x_j; \beta)$, generalise least squares estimation to maximum likelihood estimation, using iterative weighted least squares algorithm: iterate to convergence

$$\widehat{\beta} = (X^{\mathrm{T}} W X)^{-1} X^{\mathrm{T}} W z, \quad z = X\beta + W^{-1} u,$$

  where

$$X_{n\times p} \equiv X(\beta) = \frac{\partial \eta}{\partial \beta^{\mathrm{T}}}, \quad u_{n\times 1} \equiv u(\eta) = \frac{\partial \ell}{\partial \eta}, \quad W_{n\times n} \equiv W(\eta) = -\mathrm{E}\left\{\frac{\partial^2 \ell}{\partial \eta \partial \eta^{\mathrm{T}}}\right\},$$

  with ℓ the log likelihood for the data.
- Standard likelihood theory is used for confidence intervals and model comparison.
- Linear model diagnostics (residuals, leverage, Cook statistics, ...) generalise to this setting.
- Next: generalized linear models (GLMs), wide class of models with exponential family-like response distributions.

2.3 Generalized Linear Models

Motivation

- Need to generalise linear model beyond normal responses, e.g. to data with $y \in \{0, 1, \ldots, m\}$, or $y \in \{0, 1, \ldots\}$, or $y > 0$.
- Consider **exponential family** response distributions (binomial, Poisson, ...), which have an elegant unifying theory, and encompass many possibilities (in addition to the normal)
- Basic idea is to build models such that

$$\mathrm{E}(y) = \mu, \quad g(\mu) = \eta = x^{\mathrm{T}}\beta,$$

  where g is a suitable function, and $y \sim$ exponential family (almost).
- **Warnings**:
  - **Don't** confuse Generalized Linear Model (GLM) with General Linear Model (GLM, in older books, the latter is $y = X\beta + \varepsilon$, with $\mathrm{cov}(\varepsilon) = \sigma^2 V$ not diagonal);
  - **Don't** write $y = \mu + \varepsilon$, since in a GLM the distribution of ε usually depends on μ.

Generalized linear model (GLM)

- ☐ Normal linear model has three key aspects:
  - structure for covariates: **linear predictor**, $\eta = x^{\mathrm{T}}\beta$;
  - response distribution: $y \sim N(\mu, \sigma^2)$;
  - linear relation $\eta = \mu$ between $\mu = \mathrm{E}(y)$ and η.
- ☐ GLM extends last two to
  - Y has density/mass function

$$f(y;\theta,\phi) = \exp\left\{\frac{y\theta - b(\theta)}{\phi} + c(y;\phi)\right\}, \quad y \in \mathcal{Y}, \theta \in \Omega_\theta, \phi > 0, \tag{14}$$

    where
    - ▷ $\mathcal{Y}$ is the support of Y,
    - ▷ Ω_θ is the parameter space of valid values for $\theta \equiv \theta(\eta)$, and
    - ▷ the **dispersion parameter** ϕ is often known;
  - $\eta = g(\mu)$, where g is monotone **link function**
    - ▷ the **canonical link** function giving $\eta = \theta = b'^{-1}(\mu)$ has nice statistical properties;
    - ▷ but a range of link functions are possible for each distribution of Y.

Examples

Example 21 (GLM density) *Show that the moment-generating function of $f(y;\theta,\phi)$ is $M_Y(t) = \exp[\{b(\theta + t\phi) - b(\theta)\}/\phi]$, and deduce that*

$$\mathrm{E}(Y) = b'(\theta) = \mu, \quad \mathrm{var}(Y) = \phi b''(\theta) = \phi b''\{b'^{-1}(\mu)\} = \phi V(\mu);$$

the function $\mu \mapsto V(\mu)$ is known as the **variance function**.

Example 22 (Poisson distribution) *Write the Poisson mass function as a GLM density, and find its canonical link function.*

Example 23 (Normal distribution) *Write the normal density function as a GLM density, and find its canonical link function.*

Note to Example 21

- Suppose that Y has a continuous density; if not the argument below is the same, except that integrals are replaced by summations.
- Let $\Omega_\theta = \{\theta : b(\theta) < \infty\}$. Then

$$\begin{aligned} M_Y(t) &= \mathrm{E}\{\exp(tY)\} \\ &= \int e^{ty} \exp\left\{\frac{y\theta - b(\theta)}{\phi} + c(y;\phi)\right\} \mathrm{d}y \\ &= \int \exp\left\{\frac{y(\theta + t\phi) - b(\theta)}{\phi} + c(y;\phi)\right\} \mathrm{d}y. \end{aligned}$$

If $\theta + t\phi \in \Omega_\theta$, then

$$\int \exp\left\{\frac{y(\theta + t\phi) - b(\theta + t\phi)}{\phi} + c(y;\phi)\right\} \mathrm{d}y = 1,$$

so

$$M_Y(t) = \mathrm{E}\{\exp(tY)\} = \exp\left[\{b(\theta + t\phi) - b(\theta)\}/\phi\right].$$

- Hence the cumulant-generating function of Y is

$$K_Y(t) = \log M_Y(t) = \{b(\theta + t\phi) - b(\theta)\}/\phi,$$

and differentiating twice with respect to t and setting $t = 0$ yields

$$\mathrm{E}(Y) = K_Y'(t)\big|_{t=0} = b'(\theta), \quad \mathrm{var}(Y) = K_Y''(t)\big|_{t=0} = \phi b''(\theta).$$

- One can show that $b(\theta)$ is strictly convex on Ω_θ. Thus $b'(\theta)$ is a monotonic increasing function of θ, so $b'^{-1}(\cdot)$ exists and is itself monotonic, so $V(\mu) = b''\{b'^{-1}(\mu)\}$ is well-defined.

Note to Example 22

The Poisson density may be written as

$$f(y;\mu) = \exp\left(y\log\mu - \mu - \log y!\right), \quad y = 0, 1, \ldots, \quad \mu > 0,$$

which has GLM form (4) with $\theta = \log\mu$, $b(\theta) = e^\theta$, $\phi = 1$, and $c(y;\phi) = -\log y!$. The mean of y is $\mu = b'(\theta) = e^\theta = \mu$, and its variance is $b''(\theta) = e^\theta = \mu$, so the variance function is linear: $V(\mu) = \mu$.

Note to Example 23

The normal density with mean μ and variance σ^2 may be written

$$f(y;\mu,\sigma^2) = \exp\left\{-\frac{(y^2 - 2y\mu + \mu^2)}{2\sigma^2} - \tfrac{1}{2}\log(2\pi\sigma^2)\right\},$$

so

$$\theta = \mu, \quad \phi = \sigma^2, \quad b(\theta) = \tfrac{1}{2}\theta^2, \quad c(y;\phi) = -\tfrac{1}{2\phi}y^2 - \tfrac{1}{2}\log(2\pi\phi).$$

As the first and second derivatives of $b(\theta)$ are θ and 1, we have $V(\mu) = 1$; the variance function is constant.

Estimation of β

Example 24 (IWLS algorithm) *Find the components of the IWLS algorithm for a GLM.*

- If canonical link is used then $\theta_j = x_j^{\mathrm{T}}\beta$, so if ϕ is known, then

$$\begin{aligned}\ell(\beta) &= \sum_{j=1}^{n}\left\{\frac{y_j x_j^{\mathrm{T}}\beta - b(x_j^{\mathrm{T}}\beta)}{\phi} + c(y_j;\phi)\right\} \\ &= \{y^{\mathrm{T}}X\beta - K(\beta)\}/\phi + C(y;\phi),\end{aligned}$$

  say, which in terms of β is a linear exponential family with
  - **canonical parameter** $\beta_{p\times 1}$
  - **canonical statistic** $(X^{\mathrm{T}}y)_{p\times 1}$,

  and many nice properties then hold.
- If X is full rank, then $\ell(\beta)$ is (almost always) strictly concave and has a unique maximum in terms of β.
- Problem: the maximum may be at infinity in certain (rare) cases—this can arise with binomial responses: beware of $\widehat{\theta}_r \approx \pm 36$.

Note to Example 24

- To compute the quantities needed for the IWLS step $\widehat{\beta} = (X^{\mathrm{T}}WX)^{-1}X^{\mathrm{T}}W(X\beta + W^{-1}u)$, we need

$$X_{n\times p} = \frac{\partial \eta}{\partial \beta^{\mathrm{T}}}, \quad W_{n\times n} = \mathrm{diag}\{\mathrm{E}(-\partial^2 \ell_j/\partial \eta_j^2)\}, \quad u_{n\times 1} = \{\partial \ell_j/\partial \eta_j\},$$

where (with ϕ_j instead of ϕ for generality, see the next slide),

$$\ell_j(\beta) = \left\{\frac{y_j\theta_j - b(\theta_j)}{\phi_j} + c(y_j;\phi_j)\right\}, \quad b'(\theta_j) = \mu_j, \quad \eta_j = g(\mu_j) = x_j^{\mathrm{T}}\beta.$$

- First note that $\partial \eta_j/\partial \beta_r = x_{jr}$, so $X = \partial \eta/\partial \beta^{\mathrm{T}}$ is just a matrix of constants.
- We need the first and second derivatives of ℓ_j with respect to η_j, so we write

$$\frac{\partial \ell_j}{\partial \eta_j} = \frac{\partial \mu_j}{\partial \eta_j}\frac{\partial \theta_j}{\partial \mu_j}\frac{\partial \ell_j}{\partial \theta_j},$$

with

$$\frac{\partial \eta_j}{\partial \mu_j} = g'(\mu_j), \quad \frac{\partial \mu_j}{\partial \theta_j} = b''(\theta_j) = V(\mu_j), \quad \frac{\partial \ell_j}{\partial \theta_j} = \frac{y_j - b'(\theta_j)}{\phi_j},$$

which yields

$$u_j = \frac{\partial \ell_j}{\partial \eta_j} = \frac{y_j - b(\theta_j)}{g'(\mu_j)\phi_j V(\mu_j)} = \frac{y_j - \mu_j}{g'(\mu_j)\phi_j V(\mu_j)} = \frac{A(\theta_j)}{B(\theta_j)},$$

say, where $\mathrm{E}(A) = 0$. For the second derivative, we note that

$$\frac{\partial^2 \ell_j}{\partial \eta_j^2} = \frac{\partial}{\partial \eta_j}\frac{\partial \ell_j}{\partial \eta_j} = \left(\frac{\partial \mu_j}{\partial \eta_j}\frac{\partial \theta_j}{\partial \mu_j}\frac{\partial}{\partial \theta_j}\right)\frac{\partial \ell_j}{\partial \eta_j} = \frac{\partial \mu_j}{\partial \eta_j}\frac{\partial \theta_j}{\partial \mu_j}\left\{\frac{A'(\theta_j)}{B(\theta_j)} - \frac{A(\theta_j)B'(\theta_j)}{B(\theta_j)^2}\right\},$$

and on noting that $B(\theta_j)$ is non-random and $A'(\theta_j) = -b''(\theta_j) = -V(\mu_j)$, we obtain

$$w_j = \mathrm{E}\left(-\frac{\partial^2 \ell_j}{\partial \eta_j^2}\right) = \frac{1}{g'(\mu_j)}\frac{1}{V(\mu_j)}\frac{V(\mu_j)}{g'(\mu_j)\phi_j V(\mu_j)} = \frac{1}{g'(\mu_j)^2\phi_j V(\mu_j)}.$$

Note to Example 24, part II

- From above we see that the components of the score statistic $u(\beta)$ and the weight matrix $W(\beta)$ may be expressed in terms of components μ_j of the mean vector μ as

$$\begin{aligned} u_j &= \frac{\partial\theta_j}{\partial\eta_j}\frac{\partial\ell_j(\theta_j)}{\partial\theta_j} = \frac{y_j-\mu_j}{g'(\mu_j)\phi_j V(\mu_j)}, \\ w_j &= \left(\frac{\partial\theta_j}{\partial\eta_j}\right)^2 \frac{\partial^2\ell_j(\theta_j)}{\partial\theta_j^2} = \frac{1}{g'(\mu_j)^2\phi_j V(\mu_j)}, \end{aligned} \tag{15}$$

  where $g'(\mu_j) = dg(\mu_j)/d\mu_j$. Thus $\widehat{\beta}$ is obtained by iterative weighted least squares regression of response

$$z = X\beta + g'(\mu)(y-\mu) = \eta + g'(\mu)(y-\mu)$$

  on the columns of X using weights (**??**).

- By using y as an initial value for μ and $g(y)$ as an initial value for $\eta = X\beta$, we avoid needing an initial value for β.

- It may be necessary to modify y slightly for this initial step. For example if we use the log link for Poisson data, and some y_j equal zero, then we may need to replace them with some small positive value to avoid taking $\log 0$ for some components of the initial $\eta = \log y$.

Estimation of ϕ

- When ϕ unknown, it is often replaced by $\phi_j = \phi a_j$, with known a_j and a_j^{-1} treated as a weight. Then we replace the scaled deviance by the **deviance** ϕD.

