データ解析

Rによる多変量解析入門

回帰分析(I)

lec20031030 下平英寿 shimo@is.titech.ac.jp

概要

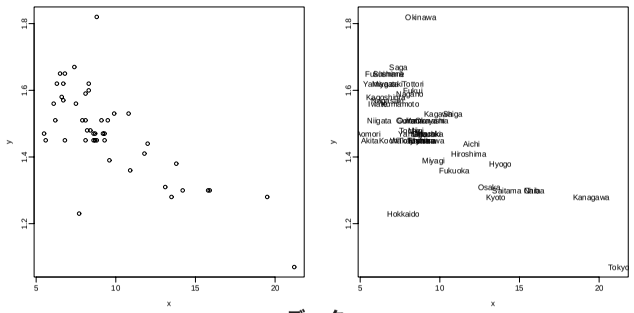
回帰分析の基礎

- 直線のあてはめ
- 回帰分析
- あてはまりのよさ
- 部分回帰

線形代数の知識，とくに「射影」を前提とする

直線のあてはめ

散布図 (scatter plot)



データ

$$(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$$

セッションファイル

edu:~shimo/class/gakubu200209/note20021020.Rt

```
> ### 散布図
> ax <- "E09504"
> X2000$jitem[ax]
                                        E09504
"最終学歴が大学・大学院卒の者の割合 "
> x <- X2000$x[,ax]
> ay <- "A05203"
> X2000$jitem[ay]
                                        A05203
"合 計 特 殊 出 生 率 "
> y <- X2000$x[,ay]
> rbind(x,y)
  Hokkaido Aomori Iwate Miyagi Akita Yamagata Fukushima Ibaraki Tochigi Gumma
x     7.70   5.50  6.10   9.60  5.60     6.30      6.50    9.30    8.20  8.1
y     1.23   1.47  1.56   1.39  1.45     1.62      1.65    1.47    1.48  1.5
  Saitama Chiba Tokyo Kanagawa Niigata Toyama Ishikawa Fukui Yamanashi Nagan
```



```
x    14.2  15.9 21.20    19.50    6.20   8.80     9.30   8.3      9.10   8.1
y     1.3   1.3  1.07     1.28    1.51   1.45     1.45   1.6      1.51   1.5
  Gifu Shizuoka Aichi  Mie Shiga Kyoto Osaka Hyogo Nara Wakayama Tottori
x 8.70     9.20 12.00 8.40 10.80 13.50 13.10 13.80 15.8     8.10    8.30
y 1.47     1.47  1.44 1.48  1.53  1.28  1.31  1.38  1.3     1.45    1.62
  Shimane Okayama Hiroshima Yamaguchi Tokushima Kagawa Ehime Kochi Fukuoka Sa
x    6.80    9.50     11.80      8.60      8.60   9.90  8.70  6.80   10.90 7.
y    1.65    1.51      1.41      1.47      1.45   1.53  1.45  1.45    1.36 1.
  Nagasaki Kumamoto Ooita Miyazaki Kagoshima Okinawa
x     6.70     7.50  7.90     6.70      6.60    8.80
y     1.57     1.56  1.51     1.62      1.58    1.82
> ## 散布図を点で描く
> plot(x,y)
> ## 散布図を県名で描く
> myplot(x,y)
```

平均，分散，標準偏差，共分散，相関

$$\bar{x} = \frac{1}{n}\sum x_i \qquad x_i\text{の平均}$$

$$\bar{y} = \frac{1}{n}\sum y_i \qquad y_i\text{の平均}$$

$$s_{xy} = \frac{1}{n-1}\sum (x_i - \bar{x})(y_i - \bar{y}) \qquad x_i\text{と}y_i\text{の共分散}$$

$$s_x^2 = \frac{1}{n-1}\sum (x_i - \bar{x})^2 = s_{xx} \qquad x_i\text{の分散}$$

$$s_x = \sqrt{\frac{1}{n-1}\sum (x_i - \bar{x})^2} \qquad x_i\text{の標準偏差}$$

$$r_{xy} = \frac{s_{xy}}{s_x s_y} = \frac{s_{xy}}{\sqrt{s_{xx} s_{yy}}} \qquad \text{相関係数}$$

```
> mymean1
function(x) sum(x)/length(x)
> mymean1(x)
[1] 9.540426
> mymean1(y)
```



```
[1] 1.472979
> myvar1
function(x,y=x) sum((x-mymean1(x))*(y-mymean1(y)))/(length(x)-1)
> sqrt(myvar1(x))
[1] 3.438950
> sqrt(myvar1(y))
[1] 0.1331380
> myvar1(x,y)/sqrt(myvar1(x)*myvar1(y))
[1] -0.7296628
> mycor1
function(x,y) myvar1(x,y)/sqrt(myvar1(x)*myvar1(y))
> mycor1(x,y)
[1] -0.7296628
```

単回帰モデル (simple regression model)

$$y = \beta_0 + \beta_1 x + \epsilon$$

$$y_1 = \beta_0 + \beta_1 x_1 + \epsilon_1$$
$$y_2 = \beta_0 + \beta_1 x_2 + \epsilon_2$$
$$\vdots$$
$$y_n = \beta_0 + \beta_1 x_n + \epsilon_n$$

- y 目的変数，従属変数，応答変数
- x 説明変数，独立変数，予測変数
- ϵ 誤差
- β_0, β_1 回帰係数，偏回帰係数

最小二乗法 (least squares method)

