一日でわかる（かな？）行列を使った回帰分析

１．パラメータの推定

$$y=\begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix},\ X=\begin{pmatrix} x_{01} & \cdots & x_{k1} \\ \vdots & \ddots & \vdots \\ x_{0n} & \cdots & x_{kn} \end{pmatrix},\ \beta=\begin{pmatrix} \beta_0 \\ \vdots \\ \beta_k \end{pmatrix},\ e=\begin{pmatrix} e_1 \\ \vdots \\ e_n \end{pmatrix},\ \begin{pmatrix} x_{01} \\ \vdots \\ x_{0n} \end{pmatrix}=\begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}$$

$$y=X\beta+e$$

$$X'e=X'(y-X\beta)=X'y-X'X\beta=0$$

$$X'X\beta=X'y$$

$$\hat{\beta}=(X'X)^{-1}X'y$$

$$y=X\hat{\beta}+\hat{e}$$

$$\hat{R}^2=1-\frac{\hat{e}'\hat{e}}{(y-\bar{y})'(y-\bar{y})}=1-\frac{S(\hat{\beta})}{(y-\bar{y})'(y-\bar{y})}$$

２．パラメータの分散の推定

$$E(e_i)=0, E(e_i{}^2)=\sigma^2, E(e_ie_j)=0, E(ee')=\sigma^2 I$$

$$\hat{\beta}=(X'X)^{-1}X'y=(X'X)^{-1}X'(X\beta+e)=(X'X)^{-1}X'X\beta+(X'X)^{-1}X'e$$

$$=\beta+(X'X)^{-1}X'e$$

$$E(\hat{\beta})=\beta$$

$$Var(\hat{\beta})=E\left[(X'X)^{-1}X'ee'X(X'X)^{-1}\right]=\sigma^2(X'X)^{-1}$$

３．カイ二乗分布

$$z=\begin{pmatrix} z_1 \\ \vdots \\ z_q \end{pmatrix}, \mu=\begin{pmatrix} \mu_1 \\ \vdots \\ \mu_q \end{pmatrix}, \Sigma=\begin{pmatrix} \sigma_{11} & \cdots & \sigma_{1q} \\ \vdots & \ddots & \vdots \\ \sigma_{q1} & \cdots & \sigma_{qq} \end{pmatrix}$$

$$z\sim N(\mu,\Sigma)\ \Rightarrow\ (z-\mu)'\Sigma^{-1}(z-\mu)\sim\chi_q$$

４．線形制約の検定（Wald 統計量）

$$Q'\beta=c \qquad Q=\begin{pmatrix} r_{01} & \cdots & r_{0q} \\ \vdots & \ddots & \vdots \\ r_{k1} & \cdots & r_{kq} \end{pmatrix},\ c=\begin{pmatrix} c_1 \\ \vdots \\ c_q \end{pmatrix}$$

の係数制約（r 個）の下で、

$$S(\beta)=e'e=(y-X\beta)'(y-X\beta)$$

$$=\hat{e}'\hat{e}+(\hat{\beta}-\beta)'X'X(\hat{\beta}-\beta)$$

$$=S(\hat{\beta})+(\hat{\beta}-\beta)'X'X(\hat{\beta}-\beta)$$

$\delta\equiv\hat{\beta}-\beta$ と置けば、

$$S(\beta) = S(\hat{\beta}) + \delta' X' X \delta$$
$$Q'\beta = Q'(\hat{\beta} - \delta) = c \Rightarrow Q'\delta = Q'\hat{\beta} - c$$
$$Min S(\beta) \quad s.t.\ Q'\beta = c \quad \Leftrightarrow \quad Min L = S(\hat{\beta}) + \delta' X' X \delta + 2\lambda' [Q'\delta - (Q'\hat{\beta} - c)]$$
$$X' X \delta + Q\lambda = 0 \ and \ Q'\delta = Q'\hat{\beta} - c$$
$$\tilde{\delta} \equiv \hat{\beta} - \tilde{\beta} = -(X'X)^{-1} Q\lambda$$
$$Q'\tilde{\delta} = -Q'(X'X)^{-1} Q\lambda = Q'\hat{\beta} - c \ \Rightarrow \ \tilde{\lambda} = -\left[Q'(X'X)^{-1}Q\right]^{-1}(Q'\hat{\beta} - c)$$
$$\tilde{\delta} = (X'X)^{-1} Q \left[Q'(X'X)^{-1}Q\right]^{-1}(Q'\hat{\beta} - c)$$