- If the model is correct and ϕ is known, then **Pearson's statistic**

$$P = \frac{1}{\phi}\sum_{j=1}^{n}\frac{(y_j-\widehat{\mu}_j)^2}{a_j V(\widehat{\mu}_j)} \mathrel{\dot\sim} \chi^2_{n-p},$$

  analogously to the sum of squares in a linear model, with $\mathrm{E}(P) \doteq n-p$.

- The MLE of ϕ can be badly behaved, so usually we prefer the method of moments estimator

$$\widehat{\phi} = \frac{1}{n-p}\sum_{j=1}^{n}(y_j-\widehat{\mu}_j)^2/\{a_j V(\widehat{\mu}_j)\},$$

  which is obtained by solving the equation $P = n-p$, based on noting that $\mathrm{E}(\chi^2_{n-p}) = n-p$.

- If the data are sparse (e.g., many small binomial or Poisson counts), then standard asymptotic results are suspect.

Example: Jacamar data

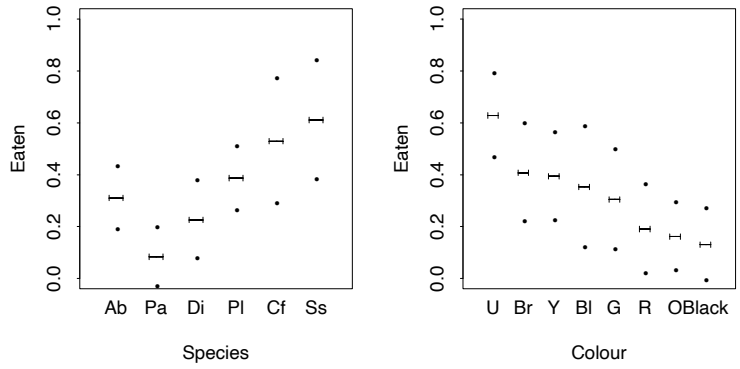
Table 3: Response (N=not sampled, S = sampled and rejected, E = eaten) of a rufous-tailed jacamar to individuals of seven species of palatable butterflies with artifically coloured wing undersides. Data from Peng Chai, University of Texas.

	Aphrissa boisduvalli N/S/E	*Phoebis argante* N/S/E	*Dryas iulia* N/S/E	*Pierella luna* N/S/E	*Consul fabius* N/S/E	*Siproeta stelenes*† N/S/E
Unpainted	0/0/14	6/1/0	1/0/2	4/1/5	0/0/0	0/0/1
Brown	7/1/2	2/1/0	1/0/1	2/2/4	0/0/3	0/0/1
Yellow	7/2/1	4/0/2	5/0/1	2/0/5	0/0/1	0/0/3
Blue	6/0/0	0/0/0	0/0/1	4/0/3	0/0/1	0/1/1
Green	3/0/1	1/1/0	5/0/0	6/0/2	0/0/1	0/0/3
Red	4/0/0	0/0/0	6/0/0	4/0/2	0/0/1	3/0/1
Orange	4/2/0	6/0/0	4/1/1	7/0/1	0/0/2	1/1/1
Black	4/0/0	0/0/0	1/0/1	4/2/2	7/1/0	0/1/0

† includes *Philaethria dido* also.

Jacamar data

Figure 2: Proportion of butterflies eaten ($\pm 2SE$) for different species and wing colour.



Jacamar data

- How does a bird respond to the species s and wing colour c of its prey?
- Response has 3 (ordered) categories: not attacked (N), attacked but then rejected (S), attacked and eaten (E)
- The data form an 8×6 layout, with a 3-category response in each cell, total m_{cs}
- Assume that the number in category E (response) is binomial:

$$R_{cs} \sim B(m_{cs}, \pi_{cs}), \quad c = 1, \ldots, 8, s = 1, \ldots, 6,$$

where c is colour and s is species, with probability that bird attacks and eats butterfly is

$$\pi_{cs} = \frac{\exp(\alpha_c + \gamma_s)}{1 + \exp(\alpha_c + \gamma_s)}, \quad c = 1, \ldots, 8, s = 1, \ldots, 6,$$

so

  - large α_c corresponds to colours that the jacamar likes to eat,
  - large γ_s corresponds to species that it likes.

- This is a GLM with response $y_{cs} = r_{cs}/m_{cs}$, $\mathrm{E}(y_{cs}) = \pi_{cs}$, and canonical (logit) link function

$$\eta = \log\{\pi/(1-\pi)\}, \quad \eta_{cs} = \alpha_c + \gamma_s.$$

Jacamar data: Analysis of deviance

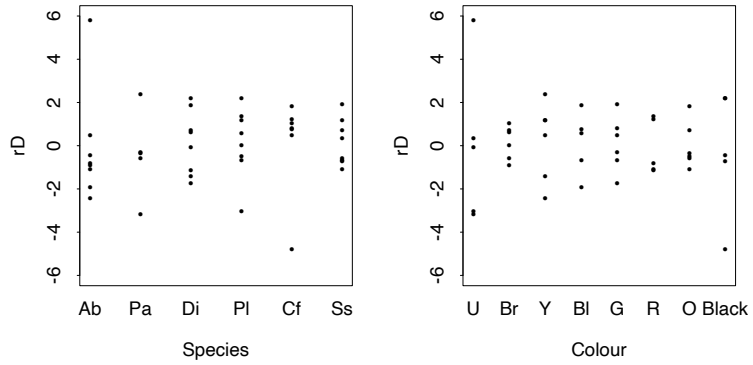
Table 4: Deviances and analysis of deviance for models fitted to jacamar data. The lower part shows results for the reduced data, without two outliers.

	Full data		Without outliers	
Terms	df	Deviance	df	Deviance
1	43	134.24	35	73.68
1+Species	38	114.59	31	46.04
1+Colour	36	108.46	28	63.20
1+Species+Colour	31	67.28	24	28.02

Terms	df	Deviance reduction	Terms	df	Deviance reduction
Species (unadj. for Colour)	5	19.64	Species (adj. for Colour)	5	41.18
Colour (adj. for Species)	7	47.31	Colour (unadj. for Species)	7	25.78
Species (unadj. for Colour)	4	27.63	Species (adj. for Colour)	4	35.18
Colour (adj. for Species)	7	18.03	Colour (unadj. for Species)	7	10.48

Jacamar data: Residuals

Figure 3: Standardized deviance residuals r_D for binomial two-way layout fitted to jacamar data.



Jacamar data: Parameter estimates

Table 5: Estimated parameters and standard errors for the jacamar data, without 2 outliers.

Aphrissa boisduvalli	*Phoebis argante*	*Dryas iulia*	*Pierella luna*	*Consul fabius*	*Siproeta stelenes*
–1.99 (0.79)	–2.22 (0.85)	–0.56 (0.67)	0.16 (0.54)	—	1.50 (0.78)

Brown	Yellow	Blue	Green	Red	Orange	Black
0.16 (0.73)	0.33 (0.68)	–0.53 (0.81)	–0.83 (0.75)	–1.93 (0.88)	–1.94 (0.85)	–1.26 (0.86)

- ☐ Interpretation
- ☐ Residual deviance: 28.02, with 24 df
- ☐ Pearson statistic: 25.58, with 24 df
- ☐ Standardized residuals in range -2.03 to 1.96: OK.

Example: Chimpanzee data

Table 6: Times in minutes taken by four chimpanzees to learn ten words.

Chimpanzee	Word									
	1	2	3	4	5	6	7	8	9	10
1	178	60	177	36	225	345	40	2	287	14
2	78	14	80	15	10	115	10	12	129	80
3	99	18	20	25	15	54	25	10	476	55
4	297	20	195	18	24	420	40	15	372	190

- A two-way layout.
- Times vary from 2 to 476 minutes — need transformation (e.g., logarithm) if use linear model.

Chimpanzee data

- How does learning time depend on word w and chimp c?
- Response is continuous and positive, so we try fitting the gamma distribution with mean μ and shape parameter ν, i.e.,

$$f(y;\mu,\nu) = \frac{1}{\Gamma(\nu)} y^{\nu-1} \left(\frac{\nu}{\mu}\right)^{\nu} \exp(-\nu y/\mu), \quad y > 0, \quad \nu, \mu > 0,$$

  so dispersion parameter is $\phi = 1/\nu$ ($\phi = \nu = 1$ for exponential).
- Possible link functions:

$$\eta = \log \mu, \text{ (log, most common)}, \quad \eta = 1/\mu, \text{ (reciprocal, canonical)}$$

- Linear model structure:

$$\eta_{cw} = \alpha_c + \gamma_w, \quad c = 1, \ldots, 4, w = 1, \ldots, 10,$$

  but the interpretation of the α_c and γ_w will depend on the link function.
- With the log link, the deviances for models 1, 1+Chimp, 1+Word, and 1+Chimp+Word are 60.38, 53.43, 21.19, and 14.97. How many df are there for each model?

Chimpanzee data: Analysis of deviance

Table 7: Analysis of deviance for models fitted to chimpanzee data.

Term	df	Deviance reduction	Term	df	Deviance reduction
Chimp (unadj. for Word)	3	6.95	Chimp (adj. for Word)	3	6.22
Word (adj. for Chimp)	9	38.46	Word (unadj. for Chimp)	9	39.19

- ☐ Method of moments estimate is $\widehat{\phi} = 0.432$, so $\widehat{\nu} = 1/\widehat{\phi} = 2.31$.
- ☐ Use F tests to assess effects of Word and Chimp, for example obtaining

$$\frac{6.22/3}{0.423} = 4.78 \mathrel{\dot\sim} F_{3,27}$$

  if there is no difference between the chimps. What is the corresponding statistic for testing differences between words?
- ☐ Residuals suggest that this model, or one with the inverse link, are both adequate, and both are better than fitting a normal linear model to the log times.

Summary

- ☐ Generalized linear models extend the classical linear model in two ways:
  - the response distribution is (almost) exponential family, so includes binomial, Poisson, gamma and other distributions in addition to the normal;
  - the relation between the linear predictor $\eta = x^{\mathrm{T}}\beta$ and the mean μ is determined by a wide range of possible link functions.
- ☐ Canonical link functions give particularly simple models and are widely used.
- ☐ Estimates of β are obtained by IWLS, which has a simple form, with no need for initial values.
- ☐ A simple estimate of the dispersion parameter ϕ is available using the method of moments.
- ☐ Models are compared using the analysis of deviance, which generalises the analysis of variance in the classical linear model.
- ☐ Standard likelihood theory results are used for inference (standard errors, confidence intervals, etc.)
- ☐ Standard diagnostics (residuals, . . .) extend in a natural way to this setting.

2.4 Proportion Data

Binary response

- Response Y has Bernoulli distribution with

$$\mathrm{P}(Y=1)=\pi, \quad \mathrm{P}(Y=0)=1-\pi, \quad 0<\pi<1.$$

  and $\mathrm{E}(Y)=\mu=\pi$, $\mathrm{var}(Y)=\pi(1-\pi)$.
- Linear link function $\pi=\eta=x^{\mathrm{T}}\beta$ can give $\pi \notin [0,1]$, so not usually a good idea.
- Y can be interpreted in terms of a hidden variable/tolerance distribution: let $Z=x^{\mathrm{T}}\gamma+\sigma\varepsilon$, where $\varepsilon \sim F$. Set $Y=I(Z>0)$, and note that

$$\pi=\mathrm{P}(Y=1)=\mathrm{P}(x^{\mathrm{T}}\gamma+\sigma\varepsilon>0)=\mathrm{P}(\varepsilon>-x^{\mathrm{T}}\gamma/\sigma)=1-F(-x^{\mathrm{T}}\beta),$$

  say. Note that $\beta=\gamma/\sigma$ is estimable, but γ and σ are not.
- The corresponding link function is given by

$$\eta=x^{\mathrm{T}}\beta=-F^{-1}(1-\pi)=g(\pi),$$

  so different choices of F yield different possible link functions.

Link functions

Tolerance distributions and corresponding link functions for binary data.

Distribution F		Link function	
Logistic	$e^u/(1+e^u)$	Logit	$\eta=\log\{\pi/(1-\pi)\}$
Normal	$\Phi(u)$	Probit	$\eta=\Phi^{-1}(\pi)$
Log Weibull	$1-\exp(-\exp(u))\}$	Log-log	$\eta=-\log\{-\log(\pi)\}$
Gumbel	$\exp\{-\exp(-u)\}$	Complementary log-log	$\eta=\log\{-\log(1-\pi)\}$

- The logit and probit links are symmetric.
- Logit (canonical link) is usual choice, good for medical studies (later), with nice interpretation, but the probit is very similar to it and may be preferred in some cases, for its relation to the normal distribution.
- The log-log and complementary log-log links are asymmetric.