誤差 $\epsilon_i = y_i - (\beta_0 + \beta_1 x_i)$

誤差の二乗和 $S = \sum_{i=1}^{n} \epsilon_i^2 = \sum_{i=1}^{n} \{y_i - (\beta_0 + \beta_1 x_i)\}^2$

$$= \sum \left\{\beta_0^2 + 2\beta_0\beta_1 x_i + \beta_1^2 x_i^2 - 2y_i\beta_0 - 2y_i x_i \beta_1 + y_i^2\right\}$$

$$= n\left\{\beta_0^2 + 2\bar{x}\beta_0\beta_1 + \overline{x^2}\beta_1^2 - 2\bar{y}\beta_0 - 2\overline{xy}\beta_1 + \overline{y^2}\right\}$$

Sが最小になるようにβ_0とβ_1を調節すると...

$$\hat{\beta}_1 = \frac{s_{xy}}{s_{xx}}, \quad \hat{\beta}_0 = \bar{y} - \hat{\beta}_1\bar{x}$$

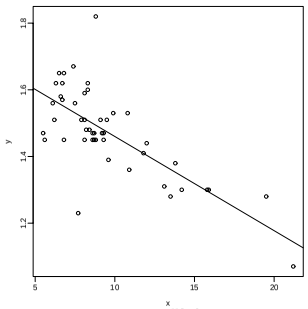
これで予測 $\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x$

数値例１

```
> b1 <- myvar1(x,y)/myvar1(x,x)
> b0 <- mymean1(y) - b1 * mymean1(x)
> coef <- c(b0,b1)
> coef
[1]  1.74248324 -0.02824869
> ## 散布図に回帰直線を描く
> plot(x,y)
> abline(b0,b1)
> ## 予測
> pred <- b0 + b1 * x # この計算では，スカラ（長さ１のベクトル）と長さ４７のベクトルを足し算している．長さの違うベクトルを足し算すると，短いほうが繰り返し用いられる．
> rbind(pred,y)
     Hokkaido   Aomori    Iwate   Miyagi    Akita Yamagata Fukushima  Ibaraki
pred 1.524968 1.587115 1.570166 1.471296 1.584291 1.564516  1.558867 1.479770
y    1.230000 1.470000 1.560000 1.390000 1.450000 1.620000  1.650000 1.470000
      Tochigi    Gumma  Saitama    Chiba    Tokyo Kanagawa  Niigata   Toyama
pred 1.510844 1.513669 1.341352 1.293329 1.143611 1.191634 1.567341 1.493895
```

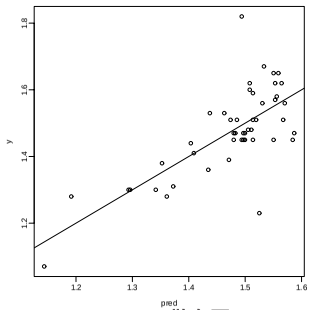


```
y    1.480000 1.510000 1.300000 1.300000 1.070000 1.280000 1.510000 1.450000
     Ishikawa    Fukui Yamanashi   Nagano     Gifu Shizuoka    Aichi      Mie
pred 1.479770 1.508019  1.485420 1.513669 1.496720 1.482595 1.403499 1.505194
y    1.450000 1.600000  1.510000 1.590000 1.470000 1.470000 1.440000 1.480000
       Shiga    Kyoto    Osaka    Hyogo     Nara Wakayama  Tottori  Shimane
pred 1.437397 1.361126 1.372425 1.352651 1.296154 1.513669 1.508019 1.550392
y    1.530000 1.280000 1.310000 1.380000 1.300000 1.450000 1.620000 1.650000
      Okayama Hiroshima Yamaguchi Tokushima   Kagawa    Ehime    Kochi  Fukuo
pred 1.474121  1.409149  1.499545  1.499545 1.462821 1.496720 1.550392 1.4345
y    1.510000  1.410000  1.470000  1.450000 1.530000 1.450000 1.450000 1.3600
        Saga Nagasaki Kumamoto    Ooita Miyazaki Kagoshima  Okinawa
pred 1.533443 1.553217 1.530618 1.519319 1.553217  1.556042 1.493895
y    1.670000 1.570000 1.560000 1.510000 1.620000  1.580000 1.820000

> ## 予測と実測値の散布図
> plot(pred,y)
> abline(0,1)
```



(x_i, y_i)**の散布図**

$y = \beta_0 + \beta_1 x$



$(\hat{y}_i, y_i)$**の散布図**

$\hat{y} = y$

$\hat{\beta}_0 = 1.74,\ \hat{\beta}_1 = -0.028$

最小二乗推定量の導出

$$\frac{\partial S}{\partial \beta_0} = -2\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i) = 0$$

$$\frac{\partial S}{\partial \beta_1} = -2\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i)x_i = 0$$

$$\sum_{i=1}^{n} y_i = n\beta_0 + \beta_1 \sum_{i=1}^{n} x_i$$

$$\sum_{i=1}^{n} x_i y_i = \beta_0 \sum_{i=1}^{n} x_i + \beta_1 \sum_{i=1}^{n} x_i^2$$

$$\begin{bmatrix} \sum y_i \\ \sum x_i y_i \end{bmatrix} = \begin{bmatrix} \sum 1 & \sum x_i \\ \sum x_i & \sum x_i^2 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$$

$$\begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} \sum 1 & \sum x_i \\ \sum x_i & \sum x_i^2 \end{bmatrix}^{-1} \begin{bmatrix} \sum y_i \\ \sum x_i y_i \end{bmatrix}$$

ベクトル表現

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, \quad \boldsymbol{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \quad \boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

