Regression II

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1. Distributional checks
   - Leverage
   - Weighted Least Squares

Set–up

- We can generalize this to

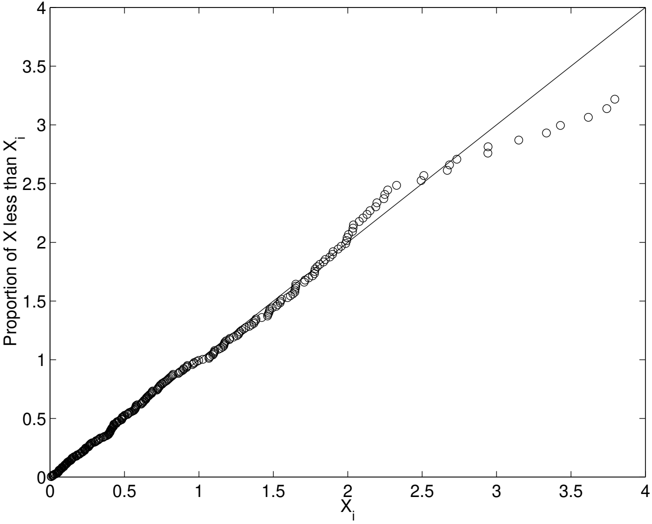
$$P(Y \leq y) = F(y)$$

and so as $n \to \infty$

$$F_n(y) \to F(y)$$

$$\begin{aligned} F^{-1}(F_n(y_i)) &\approx y_i \\ F^{-1}(\text{prop. of obs. } \leq y_i) &\approx y_i. \end{aligned}$$

QQ–plot



Set–up

- Note that
$$\mathbb{V}\mathrm{ar}\{\mathsf{e}\} = \sigma^2(\mathsf{I}_n - \mathsf{P})$$
- If $p_{ii} \approx 1$ then the variance of the ith residual is very low.
- Totally determined by X, i.e. the design matrix is forcing the ith observation to have high impact.
- The ith observation has **high leverage**.
- $\sum_{i=1}^{n} p_{ii} = p$ so the "average" is p/n and a rule of thumb is to take notice when
$$p_{ii} > \frac{2p}{n}.$$

Weighted Least Squares

- Consider the linear model

$$\mathbb{E}\{Y_i\} = \mathrm{x}_i\beta$$

and

$$\mathbb{V}\mathrm{ar}(Y_i) = \frac{\sigma^2}{w_i},$$

where w_i are known weights.
- heteroscedastic variables.
- Using least squares is no longer optimal.
- Cases with small w_i need to be downweighted with respect to the parameter estimation while those with w_i large need to be given more weight.

Weighted Least Squares

- Find an estimate for β by minimising the weighted sum of squares:

$$
\begin{aligned}
S(\beta) &= \sum_{i=1}^{n} w_i \left(Y_i - \mathrm{x}_i^T \beta \right)^2 \\
&= \sigma^2 \sum_{i=1}^{n} \frac{(Y_i - E\{Y_i\})^2}{\mathbb{V}\mathrm{ar}\{Y_i\}}
\end{aligned}
$$

Weighted Least Squares

- In vector form we then have:

$$Y = X\beta + D\epsilon$$

$$\mathbb{V}\mathrm{ar}(\epsilon) = \sigma^2 I_n$$

$$\mathbb{E}\{\epsilon\} = 0$$

and

$$D = \begin{pmatrix} \frac{1}{\sqrt{w_1}} & 0 & \dots & 0 \\ 0 & \frac{1}{\sqrt{w_2}} & \dots & 0 \\ 0 & \dots & \frac{1}{\sqrt{w_i}} & 0 \\ \dots & \dots & \dots & \dots \\ 0 & \dots & 0 & \frac{1}{\sqrt{w_n}} \end{pmatrix}$$