Logistic regression

- Commonest choice of link function for proportion data is the **logit**, which gives

$$\mathrm{P}(Y=1)=\pi=\frac{\exp(x^{\mathrm{T}}\beta)}{1+\exp(x^{\mathrm{T}}\beta)},\quad \mathrm{P}(Y=0)=1-\pi=\frac{1}{1+\exp(x^{\mathrm{T}}\beta)},$$

leading to a linear model for the **log odds** of success,

$$\log\left\{\frac{\mathrm{P}(Y=1)}{\mathrm{P}(Y=0)}\right\}=\log\left(\frac{\pi}{1-\pi}\right)=x^{\mathrm{T}}\beta,\quad \beta\in\mathbb{R}^p.$$

- The likelihood for β based on independent responses $y_1,\ldots,y_n$ with covariate vectors $x_1,\ldots,x_n$ and corresponding probabilities $\pi_1,\ldots,\pi_n$ is

$$L(\beta)=\prod_{j=1}^{n}\pi_j^{y_j}(1-\pi_j)^{1-y_j}=\cdots=\frac{\exp\left(\sum_{j=1}^{n}y_jx_j^{\mathrm{T}}\beta\right)}{\prod_{j=1}^{n}\left\{1+\exp\left(x_j^{\mathrm{T}}\beta\right)\right\}},$$

which is a regular exponential family with $s(y)=X^{\mathrm{T}}y$ and log likelihood

$$\ell(\beta)=(X^{\mathrm{T}}y)^{\mathrm{T}}\beta-\sum_{j=1}^{n}\log\left\{1+\exp\left(x_j^{\mathrm{T}}\beta\right)\right\},\quad \beta\in\mathbb{R}^p,$$

known as the **logistic regression model**.

Nodal involvement data

Data on nodal involvement: 53 patients with prostate cancer have nodal involvement (r), with five binary covariates age, stage, etc.

m	r	age	stage	grade	xray	acid
6	5	0	1	1	1	1
6	1	0	0	0	0	1
4	0	1	1	1	0	0
4	2	1	1	0	0	1
4	0	0	0	0	0	0
3	2	0	1	1	0	1
3	1	1	1	0	0	0
3	0	1	0	0	0	1
3	0	1	0	0	0	0
2	0	1	0	0	1	0
2	1	0	1	0	0	1
2	1	0	0	1	0	0
1	1	1	1	1	1	1
⋮	⋮	⋮	⋮	⋮	⋮	
1	1	0	0	1	0	1
1	0	0	0	0	1	1
1	0	0	0	0	1	0

Deviances for nodal involvement models

Scaled deviances D for 32 logistic regression models for nodal involvement data. $+$ denotes a term included in the model.

age	st	gr	xr	ac	df	D	age	st	gr	xr	ac	df	D
					52	40.71	+	+	+			49	29.76
+					51	39.32	+	+		+		49	23.67
	+				51	33.01	+	+			+	49	25.54
		+			51	35.13	+		+	+		49	27.50
			+		51	31.39	+		+		+	49	26.70
				+	51	33.17	+			+	+	49	24.92
+	+				50	30.90		+	+	+		49	23.98
+		+			50	34.54		+	+		+	49	23.62
+			+		50	30.48		+		+	+	49	19.64
+				+	50	32.67			+	+	+	49	21.28
	+	+			50	31.00	+	+	+	+		48	23.12
	+		+		50	24.92	+	+	+		+	48	23.38
	+			+	50	26.37	+	+		+	+	48	19.22
		+	+		50	27.91	+		+	+	+	48	21.27
		+		+	50	26.72		+	+	+	+	48	18.22
			+	+	50	25.25	+	+	+	+	+	47	18.07

Model selection

- ☐ We have 32 competing models, and would like to select the 'best', or a few 'near-best'.
- ☐ In general we have 2^p models, so automatic selection of some sort is helpful.
- ☐ Could use likelihood ratio tests (differences of deviances) to compare competing models, but this involves many correlated tests, so may lead to spurious results.
- ☐ Usually minimise an information criterion, which accounts for the number of parameters in each model, such as

$$\mathrm{AIC} \equiv D + 2p, \quad \mathrm{BIC} \equiv D + p \log n,$$

  where D is the deviance.
- ☐ Recall their properties, with p fixed and as $n \to \infty$:
  - AIC tends to overfit, i.e., it has a positive probability of choosing a model that is too complex,;
  - BIC applies a stronger penalty, so *if the true model is among those fitted*, it will choose it with probability one;
  - BIC usually yields less complex models than AIC, but they may predict less well.
- ☐ There are many other information criteria, but these are most used in practice.

Example: Nodal involvement

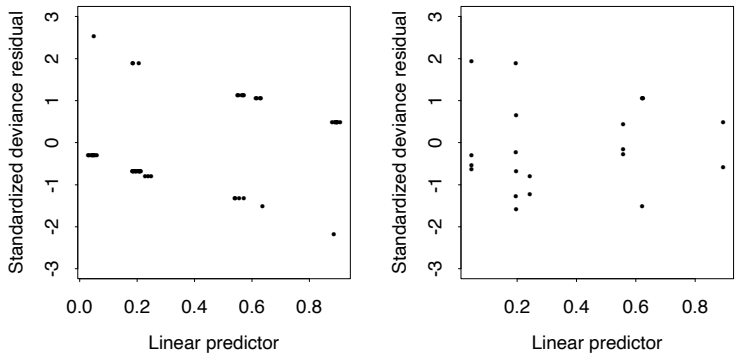
- Model with lowest AIC has stage, xray, acid:

$$x^{\mathrm{T}}\widehat{\beta} = -3.05 + 1.65 I_{\mathsf{stage}} + 1.91 I_{\mathsf{xray}} + 1.64 I_{\mathsf{acid}},$$

  where $I_{\mathsf{stage}} = 1$ indicates that stage takes its higher level, etc.
- Interpretation of this model:
  - for an individual with stage, xray and acid at their lowest levels, the fitted probability of nodal involvement is $e^{-3.05}/(1 + e^{-3.05}) \doteq 0.045$ (though there are no such people in the data, so this involves extrapolation);
  - for someone with only $I_{\mathsf{stage}} = 1$, the odds of nodal involvement are $e^{-3.05+1.65} = e^{-1.4} \doteq 0.25$, a probability of 0.2;
  - for someone with $I_{\mathsf{stage}} = I_{\mathsf{xray}} = I_{\mathsf{acid}} = 1$, the odds of nodal involvement are $e^{-3.05+1.65+1.91+1.64} \doteq 8.6$, a probability of 0.9;
- Problems with interpretation of residual deviance of 19.64: how many df? — can amalgamate independent binary responses with same covariates.
- Likewise problems with residuals ...

Nodal involvement residuals

Figure 4: Standardized deviance residuals for nodal involvement data, for ungrouped responses (left) and grouped responses (right).



Summary

- ☐ Proportion data are often modelled using the Bernoulli/binomial response distributions.
- ☐ Link functions (logit, probit, ...) have interpretations in terms of underlying continuous variables that have been dichotomized.
- ☐ The canonical and most commonly-used link is the logit, and fitting using this yields logistic regression, in which
  - the canonical parameter is the log odds;
  - classical data structures (e.g., the 2×2 table) have nice interpretations.
- ☐ The deviance can be used to compare models (so can AIC, BIC, ...), but using its absolute value to assess fit can be dangerous (exercise).
- ☐ Residuals for binary data are not very informative.

2.5 Count Data

Types of count data

- ☐ $y \in \{0, 1, 2, \ldots\}$, perhaps with upper bound m, depending on sampling scheme:
  - counts, with no fixed total;
  - m individuals, subdivided into various categories:
    - ▷ **nominal response**—unordered categories (gender, nationality, ...)
    - ▷ **ordinal response**—ordered categories (pain level, spiciness of curry, ...)
- ☐ Simplest models:
  - single unbounded response, or Poisson approximation to binomial, takes $Y \sim \text{Pois}(\mu)$;
  - group of responses $(Y_1, \ldots, Y_d)$ with fixed total $\sum Y_j = m$ has multinomial distribution, probabilities $(\pi_1, \ldots, \pi_d)$ and denominator m.
- ☐ Previous examples:
  - Doll and Hill data on smoking had response y Poisson with $\mu = T\lambda(x; \beta)$;
  - Jacamar data had ordinal (?) response N/S/E with total N+S+E fixed—multinomial with $d = 3$

Poisson and multinomial distributions

- $Y \sim \text{Pois}(\mu)$ implies that

$$f(y;\mu) = \frac{\mu^y}{y!}e^{-\mu}, \quad y = 0, 1, 2, \ldots, \quad \mu > 0.$$

- Exponential family with natural parameter $\theta = \log \mu$, GLM with canonical logarithmic link, $x^{\mathrm{T}}\beta = \eta = \log \mu$.
- If Y is number of events in Poisson process of rate λ observed for period of length T, then $\mu = \lambda T$ and we set $\eta = x^{\mathrm{T}}\beta + \log T$
  - **offset** $\log T$ is fixed part of linear predictor η
- If $Y_r \overset{\text{ind}}{\sim} \text{Pois}(\mu_r)$, $r = 1, \ldots, d$, then the joint distribution of $Y_1, \ldots, Y_d$ given $Y_1 + \cdots + Y_d = m$ is **multinomial,** with denominator m, and probabilities

$$\pi_1 = \frac{\mu_1}{\sum_{r=1}^d \mu_r}, \quad \ldots, \quad \pi_d = \frac{\mu_d}{\sum_{r=1}^d \mu_r}.$$

- If $(Y_1, \ldots, Y_d) \sim \text{Mult}(m; \pi_1, \ldots, \pi_d)$, then marginal and conditional distributions, e.g., of

$$(Y_1 + Y_2, Y_3 + Y_4 + Y_5, Y_6, \ldots, Y_d), \quad (Y_1, Y_2, Y_4) \mid (Y_3, Y_5, \ldots, Y_d),$$

  are also multinomial.

Log-linear and logistic regressions

- Special case: if $d = 2$, then

$$Y_2 \mid Y_1 + Y_2 = m \quad \sim \quad B\left(m, \pi = \frac{\mu_2}{\mu_1 + \mu_2}\right)$$

- If $\mu_1 = \exp(\gamma + x_1^{\mathrm{T}}\beta)$, $\mu_2 = \exp(\gamma + x_2^{\mathrm{T}}\beta)$, then

$$\pi = \frac{\exp(\gamma + x_2^{\mathrm{T}}\beta)}{\exp(\gamma + x_1^{\mathrm{T}}\beta) + \exp(\gamma + x_2^{\mathrm{T}}\beta)} = \frac{\exp\{(x_2 - x_1)^{\mathrm{T}}\beta\}}{1 + \exp\{(x_2 - x_1)^{\mathrm{T}}\beta\}},$$

  which corresponds to a logistic regression model for Y_2 with denominator m and probability π.
- Can estimate β using log linear model or logistic model—but can't estimate γ from logistic model.

Premier League data

```
> soccer
    month day year       team1       team2 score1 score2
1     Aug  19 2000    Charlton ManchesterC      4      0
2     Aug  19 2000     Chelsea     WestHam      4      2
3     Aug  19 2000    Coventry   Middlesbr      1      3
4     Aug  19 2000       Derby Southampton      2      2
5     Aug  19 2000       Leeds     Everton      2      0
6     Aug  19 2000   Leicester  AstonVilla      0      0
7     Aug  19 2000   Liverpool    Bradford      1      0
8     Aug  19 2000  Sunderland     Arsenal      1      0
9     Aug  19 2000   Tottenham     Ipswich      3      1
10    Aug  20 2000 ManchesterU   Newcastle      2      0
11    Aug  21 2000     Arsenal   Liverpool      2      0
12    Aug  22 2000    Bradford     Chelsea      2      0
13    Aug  22 2000     Ipswich ManchesterU      1      1
14    Aug  22 2000   Middlesbr   Tottenham      1      1
15    Aug  23 2000     Everton    Charlton      3      0
16    Aug  23 2000 ManchesterC  Sunderland      4      2
17    Aug  23 2000   Newcastle       Derby      3      2
18    Aug  23 2000 Southampton    Coventry      1      2
19    Aug  23 2000     WestHam   Leicester      0      1
20    Aug  26 2000     Arsenal    Charlton      5      3
 ...
```


Premier League data

- 380 soccer matches in English Premier League in 2000–2001 season.
- Data: home score y_{ij}^h and away score y_{ij}^a when team i is at home to team j, for $i, j, = 1, \ldots, 20$, $i \neq j$.
- Treat these as Poisson counts with means

$$\mu_{ij}^h = \exp(\Delta + \alpha_i - \beta_j), \quad \mu_{ij}^a = \exp(\alpha_j - \beta_i)$$

  where
  - Δ represents the home advantage;
  - α_i and β_i represent the offensive and defensive strengths of team i.
- Two possibilities for fitting:
  - Poisson GLM, with 39 parameters;
  - binomial GLM, with 20 parameters.