係数 β の制約が真の場合（$Q'\beta = c$ ）、その分布 φ（正規分布とは限らない）は、

$$\hat{\beta} \sim \varphi\left(\beta, \sigma^2 (X'X)^{-1}\right)$$
$$Q'\hat{\beta} \sim \varphi\left(c, \sigma^2 Q'(X'X)^{-1} Q\right)$$
$$(Q'\hat{\beta} - c)' \left[\sigma^2 Q'(X'X)^{-1} Q\right]^{-1} (Q'\hat{\beta} - c) \sim \chi_r \ \ if \ n \to \infty$$

$$S(\beta) = S(\hat{\beta}) + (\hat{\beta} - \beta)' X'X (\hat{\beta} - \beta)$$

なので、

$$\begin{aligned} S(\tilde{\beta}) - S(\hat{\beta}) &= (\hat{\beta} - \tilde{\beta})' X'X (\hat{\beta} - \tilde{\beta}) = \tilde{\delta}' X' X \tilde{\delta} \\ &= (Q'\hat{\beta} - c)' \left[Q'(X'X)^{-1}Q\right]^{-1} Q'(X'X)^{-1} X'X (X'X)^{-1} Q \left[Q'(X'X)^{-1}Q\right]^{-1} (Q'\hat{\beta} - c) \\ &= (Q'\hat{\beta} - c)' \left[Q'(X'X)^{-1}Q\right]^{-1} (Q'\hat{\beta} - c) \end{aligned}$$

したがって、

$$\frac{S(\tilde{\beta}) - S(\hat{\beta})}{\sigma^2} = (Q'\hat{\beta} - c)' \left[\sigma^2 Q'(X'X)^{-1} Q\right]^{-1} (Q'\hat{\beta} - c) \sim \chi_r \ \ if \ n \to \infty$$

この結果を使えば、

$$W \equiv \frac{(N-k-1)(\hat{R}^2 - \tilde{R}^2)}{1 - \hat{R}^2} = (N-k-1)\frac{(1-\tilde{R}^2) - (1-\hat{R}^2)}{1-\hat{R}^2}$$
$$= (N-k-1)\frac{\dfrac{S(\tilde{\beta})}{(y-\bar{y})'(y-\bar{y})} - \dfrac{S(\hat{\beta})}{(y-\bar{y})'(y-\bar{y})}}{\dfrac{S(\hat{\beta})}{(y-\bar{y})'(y-\bar{y})}} = \frac{S(\tilde{\beta}) - S(\hat{\beta})}{\dfrac{S(\hat{\beta})}{N-k-1}} = \frac{S(\tilde{\beta}) - S(\hat{\beta})}{\hat{\sigma}^2}$$

したがって（N－k－1 のかわりに N でもよい）、

$$W = \frac{S(\tilde{\beta}) - S(\hat{\beta})}{\hat{\sigma}^2} \to \frac{S(\tilde{\beta}) - S(\hat{\beta})}{\sigma^2} \sim \chi_r \ \ if \ n \to \infty$$