Weighted Least Squares

- We then multiply through the linear equation by

$$
\begin{aligned}
\mathsf{D}^{-1}\mathsf{Y} &= \mathsf{D}^{-1}\mathsf{X}\beta + \epsilon \\
\tilde{\mathsf{Y}} &= \tilde{\mathsf{X}}\beta + \epsilon \\
\mathbb{V}\mathrm{ar}\{\epsilon\} &= \sigma^2 \mathsf{I}_n \\
\mathbb{E}\{\epsilon\} &= 0 \qquad (1)
\end{aligned}
$$

This is recognizable as a liner model. The β estimate is given by

$$
\begin{aligned}
\hat{\beta} &= \left(\tilde{\mathsf{X}}^T\tilde{\mathsf{X}}\right)^{-1}\tilde{\mathsf{X}}^T\tilde{\mathsf{Y}} \\
&= \left(\left(\mathsf{D}^{-1}\mathsf{X}\right)^T\left(\mathsf{D}^{-1}\mathsf{X}\right)\right)^{-1} \\
&\quad \left(\mathsf{D}^{-1}\mathsf{X}\right)^T\mathsf{D}^{-1}\mathsf{Y} \\
&= \left(\mathsf{X}^T\mathsf{V}\mathsf{X}\right)^{-1}\mathsf{X}^T\mathsf{V}\mathsf{Y} \qquad (2)
\end{aligned}
$$

where $\mathsf{V} = \mathsf{D}^{-2}$.

Testing in the Least Squares Set–Up

- Assume that $\boldsymbol{Y} \sim N(X\beta, \sigma^2 \mathrm{I}_n)$.
- Definition: If $\mathrm{Z} \sim N(\boldsymbol{\mu}, \mathrm{I}_n)$ where $\boldsymbol{\mu} \neq 0$ then $\mathrm{Z}^T\mathrm{Z}$ is said to have a non-central χ^2 distribbution on n d. o. f. and non-centrality parameter $\delta > 0$ given by $\delta^2 = \mu^T\mu$.
- $\mu = 0 \Rightarrow \chi^2_n$ as the non-centrality parameter is then zero.
- We normally for the general distribution write $U = \mathrm{Z}^T\mathrm{Z} \sim \chi^2_n(\delta)$.
- The distribution of $\mathrm{Z}^T\mathrm{Z}$ depends on μ only via δ.
- $\mathbb{E}(U) = n + \delta^2$.
- $\mathbb{V}\mathrm{ar}(U) = 2n + 4\delta^2$
- If $U_i \sim \chi^2_{n_i}(\delta_i)$ for $i = 1, \ldots k$ and if the $\{U_i\}$ are all independent then

$$\sum_{i=1}^{k} U_i \sim \chi^2_n(\delta),$$

where $n = \sum_{i=1}^k n_i$ and $\delta^2 = \sum_{i=1}^k \delta_i^2$.

Testing in the Least Squares Set–Up

- Lemma: If $\mathrm{Z} \sim N(\boldsymbol{\mu}, \mathrm{I}_n)$ and if A is a $n \times n$ symmetric and idempotent matrix of rank r then

$$\mathrm{Z}^T \mathrm{AZ} \sim \chi_n^2(\delta),$$

where $\delta^2 = \mu^T A \mu$.
Proof: Let A be a symmetric idempotent matrix ($A^2 = A$). Then A has r eigenvalues that are unity, and $n - r$ eigenvalues that are zero. Because A is symmetric there is an orthogonal $P^T P = \mathrm{I}_n$ matrix P st

$$P^T A P = D,$$

where D is diagonal with r ones and $n - r$ zeros down the diagonal.
Let $\mathrm{V} = P^T \mathrm{Z}$. Then

$$\mathrm{V} \sim N(P^T \mu, \mathrm{I}_n).$$

Testing in the Least Squares Set–Up

- Furthermore it follows that

$$
\begin{aligned}
Z^T A Z &= (PV)^T A(PV) \\
&= V^T P^T A P V \\
&= V^T D V \\
&= V^T D^T D V \\
&= (DV)^T (DV) \\
&= \text{sum of squares of } r \text{ components} \\
&= \chi^2_r(d),
\end{aligned}
$$

for some d. In fact
$d^2 = \mathbb{E}(DV)^T \mathbb{E}(DV) = (DP^T\mu)^T(DP^T\mu) = \mu^T PDP^T\mu = \mu^T A\mu.$