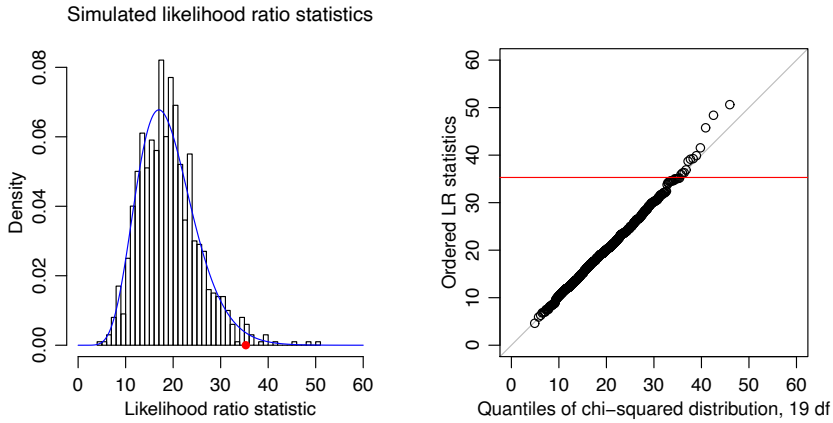
Premier League data: Analysis of deviance

Poisson model			Binomial model		
Terms	df	Deviance reduction	Terms	df	Deviance reduction
Home	1	33.58	Home	1	33.58
Defence	19	39.21	Team	19	79.63
Offence	19	58.85			
Residual	720	801.08	Residual	332	410.65

- ☐ There's a strong effect of playing at home, and lots of evidence of differences among the teams—more in offence than defence.
- ☐ Both residual deviances are a little large, but since the counts are small, we don't expect the large-sample χ^2 distribution to apply well to the residual deviance.
- ☐ Simulations from the fitted model suggest that the residual deviances are not unusually large, so there's no evidence of a lack of fit.

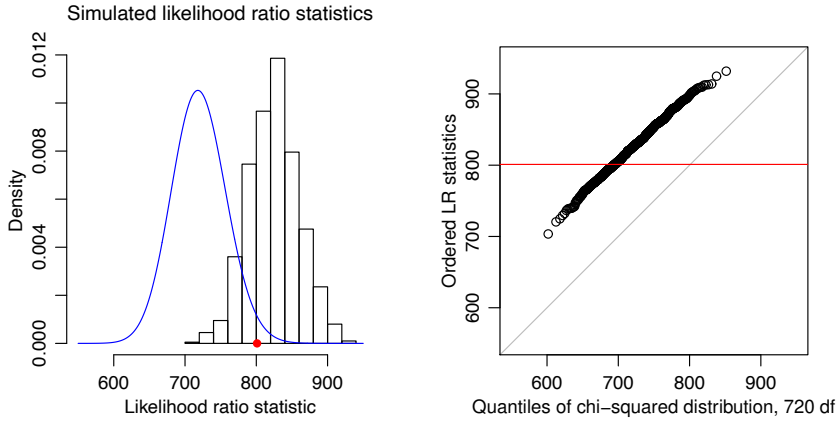
Premier League data: Null deviance for defence effect

Defence effect deviance (in red) for the Poisson model is large(ish) relative to χ^2_{19} distribution, but the asymptotics seem OK, based on simulations from a model without this effect (i.e., `Home + Offence`). It seems we can trust asymptotic distributions for differences of deviances, even though the counts are small.



Premier League data: Residual deviance

Residual deviance of 801 (in red) for the Poisson model seems large(ish) relative to χ^2_{720} distribution, but the asymptotics are suspect because most of the counts are small. Comparison of observed deviance with χ^2_{720} distribution shows that 801 is in fact somewhat smaller than average for datasets simulated from the fitted model.



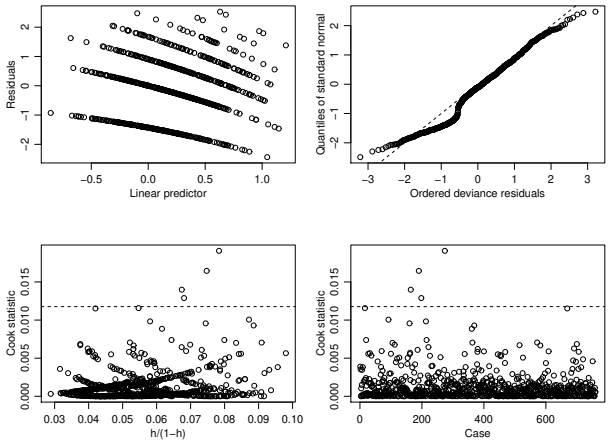
Premier League data: Estimates

	Overall (δ)	Offensive (α)	Defensive (β)
Manchester United	0.39	0.22	0.15
Liverpool	0.13	0.12	−0.08
Arsenal	—	0.04	—
Chelsea	−0.09	0.08	−0.22
Leeds	−0.10	0.02	−0.17
Ipswich	−0.16	−0.10	−0.13
Sunderland	−0.33	−0.31	−0.10
Aston Villa	−0.48	−0.31	−0.15
West Ham	−0.53	−0.33	−0.30
Middlesborough	−0.53	−0.35	−0.17
Charlton	−0.55	−0.21	−0.43
Tottenham	−0.58	−0.28	−0.38
Newcastle	−0.59	−0.35	−0.30
Southampton	−0.60	−0.45	−0.25
Everton	−0.75	−0.32	−0.46
Leicester	−0.77	−0.47	−0.31
Manchester City	−0.90	−0.40	−0.56
Coventry	−0.93	−0.53	−0.52
Derby	−0.93	−0.51	−0.45
Bradford	−1.29	−0.71	−0.62
SEs	0.29	0.20	0.20

Home advantage: $\widehat{\Delta} = 0.37$ (0.07), $\exp(\widehat{\Delta}) = 1.45$.

Premier League data: Assessment of fit

Diagnostic plots for fitted model: residuals against $\widehat{\eta}$ (top left); normal QQ-plot of residuals (top right); Cook statistic C_j against leverage ratio $h_j/(1-h_j)$ (lower left); Cook statistic C_j against case number (lower right).



2.7 Contingency Tables

Sampling schemes

- A **contingency table** contains individuals (sampling units) cross-classified by various categorical variables.
  - Example: the jacamar data cross-classify butterflies by

    $$6 \text{ species} \times 8 \text{ colours} \times 3 \text{ fates}$$

    for a total of 144 categories, each with its number of butterflies $0, 1, \ldots, 14$.
- The sampling scheme underlying a table may fix certain totals. Suppose a pollster wants to find out how people will vote. She might
  - wait in the street for a morning, and get opinions from those people willing to talk to her;
  - wait until she has the views of a fixed number, say m, of people;
  - wait until she has the views of fixed numbers of men and women.

Example 25 *Find the likelihoods for each of these sampling schemes, under (unrealistic!) assumptions of independence of voters.*

Note to Example 25

- An $R \times C$ table arises by randomly sampling a population over a fixed period and then classifying the resulting individuals.
- In the first scheme there are no constraints on the row and column totals, and a simple model is that the count in the (r, c) cell, y_{rc}, has a Poisson distribution with mean μ_{rc}. The resulting likelihood is

$$\prod_{r,c} \left\{ \frac{\mu_{rc}^{y_{rc}}}{y_{rc}!} e^{-\mu_{rc}} \right\};$$

  this is simply the Poisson likelihood for the counts in the RC groups.
- The pollster may set out with the intention of interviewing a fixed number m of individuals, stopping only when $\sum_{rc} y_{rc} = m$. In this case the data are multinomially distributed, with likelihood

$$\frac{m!}{\prod_{r,c} y_{rc}!} \prod_{r,c} \pi_{rc}^{y_{rc}}, \quad \sum_{r,c} \pi_{rc} = 1,$$

  with $\pi_{rc} = \mu_{rc} / \sum_{s,t} \mu_{st}$ the probability of falling into the (r, c) cell.
- A third scheme is to interview fixed numbers of men and of women, thus fixing the row totals $m_r = \sum_c y_{rc}$ in advance. In effect this treats the row categories as subpopulations, and the column categories as the response. This yields independent multinomial distributions for each row, and product multinomial likelihood

$$\prod_{r} \left\{ \frac{m_r!}{\prod_c y_{rc}!} \prod_c \pi_{rc}^{y_{rc}} \right\}, \quad \sum_c \pi_{1c} = \cdots = \sum_c \pi_{Rc} = 1,$$

  in which $\pi_{rc} = \mu_{rc} / \sum_t \mu_{rt}$.

Contingency tables and Poisson response models

- Multinomial models can be fitted using Poisson errors, provided the appropriate baseline terms are always included in the linear predictor.
- Write the data as two-way layout, with C columns and R rows with fixed totals (e.g., $6 \times 8 = 48$ rows each with 3 columns for the jacamar data).
- Consider Poisson model with means $\mu_{rc} = \exp(\gamma_r + x_{rc}^{\mathrm{T}} \beta)$:
  - the row parameters $\gamma_1, \ldots \gamma_R$ are **nuisance parameters**, not of interest;
  - we want inference for the **parameter of interest**, β.
- Corresponding multinomial model has fixed row totals m_r and probabilities

$$\pi_{rc} = \frac{\mu_{rc}}{\sum_{d=1}^{C} \mu_{rd}} = \frac{\exp(\gamma_r + x_{rc}^{\mathrm{T}} \beta)}{\sum_{d=1}^{C} \exp(\gamma_r + x_{rd}^{\mathrm{T}} \beta)} = \frac{\exp(x_{rc}^{\mathrm{T}} \beta)}{\sum_{d=1}^{C} \exp(x_{rd}^{\mathrm{T}} \beta)},$$

  for $r = 1, \ldots, R$, $c = 1, \ldots, C$; i.e., one multinomial variable for each row.
- The resulting multinomial log likelihood is

$$\begin{aligned} \ell_{\mathrm{Mult}}(\beta; y \mid m) &\equiv \sum_{r=1}^{R} \sum_{c=1}^{C} y_{rc} \log \pi_{rc} \\ &= \sum_{r=1}^{R} \left\{ \sum_{c=1}^{C} y_{rc} x_{rc}^{\mathrm{T}} \beta - m_r \log \left(\sum_{d=1}^{C} e^{x_{rd}^{\mathrm{T}} \beta} \right) \right\}. \end{aligned}$$

Contingency tables and Poisson response models, II

Lemma 26 *If parameters τ_r for the row margins are included in the above setup, then we can write*

$$\ell_{\text{Poiss}}(\beta, \tau) = \ell_{\text{Poiss}}(\tau; m) + \ell_{\text{Mult}}(\beta; y \mid m).$$

- Implications:
  - the MLEs of β and τ based on the LHS are the same as those from separate maximisations of the terms on the right:
    - $\widehat{\beta}$ equals the MLE for the multinomial model,
    - $\widehat{\tau}_r = m_r$
  - the observed and expected information matrices for β, τ are block diagonal.
  - SEs based on the multinomial and Poisson models are equal (exercise).
- General conclusion: inferences on β are the same for multinomial and Poisson models,

  provided the parameters associated to the margins fixed under the multinomial model, i.e., the γ_r, are included in the Poisson fit.

Note to Lemma 26

- The Poisson model has no conditioning, so with $\log \mu_{rc} = \gamma_r + x_{rc}^{\mathrm{T}}\beta$ the log likelihood is

$$\ell_{\text{Poiss}}(\beta, \gamma) \equiv \sum_{r,c} (y_{rc} \log \mu_{rc} - \mu_{rc}) = \sum_{r=1}^{R} \left(m_r \gamma_r + \sum_{c=1}^{C} y_{rc} x_{rc}^{\mathrm{T}}\beta - e^{\gamma_r} \sum_{c=1}^{C} e^{x_{rc}^{\mathrm{T}}\beta} \right).$$

- Now we reparametrise in terms of the row totals $\tau_r = \sum_c \mu_{rc}$, noting that

$$\tau_r = e^{\gamma_r} \sum_{c=1}^{C} e^{x_{rc}^{\mathrm{T}}\beta}, \quad \gamma_r = \log \tau_r - \log \left\{ \sum_{c=1}^{C} \exp(x_{rc}^{\mathrm{T}}\beta) \right\},$$

so

$$\begin{aligned} \ell_{\text{Poiss}}(\beta, \tau) &\equiv \sum_{r=1}^{R} (m_r \log \tau_r - \tau_r) + \sum_{r=1}^{R} \left\{ \sum_{c=1}^{C} y_{rc} x_{rc}^{\mathrm{T}}\beta - m_r \log \left(\sum_{c=1}^{C} e^{x_{rc}^{\mathrm{T}}\beta} \right) \right\}, \\ &= \ell_{\text{Poiss}}(\tau; m) + \ell_{\text{Mult}}(\beta; y \mid m), \end{aligned}$$

which is the log likelihood corresponding to

- independent Poisson row totals m_r with means τ_r, and, independent of this,
- the multinomial log likelihood for the contingency table.

Jacamar data

Response (N=not sampled, S = sampled and rejected, E = eaten) of a rufous-tailed jacamar to individuals of seven species of palatable butterflies with artifically coloured wing undersides. Data from Peng Chai, University of Texas.

	Aphrissa boisduvalli N/S/E	*Phoebis argante* N/S/E	*Dryas iulia* N/S/E	*Pierella luna* N/S/E	*Consul fabius* N/S/E	*Siproeta stelenes*† N/S/E
Unpainted	0/0/14	6/1/0	1/0/2	4/1/5	0/0/0	0/0/1
Brown	7/1/2	2/1/0	1/0/1	2/2/4	0/0/3	0/0/1
Yellow	7/2/1	4/0/2	5/0/1	2/0/5	0/0/1	0/0/3
Blue	6/0/0	0/0/0	0/0/1	4/0/3	0/0/1	0/1/1
Green	3/0/1	1/1/0	5/0/0	6/0/2	0/0/1	0/0/3
Red	4/0/0	0/0/0	6/0/0	4/0/2	0/0/1	3/0/1
Orange	4/2/0	6/0/0	4/1/1	7/0/1	0/0/2	1/1/1
Black	4/0/0	0/0/0	1/0/1	4/2/2	7/1/0	0/1/0

† includes *Philaethria dido* also.