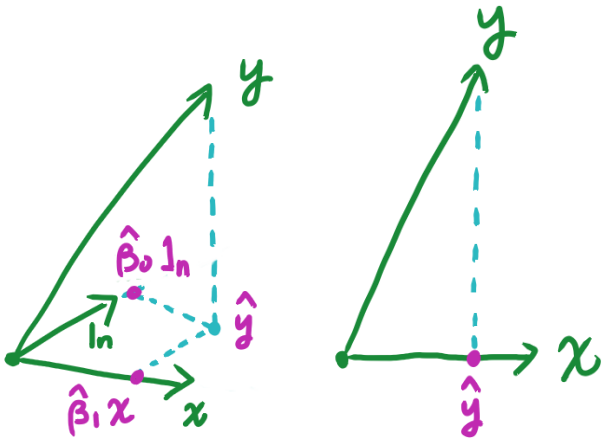
$$\boldsymbol{y} = \beta_0 \mathbf{1}_n + \beta_1 \boldsymbol{x} + \boldsymbol{\epsilon}$$

$$= \left[\mathbf{1}_n, \boldsymbol{x}\right] \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} + \boldsymbol{\epsilon}$$

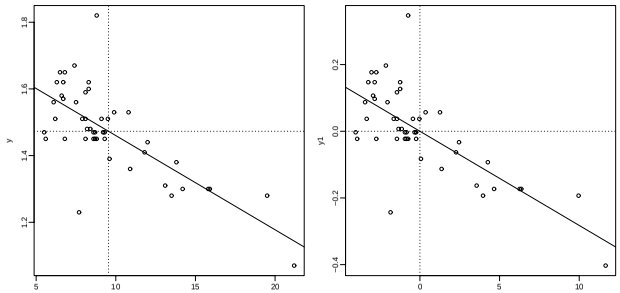
$$= \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

$\boldsymbol{X} = \left[\mathbf{1}_n, \boldsymbol{x}\right]$, $\boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix}$, $S = \|\boldsymbol{\epsilon}\|^2 = \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}\|^2$**の最小化**

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



中心化 (centering)



$\bar{x} = 9.54, \bar{y} = 1.47$

$\bar{x} = 0, \bar{y} = 0$

$x_i \leftarrow x_i - \bar{x}, \quad y_i \leftarrow y_i - \bar{y}$

$$y_i = \beta_1 x_i + \epsilon_i$$

$$\boldsymbol{y} = \beta_1 \boldsymbol{x} + \boldsymbol{\epsilon}$$

$\|\boldsymbol{y} - \beta_1 \boldsymbol{x}\|^2$**の最小化は**$\boldsymbol{y}$**の**$\boldsymbol{x}$**への射影**

$$\hat{\boldsymbol{y}} = \hat{\beta}_1 \boldsymbol{x} = \left(\frac{\boldsymbol{x}}{\|\boldsymbol{x}\|}\right)\left(\frac{\boldsymbol{x}}{\|\boldsymbol{x}\|}\right)' \boldsymbol{y} = \left(\frac{\boldsymbol{x}'\boldsymbol{y}}{\|\boldsymbol{x}\|^2}\right)\boldsymbol{x}$$

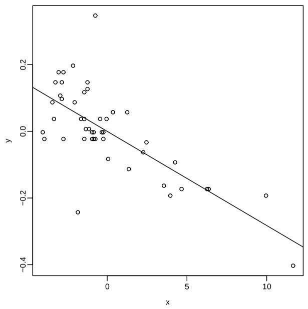
$$S_{xx} = \sum x_i^2 = \boldsymbol{x}'\boldsymbol{x} = \|\boldsymbol{x}\|^2, \quad S_{xy} = \sum x_i y_i = \boldsymbol{x}'\boldsymbol{y}$$

$$\hat{\beta}_1 = \frac{S_{xy}}{S_{xx}} = \frac{\boldsymbol{x}'\boldsymbol{y}}{\|\boldsymbol{x}\|^2}$$

```
> n <- length(y)
> n
[1] 47
> i <- rep(1,n)
> i
 [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
[39] 1 1 1 1 1 1 1 1 1
> i %*% x / n
         [,1]
[1,] 9.540426
> i %*% y / n
         [,1]
[1,] 1.472979
> x <- x - i * (i %*% x / n)
> y <- y - i * (i %*% y / n)
> mymean1(x)
[1] -1.530690e-15
> mymean1(y)
```



```
[1] -1.842498e-16
> (x %*% y)/(x %*% x)  # = b1
            [,1]
[1,] -0.02824869
> plot(x,y)
> abline(0,(x %*% y)/(x %*% x) )
```



回帰分析

重回帰モデル (multiple regression model)

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_p x_p + \epsilon$$

$$\boldsymbol{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \quad \boldsymbol{x}_k = \begin{bmatrix} x_{1k} \\ \vdots \\ x_{nk} \end{bmatrix}, \quad \boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_p \end{bmatrix}$$

$$\boldsymbol{y} = \beta_0 \boldsymbol{1}_n + \beta_1 \boldsymbol{x}_1 + \cdots + \beta_p \boldsymbol{x}_p + \boldsymbol{\epsilon}$$

$$\boldsymbol{X} = [\boldsymbol{1}_n, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_p] = \begin{bmatrix} 1 & x_{11} & \ldots & x_{1p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & \ldots & x_{np} \end{bmatrix}$$

$$\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

射影

$$\|\boldsymbol{\epsilon}\|^2 = \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}\|^2$$

を最小にするには

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

ハット行列（射影行列）

$$\boldsymbol{H} = \boldsymbol{X}(\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'$$

$\boldsymbol{1}_n, \boldsymbol{x}_1, \ldots, \boldsymbol{x}_p$ の張る空間への $\boldsymbol{y}$ の射影

$$\hat{\boldsymbol{y}} = \boldsymbol{H}\boldsymbol{y}$$

もし $\boldsymbol{X}'\boldsymbol{X}$ が退化している場合には

$$\hat{\boldsymbol{y}} = \boldsymbol{X}\boldsymbol{X}^{+}\boldsymbol{y}$$

導出

$$\|\boldsymbol{\epsilon}\|^2 = (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})'(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta})$$
$$= \boldsymbol{y}'\boldsymbol{y} - 2\boldsymbol{\beta}'\boldsymbol{X}'\boldsymbol{y} + \boldsymbol{\beta}'(\boldsymbol{X}'\boldsymbol{X})\boldsymbol{\beta}$$