Testing in the Least Squares Set–Up

- Lemma: If $\mathrm{Z} \sim N(\boldsymbol{\mu}, \mathrm{I}_n)$ and A_1 and A_2 are symmetric idempotent matrices such that $A_1 A_2 = 0$ then $\mathrm{Z}^T A_1 \mathrm{Z}$ and $\mathrm{Z}^T A_2 \mathrm{Z}$ are independent.
  Proof: $\mathrm{Z}^T A_i \mathrm{Z} = (A_i Z)^T (A_i Z)$ for $i = 1, 2$. Consider the two vectors $A_1 Z$ and $A_2 Z$ then

$$\mathbb{C}\mathrm{ov}\{A_1 Z, A_2 Z\} = A_1 \,\mathbb{C}\mathrm{ov}(Z) A_2^T \tag{3}$$

$$= A_1 \mathrm{I} A_2 = 0. \tag{4}$$

  This means that every component of $A_1 Z$ is uncorrelated with every component of $A_2 Z$. By normality this means that the components are independent.

- Corollary: If $A_1, \ldots, A_k$ are symmetric and idempotent and if $A_i A_j = 0$ for $i \neq j$ then $\{\mathrm{Z}^T A_i \mathrm{Z}\}$ are mutually independent.

Testing in the Least Squares Set–Up

- Lemma: If $A_1, \ldots A_k$ are symmetric $n \times n$ matrices such that $\sum A_i = \mathrm{I}$ and such that $\mathrm{rank}(A_i) = r_i$ then the following are equivalent:

  (a) $\sum_i r_i = n$
  (b) $A_i A_j = 0 \;\; i \neq j$
  (c) A_i are idempotent for $i = 1, \ldots, k$.

Testing in the Least Squares Set–Up

- If

$$Z \sim N(\mu, I_n)$$

and

$$\sum_i A_i = I_n$$

where A_i with ranks r_i are symmetric $n \times n$ matrices such that at least one of

1. $\sum_i r_i = n$
2. $A_i A_j = 0$ for $i \neq j$
3. A_i are idempotent.

holds (and therefore all of them, proof omitted) then

$$Z^T A_i Z$$

are independent

$$\chi^2_{r_i}(\delta_i)$$

where $\delta_i^2 = \mu^T A_i \mu$.

Testing in the Least Squares Set–Up

- Proof: A_i are assumed to be idempotent. By the lemma this means

$$Z^T A_i Z \sim \chi^2_{r_i}(\delta_i).$$

Because they are mutually orthogonal by assumption this implies that

$$\mathsf{Z}^T \mathsf{A}_i \mathsf{Z}$$

are independent.

Testing in the Least Squares Set–Up

- Assume we want to test the hypothesis

$$\mathrm{H}_0 : \ \mathrm{A}\beta = 0$$

versus

$$\mathrm{H}_1 : \ \mathrm{A}\beta \neq 0$$

where $\mathrm{rank}\mathrm{A} = s = p - p_0$.