Jacamar data: Models

- Let factors F, S, C represent the 3 fates, the 6 species, and the 8 colours.
- The models $C * S$, $C * S + F$, and $C * S + C * F$ mean we set

$$\log \mu_{csf} = \alpha_{cs}, \quad \log \mu_{csf} = \alpha_{cs} + \gamma_f, \quad \log \mu_{csf} = \alpha_{cs} + \gamma_{cf}.$$

- The vector of probabilities corresponding to the model with terms $C * S$ is

$$(\pi_{cs1}, \pi_{cs2}, \pi_{cs3}) = \left(\frac{\mu_{cs1}}{\sum_{f=1}^{3} \mu_{csf}}, \frac{\mu_{cs2}}{\sum_{f=1}^{3} \mu_{csf}}, \frac{\mu_{cs3}}{\sum_{f=1}^{3} \mu_{csf}} \right) = (\tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3}),$$

  and that corresponding to the model with terms $C * S + F$ is

$$\begin{aligned} (\pi_{cs1}, \pi_{cs2}, \pi_{cs3}) &= \left(\frac{\mu_{cs1}}{\sum_{f=1}^{3} \mu_{csf}}, \frac{\mu_{cs2}}{\sum_{f=1}^{3} \mu_{csf}}, \frac{\mu_{cs3}}{\sum_{f=1}^{3} \mu_{csf}} \right) \\ &= \frac{1}{e^{\gamma_1} + e^{\gamma_2} + e^{\gamma_3}} \left(e^{\gamma_1}, e^{\gamma_2}, e^{\gamma_3} \right). \end{aligned}$$

- Exercise: similar computations for $C * S + C * F$ and $C * S + C * F + S * F$.

Jacamar data: Analysis of deviance

Deviances for log-linear models fitted to jacamar data.

Terms	df	Deviance
$C * S$	88	259.42
$C * S + F$	86	173.86
$C * S + C * F$	72	139.62
$C * S + S * F$	76	148.23
$C * S + C * F + S * F$	62	90.66
$C * S * F$	0	0

- ☐ The null model $C * S$ is not of interest.
- ☐ The first model it is sensible to fit is $C * S + F$.
- ☐ The best model seems to be $C * S + C * F + S * F$, corresponding to independent effects of species and colour, though its deviance is high (but remember the two outlying cells!)

2.8 Ordinal Responses

Pneumoconiosis data

Period of exposure x and prevalence of pneumoconiosis amongst coalminers.

	Period of exposure (years)							
	5.8	15	21.5	27.5	33.5	39.5	46	51.5
Normal	98	51	34	35	32	23	12	4
Present	0	2	6	5	10	7	6	2
Severe	0	1	3	8	9	8	10	5

- ☐ Here

$$\text{Normal} \quad < \quad \text{Present} \quad < \quad \text{Severe},$$

so these are ordinal responses with $d = 3$ categories and the total in each group (corresponding to each period of exposure) fixed.

- ☐ We imagine that the assigned category stems from an underlying continuous variable, even if this cannot be quantified very well.

Models

- Assume we have n independent individuals whose responses $I_1, \ldots, I_n$ fall into the set $\{1, \ldots, L\}$, corresponding to L ordered categories, and that

$$\gamma_l = \mathrm{P}(I_j \leq l) = \pi_1 + \cdots + \pi_l, \quad l = 1, \ldots, L, \quad \gamma_L = 1,$$

- The corresponding likelihood is $\prod_{j=1}^{n} \pi_{I_j}$, where usually the contribution $\pi_{I_j} \equiv \pi_{I_j}(\eta_j)$ for individual j will depend on covariates x_j through a linear predictor $\eta_j = x_j^{\mathrm{T}}\beta$.
- We often want the interpretation of the parameters not to change if we merge adjacent categories, and we can do this using an underlying tolerance distribution, with

$$I_j = l \quad \Leftrightarrow \quad x_j^{\mathrm{T}}\beta + \varepsilon_j \in (\zeta_{l-1}, \zeta_l], \quad \zeta_0 = -\infty < \zeta_1 < \cdots < \zeta_{L-1} < \zeta_L = \infty,$$

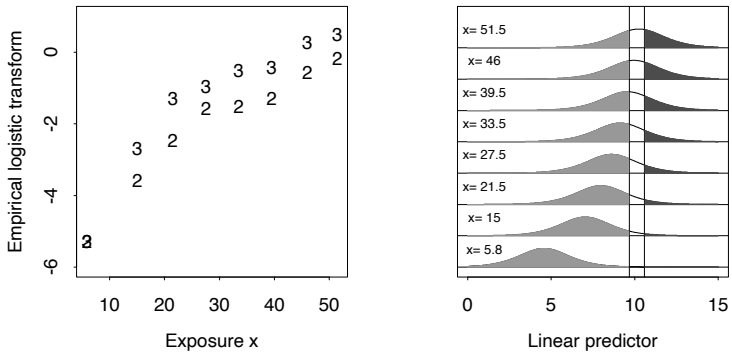
  where the tolerance distribution F of ε_j is often taken to be logistic, giving the **proportional odds model**, in which

$$\pi_l(x_j^{\mathrm{T}}\beta) = \mathrm{P}(\zeta_{l-1} < x_j^{\mathrm{T}}\beta + \varepsilon \leq \zeta_l) = F(\zeta_l - x_j^{\mathrm{T}}\beta) - F(\zeta_{l-1} - x_j^{\mathrm{T}}\beta), \quad l = 1, \ldots, L;$$

  here $\zeta_1, \ldots, \zeta_{L-1}$ are aliased with an intercept β_0 and are not usually of interest.
- Another standard tolerance distribution is $F(u) = 1 - \exp\{-\exp(u)\}$.
- To fit, we just apply IWLS to the multinomial likelihood $\prod_{j=1}^{n} \pi_{I_j}$.

Pneumoconiosis data

Pneumoconiosis data analysis, showing how the implied fitted logistic distributions depend on x. Left: plots of empirical logistic transforms for comparing categories 1 with $2+3$ and $1+2$ with 3; the nonlinearity suggests using $\log x$ as covariate. Right: fitted model, showing probabilities for the three groups with an underlying logistic distribution.



Comments on count data

- ☐ Log-linear models are mathematically elegant and useful defaults for count data, with close links to logistic regression, based on the relation between the Poisson and multinomial distributions.
- ☐ Interpretation of log-linear models can be difficult, especially for contingency tables, because marginal and conditional parameters cannot be disentangled.
- ☐ Other models exist that are less elegant mathematically, but are more interpretable statistically.
- ☐ Also possible to fit models for ordinal data, using multinomial models and tolerance distribution interpretation used for binomial data.

2.9 Overdispersion slide 166

Overdispersion

- ☐ Often find that discrete response data are more variable than might be expected from a simple Poisson or binomial model, so we see
  - residual deviances larger than expected
  - residuals more variable than expected under the model

  but otherwise no evidence of systematic lack of fit
- ☐ This is **overdispersion**, perhaps due to effect of unmeasured explanatory variables on the responses.

UK monthly AIDS reports 1983–1992

Diagnosis period		Reporting-delay interval (quarters):									Total reports to end
Year	Quarter	$0^\dagger$	1	2	3	4	5	6	$\cdots$	$\geq$14	of 1992
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
1988	1	31	80	16	9	3	2	8	$\cdots$	6	174
	2	26	99	27	9	8	11	3	$\cdots$	3	211
	3	31	95	35	13	18	4	6	$\cdots$	3	224
	4	36	77	20	26	11	3	8	$\cdots$	2	205
1989	1	32	92	32	10	12	19	12	$\cdots$	2	224
	2	15	92	14	27	22	21	12	$\cdots$	1	219
	3	34	104	29	31	18	8	6	$\cdots$		253
	4	38	101	34	18	9	15	6	$\cdots$		233
1990	1	31	124	47	24	11	15	8	$\cdots$		281
	2	32	132	36	10	9	7	6	$\cdots$		245
	3	49	107	51	17	15	8	9	$\cdots$		260
	4	44	153	41	16	11	6	5	$\cdots$		285
1991	1	41	137	29	33	7	11	6	$\cdots$		271
	2	56	124	39	14	12	7	10	$\cdots$		263
	3	53	175	35	17	13	11	2			306
	4	63	135	24	23	12	1				258
1992	1	71	161	48	25	5					310
	2	95	178	39	6						318
	3	76	181	16							273
	4	67	66								133

AIDS data

- ☐ UK monthly reports of AIDS diagnoses 1983–1992, with reporting delay up to several years!
- ☐ Example of incomplete contingency table (very common in insurance)
- ☐ Chain-ladder model: number of reports in row j and column k is Poisson, with mean

$$\mu_{jk} = \exp(\alpha_j + \beta_k).$$

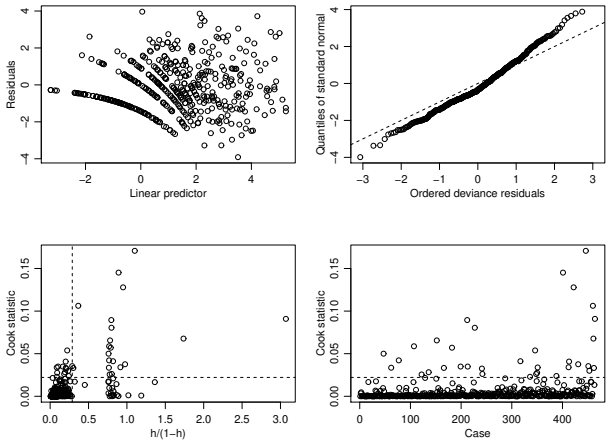
- ☐ Analysis of deviance:

Model	df	Deviance reduction	df	Deviance
			464	14184.3
Time (rows)	37	6114.8	427	8069.5
Delay (cols)	14	7353.0	413	716.5

- ☐ Residual deviance is obviously far too large for a Poisson model to be OK, but the model is also too complex, since we expect smooth variation in the α_j.
- ☐ Residuals on next page show no obvious problems, just generic overdispersion.

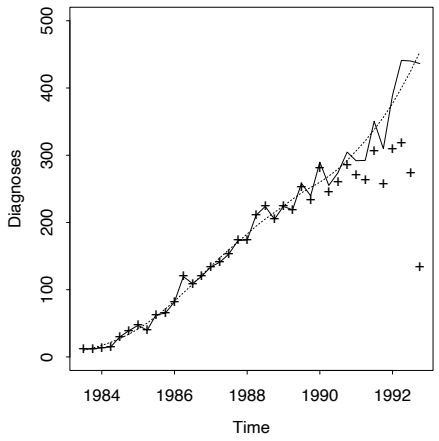
AIDS data: Assessment of fit

Diagnostic plots for fitted model: residuals against $\widehat{\eta}$ (top left); normal QQ-plot of residuals (top right); Cook statistic C_j against leverage ratio $h_j/(1-h_j)$ (lower left); Cook statistic C_j against case number (lower right).



AIDS data

- ☐ Data (+) and predicted true numbers based on simple Poisson model (solid) and GAM (dots).
- ☐ The Poisson model and data agree up to where data start to be missing.



Dealing with overdispersion

- Two basic approaches:
  - parametric modelling
  - quasi-likelihood estimation, based only on the variance function

Example 27 (Linear and quadratic variance functions) *Suppose that, conditional on* $\varepsilon > 0$, $Y \sim \text{Pois}(\mu\varepsilon)$, *where* $\text{E}(\varepsilon) = 1$ *and* $\text{var}(\varepsilon) = \xi$. *Show that this can lead to either linear or quadratic variance functions, but a lot of data may be needed to distinguish them.*

Comparison of variance functions for overdispersed count data. The linear and quadratic variance functions are $V_L(\mu) = (1 + \xi_L)\mu$ and $V_Q(\mu) = \mu(1 + \xi_Q\mu)$, with $\xi_L = 0.5$ and ξ_Q chosen so that $V_L(15) = V_Q(15)$.

μ	1	2	5	10	15	20	30	40	60
Linear	1.5	3.0	7.5	15.0	22.5	30	45	60	90
Quadratic	1.0	2.1	5.8	13.3	22.5	33	60	93	180

Note to Example 27

Let ε have unit mean and variance $\xi > 0$, and to be concrete suppose that conditional on ε, Y has the Poisson distribution with mean $\mu\varepsilon$. Then

$$\text{E}(Y) = \text{E}_\varepsilon\left\{\text{E}(Y \mid \varepsilon)\right\}, \quad \text{var}(Y) = \text{var}_\varepsilon\left\{\text{E}(Y \mid \varepsilon)\right\} + \text{E}_\varepsilon\left\{\text{var}(Y \mid \varepsilon)\right\},$$

so the response has mean and variance

$$\text{E}(Y) = \text{E}_\varepsilon(\mu\varepsilon) = \mu, \quad \text{var}(Y) = \text{var}_\varepsilon(\mu\varepsilon) + \text{E}_\varepsilon(\mu\varepsilon) = \mu(1 + \xi\mu).$$

If on the other hand the variance of ε is ξ/μ, then $\text{var}(Y) = (1 + \xi)\mu$. In both cases the variance of Y is greater than its value under the standard Poisson model, for which $\xi = 0$. In the first case the variance function is quadratic, and in the second it is linear.