これを $\boldsymbol{\beta}$ で微分して

$$\frac{\partial \|\boldsymbol{\epsilon}\|^2}{\partial \boldsymbol{\beta}} = -2\boldsymbol{X}'\boldsymbol{y} + 2\boldsymbol{X}'\boldsymbol{X}\boldsymbol{\beta} = 0$$

すなわち正規方程式(normal equation)

$$\boldsymbol{X}'\boldsymbol{X}\boldsymbol{\beta} = \boldsymbol{X}'\boldsymbol{y}$$

これを解いて

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

もし $\boldsymbol{X}'\boldsymbol{X}$ が退化している場合には

$$\hat{\boldsymbol{\beta}} = \boldsymbol{X}^{+}\boldsymbol{y}$$

回帰分析のプログラミング

- 入力: $\boldsymbol{X}$ と $\boldsymbol{y}$
- 回帰係数の推定: $\hat{\boldsymbol{\beta}} = (\boldsymbol{X}'\boldsymbol{X})^{-1}\boldsymbol{X}'\boldsymbol{y}$ または $\hat{\boldsymbol{\beta}} = \boldsymbol{X}^{+}\boldsymbol{y}$
- 数値計算の方法：逆行列，QR分解，特異値分解などいろいろありえる
- 予測値: $\hat{\boldsymbol{y}} = \boldsymbol{X}\hat{\boldsymbol{\beta}}$
- 残差: $\boldsymbol{e} = \boldsymbol{y} - \hat{\boldsymbol{y}}$
- 出力: $\hat{\boldsymbol{\beta}}$, $\hat{\boldsymbol{y}}$, $\boldsymbol{e}$

演習問題（myfunc20020919.Rのmylsfitを参考にしてもよい．）

数値例２

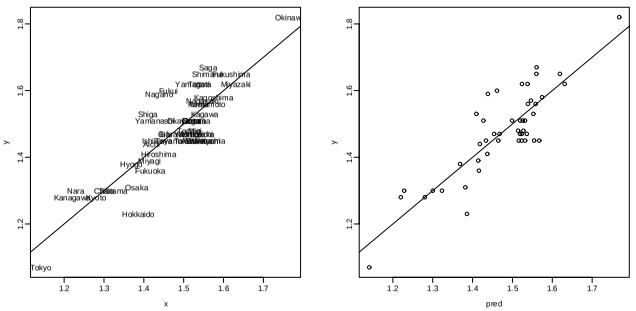
```
> ## 多変量で線形
> ax <- c("E09504","A0410302","C01301","B02101"); x <- X2000$x[,ax]
> ay <- "A05203"; y <- X2000$x[,ay]
> X2000$jitem[c(ax,ay)]
                              E09504                                  A0410302
"最終学歴が大学・大学院卒の者の割合 " "未　婚　者　割　合［20〜24歳・女］ "
                              C01301                                    B02101
           "県民１人当たり県民所得　"                 "年　平　均　気　温　"
                              A05203
             "合 計 特 殊 出 生 率　"
> f <- mylsfit(x,y)
> f$tsummary
, ,  = Y


                 Estimate      Std.Err     t-value      Pr(>|t|)
  Intercept  3.636118e+00 6.108140e-01  5.9529052 4.642519e-07
  E09504    -1.655659e-02 6.570354e-03 -2.5198932 1.562857e-02
```



```
  A0410302  -2.727500e-02 7.438516e-03 -3.6667262 6.850351e-04
  C01301     1.228960e-05 4.635665e-05  0.2651098 7.922217e-01
  B02101     2.012511e-02 5.098161e-03  3.9475245 2.951848e-04

> f$fsummary
  Mean Sum Sq R Squared  F-value Df 1 Df 2       Pr(>F)
Y  0.07061925 0.7431179 30.37478    4   42 6.678249e-12
> x1 <- cbind(rep(1,length(y)),x)
> coef <- solve(t(x1) %*% x1) %*% (t(x1) %*% y)
> coef

                  [,1]
          3.636118e+00
  E09504   -1.655659e-02
  A0410302 -2.727500e-02
  C01301    1.228960e-05
  B02101    2.012511e-02
> pred <- x1 %*% coef
> t(cbind(pred,y))
```

```
  Hokkaido   Aomori    Iwate   Miyagi    Akita Yamagata Fukushima  Ibaraki
  1.385854 1.518977 1.538630 1.414345 1.515823 1.524002  1.619096 1.467897
y 1.230000 1.470000 1.560000 1.390000 1.450000 1.620000  1.650000 1.470000
   Tochigi    Gumma  Saitama    Chiba    Tokyo Kanagawa  Niigata   Toyama
  1.514316 1.531548 1.323061 1.300365 1.140643 1.219962 1.525388 1.464334
y 1.480000 1.510000 1.300000 1.300000 1.070000 1.280000 1.510000 1.450000
  Ishikawa    Fukui Yamanashi   Nagano     Gifu Shizuoka    Aichi      Mie
  1.433561 1.461327  1.427325 1.438374 1.453923 1.535835 1.418394 1.527675
y 1.450000 1.600000  1.510000 1.590000 1.470000 1.470000 1.440000 1.480000
    Shiga    Kyoto    Osaka    Hyogo     Nara Wakayama  Tottori  Shimane
  1.409378 1.280022 1.381912 1.368422 1.228403 1.554402 1.538035 1.559977
y 1.530000 1.280000 1.310000 1.380000 1.300000 1.450000 1.620000 1.650000
   Okayama Hiroshima Yamaguchi Tokushima   Kagawa    Ehime    Kochi  Fukuoka
  1.499213  1.436992   1.52368  1.523004 1.552604 1.531791 1.567354 1.415729
y 1.510000  1.410000   1.47000  1.450000 1.530000 1.450000 1.450000 1.360000
     Saga Nagasaki Kumamoto    Ooita Miyazaki Kagoshima  Okinawa
  1.560404 1.546608 1.558161 1.519602 1.631219  1.574310 1.768123
y 1.670000 1.570000 1.560000 1.510000 1.620000  1.580000 1.820000
> myplot(pred,y)
```

```
> abline(0,1)
> plot(pred,y)
> abline(0,1)
```