- Under H_0 we get the simpler linear model

$$E\{\mathrm{Y}\} = \mathrm{X}_0\beta_0$$

where β_0 is $p_0 \times 1$. New hat matrix:

$$\mathrm{P}_0 = \mathrm{X}_0\left(\mathrm{X}_0^T\mathrm{X}_0\right)^{-1}\mathrm{X}_0^T.$$

Testing in the Least Squares Set–Up

- $\boldsymbol{P}_0$ has trace p_0.
- Consider the likelihood ratio:

$$t = \frac{\text{maximum liklihood under } H_1}{\text{maximum liklihood under } H_0}$$

- From MLE we get a biased estimate of σ and the least squares estimates of $\widehat{\boldsymbol{\beta}}$.
- Plugging in:

$$t = \left(\frac{\widehat{\sigma}^2_{ML,0}}{\widehat{\sigma}^2_{ML}} \right)^{\frac{n}{2}}.$$

- Consider a monotonic increasing function of t:

$$f(t) = \frac{n-p}{p-p_0}\left(t^{2/n} - 1\right),$$

or

$$F = \frac{n-p}{p-p_0}\frac{RSS_0 - RSS}{RSS}.$$

Testing in the Least Squares Set–Up

- Use the Fisher-Cochran theorem:

$$\mathsf{I}_n = (\mathsf{I}_n - \mathsf{P}) + (\mathsf{P} - \mathsf{P}_0) + \mathsf{P}_0$$

with ranks

$$n = (n - p) + (p - p_0) + p_0.$$

Let

$$\begin{aligned} \mathsf{A}_1 &= (\mathsf{I}_n - \mathsf{P}) \\ \mathsf{A}_2 &= (\mathsf{P} - \mathsf{P}_0) \\ \mathsf{A}_3 &= \mathsf{P}_0 \end{aligned}$$

These are are symmetric and idempotent.

Testing in the Least Squares Set–Up

- We may write $\mathsf{P}_0 = \mathsf{X}\mathsf{B}$ for some B of constants. Let

$$\mathsf{Z} = \frac{1}{\sigma}\mathsf{Y}$$

Note

$$RSS = \mathsf{Y}^T \mathsf{A}_1 \mathsf{Y} = \sigma^2 \mathsf{Z}^T \mathsf{A}_1 \mathsf{Z},$$

$$RSS_0 - RSS = \mathsf{Y}^T \mathsf{A}_2 \mathsf{Y} = \sigma^2 \mathsf{Z}^T \mathsf{A}_2 \mathsf{Z}$$

and so with NTA by the Fisher-Cochran theorem

$$RSS/\sigma^2 \sim \chi^2_{n-p}$$

and

$$(RSS_0 - RSS)/\sigma^2 \sim \chi^2_{p-p_0}$$

independently (the non-centrality parameters vanish.)

Testing in the Least Squares Set–Up

- We then have

$$
\begin{aligned}
F &= \frac{\sigma^2}{\sigma^2}\frac{n-p}{p-p_0}\frac{RSS_0 - RSS}{RSS} \\
&\sim \frac{\chi^2_{p-p_0}/(p-p_0)}{\chi^2_{n-p}/(n-p)} \\
&\sim F_{p-p_0,n-p}
\end{aligned}
$$

- Decompose the **total sum of squares** by

$$
\begin{aligned}
\mathrm{Y}^T\mathrm{Y} &= \mathrm{Y}^T(\mathrm{I}_n - \mathrm{P})\mathrm{Y} \\
&+ \mathrm{Y}^T(\mathrm{P}-\mathrm{P}_0)\mathrm{Y} + \mathrm{Y}^T\mathrm{P}_0\mathrm{Y}
\end{aligned}
$$

These are the **total sum of squares** (TSS), **residual sum of squares** (RSS), **sum of squares for testing** H_0 and the sum of squares due reduction due to β_0. This can be summarized in an ANOVA (ANalysis Of VAriance) table.