Negative binomial model

Example 28 (Negative binomial) *In Example 27, if ε is gamma with shape parameter $1/\nu$, show that*

$$f(y;\mu,\nu) = \frac{\Gamma(y+\nu)}{\Gamma(\nu)y!}\frac{\nu^\nu \mu^y}{(\nu+\mu)^{\nu+y}}, \quad y = 0,1,\ldots, \quad \mu,\nu > 0,$$

and that quadratic and linear variance functions are obtained on setting $\nu = 1/\xi$ and $\nu = \mu/\xi$ respectively.
The log link function $\log\mu = x^{\mathrm{T}}\beta$ is most natural.
ξ is estimated by maximum likelihood or through Pearson's statistic.

Example 29 (AIDS data)

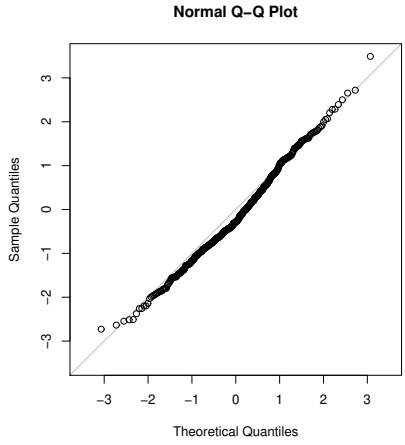
- *MLE $\widehat{\xi}_Q = 22.7$ (5.5)*
- *Analysis of Deviance (with $\widehat{\xi}_Q$ fixed):*

Model	*df*	*Deviance reduction*	*df*	*Deviance*
			464	*7998.3*
Time (rows)	*37*	*3582.5*	*427*	*4415.8*
Delay (cols)	*14*	*3892.2*	*413*	*523.6*

- *Still somewhat overdispersed?*

AIDS data: Deviance residuals for NB model

Clear improvement over previous plots, even if not perfect.



Quasi-likelihood

- Recall two basic assumptions for the linear model:
  - the responses are uncorrelated with means $\mu_j = x_j^{\mathrm{T}}\beta$ and equal variances σ^2;
  - in addition to this, the responses are normally distributed.
- To avoid parametric modelling, we generalise the second-order assumptions, to

$$\mathrm{E}(Y_j) = \mu_j, \quad \mathrm{var}(Y_j) = \phi_j V(\mu_j), \quad g(\mu_j) = \eta_j = x_j^{\mathrm{T}}\beta,$$

  where the variance function $V(\cdot)$ and the link function are taken as known.
- We obtain estimates $\tilde{\beta}$ by solving the estimating equation

$$h(\beta; Y) = X^{\mathrm{T}}u(\beta) = \sum_{j=1}^{n} x_j u_j(\beta) = \sum_{j=1}^{n} x_j \frac{Y_j - \mu_j}{g'(\mu_j)\phi_j V(\mu_j)} = 0.$$

- If the mean structure is correct, then $\mathrm{E}(Y_j) = \mu_j$, so $\mathrm{E}\{h(\beta; Y)\} = 0$, and under mild conditions $\tilde{\beta}$ is consistent (but maybe not efficient) as $n \to \infty$.

Quasi-likelihood II

Recall that the general variance of an estimator $\tilde{\beta}$ defined by an estimating equation $h(\beta; Y)_{p\times 1} = 0_p$ has sandwich form

$$\mathrm{E}\left\{-\frac{\partial h(\beta; Y)}{\partial \beta^{\mathrm{T}}}\right\}^{-1} \mathrm{var}\left\{h(\beta; Y)\right\} \mathrm{E}\left\{-\frac{\partial h(\beta; Y)^{\mathrm{T}}}{\partial \beta}\right\}^{-1}.$$

Lemma 30 *If $V(\mu)$ is correctly specified, then $\mathrm{var}(\tilde{\beta}) \doteq (X^{\mathrm{T}}WX)^{-1}$, where W is diagonal with (j, j) element $\{g'(\mu_j)^2\phi_j V(\mu_j)\}^{-1}$.*

- If $\phi_j = \phi a_j$, with known $a_j > 0$ and unknown $\phi > 0$, then we obtain
  - $\tilde{\beta}$ by fitting the GLM with variance function $V(\mu)$ and link $g(\mu)$;
  - standard errors by multiplying the standard errors for this fit by $\widehat{\phi}^{1/2}$, where

$$\widehat{\phi} = \frac{1}{n-p}\sum_{j=1}^{n} \frac{(y_j - \widehat{\mu}_j)^2}{a_j g'(\mu_j)^2 V(\widehat{\mu}_j)}.$$

Note to Lemma 30

- Note first that we can write

$$u_j(\beta) \equiv u_j(\mu_j) = \frac{A_j(\mu_j)}{B_j(\mu_j)},$$

where $A_j(\mu_j) = Y_j - \mu_j$ and $B_j(\mu_j) = g'(\mu_j)\phi_j V(\mu_j)$. Only A_j is random and $\mathrm{E}\{A_j(\mu_j)\} = 0$. Hence if we let prime denote derivative with respect to μ_j,

$$\frac{\partial u_j(\mu_j)}{\partial \mu_j} = \frac{A_j'(\mu_j)}{B_j(\mu_j)} - \frac{A_j(\mu_j)B_j'(\mu_j)}{B_j^2(\mu_j)}$$

has expectation $\mathrm{E}\{A_j'(\mu_j)\}/B_j(\mu_j) = -1/B_j(\mu_j)$.

- We require $\mathrm{E}\{-\partial h(\beta;Y)/\partial\beta^{\mathrm{T}}\}$ and $\mathrm{var}\{h(\beta;Y)\}$. Now

$$\frac{\partial u_j(\beta)}{\partial \beta^{\mathrm{T}}} = \frac{\partial \eta_j}{\partial \beta^{\mathrm{T}}}\frac{\partial \mu_j}{\partial \eta_j}\frac{\partial u_j(\beta)}{\partial \mu_j} = x_j^{\mathrm{T}}\frac{1}{g'(\mu_j)}u_j'(\mu_j),$$

which gives

$$\mathrm{E}\left\{-\frac{\partial h(\beta;Y)}{\partial \beta^{\mathrm{T}}}\right\} = -\sum_{j=1}^{n} x_j \mathrm{E}\left\{\frac{\partial u_j(\beta)}{\partial \beta^{\mathrm{T}}}\right\} = \sum_{j=1}^{n} x_j x_j^{\mathrm{T}}\frac{1}{g'(\mu_j)^2\phi_j V(\mu_j)} = X^{\mathrm{T}}WX,$$

where W is the $n \times n$ diagonal matrix with jth element $\{g'(\mu_j)^2\phi_j V(\mu_j)\}^{-1}$. Moreover if in addition the variance function has been correctly specified, then $\mathrm{var}(Y_j) = \phi_j V(\mu_j)$, and hence

$$\mathrm{var}\{h(\beta;Y)\} = X^{\mathrm{T}}\mathrm{var}\{u(\beta)\}X = \sum_{j=1}^{n} x_j x_j^{\mathrm{T}}\frac{\mathrm{var}(Y_j)}{g'(\mu_j)^2\phi_j^2 V(\mu_j)^2} = X^{\mathrm{T}}WX.$$

Thus the sandwich equals $(X^{\mathrm{T}}WX)^{-1}$.

- Had the variance function been wrongly specified, the variance matrix of $\tilde{\beta}$ would have been $(X^{\mathrm{T}}WX)^{-1}(X^{\mathrm{T}}W'X)(X^{\mathrm{T}}WX)^{-1}$, where W' is a diagonal matrix involving the true and assumed variance functions. Only if the variance function has been chosen very badly will this sandwich matrix differ greatly from $(X^{\mathrm{T}}WX)^{-1}$, which therefore provides useful standard errors unless a plot of absolute residuals against fitted means is markedly non-random. In that case the choice of variance function should be reconsidered.

Quasi-likelihood III

- Under an exponential family model, $h(\beta; Y)$ is the score statistic, so $\tilde{\beta}$ is the MLE and is efficient (i.e., it has the smallest possible variance in large samples).
- If not, inference is valid provided g and V are correctly chosen, and $\tilde{\beta}$ is optimal among estimators based on linear combinations of the $Y_j - \mu_j$, by extending the Gauss–Markov theorem.
- In fact we can define a **quasi-likelihood** Q and its score through

$$Q(\beta; Y) = \sum_{j=1}^{n} \int_{Y_j}^{\mu_j} \frac{Y_j - u}{\phi a_j V(u)} \, \mathrm{d}u, \quad h(\beta; Y) = \frac{\partial}{\partial \beta} Q(\beta; Y),$$

  and a (quasi-)deviance as $D = -2\phi Q(\beta; Y)$.
- To compare models A, B with numbers of parameters $p_B < p_A$ and deviances $D_B > D_A$, we use the fact that

$$\frac{(D_B - D_A)/(p_A - p_B)}{\widehat{\phi}_A} \quad \dot{\sim} \quad F_{p_A - p_B, n - p_A},$$

  if the simpler model B is adequate. This is easy in R.