数値例３

```
> ###  まず単回帰，それからダミー変数 （２）
> ## 単回帰
> ax <- "C01301"; ay <- "C04602"
> X2000$jitem[c(ax,ay)]
                                C01301
                    "県民１人当たり県民所得　"
                                C04602
"個 人 預 貯 金 残 高（人口１人当たり） "
> X2000$junit[c(ax,ay)]
                  C01301                    C04602
   "(千円:thousand yen)" "(万円:10 thousand yen)"
> x <- X2000$x[,ax,drop=F]
> y <- X2000$x[,ay,drop=F]
> f <- mylsfit(x,y)
> f$tsummary
, ,  = C04602
```

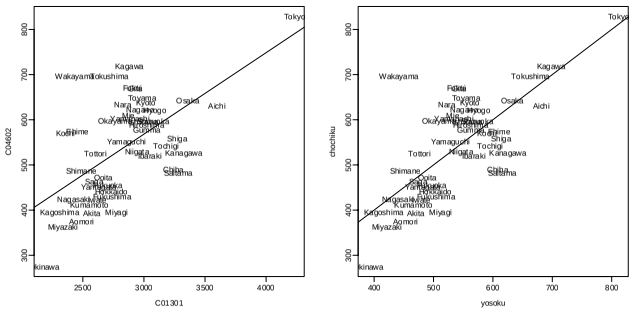


```
             Estimate      Std.Err   t-value     Pr(>|t|)
  Intercept 26.9369511 102.88756993 0.2618096 7.946630e-01
  C01301     0.1804065   0.03580613 5.0384246 8.093436e-06

> f$fsummary
      Mean Sum Sq R Squared  F-value Df 1 Df 2       Pr(>F)
C04602    90.60172 0.3606658 25.38572    1   45 8.093436e-06
> myplot(x,y)
> abline(f)
> ## ダミー変数
> nihonregion[,"shikoku"]
 Hokkaido    Aomori     Iwate    Miyagi     Akita  Yamagata Fukushima    Ibara
        0         0         0         0         0         0         0
  Tochigi     Gumma   Saitama     Chiba     Tokyo  Kanagawa   Niigata     Toya
        0         0         0         0         0         0         0
 Ishikawa     Fukui Yamanashi    Nagano      Gifu  Shizuoka     Aichi
        0         0         0         0         0         0         0
    Shiga     Kyoto     Osaka     Hyogo      Nara  Wakayama   Tottori   Shima
```

```
        0         0         0         0         0         0         0
  Okayama Hiroshima Yamaguchi Tokushima    Kagawa     Ehime     Kochi   Fukuo
        0         0         0         1         1         1         1
     Saga  Nagasaki  Kumamoto     Ooita  Miyazaki Kagoshima   Okinawa
        0         0         0         0         0         0         0
> x <- cbind(X2000$x[,ax,drop=F],nihonregion[,"shikoku",drop=F])
> t(x)
       Hokkaido Aomori Iwate Miyagi Akita Yamagata Fukushima Ibaraki Tochig
C01301      2731   2489  2619   2776  2574     2629      2737    3047    318
shikoku        0      0     0      0     0        0         0       0      0
       Gumma Saitama Chiba Tokyo Kanagawa Niigata Toyama Ishikawa Fukui
C01301  3022    3280  3243  4230     3326    2941   2982     2996  2904
shikoku    0       0     0     0        0       0      0        0     0
       Yamanashi Nagano Gifu Shizuoka Aichi  Mie Shiga Kyoto Osaka Hyogo Nar
C01301       2885   2969 2931     3073  3598 2874  3271  3015  3359  3088 282
shikoku         0      0    0        0     0    0     0     0     0     0
       Wakayama Tottori Shimane Okayama Hiroshima Yamaguchi Tokushima Kagawa
C01301     2436    2604    2485    2764       3019      2855      2716   288
shikoku       0       0       0       0          0         0         1     1
```

```
        Ehime Kochi Fukuoka Saga Nagasaki Kumamoto Ooita Miyazaki Kagoshima
C01301   2456  2357    2703 2589     2426     2552  2664     2336       2311
shikoku     1     1       0    0        0        0     0        0          0
        Okinawa
C01301     2183
shikoku       0
> f <- mylsfit(x,y)
> f$tsummary
, ,  = C04602


             Estimate     Std.Err    t-value     Pr(>|t|)
  Intercept -59.1667194 92.49159483 -0.6396983 5.256857e-01
  C01301      0.2057250  0.03192249  6.4445142 7.486358e-08
  shikoku   163.9675326 42.22411062  3.8832679 3.422263e-04

> f$fsummary
      Mean Sum Sq R Squared  F-value Df 1 Df 2     Pr(>F)
C04602     79.0721 0.5238522 24.20414    2   44 8.1343e-08
```

```
> myplot(f$pred,y,xlab="yosoku",ylab="chochiku")
> abline(0,1)
```




```
> ###  まず単回帰，それからダミー変数（１）
> ## 単回帰
> ax <- "C01301"; ay <- "C04602"
> X2000$jitem[c(ax,ay)]
                                C01301
                    "県民１人当たり県民所得　"
                                C04602
"個 人 預 貯 金 残 高（人口１人当たり） "
> x <- X2000$x[,ax,drop=F]
> y <- X2000$x[,ay,drop=F]
> f <- mylsfit(x,y)
> f$tsummary
, ,  = C04602


             Estimate      Std.Err   t-value     Pr(>|t|)
  Intercept 26.9369511 102.88756993 0.2618096 7.946630e-01
  C01301     0.1804065   0.03580613 5.0384246 8.093436e-06
```

