Breusch-Pagan's test - complete version

$\binom{x_1}{Y_1},\dots,\binom{x_n}{Y_n} \overset{iid}{\sim}$ normal linear model, $\operatorname{var}(Y_i|X_i) = \sigma^2\tau_i(\beta,\lambda)$

τ_i given functions $\mathbb{R}\to(0,\infty)$ that do not dep. on Y $\quad E(Y_i|x_i) = x_i'\beta \qquad \theta = (\beta^T,\sigma^2,\lambda^T)^T \in \mathbb{R}^{k+1+\ell}$

$\tau_i(\beta,0) = 1$. Rao's score test $H_0: \lambda = 0$, $H_1: \lambda \neq 0$.

$$L(\theta) = c\,\frac{1}{\sigma^n\sqrt{\prod\tau_i}}\exp\left\{-\frac{1}{2\sigma^2}\sum\frac{(y_i - x_i'\beta)^2}{\tau_i}\right\} \qquad e_i := y_i - x_i'\beta$$

$$\ell(\theta) = \log c - \frac{n}{2}\log\sigma^2 - \frac{1}{2}\sum\log\tau_i - \frac{1}{2\sigma^2}\sum\frac{e_i^2}{\tau_i}$$

$$\frac{\partial\ell(\theta)}{\partial\beta} = -\frac{1}{2}\sum\frac{\partial\log\tau_i}{\partial\beta} + \frac{1}{2\sigma^2}\Big[\sum\frac{2e_ix_i}{\tau_i} + \frac{1}{2\sigma^2}\sum\left(\frac{e_i}{\sqrt{\tau_i}}\right)^2\frac{\partial\log\tau_i}{\partial\beta}$$

$$= \frac{1}{\sigma^2}\sum\frac{e_ix_i}{\tau_i} + \frac{1}{2}\sum\left(\left(\frac{e_i}{\sigma\sqrt{\tau_i}}\right)^2 - 1\right)\frac{\partial\log\tau_i}{\partial\beta}$$

$$\frac{\partial}{\partial\beta}\left(\frac{e_i}{\sigma\sqrt{\tau_i}}\right)^2 = \frac{2}{\sigma}\left(\frac{e_i}{\sigma\sqrt{\tau_i}}\right)\cdot\frac{\left(-x_i\sqrt{\tau_i} - \frac{e_i}{2\sqrt{\tau_i}}\frac{\partial\tau_i}{\partial\beta}\right)}{\tau_i} = -\left(\frac{2e_ix_i}{\tau_i\sigma^2} + \frac{e_i^2}{\tau_i^2\sigma^2}\cdot\frac{\partial\tau_i}{\partial\beta}\right)$$

$$\frac{\partial\ell(\theta)}{\partial\sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^4}\sum\frac{e_i^2}{\tau_i} = -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^2}\sum\left(\frac{e_i}{\sigma\sqrt{\tau_i}}\right)^2$$

$$\frac{\partial}{\partial\lambda}\left(\frac{e_i}{\sigma\sqrt{\tau_i}}\right)^2 = -\frac{e_i^2}{\sigma^2}\cdot\frac{1}{\tau_i^2}\frac{\partial\tau_i}{\partial\lambda} = -\left(\frac{e_i}{\sigma\sqrt{\tau_i}}\right)^2\frac{\partial\log\tau_i}{\partial\lambda}$$

$$\frac{\partial\ell(\theta)}{\partial\lambda} = -\frac{1}{2}\sum\frac{\partial\log\tau_i}{\partial\lambda} + \frac{1}{2}\sum\left(\frac{e_i}{\sigma\sqrt{\tau_i}}\right)^2\frac{\partial\log\tau_i}{\partial\lambda} = \frac{1}{2}\sum\left(\left(\frac{e_i}{\sigma\sqrt{\tau_i}}\right)^2 - 1\right)\frac{\partial\log\tau_i}{\partial\lambda}$$

$$\frac{\partial}{\partial\beta^T}\frac{e_i}{\tau_i} = \frac{-x_i'\tau_i - e_i\,\partial\tau_i/\partial\beta'}{\tau_i^2} = -\left(\frac{x_i'}{\tau_i} + \frac{e_i}{\tau_i^2}\frac{\partial\tau_i}{\partial\beta'}\right)$$

$$\frac{\partial}{\partial\lambda^T}\frac{e_i}{\tau_i} = -\frac{e_i}{\tau_i^2}\frac{\partial\tau_i}{\partial\lambda^T}$$