AIDS example

```
> aids.ql <- glm(y~factor(time)+factor(delay),family=quasipoisson,data=aids.in)
> anova(aids.ql,test="F")
Analysis of Deviance Table

Model: quasipoisson, link: log

Response: y

Terms added sequentially (first to last)


             Df Deviance Resid. Df Resid. Dev       F    Pr(>F)
NULL                           464    14184.3
factor(time)  37   6114.8       427     8069.5  92.638 < 2.2e-16 ***
factor(delay) 14   7353.0       413      716.5 294.402 < 2.2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Summary

- ☐ Overdispersion is widespread in count and proportion data.
- ☐ We deal with it either by
  - parametric modelling, or
  - quasi-likelihood (QL) estimation, which involves assumptions only on the mean-variance relationship.
- ☐ QL estimators equal the ML ones, but SEs are inflated by $\widehat{\phi}^{1/2}$.
- ☐ (Quasi-)deviance can also be defined, and used for model comparison, with F tests replacing χ^2 tests.

3 Regularisation slide 180

3.1 Basic Notions slide 181

Tall and wide regressions

- So far we have supposed that we have a **tall regression**:
  - the number of units n exceeds the number of variables p,
  - the design matrix X has rank p.
- In many 'modern' settings we instead have a **wide regression**:
  - n and p are comparable, $p > n$, maybe even $p \gg n$;
  - in genomics, for example (typically) $n = O(10^2, 10^3)$, $p = O(10^5, 10^6)$;
  - hence $\text{rank}(X) = \min(n, p) = n$.
- Even tall X may be 'almost singular', making β 'almost inestimable'.
- Solutions:
  - subset selection (drop certain columns of X);
  - seek different good explanations of response variation, not single model;
  - regularisation (often with prediction in mind).
- Certain regularisation methods (e.g., lasso) also perform subset selection.

Different good explanations

- With $p > n$, perhaps $p \gg n$, X is rank-deficient and many β may give $X\beta = y$.
- To find important variables we include intrinsic variables (gender, ...) in all models, and then
  - choose some k (preferably ≤ 15) such that $k < n$ and suppose that $p < k^a$ (let $a = 3$ for easy visualisation);
  - assign each variable to a cell of a hyper-cube with coordinates $\{1, \ldots, k\}^a$;
  - fit a linear model containing each set of k variables corresponding to the ak^{a-1} rows, columns, ... of the cube, so each variable appears in a distinct models;
  - for each such model, retain the two variables that are most significant.
- Iterate the above procedure, retaining only the most significant variables at each stage, aiming for a final set of 10–20 variables, for which a careful analysis is performed, perhaps leading to several different good explanations of the response variation.
- Some cells of the hyper-cube may be empty, and important variables might be assigned to several cells.
- The above design is a form of **balanced incomplete block design (BIBD)** (with k^a treatments and ak^{a-1} blocks).
- See Cox and Battey (2017, PNAS)

Collinearity

- Columns of X **collinear** if there exists a non-zero $v_{p\times 1}$ such that $Xv = 0$, i.e., rank$(X) < p$, so there is no unique $\widehat{\beta}$ minimising $\|y - X\beta\|^2$.
- Software deals with this by dropping columns of X, but it may be better to write $X\beta = XC\gamma$, where XC is full rank and γ has a clear interpretation.
- If X is nearly collinear, its SVD $U_{n\times n}D_{n\times p}V^{\mathrm{T}}_{p\times p}$, with $d_1 \geq \cdots \geq d_p \geq 0$, gives

$$\widehat{\beta} = (X^{\mathrm{T}}X)^{-1}X^{\mathrm{T}}y = VD_{-}^{\mathrm{T}}U^{\mathrm{T}}y = \sum_{r=1}^{p}(u_r^{\mathrm{T}}y/d_r)v_r,$$

  so $\widehat{\beta}$ is a linear combination of the vectors v_r with coefficients $u_r^{\mathrm{T}}y/d_r$. As $\mathrm{var}(U^{\mathrm{T}}y) = \sigma^2 I_n$,

$$\mathrm{var}(\widehat{\beta}) = \sigma^2 VD_{-}^{\mathrm{T}}D_{-}V^{\mathrm{T}} = \sigma^2\sum_{r=1}^{p} d_r^{-2}v_r v_r^{\mathrm{T}},$$

  i.e., $\widehat{\beta}$ is unstable in the directions corresponding to the v_r with small singular values d_r.
- In numerical analysis, collinearity often measured using **condition number** $(d_1/d_p)^{1/2}$, but its statistical meaning is unclear.

Regularisation

- Stop $\widehat{\beta}$ from fluctuating too wildly in directions with small eigenvalues d_r, by adding a non-negative penalty $p_\lambda(\beta)$ and choosing β to minimise the **penalised sum of squares**

$$\|y - X\beta\|^2 + p_\lambda(\beta). \tag{16}$$

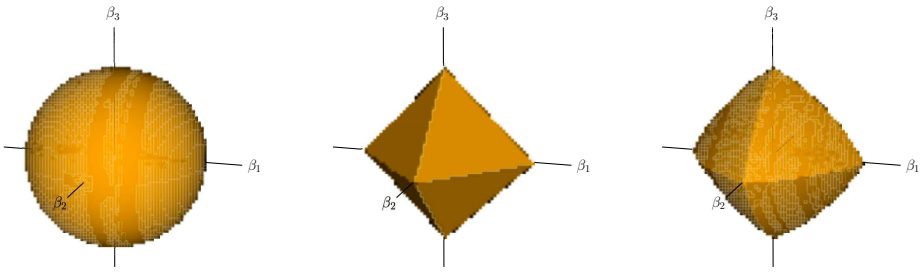
- The strength of the penalty depends on a positive parameter λ that constrains β more as λ increases.
- Often $p_\lambda(\beta) = \lambda p(\beta)$, where, for example,
  - $p(\beta) = \|\beta\|_2^2 = \sum_{r=1}^{p}\beta_r^2$ gives **ridge regression** (aka Tikhonov regularisation);
  - $p(\beta) = \|\beta\|_1 = \sum_{r=1}^{p}|\beta_r|$ gives the **lasso** (aka L_1 regularisation);
  - $p(\beta) = (1-\alpha)\|\beta\|_2^2 + \alpha\|\beta\|_1$ for $0 \leq \alpha \leq 1$ gives the **elastic net**;
  - $p(\beta) = \sum_{g=1}^{G} p_g^{1/2}\|\beta_g\|_2$, with β_g being $p_g \times 1$ sub-vectors of β, gives the **grouped lasso**, which penalises factors with parameters β_g.
- It is useful to see regularisation through the lens of Bayesian inference, with the regularising term equivalent to the prior density.

Bound form

- Equivalently we can take the **bound form** of the minimisation problem, i.e.,

$$\text{minimise}_\beta \quad \|y - X\beta\|_2^2 \quad \text{subject to} \quad p(\beta) \leq t,$$

  for some $t \geq 0$, where setting $t = \infty$ just gives the least squares estimates.
- Below: constraint balls for ridge (left), lasso (centre) and elastic-net (right) regularisation. The sharp corners of the last two allow for variable selection as well as shrinkage.



Bayesian setting

- Treat all unknowns as random variables, and compute conditional distribution of unobserved unknowns conditional on observed unknowns.
- Requires prior density on β, and if σ^2 is known, then a simple combination of **data model** and **prior model** is

$$y \mid \beta, \sigma^2 \sim \mathcal{N}(X\beta, \sigma^2 I_n), \quad \beta \mid \sigma^2 \sim \mathcal{N}_p(\beta_*, \sigma^2 V_*), \tag{17}$$

  where the prior model is determined by β_* and V_*.
- Full specification would require prior on σ^2, but we don't need this.
- Let $\equiv$ mean we have dropped additive constants not involving the argument of a density.
- The log multivariate normal density is

$$\begin{aligned} \log f(x \mid \mu, \Omega) &= -\frac{m}{2}\log 2\pi - \frac{1}{2}\log|\Omega| - \frac{1}{2}(x-\mu)^{\mathrm{T}}\Omega^{-1}(x-\mu) \\ &\equiv x^{\mathrm{T}}\Omega^{-1}\mu - \frac{1}{2}x^{\mathrm{T}}\Omega^{-1}x \\ &\equiv Q(x) = x^{\mathrm{T}}a - \frac{1}{2}x^{\mathrm{T}}Bx, \end{aligned}$$

  say, and as $\exp Q(x)$ is proportional to a unique probability density function,

$$\mathrm{E}(X) = \mu = B^{-1}a, \quad \mathrm{var}(X) = \Omega = B^{-1}, \quad \text{where } B \text{ is the } \textbf{precision matrix}.$$

Bayesian linear model I

- The model (6) gives

$$\begin{aligned}\log f(\beta \mid y, \sigma^2) &= \log\left\{\frac{f(y \mid \beta, \sigma^2) f(\beta \mid \sigma^2)}{f(y \mid \sigma^2)}\right\} \\ &\equiv \log f(y \mid \beta, \sigma^2) + \log f(\beta \mid \sigma^2) \\ &\equiv -\frac{(y - X\beta)^{\mathrm{T}}(y - X\beta)}{2\sigma^2} - \frac{(\beta - \beta_*)^{\mathrm{T}} V_*^{-1}(\beta - \beta_*)}{2\sigma^2} \\ &\propto \|y - X\beta\|_2^2 + (\beta - \beta_*)^{\mathrm{T}} V_*^{-1}(\beta - \beta_*).\end{aligned}$$

- Comparison with (5) shows that $p_\lambda(\beta)$ represents prior beliefs about the likely values of β: before seeing the data, the most plausible value is β_*, with precision V_*^{-1}.
- Dropping more constants,

$$\begin{aligned}\log f(\beta \mid y, \sigma^2) &\equiv \frac{1}{\sigma^2}\left\{\beta^{\mathrm{T}} X^{\mathrm{T}} y - \beta^{\mathrm{T}}(X^{\mathrm{T}} X)\beta/2 + \beta^{\mathrm{T}} V_*^{-1}\beta_* - \beta^{\mathrm{T}} V_*^{-1}\beta/2\right\} \\ &= \frac{1}{2\sigma^2}\left\{2\beta^{\mathrm{T}}(X^{\mathrm{T}} y + V_*^{-1}\beta_*) - \beta^{\mathrm{T}}(X^{\mathrm{T}} X + V_*^{-1})\beta\right\}, \qquad (18)\end{aligned}$$

  which is $Q(x)$ with x, a and B replaced by β, $(X^{\mathrm{T}} y + V_*^{-1}\beta_*)/\sigma^2$ and $(X^{\mathrm{T}} X + V_*^{-1})/\sigma^2$.
- Hence $f(\beta \mid y, \sigma^2)$ is multivariate normal with mean vector and variance matrix

$$\mathrm{E}(\beta \mid y, \sigma^2) = (X^{\mathrm{T}} X + V_*^{-1})^{-1}(X^{\mathrm{T}} y + V_*^{-1}\beta_*), \quad \mathrm{var}(\beta \mid y, \sigma^2) = \sigma^2 (X^{\mathrm{T}} X + V_*^{-1})^{-1}.$$

Bayesian linear model II

- The **maximum a posteriori (MAP) estimator** of β is $\mathrm{E}(\beta \mid y, \sigma^2)$, and the MAP estimator of $A_{q\times p}\beta$ is $A\mathrm{E}(\beta \mid y, \sigma^2)$, which has a posterior normal density.
- When $X^{\mathrm{T}} X$ is invertible,

$$\tilde{\beta} = \mathrm{E}(\beta \mid y, \sigma^2) = (X^{\mathrm{T}} X + V_*^{-1})^{-1}(X^{\mathrm{T}} X\widehat{\beta} + V_*^{-1}\beta_*)$$

  is an average of $\widehat{\beta}$ and β_*, weighted by $X^{\mathrm{T}} X$ and V_*^{-1}.
- The posterior precision matrix

$$\mathrm{var}(\beta \mid y, \sigma^2)^{-1} = X^{\mathrm{T}} X/\sigma^2 + V_*^{-1}/\sigma^2$$

  adds the Fisher information and the prior precision matrix, V_*^{-1}/σ^2.
- High precision corresponds to small variance, and conversely:
  - letting $V_*^{-1} \to 0$ yields an improper prior density; and
  - for large V_*^{-1} the posterior precision is essentially determined by the prior precision.

  Thus the prior density regularises $\widehat{\beta}$ by including β_* and V_*.

Improper prior density

- We only need V_* to add information in directions corresponding to small singular values of X, so we might use an **improper prior** in which V_* is singular:

$$f(\beta \mid \sigma^2) = \frac{1}{(2\pi)^{p/2}|V_*|_+^{1/2}} \exp\left\{-(\beta-\beta_*)^{\mathrm{T}} V_*^- (\beta-\beta_*)/(2\sigma^2)\right\}, \tag{19}$$

  where V_* has spectral decomposition ED_*E^{T},
  - $|V_*|_+$ denotes the product of the non-zero elements of D_*, and
  - $V_*^- = \sum_{r:d_{*r}>0} e_r e_r^{\mathrm{T}}/d_{*r}$ is a generalized inverse of V_*.
- Below we write V_*^- even when V_* is invertible.
- (8) is improper because it is not integrable in the directions of the columns of E for which the corresponding d_r^* equal zero, but we need only that the posterior density of β be proper, i.e., that the posterior precision matrix

$$\mathrm{var}(\beta \mid y, \sigma^2)^{-1} = X^{\mathrm{T}}X/\sigma^2 + V_*^-/\sigma^2$$

  is invertible.

Empirical Bayes

- Use the data to estimate the prior: construct estimators using Bayesian arguments, but assess their properties using classical criteria (bias, MSE, ...)
- The estimator $\tilde{\beta} = \mathrm{E}(\beta \mid y, \sigma^2)$ has mean and variance

$$\begin{aligned} \mathrm{E}(\tilde{\beta} \mid \beta) &= (X^{\mathrm{T}}X + V_*^-)^{-1}(X^{\mathrm{T}}X\beta + V_*^-\beta_*) \\ &= \beta + (X^{\mathrm{T}}X + V_*^-)^{-1}V_*^-(\beta_* - \beta), \\ \mathrm{var}(\tilde{\beta} \mid \beta) &= \sigma^2(X^{\mathrm{T}}X + V_*^-)^{-1}X^{\mathrm{T}}X(X^{\mathrm{T}}X + V_*^-)^{-1}. \end{aligned} \tag{20}$$

- Hence $\tilde{\beta}$
  - is biased unless $\beta_* = \beta$,
  - has smaller variance than $\widehat{\beta}$,

  so maybe there is a bias-variance tradeoff when estimating $A\beta$.
- If we write $\mu = \mathrm{E}(\tilde{\beta} \mid \beta)$, then the MSE is

$$\begin{aligned} \mathrm{E}\left(\|A\tilde{\beta} - A\beta\|^2 \mid \beta\right) &= \mathrm{E}\{(\tilde{\beta}-\beta)^{\mathrm{T}}A^{\mathrm{T}}A(\tilde{\beta}-\beta) \mid \beta\} \\ &= \mathrm{E}\left[\mathrm{tr}\left\{A(\tilde{\beta}-\beta)(\tilde{\beta}-\beta)^{\mathrm{T}}A^{\mathrm{T}}\right\} \mid \beta\right] \\ &= \mathrm{tr}\left[\mathrm{E}\left\{A(\tilde{\beta}-\mu+\mu-\beta)(\tilde{\beta}-\mu+\mu-\beta)^{\mathrm{T}}A^{\mathrm{T}} \mid \beta\right\}\right]. \end{aligned}$$

Empirical Bayes II

- The expectation above is

$$A\left\{\mathrm{var}(\tilde{\beta} \mid \beta) + (X^{\mathrm{T}}X + V_*^-)^{-1}V_*^-(\beta - \beta_*)(\beta - \beta_*)^{\mathrm{T}}V_*^-(X^{\mathrm{T}}X + V_*^-)^{-1}\right\}A^{\mathrm{T}},$$

  giving the MSE when estimating a fixed β.
- Taking expectations over the prior model for β gives

$$\mathrm{E}\left(\|A\tilde{\beta} - A\beta\|^2\right) = \sigma^2\mathrm{tr}\left\{A(X^{\mathrm{T}}X + V_*^-)^{-1}A^{\mathrm{T}}\right\}, \tag{21}$$

  which is larger than $A\mathrm{var}(\tilde{\beta} \mid \beta)A^{\mathrm{T}}$ and does not depend on β_*.
- This computation uses only the mean and variance, so holds under second-order assumptions.
- From now on we set $\beta_* = 0$, unless we state otherwise.

Equivalent degrees of freedom

- If we set $\beta_* = 0$, then the fitted values are

$$\tilde{y} = X\tilde{\beta} = X(X^{\mathrm{T}}X + V_*^-)^{-1}X^{\mathrm{T}}y = H_*y,$$

  say.
- We define the **equivalent degrees of freedom** of the fit as

$$\mathrm{edf} = \mathrm{tr}(H_*) = \mathrm{tr}\{X(X^{\mathrm{T}}X + V_*^-)^{-1}X^{\mathrm{T}}\} = p - \mathrm{tr}\{(X^{\mathrm{T}}X + V_*^-)^{-1}V_*^-\},$$

- This is lower than p unless $V_*^- = 0$, so regularisation reduces the degrees of freedom by an amount that depends on V_*.
- The penalised estimate is a linear function of the unpenalised one (if it exists), as we can write

$$\tilde{\beta} = (X^{\mathrm{T}}X + V_*^-)^{-1}X^{\mathrm{T}}X\widehat{\beta} = P_*\widehat{\beta},$$

  say. As

$$\mathrm{edf} = \mathrm{tr}(H_*) = \mathrm{tr}(P_*),$$

  this gives an alternative formula useful in complex models.

How much penalisation?

- ☐ Often V_*^- depends on some $\lambda > 0$ that must be chosen, as well as σ^2, which is usually estimated by a (penalised) residual sum of squares.
- ☐ To estimate λ, we compare y_j with its predicted value $\widehat{y}_{\lambda,j}^- = x_j^{\mathrm{T}}\widehat{\beta}_{\lambda,-j}$, where $\widehat{\beta}_{\lambda,-j}$ is

$$\widehat{\beta}_\lambda = (X^{\mathrm{T}}X + V_*^-)^{-1}X^{\mathrm{T}}y$$

  computed with the jth rows x_j and y_j of X and y omitted.
- ☐ Using Lemma 14, the **leave-one-out cross-validation** sum of squares is then

$$\mathrm{CV}_\lambda = \sum_{j=1}^n (y_j - \widehat{y}_{\lambda,j}^-)^2 = \|y - \widehat{y}_\lambda^-\|^2 = \sum_{j=1}^n \frac{(y_j - \widehat{y}_{\lambda,j})^2}{(1-h_{\lambda,jj})^2},$$

  where $\widehat{y}_{\lambda,j}$ is the jth element of the complete-data fitted value $H_\lambda y$ and $h_{\lambda,jj}$ is the jth diagonal element of $H_\lambda = X(X^{\mathrm{T}}X + V_*^-)^{-1}X^{\mathrm{T}}$ for the overall fit.
- ☐ More often we use the **generalized cross-validation** criterion

$$\mathrm{GCV}_\lambda = \sum_{j=1}^n \frac{(y_j - \widehat{y}_{\lambda,j})^2}{\{1 - \mathrm{tr}(H_\lambda)/n\}^2}.$$

- ☐ Whichever criterion is used, it is typically minimised numerically over a grid of values of λ.

REML

- ☐ Cross-validation makes only second-order assumptions.
- ☐ Under normality, the marginal density of y is $\mathcal{N}\{X\beta_*, \sigma^2(I_n + XV_*X^{\mathrm{T}})\}$, so we could estimate β_*, σ^2 and λ by maximising the corresponding likelihood.
- ☐ If n and p are large, this results in biased estimates of λ and σ^2, so we prefer to eliminate β_*, resulting in a **log restricted likelihood** whose form is given below, with $W_\lambda^{-1} = I_n + XV_*X^{\mathrm{T}}$.

Lemma 31 *In a model in which $y \sim \mathcal{N}(X\beta, \sigma^2 W_\lambda^{-1})$, where W_λ depends on a parameter λ, a log restricted likelihood for σ^2 and λ is*

$$\ell_{\mathrm{REML}}(\sigma^2, \lambda) \equiv \frac{1}{2}\log(|W_\lambda|/|X^{\mathrm{T}}W_\lambda X|) - \frac{n-p}{2}\log\sigma^2 - \frac{1}{2\sigma^2}(y - \widehat{y}_\lambda)^{\mathrm{T}}W_\lambda(y - \widehat{y}_\lambda),$$

where $\widehat{\beta}_\lambda = (X^{\mathrm{T}}W_\lambda X)^{-1}X^{\mathrm{T}}W_\lambda y$ and $\widehat{y}_\lambda = X\widehat{\beta}_\lambda$. For fixed λ the restricted maximum likelihood estimator of σ^2 is therefore

$$\widehat{\sigma}_\lambda^2 = \frac{1}{n-p}(y - \widehat{y}_\lambda)^{\mathrm{T}}W_\lambda(y - \widehat{y}_\lambda),$$

and the resulting profile log restricted likelihood for λ is

$$\ell_{\mathrm{p}}(\lambda) \equiv \frac{1}{2}\log(|W_\lambda|/|X^{\mathrm{T}}W_\lambda X|) - \frac{(n-p)}{2}\log\widehat{\sigma}_\lambda^2.$$

Note on Lemma 31

- Suppose that $f(y;\alpha,\beta)$ depends on two parameters, that interest is focused on α, and that for fixed α there is a minimal sufficient statistic s_α for β. Then $f(y;\alpha,\beta) = f(y \mid s_\alpha;\alpha) f(s_\alpha;\alpha,\beta)$, and since the first density on the right is a proper conditional density not depending on β, we can use it for inference on α, in the form

$$\log f(y \mid s_\alpha;\alpha) = \log f(y;\alpha,\beta) - \log f(s_\alpha;\alpha,\beta).$$

  As the left-hand side of this expression does not depend on β, we may be able to simplify the right-hand side by an astute choice of β.

- In the normal model we take $\alpha = (\sigma^2,\lambda)$. If α is fixed, then $s_\alpha = \widehat{\beta}_\alpha = (X^{\mathrm{T}} W_\lambda X)^{-1} X^{\mathrm{T}} W_\lambda y$ is sufficient for β; its distribution is $\mathcal{N}_p\{\beta, \sigma^2 (X^{\mathrm{T}} W_\lambda X)^{-1}\}$. Hence

$$\ell_{\mathrm{REML}}(\sigma^2,\lambda) = \log f(y \mid \widehat{\beta}_\lambda;\sigma^2,\lambda) = \log f(y;\sigma^2,\lambda,\beta) - \log f(\widehat{\beta}_\lambda;\sigma^2,\lambda,\beta)$$

  which equals

$$\begin{aligned} -\frac{n}{2}\log\sigma^2 \quad &+ \quad \tfrac{1}{2}\log|W_\lambda| - \frac{1}{2\sigma^2}(y - X\beta)^{\mathrm{T}} W_\lambda (y - X\beta) \\ &+ \quad \frac{p}{2}\log\sigma^2 - \tfrac{1}{2}\log|X^{\mathrm{T}} W_\lambda X| + \frac{1}{2\sigma^2}(\widehat{\beta}_\lambda - \beta)^{\mathrm{T}} X^{\mathrm{T}} W_\lambda X (\widehat{\beta}_\lambda - \beta), \end{aligned}$$

  or equivalently, on setting $\beta = 0$ and $\widehat{y}_\lambda = X\widehat{\beta}_\lambda$,

$$\tfrac{1}{2}\log(|W_\lambda|/|X^{\mathrm{T}} W_\lambda X|) - \frac{(n-p)}{2}\log\sigma^2 - \frac{1}{2\sigma^2}\left(y^{\mathrm{T}} W_\lambda y - \widehat{y}_\lambda^{\mathrm{T}} X^{\mathrm{T}} W_\lambda \widehat{y}_\lambda\right).$$

- The last term reduces to the given form because $\widehat{y}_\lambda^{\mathrm{T}} W_\lambda (y - \widehat{y}_\lambda) = 0$, so the term in brackets in the last displayed equation is the residual sum of squares $(y - \widehat{y}_\lambda)^{\mathrm{T}} W_\lambda (y - \widehat{y}_\lambda)$.

- The restricted maximum likelihood estimator $\widehat{\sigma}^2_\lambda$ and the profile log restricted likelihood for λ are obtained by maximising $\ell_{\mathrm{REML}}(\sigma^2,\lambda)$, for fixed λ and then dropping constant terms from $\ell_{\mathrm{REML}}(\widehat{\sigma}^2_\lambda,\lambda)$.

3.2 Simple Applications

Ridge regression

- Used for prediction when X is close to singular.
- If the first column of X is 1_n, we set $\beta_* = 0$ and $V_*^- = \lambda S = \lambda \mathrm{diag}(0, I_{p-1})$, giving

$$\widehat{\beta}_\lambda = (X^{\mathrm{T}} + \lambda S)^{-1} X^{\mathrm{T}} y, \quad \widehat{y}_\lambda = X\widehat{\beta}_\lambda = X(X^{\mathrm{T}} + \lambda S)^{-1} X^{\mathrm{T}} y = H_\lambda y,$$

  and effective degrees of freedom

$$\mathrm{edf}_\lambda = \mathrm{tr}(H_\lambda) = \mathrm{tr}\{(X^{\mathrm{T}}X + \lambda S)^{-1} X^{\mathrm{T}} X\} = \sum_{r=1}^{p} \frac{1}{1 + \lambda \delta_r},$$

  where $\delta_p \geq \cdots \geq \delta_2 > \delta_1 = 0$ are the eigenvalues of $(X^{\mathrm{T}}X)^{-1/2} S (X^{\mathrm{T}}X)^{-1/2}$.
- As λ increases from zero to infinity, edf_λ decreases from $p = \mathrm{rank}(X)$ to 1. The two are equivalent, but edf_λ is more easily interpreted, because it is not related to the scale of X.
- The inverse exists even if $X^{\mathrm{T}}X$ is singular, but if it is invertible then

$$\widehat{\beta}_\lambda = (X^{\mathrm{T}}X + \lambda S)^{-1}(X^{\mathrm{T}}X + \lambda S - \lambda S)(X^{\mathrm{T}}X)^{-1} X^{\mathrm{T}} y = \widehat{\beta} - \lambda (X^{\mathrm{T}}X + \lambda S)^{-1} S \widehat{\beta},$$

  so as $\lambda \to \infty$ all the elements of $\widehat{\beta}_\lambda$ tend to zero, other than the first. This corresponds to reducing the prior variance to zero, thereby giving the data themselves less and less influence on the elements of $\widehat{\beta}_\lambda$ other than the first, and thus stabilises the estimator.

Example: Cement data