Testing in the Least Squares Set–Up

- Then

Source	d.o.f.	Sum of Squares	Mean squares	F
Red	$p-s$	$\underline{y}^T \mathrm{P}_0 \underline{y}$		
H_0	s	$\underline{y}^T(\mathrm{P}-\mathrm{P}_0)\underline{y}$	$M_1 = \frac{\underline{y}^T(\mathrm{P}-\mathrm{P}_0)\underline{y}}{s}$	$\frac{M_1}{M_2}$
Residual	$n-p$	$\underline{y}^T(\mathrm{I}-\mathrm{P})\underline{y}$	$M_2 = \frac{\underline{y}^T(\mathrm{I}-\mathrm{P})\underline{y}}{n-p}$	
total	n	$\underline{y}^T\underline{y}$		

- $M_2 = \frac{RSS}{n-p}$ is an *unbiased* estimate of σ^2.
- Reject the null hypothesis at level α if

$$F > f_\alpha$$

where

$$P(F_{s,n-p} > f_\alpha) = \alpha.$$

Assumptions in the Least Squares Set–Up

- Four basic assumptions inherent in the Gaussian linear regression model:
- Linearity: $\mathbb{E}\{Y\}$ is linear in X.
- Homoskedasticity: $\mathbb{V}\mathrm{ar}\{\epsilon_j\} = \sigma^2$ for all j.
- Gaussian Distribution: errors are normally distributed.
- Uncorrelated Errors: ϵ_i uncorrelated with ϵ_j for $i \neq j$.
- When one of these assumptions fails clearly, then Gaussian linear regression is inappropriate as a model for the data.
- Isolated problems, such as outliers and influential observations also deserve investigation. They may or may not decisively affect model validity.

Assumptions in the Least Squares Set–Up

- Scientific reasoning: impossible to validate model assumptions.
- Cannot prove that the assumptions hold. Can only provide evidence in favour (or against!) them.
- Strategy: Find implications of each assumption that we can check graphically (mostly concerning residuals).
- Construct appropriate plots and assess them (requires experience).
- 'Magical Thinking': Beware of overinterpreting plots!

Outliers

- An outlier is an observation that does not conform to the general pattern of the rest of the data.
- We *standardise* the residuals through:

$$r_i = \frac{e_i}{\sqrt{s^2(1 - p_{ii})}}$$

where

$$s^2 = \frac{RSS}{n - p}.$$

s^2 has $n - p$ degrees of freedom, and note that r_i is *not* student t.

Outliers (more)

- Outliers may be influential: they “stand out” in the “y-dimension”.
- However an observation may also be influential because of unusual values in the “x–dimension”.
- Such influential observations cannot be so easily detected through plots. But we may wish to automatically detect problems.
- How to find cases having strong effect on fitted model?
- Idea: see effect when case j , i.e., (x_j^T, Y_j) is not kept.
- Let $\boldsymbol{\beta}_{-j}$ be the LSE when model is fitted to data without case j and let $\widehat{\mathrm{Y}}_{-j} = \mathrm{X}\boldsymbol{\beta}_{-j}$ be the fitted value.

Outliers (more)

- Define Cook's distance

$$C_j = \frac{1}{ps^2} \left\{ \widehat{Y} - \widehat{Y}_{-j} \right\}^T \left\{ \widehat{Y} - \widehat{Y}_{-j} \right\}.$$

- This measures the scaled distance between the predictions and recall

$$s^2 = \frac{1}{n-p} \|Y - \widehat{Y}\|^2.$$

- It is possible to show that

$$C_j = \frac{r_j^2 p_{jj}}{p(1-p_{jj})},$$

and thus it can be seen that a large C_j implies and/or large r_j and/or large p_{jj}.

Outliers (more)

- Cases with $C_j > 8/(n-2p)$ are considered large.
- We therefore plot C_j against j and compare with this cut-off.

Diagnostics

- We plot $\boldsymbol{Y}$ against columns of $\boldsymbol{X}$ to check for linearity and outliers.
- We plot the standardized residuals r against the columns of $\boldsymbol{X}$.
- We plot the standardized residuals r against covariates we left out.
- We plot r against $\widehat{\mathrm{Y}}$ to check homoscedasticity.
- We make qq plots to check distribution.
- We make the Cook distance plot to check for influential observations.