$$\frac{\partial^2\ell(\theta)}{\partial\beta\partial\beta^T} = -\frac{1}{\sigma^2}\sum\frac{x_ix_i'}{\tau_i} - \frac{1}{\sigma^2}\sum\frac{x_ie_i}{\tau_i}\frac{\partial\log\tau_i}{\partial\beta^T} + \frac{1}{2}\sum\frac{\partial\log\tau_i}{\partial\beta}\left(-\frac{2e_ix_i'}{\tau_i\sigma^2} - \frac{e_i^2}{\sigma^2\tau_i}\frac{\partial\log\tau_i}{\partial\beta^T}\right) + \frac{\partial^2\log\tau_i}{\partial\beta\partial\beta^T}\ !$$

$$+\frac{1}{2}\sum\left[\left(\frac{e_i}{\sigma\sqrt{\tau_i}}\right)^2 - 1\right]\cdot\frac{\partial^2\log\tau_i}{\partial\beta\partial\beta^T}$$

vanishes in expectation

$$\frac{\partial^2\ell(\theta)}{\partial\beta\partial\sigma^2} = -\frac{1}{\sigma^4}\sum\frac{e_ix_i}{\tau_i} - \frac{1}{2\sigma^4}\sum\frac{e_i^2}{\tau_i}\frac{\partial\log\tau_i}{\partial\beta}$$

$$\frac{\partial^2\ell(\theta)}{\partial\beta\partial\lambda^T} = -\frac{1}{\sigma^2}\sum x_i\frac{e_i}{\tau_i}\frac{\partial\log\tau_i}{\partial\lambda^T} + \frac{1}{2}\sum\frac{\partial\log\tau_i}{\partial\beta}\cdot\left(-\left(\frac{e_i}{\sigma\sqrt{\tau_i}}\right)^2\frac{\partial\log\tau_i}{\partial\lambda^T}\right) + \frac{1}{2}\sum\left(\left(\frac{e_i}{\sigma\sqrt{\tau_i}}\right)^2 - 1\right)\cdot\frac{\partial^2\log\tau_i}{\partial\beta\partial\lambda^T}$$

$$\frac{\partial^2\ell(\theta)}{\partial\sigma^2\partial\sigma^2} = \frac{n}{2\sigma^4} - \frac{1.2}{2\sigma^6}\sum\left(\frac{e_i}{\sqrt{\tau_i}}\right)^2$$

$$\frac{\partial^2\ell(\theta)}{\partial\sigma^2\partial\lambda^T} = -\frac{1}{2\sigma^2}\sum\left(\frac{e_i}{\sigma\sqrt{\tau_i}}\right)^2\frac{\partial\log\tau_i}{\partial\lambda^T}$$

$$\frac{\partial^2\ell(\theta)}{\partial\lambda\partial\lambda^T} = \frac{1}{2}\sum\frac{\partial\log\tau_i}{\partial\lambda}\cdot\left(-\left(\frac{e_i}{\sigma\sqrt{\tau_i}}\right)^2\frac{\partial\log\tau_i}{\partial\lambda^T}\right) + \frac{1}{2}\sum\left(\left(\frac{e_i}{\sigma\sqrt{\tau_i}}\right)^2 - 1\right)\frac{\partial^2\log\tau_i}{\partial\lambda\partial\lambda^T}$$

$E\left(\frac{e_i}{\sigma\sqrt{\tau_i}}\right)^2 = 1 \qquad E e_i = 0 \quad \Rightarrow$ Fisher information matrix

$W = \operatorname{diag}\tau_i^{-1}$

$D_\beta = \frac{\partial\log\tau}{\partial\beta^T}$ ← $n\times k$ matrix

$D_\lambda = \frac{\partial\log\tau}{\partial\lambda^T}$ ← $n\times\ell$ matrix

$$J_n(\theta) = \begin{pmatrix} \frac{1}{\sigma^2}X'WX + \frac{1}{2}D_\beta'D_\beta & \frac{1}{2\sigma^2}D_\beta'\mathbb{1} & \frac{1}{2}D_\beta'D_\lambda \\ \frac{1}{2\sigma^2}\mathbb{1}'D_\beta & n/2\sigma^4 & \frac{1}{2\sigma^2}\mathbb{1}'D_\lambda \\ \frac{1}{2}D_\lambda'D_\beta & \frac{1}{2\sigma^2}D_\lambda'\mathbb{1} & \frac{1}{2}D_\lambda'D_\lambda \end{pmatrix}$$

under H_0: $\tilde{\lambda} = 0$, $\tilde{\beta} = (X'X)^{-1}X'Y$, $\tilde{\sigma}^2 = \frac{1}{m}\sum \tilde{e}_i^2 = \frac{1}{2}\sum (Y_i - x_i'\tilde{\beta})^2$ (stan... norm... homos...)