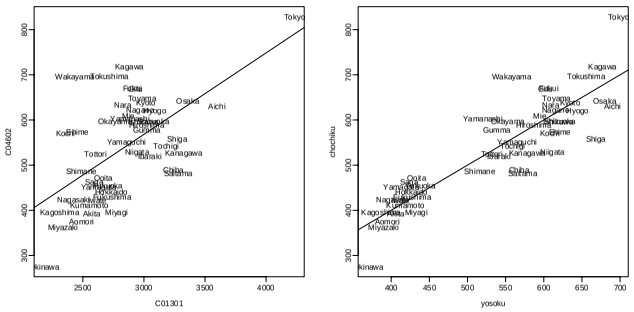
```
> f$fsummary
      Mean Sum Sq R Squared  F-value Df 1 Df 2       Pr(>F)
C04602    90.60172 0.3606658 25.38572    1   45 8.093436e-06
> myplot(x,y)
> abline(f)
> ## 中心化してダミー変数を使う
> x <- x - mean(x)
> y <- y - mean(y)
> x <- cbind(x,nihonregion)
> x
             C01301 tohoku kanto shinetsu tokai kinki chugoku shikoku kyush
Hokkaido  -118.659574      1     0        0     0     0       0       0
Aomori    -360.659574      1     0        0     0     0       0       0
Iwate     -230.659574      1     0        0     0     0       0       0
Miyagi     -73.659574      1     0        0     0     0       0       0
Akita     -275.659574      1     0        0     0     0       0       0
Yamagata  -220.659574      1     0        0     0     0       0       0
Fukushima -112.659574      1     0        0     0     0       0       0
```

```
Ibaraki     197.340426      0     1        0     0     0       0       0
Tochigi     331.340426      0     1        0     0     0       0       0
Gumma       172.340426      0     1        0     0     0       0       0
Saitama     430.340426      0     1        0     0     0       0       0
Chiba       393.340426      0     1        0     0     0       0       0
Tokyo      1380.340426      0     1        0     0     0       0       0
Kanagawa    476.340426      0     1        0     0     0       0       0
Niigata      91.340426      0     0        1     0     0       0       0
Toyama      132.340426      0     0        1     0     0       0       0
Ishikawa    146.340426      0     0        1     0     0       0       0
Fukui        54.340426      0     0        1     0     0       0       0
Yamanashi    35.340426      0     1        0     0     0       0       0
Nagano      119.340426      0     0        1     0     0       0       0
Gifu         81.340426      0     0        0     1     0       0       0
Shizuoka    223.340426      0     0        0     1     0       0       0
Aichi       748.340426      0     0        0     1     0       0       0
Mie          24.340426      0     0        0     1     0       0       0
Shiga       421.340426      0     0        0     0     1       0       0
Kyoto       165.340426      0     0        0     0     1       0       0
```

```
Osaka       509.340426      0     0        0     0     1       0       0
Hyogo       238.340426      0     0        0     0     1       0       0
Nara        -22.659574      0     0        0     0     1       0       0
Wakayama   -413.659574      0     0        0     0     1       0       0
Tottori    -245.659574      0     0        0     0     0       1       0
Shimane    -364.659574      0     0        0     0     0       1       0
Okayama     -85.659574      0     0        0     0     0       1       0
Hiroshima   169.340426      0     0        0     0     0       1       0
Yamaguchi     5.340426      0     0        0     0     0       1       0
Tokushima  -133.659574      0     0        0     0     0       0       1
Kagawa       31.340426      0     0        0     0     0       0       1
Ehime      -393.659574      0     0        0     0     0       0       1
Kochi      -492.659574      0     0        0     0     0       0       1
Fukuoka    -146.659574      0     0        0     0     0       0       0
Saga       -260.659574      0     0        0     0     0       0       0
Nagasaki   -423.659574      0     0        0     0     0       0       0
Kumamoto   -297.659574      0     0        0     0     0       0       0
Ooita      -185.659574      0     0        0     0     0       0       0
Miyazaki   -513.659574      0     0        0     0     0       0       0
```

```
Kagoshima -538.659574      0     0        0     0     0       0       0
Okinawa   -666.659574      0     0        0     0     0       0       0
> f <- mylsfit(x,y,intercept=F)  # 定数項は含めないで回帰分析
> f$tsummary
, ,  = C04602


             Estimate     Std.Err    t-value     Pr(>|t|)
  C01301     0.1320462  0.03475661  3.7991678 5.099313e-04
  tohoku   -98.8497878 22.79470611 -4.3365239 1.027886e-04
  kanto    -25.7297094 25.16274109 -1.0225321 3.129950e-01
  shinetsu  58.3071977 25.97661830  2.2446031 3.069535e-02
  tokai     50.2255783 30.22020273  1.6619868 1.047444e-01
  kinki     71.3354400 24.03080205  2.9685002 5.157827e-03
  chugoku   23.1530379 25.95441651  0.8920654 3.779721e-01
  shikoku  131.8024396 29.99034941  4.3948284 8.608699e-05
  kyushu   -83.2049623 24.21735814 -3.4357572 1.444296e-03

> f$fsummary
```

```
       Mean Sum Sq R Squared  F-value Df 1 Df 2       Pr(>F)
C04602     57.4674 0.7827953 15.21668    9   38 4.247037e-10
> my <- mean(X2000$x[,ay])
> myplot(f$pred+my,y+my,xlab="yosoku",ylab="chochiku")
> abline(0,1)
```