```
> cement
   x1 x2 x3 x4     y
1   7 26  6 60  78.5
2   1 29 15 52  74.3
3  11 56  8 20 104.3
4  11 31  8 47  87.6
5   7 52  6 33  95.9
6  11 55  9 22 109.2
7   3 71 17  6 102.7
8   1 31 22 44  72.5
9   2 54 18 22  93.1
10 21 47  4 26 115.9
11  1 40 23 34  83.8
12 11 66  9 12 113.3
13 10 68  8 12 109.4
```

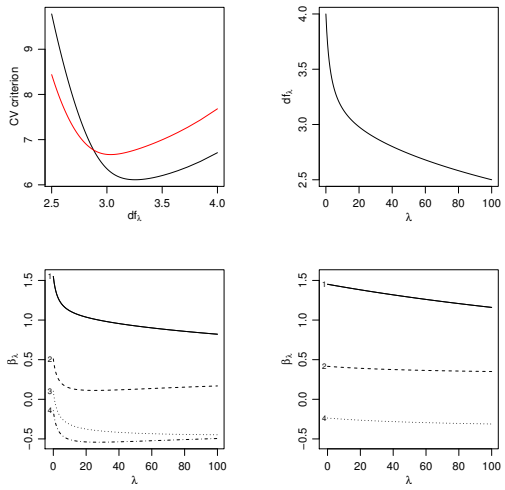
Example: Cement data

	Full model		Reduced model	
Parameter	Estimate	Standard error	Estimate	Standard error
β_0	62.41	70.07	71.64	14.14
β_1	1.55	0.74	1.45	0.12
β_2	0.51	0.72	0.42	0.19
β_3	0.10	0.75		
β_4	–0.14	0.71	–0.24	0.17

- ☐ The next slide shows results for ridge fits for these models.
- ☐ Looks like 3 df is optimal for prediction.
- ☐ Software often preprocesses X and y by either
  - centering both, by subtracting column means, or
  - centering y and centering and scaling X, so the column means are zero and the column variances are unity.
- ☐ The singular values for the centred X matrix are 78.8, 28.5, 12.2, 1.7, and those for the centred and scaled X matrix are 5.18, 4.35, 1.50, 0.14, so it matters which is used.
- ☐ The singular values for the (centred) reduced matrix are 78.8, 19.8 and 9.15.
- ☐ The shrinkage due to increasing λ occurs more slowly for the reduced model.

Example: Cement data/Ridge analysis

Top left: CV (black) and GCV (red) as functions of degrees of freedom df_λ. Top right: dependence of df_λ on λ. Bottom left: $\widehat{\beta}_\lambda$ as a function of λ, with all four covariates. Bottom right: $\widehat{\beta}_\lambda$ as a function of λ, with x_1, x_2, and x_4 only.



Comments

- ☐ The literature on ridge regression is very large and very dispersed, with many variants and many connections to ML techniques.
- ☐ Be careful with software: any pre-processing of X is not always described.