$$\Rightarrow \left.\frac{\partial \ell(\theta)}{\partial \theta}\right|_{(\tilde{\beta},\tilde{\sigma}^2,\tilde{\lambda})} = \left(\mathbb{0}^T, 0, \frac{1}{2}\sum\left(\left(\frac{\tilde{e}_i}{\tilde{\sigma}}\right)^2 - 1\right)\underbrace{\frac{\partial \log \tau_i}{\partial \lambda}}\Big|_{\lambda=0} \right)^T$$

$$R_m := \left.\frac{\partial \ell(\theta)}{\partial \theta^T}\right|_{\tilde{\beta},\tilde{\sigma}^2,0} \cdot \left[J_m(\tilde{\theta})\right]^{-1} \left.\frac{\partial \ell(\theta)}{\partial \theta}\right|_{\tilde{\beta},\tilde{\sigma}^2,0} \xrightarrow[H_0]{d} \chi^2_\ell$$

- Special case: $\tau_i(\beta,\lambda) = \exp\{\lambda . x_i'\beta\} = \exp\{\lambda . E[Y_i|X_i]\}$ for $\lambda \in \mathbb{R}$

Then $D_\lambda = X\beta$, $D_\beta = \lambda X$, under $H_0: \lambda = 0$ we have $D_\beta = \mathbb{0}_{m\times k}$, and

$$J_m = \left(\begin{array}{cc|c} \frac{1}{\sigma^2}X'X & \mathbb{0} & \mathbb{0} \\ \mathbb{0}' & \frac{m}{2\sigma^4} & \frac{\mathbb{1}'X\beta}{2\sigma^2} \\ \hline \mathbb{0}' & \frac{\beta'X'\mathbb{1}}{2\sigma^2} & \frac{1}{2}\beta'X'X\beta \end{array}\right) \qquad \left.\frac{\partial \ell(\theta)}{\partial \theta}\right|_{\tilde{\theta}} = \left(\mathbb{0}^T, 0, \frac{1}{2\tilde{\sigma}^2}\sum(\tilde{e}_i^2 - \tilde{\sigma}^2)\hat{Y}_i\right)^T$$

and we need only the $(k+2, k+2)$-element of $J_m(\tilde{\theta})^{-1}$. Invert the partitioned matrix using $\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} \cdot & \cdot \\ \cdot & (D - CA^{-1}B)^{-1} \end{pmatrix}$ to get

$$\left[J_m(\tilde{\theta})\right]^{-1}_{k+2,k+2} = \left[\frac{1}{2}\tilde{\beta}'X'X\tilde{\beta} - \left(\mathbb{0}' \;\; \frac{\tilde{\beta}'X'\mathbb{1}}{2\tilde{\sigma}^2}\right)\begin{pmatrix} \sigma^2(X'X)^{-1} & \mathbb{0} \\ \mathbb{0}' & \frac{2\tilde{\sigma}^4}{m} \end{pmatrix}\begin{pmatrix} \mathbb{0} \\ \frac{\mathbb{1}'X\tilde{\beta}}{2\tilde{\sigma}^2} \end{pmatrix} \right]^{-1}$$

$$= \left(\frac{1}{2}\hat{Y}'\hat{Y} - \frac{1}{2m}(\hat{Y}'\mathbb{1})^2\right)^{-1} = \left(\frac{1}{2}\sum(\hat{Y}_i - \bar{\hat{Y}})^2\right)^{-1}$$

Because $\sum \tilde{e}_i^2 = m\tilde{\sigma}^2$ we can write $\sum(\tilde{e}_i^2 - \tilde{\sigma}^2)\hat{Y}_i = \sum \tilde{e}_i^2 \hat{Y}_i - \frac{1}{m}\sum\tilde{e}_i^2 . \sum\hat{Y}_i$ and

$$= \sum \tilde{e}_i^2(\hat{Y}_i - \bar{\hat{Y}})$$

$$R_m = \frac{1}{2(\tilde{\sigma}^2)^2} \cdot \frac{\left(\sum (Y_i - x_i'\tilde{\beta})^2(x_i'\tilde{\beta} - \bar{\hat{Y}})\right)^2}{\sum(\hat{Y}_i - \bar{\hat{Y}})^2} = \frac{\left(\sum (Y_i - \hat{Y}_i)(\hat{Y}_i - \bar{\hat{Y}})\right)^2}{2(\tilde{\sigma}^2)^2\sum(\hat{Y}_i - \bar{\hat{Y}})^2} \underset{as}{\overset{H_0}{\sim}} \chi^2_1$$