数値例４

```
> ### 多項式回帰
> psinit("20021020k04sp1.eps",pty="s")
> ax <- "B02304"; ay <- "B02102"
> X2000$jitem[c(ax,ay)]
                                        B02304
                        "雪　　日　　数（年　間）　"
                                        B02102
"最　高　気　温（日最高気温の月平均の最高値）　"
> X2000$junit[c(ax,ay)]
 B02304  B02102
 "(日)" "(° C)"
> x <- X2000$x[,ax]
> y <- X2000$x[,ay]
> myplot(x,y)
> ## 線形回帰（１次式）
> f1 <- mylsfit(x,y)
> f1$coefficients
```



```
                    Y
  Intercept 33.17502116
  X         -0.01808129
> f1$tsummary
, ,  = Y


              Estimate     Std.Err    t-value     Pr(>|t|)
  Intercept 33.17502116 0.260778107 127.215515 3.462132e-59
  X         -0.01808129 0.005409449  -3.342537 1.678815e-03

> f1$fsummary
  Mean Sum Sq R Squared  F-value Df 1 Df 2      Pr(>F)
Y    1.304014 0.1988971 11.17256    1   45 0.001678815
> abline(f1)
> ## 多項式回帰（２次式）
> xx <- cbind(x,x^2)
> dimnames(xx)[[2]] <- c("x","x^2")
> t(xx)
```

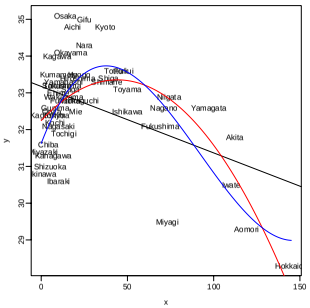
```
    Hokkaido Aomori Iwate Miyagi Akita Yamagata Fukushima Ibaraki Tochigi Gun
x        145    119   110     73   112        97         69       10       13
x^2    21025  14161 12100   5329 12544      9409       4761      100      169
    Saitama Chiba Tokyo Kanagawa Niigata Toyama Ishikawa Fukui Yamanashi Naga
x         9     4     7        7       74     50       50     48         13
x^2      81    16    49       49     5476   2500     2500   2304        169    5
    Gifu Shizuoka Aichi Mie Shiga Kyoto Osaka Hyogo Nara Wakayama Tottori
x     25        5    18  20    39    37    14    22   25        13       43
x^2  625       25   324 400  1521  1369   196   484  625       169     1849
    Shimane Okayama Hiroshima Yamaguchi Tokushima Kagawa Ehime Kochi Fukuoka
x        38       17        21         22         12      9    10     8      14
x^2    1444      289       441        484        144     81   100    64     196
    Saga Nagasaki Kumamoto Ooita Miyazaki Kagoshima Okinawa
x     17       10        10     6        1         5       0
x^2  289      100       100    36        1        25       0
> f2 <- mylsfit(xx,y)
> f2$coefficients
```

```
                    Y
  Intercept 32.2452328361
  x          0.0502327170
  x^2       -0.0005693289
> f2$tsummary
, ,  = Y


               Estimate      Std.Err    t-value     Pr(>|t|)
  Intercept 32.2452328361 0.2895669764 111.356734 1.396604e-55
  x          0.0502327170 0.0149957168   3.349804 1.667099e-03
  x^2       -0.0005693289 0.0001193666  -4.769583 2.055703e-05

> f2$fsummary
  Mean Sum Sq R Squared  F-value Df 1 Df 2       Pr(>F)
Y    1.070696 0.4719236 19.66064    2   44 7.931007e-07
> xs <- seq(min(x),max(x),length=300)
> ys <- cbind(1,xs,xs^2) %*% f2$coefficients
> lines(xs,ys,col=2)
> ## 多項式回帰（３次式）
```

```
> xx <- cbind(x,x^2,x^3)
> dimnames(xx)[[2]] <- c("x","x^2","x^3")
> f3 <- mylsfit(xx,y)
> f3$coefficients
```

```
                    Y
  Intercept  3.162375e+01
  x          1.227429e-01
  x^2       -2.052218e-03
  x^3        7.450801e-06
> f3$tsummary
, ,  = Y


               Estimate      Std.Err   t-value     Pr(>|t|)
  Intercept  3.162375e+01 3.621251e-01 87.328250 4.800261e-50
  x          1.227429e-01 3.122303e-02  3.931166 3.026254e-04
  x^2       -2.052218e-03 5.806757e-04 -3.534189 9.925295e-04
  x^3        7.450801e-06 2.862603e-06  2.602806 1.263671e-02
```

```
> f3$fsummary
  Mean Sum Sq R Squared  F-value Df 1 Df 2       Pr(>F)
Y    1.006674 0.5437978 17.08548    3   43 1.877689e-07
> xs <- seq(min(x),max(x),length=300)
> ys <- cbind(1,xs,xs^2,xs^3) %*% f3$coefficients
> lines(xs,ys,col=4)
> dev.off()
null device
          1
```



あてはまりのよさ

重相関係数

y_iと$\hat{y}_i$の相関を重相関係数Rと呼ぶ．
重相関係数の二乗R^2は決定係数と呼ばれる．

$$R = \frac{S_{y\hat{y}}}{\sqrt{S_{yy}S_{\hat{y}\hat{y}}}}$$

$$S_{y\hat{y}} = \sum(y_i - \bar{y})(\hat{y}_i - \bar{y}), S_{yy} = \sum(y_i - \bar{y})^2, S_{\hat{y}\hat{y}} = \sum(\hat{y}_i - \bar{y})^2$$