制約がひとつだけ $\beta_i = 0$ の場合、$\sqrt{W} = t \sim N(0,1) \ if \ n \to \infty$

付１．残差回帰（Frisch-Waugh 定理）

説明変数を二つのグループに分けると、

$$X = \begin{pmatrix} X_1 & X_2 \end{pmatrix} \qquad \beta = \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix}$$

$$y = X\beta + e = \begin{pmatrix} X_1 & X_2 \end{pmatrix}\begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} + e = X_1\beta_1 + X_2\beta_2 + e$$

$$X'y = X'X\hat{\beta} + X'\hat{e} = X'X\hat{\beta} = \begin{pmatrix} X_1' \\ X_2' \end{pmatrix}\begin{pmatrix} X_1 & X_2 \end{pmatrix}\begin{pmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \end{pmatrix} = \begin{pmatrix} X_1'X_1 & X_1'X_2 \\ X_2'X_1 & X_2'X_2 \end{pmatrix}\begin{pmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \end{pmatrix}$$

$$\begin{pmatrix} X_1'y \\ X_2'y \end{pmatrix} = \begin{pmatrix} X_1'X_1\hat{\beta}_1 + X_1'X_2\hat{\beta}_2 \\ X_2'X_1\hat{\beta}_1 + X_2'X_2\hat{\beta}_2 \end{pmatrix}$$

となる。

まず、β_1 の推計値を求めれば、

$$X_1'y = X_1'X_1\hat{\beta}_1 + X_1'X_2\hat{\beta}_2$$

$$X_1'X_1\hat{\beta}_1 = X_1'y - X_1'X_2\hat{\beta}_2$$

$$\hat{\beta}_1 = \left(X_1'X_1\right)^{-1}\left(X_1'y - X_1'X_2\hat{\beta}_2\right)$$

$$X_2'y = X_2'X_1\hat{\beta}_1 + X_2'X_2\hat{\beta}_2 = X_2'X_1\left(X_1'X_1\right)^{-1}\left(X_1'y - X_1'X_2\hat{\beta}_2\right) + X_2'X_2\hat{\beta}_2$$

$$\left[X_2'X_2 - X_2'X_1\left(X_1'X_1\right)^{-1}X_1'X_2\right]\hat{\beta}_1 = \left[X_2' - X_2'X_1\left(X_1'X_1\right)^{-1}X_1'\right]y$$

$$\hat{\beta}_1 = \left[X_2'X_2 - X_2'X_1\left(X_1'X_1\right)^{-1}X_1'X_2\right]^{-1}\left[X_2' - X_2'X_1\left(X_1'X_1\right)^{-1}X_1'\right]y$$

$$= \left[X_2'\left[I_n - X_1\left(X_1'X_1\right)^{-1}X_1'\right]X_2\right]^{-1}X_2'\left[I_n - X_1\left(X_1'X_1\right)^{-1}X_1'\right]y$$

$$M_1 = I_n - X_1(X_1'X_1)^{-1}X_1' \qquad M_1 = M_1' \quad M_1 = M_1^p$$

に注意すれば、β_2 の推計値は、

$$\hat{\beta}_2 = \left(X_2'M_1X_2\right)^{-1}X_2'M_1y$$

$$= \left(X_2'M_1'M_1X_2\right)^{-1}X_2'M_1'y = \left(X_2'M_1'M_1X_2\right)^{-1}X_2'M_1'M_1y$$

すなわち、

$$y = \beta_2 M_1X_2 + e \quad or \quad M_1y = \beta_2 M_1X_2 + e$$

という回帰を行えばよい。

$$X_2 = \left[X_1(X_1'X_1)^{-1}X_1' + I_n - X_1(X_1'X_1)^{-1}X_1'\right]X_2 = \hat{X}_2 + \left[I_n - X_1(X_1'X_1)^{-1}X_1'\right]X_2$$

$$= \hat{X}_2 + M_1X_2$$

から、M_1X_2 が X_2 を X_1 で回帰した残差であることがわかる。

付２．平均からの乖離を用いた回帰＝残差回帰の一種

X_1 を要素が全て 1 の縦ベクトル、X_2 を変数の数が k の $n\times k$ 行列 X_k とした場合、

$$y = X\beta + e = \begin{pmatrix} 1_n & X_k \end{pmatrix}\begin{pmatrix} \beta_0 \\ \beta_k \end{pmatrix} + e = 1_n\beta_0 + X_k\beta_k + e \qquad X = \begin{pmatrix} 1_n & X_k \end{pmatrix} \qquad 1_n = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}$$