Example 19. $X_1, \dots, X_m \overset{iid}{\sim} \text{Mult}(1, p) \qquad p = (p_1, \dots, p_k)^T \qquad p_k = 1 - \sum_{\ell=1}^{k-1} p_\ell$

$H_0: p = p_0 \quad H_1: p \neq p_0 \qquad N_\ell := \sum_{i=1}^{m} X_{i\ell}$

$$L(p) = \prod_{i=1}^{m} \left(\prod_{\ell=1}^{k-1} p_\ell^{X_{i\ell}} \right) \cdot \left(1 - \sum_{\ell=1}^{k-1} p_\ell\right)^{1-\sum_{\ell=1}^{k-1} X_{i\ell}} = \prod_{\ell=1}^{k-1} p_\ell^{N_\ell} \cdot \left(1 - \sum p_\ell\right)^{N_k}$$

$$\ell(p) = \sum N_\ell \log p_\ell + N_k \log\left(1 - \sum p_\ell\right)$$

$$\frac{\partial \ell(p)}{\partial p} = \left(\frac{N_\ell}{p_\ell} - \frac{N_k}{1 - \sum p_\ell} \right)_{\ell=1}^{k-1} \overset{!}{=} 0 \quad \Rightarrow \quad p_k := 1 - \sum_\ell p_\ell$$

$$\frac{N_\ell}{p_\ell} - \frac{N_k}{p_k} = 0$$

$$p_\ell = p_k \frac{m_\ell}{N_k} \quad \Big/ \sum_{\ell=1}^{k-1}$$

$$1 - p_k = p_k \left(\frac{m - N_k}{N_k} \right)$$

$$\hat{p}_k = \frac{N_k}{m} \Rightarrow \hat{p}_\ell = \frac{N_\ell}{N}$$

$$\left[\frac{\partial^2 \ell(p)}{\partial p \partial p^T} \right]_{\ell, l} = \begin{cases} -\frac{N_\ell}{p_\ell^2} - \frac{N_k}{(p_k)^2} & \ell = l \\ -\frac{N_k}{(p_k)^2} & \ell \neq l \end{cases}$$

$$\frac{\partial^2 \ell(p)}{\partial p \partial p^T} = -\,\text{diag}\left(\frac{N_\ell}{p_\ell^2} \right) - \mathbb{1}\mathbb{1}^T \cdot \frac{N_k}{p_k^2}$$

$$I(p) = \left[\text{diag}\left(\frac{m}{p_\ell} \right) + \mathbb{1}\mathbb{1}^T \frac{m}{p_k} \right]^{(m)}$$

<u>LR</u> $:= 2(\ell(\hat{p}) - \ell(p_0)) = 2\left(\sum N_\ell \log \hat{p}_\ell + N_k \log\left(\frac{N_k}{m}\right) - \sum N_\ell \log p_{0\ell} - N_k \log p_{0k} \right)$

$$= 2\left(\sum_{\ell=1}^{k} N_\ell \log \frac{N_\ell}{m p_{0\ell}} \right) \underset{H_0}{\overset{as}{\sim}} \chi^2_{k-1}$$

$$I(p_0)^{(m)} = \text{diag}\left(\frac{m}{p_{\ell 0}} \right) + \mathbb{1}\mathbb{1}^T \frac{m}{p_{k0}}$$

Sherman–Morrison formula

$$(A + u v^T)^{-1} = A^{-1} - \frac{A^{-1} u v^T A^{-1}}{1 + v^T A^{-1} u}$$

$$A = \text{diag}\left(\frac{m}{p_{\ell 0}} \right) \qquad u = v = \mathbb{1} \cdot \sqrt{\frac{m}{p_{k0}}}$$

$$I(p_0)^{-1} = \text{diag}\left(\frac{p_{\ell 0}}{m} \right) - \frac{\text{diag}\left(\frac{p_{\ell 0}}{m}\right) \frac{m}{p_{k0}} \mathbb{1}\mathbb{1}^T \text{diag}\left(\frac{p_{\ell 0}}{m}\right)}{1 + \frac{m}{p_{k0}} \mathbb{1}^T \text{diag}\left(\frac{p_{\ell 0}}{m}\right) \mathbb{1}}$$

$$= \text{diag}\left(\frac{p_{\ell 0}}{m} \right) - \frac{m}{p_{k0}} \left(\frac{p_{\ell 0} p_{l 0}}{m^2} \right)_{\ell, l=1}^{k-1} \frac{1}{1 + \frac{m}{p_{k0}} \sum \frac{p_{\ell 0}}{m}}$$

$$= \text{diag}\left(\frac{p_{\ell 0}}{m} \right) - \left(\frac{p_{\ell 0} p_{l 0}}{m} \right)_{\ell, l=1}^{k-1}$$

$$\frac{\partial \ell}{\partial p}(p_0) = \left(\frac{N_\ell}{p_{0\ell}} - \frac{N_k}{p_{0k}} \right)_{\ell=1}^{k-1}$$

$$R_m := \frac{\partial \ell}{\partial p}(p_0)^T I(p_0)^{-1} \frac{\partial \ell}{\partial p}(p_0)$$

$$= \left(\frac{N}{p_0} - \frac{N_k}{p_{0k}} \right)^T \left(\text{diag}\left(\frac{p_0}{m} \right) - \frac{p_0 p_0^T}{m} \right) \left(\frac{N}{p_0} - \frac{N_k}{p_{0k}} \right)$$

$$N = \begin{pmatrix} N_1 \\ \vdots \\ N_{k-1} \end{pmatrix}$$

$$= \frac{1}{m} \left[\sum \left(\frac{N_\ell}{p_{0\ell}} - \frac{N_k}{p_{0k}} \right)^2 p_{0\ell} - \left(\sum \left(\frac{N_\ell}{p_{0\ell}} - \frac{N_k}{p_{0k}} \right) p_{0\ell} \right)^2 \right]$$

$$= \frac{1}{m} \left(I - II^2 \right)$$

$$II = \sum \left(\frac{N_\ell}{p_{0\ell}} - \frac{N_k}{p_{0k}} \right) p_{0\ell} = \sum N_\ell - \frac{N_k}{p_{0k}} \sum p_{0\ell} = m - N_k - \frac{N_k}{p_{0k}}(1 - p_{0k}) = m - N_k + N_k - \frac{N_k}{p_{0k}} =$$

$$= \frac{m p_{0k} - N_k}{p_{0k}}.$$

…19 contd. $I = \sum \left(\frac{N_k}{p_{0k}} - \frac{N_k}{p_{0k}} - m + m \right)^2 p_{0k} = \sum \frac{(N_k - m p_{0k})^2}{p_{0k}} + \sum \frac{(N_k - m p_{0k})^2 p_{0k}}{p_{0k}^2}$

$- \sum 2 \frac{N_k - m p_{0k}}{p_{0k}} \cdot \frac{N_k - m p_{0k}}{p_{0k}} \cdot p_{0k} = \sum \frac{(N_k - m p_{0k})^2}{p_{0k}} + \frac{(N_k - p_{0k} m)^2}{p_{0k}^2}(1 - p_{0k}) -$

$- 2 \frac{N_k - m p_{0k}}{p_{0k}} (m - N_k - m(1 - p_{0k})) = \sum \frac{(N_k - m p_{0k})^2}{p_{0k}} + \frac{(N_k - m p_{0k})^2}{p_{0k}} \left(\frac{1}{p_{0k}} - 1 + 2 \right)$

$R_m = \frac{1}{m}(I - II^2) = \frac{1}{m} \left(\sum \frac{(N_k - m p_{0k})^2}{p_{0k}} + \frac{(N_k - m p_{0k})^2}{p_{0k}} \left(\frac{1}{p_{0k}} + 1 - \frac{1}{p_{0k}} \right) \right)$

$= \frac{1}{m} \sum_{k=1}^{k} \frac{(N_k - m p_{0k})^2}{p_{0k}} \overset{as}{\underset{H_0}{\sim}} \chi^2_{k-1}$

$W_m = \left(\frac{N}{m} - p_0 \right)' I \left(\frac{N}{m} \right) \left(\frac{N}{m} - p_0 \right) = \left(\frac{N}{m} - p_0 \right)' \left(\mathrm{diag}\left(\frac{m^2}{N} \right) + 11^T \frac{m^2}{N_k} \right) \left(\frac{N}{m} - p_0 \right)$

$= m^2 \cdot \left[\sum \frac{(N_k - m p_{0k})^2}{N_k m^2} + \frac{1}{N_k} \left[\sum \left(\frac{N_k}{m} - p_{0k} \right) \right]^2 \right] = \sum \frac{(N_k - m p_{0k})^2}{N_k} + \frac{m^2}{N_k} \left(\frac{m - N_k}{m} - (1 - p_{0k}) \right)^2$

$= \sum \frac{(N_k - m p_{0k})^2}{N_k} + \frac{m^2}{N_k} \frac{(N_k - m p_{0k})^2}{m^2} = \sum_{k=1}^{k} \frac{(N_k - m p_{0k})^2}{N_k} \overset{as}{\underset{H_0}{\sim}} \chi^2_{k-1}.$