$$M_0 = I_n - 1_n(1_n'1_n)^{-1}1_n' = I_n - \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}\frac{1}{n}\begin{pmatrix} 1 & \dots & 1 \end{pmatrix} = \begin{pmatrix} 1-\frac{1}{n} & -\frac{1}{n} & \dots & -\frac{1}{n} \\ -\frac{1}{n} & 1-\frac{1}{n} & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ -\frac{1}{n} & \dots & \dots & 1-\frac{1}{n} \end{pmatrix}$$

説明変数・被説明変数の平均を

$$\frac{\sum_{l=1}^{n} x_{il}}{n} = \bar{x}_i, \quad \frac{\sum_{l=1}^{n} y_l}{n} = \bar{y}$$ と置けば、

$$\tilde{X}_k = M_0 X_k = \begin{pmatrix} 1-\frac{1}{n} & -\frac{1}{n} & \dots & -\frac{1}{n} \\ -\frac{1}{n} & 1-\frac{1}{n} & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ -\frac{1}{n} & \dots & \dots & 1-\frac{1}{n} \end{pmatrix}\begin{pmatrix} x_{11} & x_{21} & \dots & x_{k1} \\ x_{12} & x_{22} & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ x_{1n} & \dots & \dots & x_{kn} \end{pmatrix} = \begin{pmatrix} x_{11}-\bar{x}_1 & x_{21}-\bar{x}_2 & \dots & x_{k1}-\bar{x}_k \\ x_{12}-\bar{x}_1 & x_{22}-\bar{x}_2 & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ x_{1n}-\bar{x}_1 & \dots & \dots & x_{kn}-\bar{x}_k \end{pmatrix}$$

$$= X_k - \bar{X}_k$$

$$\tilde{y} = M_0 y = \begin{pmatrix} 1-\frac{1}{n} & -\frac{1}{n} & \dots & -\frac{1}{n} \\ -\frac{1}{n} & 1-\frac{1}{n} & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ -\frac{1}{n} & \dots & \dots & 1-\frac{1}{n} \end{pmatrix}\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} y_1-\bar{y} \\ y_2-\bar{y} \\ \vdots \\ y_n-\bar{y} \end{pmatrix} = y - \bar{y} \qquad \bar{X}_k = \begin{pmatrix} \bar{x}_1 & \dots & \bar{x}_k \\ \vdots & \ddots & \vdots \\ \bar{x}_1 & \dots & \bar{x}_k \end{pmatrix}, \quad \bar{y} = \begin{pmatrix} \bar{y} \\ \vdots \\ \bar{y} \end{pmatrix}$$

$$y = \tilde{X}_k\beta_k + e \qquad or \quad \tilde{y} = \tilde{X}_k\beta_k + e$$

$$\tilde{\beta}_k = (\tilde{X}_k'\tilde{X}_k)^{-1}\tilde{X}_k'y \quad or \quad \tilde{\beta}_k = (\tilde{X}_k'\tilde{X}_k)^{-1}\tilde{X}_k'\tilde{y} = (\tilde{X}_k'\tilde{X}_k)^{-1}\tilde{X}_k'y$$

当然ながら、変数処理前の回帰分析

$$y = X\beta + e = \begin{pmatrix} 1_n & X_k \end{pmatrix}\begin{pmatrix} \beta_0 \\ \beta_k \end{pmatrix} + e \qquad \hat{\beta} = \begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_k \end{pmatrix} = \left(X'X\right)^{-1}X'$$

による回帰係数と、説明変数（と被説明変数）の平均からの乖離による回帰係数は同じ

$$\tilde{\beta}_k = \hat{\beta}_k$$

となる。