すべての要素が$\bar{y}$のベクトル$\bar{\boldsymbol{y}} = \bar{y}1_n$を用いて
中心化$\boldsymbol{y} \leftarrow \boldsymbol{y} - \bar{\boldsymbol{y}}$，$\hat{\boldsymbol{y}} \leftarrow \hat{\boldsymbol{y}} - \bar{\boldsymbol{y}}$をおこなうと

$$R = \frac{\boldsymbol{y}'\hat{\boldsymbol{y}}}{\|\boldsymbol{y}\| \cdot \|\hat{\boldsymbol{y}}\|}$$

あてはまりの良さをRまたはR^2で判断する．

とくに単回帰の場合のRはx_iとy_iの相関係数である．


```
> ### 重相関係数
> ## 数値例４（１次式）
> t(round(cbind(f1$pred,y),2))
  Hokkaido Aomori Iwate Miyagi Akita Yamagata Fukushima Ibaraki Tochigi Gumma
Y    30.55  31.02 31.19  31.86 31.15    31.42     31.93   32.99   32.94 33.03
y    28.30  29.30 30.50  29.50 31.80    32.60     32.10   30.60   31.90 32.60
  Saitama Chiba Tokyo Kanagawa Niigata Toyama Ishikawa Fukui Yamanashi Nagano
Y   33.01  33.1 33.05    33.05   31.84  32.27    32.27 32.31     32.94  31.89
y   33.20  31.6 32.40    31.30   32.90  33.10    32.50 33.60     33.30  32.60
   Gifu Shizuoka Aichi   Mie Shiga Kyoto Osaka Hyogo  Nara Wakayama Tottori
Y 32.72    33.08 32.85 32.81 32.47 32.51 32.92 32.78 32.72    32.94    32.4
y 35.00    31.00 34.80 32.50 33.40 34.80 35.10 33.50 34.30    32.90    33.6
  Shimane Okayama Hiroshima Yamaguchi Tokushima Kagawa Ehime Kochi Fukuoka
Y   32.49    32.87      32.8     32.78     32.96  33.01 32.99 33.03   32.92
y   33.30    34.10      33.4     32.80     33.20  34.00 33.00 32.20   32.80
   Saga Nagasaki Kumamoto Ooita Miyazaki Kagoshima Okinawa
Y 32.87    32.99    32.99 33.07    33.16     33.08   33.18
y 33.10    32.10    33.50 32.50    31.40     32.40   30.80
```

```
> cor(x,y)
[1] -0.4459788
> mycor1(f1$pred,y)
[1] 0.4459788
> cor(x,y)^2
[1] 0.1988971
> mycor1(f1$pred,y)^2
[1] 0.1988971
> f1$fsummary
  Mean Sum Sq R Squared  F-value Df 1 Df 2      Pr(>F)
Y    1.304014 0.1988971 11.17256    1   45 0.001678815
> ## 数値例４（２次式）
> mycor1(f2$pred,y)
[1] 0.686967
> mycor1(f2$pred,y)^2
[1] 0.4719236
> f2$fsummary
  Mean Sum Sq R Squared  F-value Df 1 Df 2       Pr(>F)
Y    1.070696 0.4719236 19.66064    2   44 7.931007e-07
```

```
> ## 数値例４（３次式）
> mycor1(f3$pred,y)
[1] 0.7374264
> mycor1(f3$pred,y)^2
[1] 0.5437978
> f3$fsummary
  Mean Sum Sq R Squared  F-value Df 1 Df 2       Pr(>F)
Y    1.006674 0.5437978 17.08548    3   43 1.877689e-07
```

残差 (residual)

$$e_i = y_i - \hat{y}_i, \quad i = 1, \ldots, n$$

$$\boldsymbol{e} = \begin{bmatrix} e_1 \\ \vdots \\ e_n \end{bmatrix}, \quad \boldsymbol{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \quad \hat{\boldsymbol{y}} = \begin{bmatrix} \hat{y}_1 \\ \vdots \\ \hat{y}_n \end{bmatrix}$$

$$\boldsymbol{e} = \boldsymbol{y} - \hat{\boldsymbol{y}}$$

ハット行列を用いると

$$\boldsymbol{e} = (\boldsymbol{I}_n - \boldsymbol{H})\boldsymbol{y}$$

$\boldsymbol{HX} = \boldsymbol{X}$なので$\boldsymbol{X}'\boldsymbol{e} = \boldsymbol{X}'(\boldsymbol{I}_n - \boldsymbol{H})\boldsymbol{y} = 0$．とくに

$$1_n'\boldsymbol{e} = 0, \quad \hat{\boldsymbol{y}}'\boldsymbol{e} = 0$$

ピタゴラスの定理

$$\|\boldsymbol{y}\|^2 = \|\hat{\boldsymbol{y}} + \boldsymbol{e}\|^2 = \|\hat{\boldsymbol{y}}\|^2 + 2\hat{\boldsymbol{y}}'\boldsymbol{e} + \|\boldsymbol{e}\|^2 = \|\hat{\boldsymbol{y}}\|^2 + \|\boldsymbol{e}\|^2$$


```
> ### 残差
> e <- y-f1$pred
> t(round(e,2))

  Hokkaido Aomori Iwate Miyagi Akita Yamagata Fukushima Ibaraki Tochigi Gu
Y    -2.25  -1.72 -0.69  -2.36  0.65     1.18      0.17   -2.39   -1.04 -0

  Saitama Chiba Tokyo Kanagawa Niigata Toyama Ishikawa Fukui Yamanashi Naga
Y    0.19  -1.5 -0.65    -1.75    1.06   0.83     0.23  1.29      0.36    0

  Gifu Shizuoka Aichi   Mie Shiga Kyoto Osaka Hyogo Nara Wakayama Tottori
Y 2.28    -2.08  1.95 -0.31  0.93  2.29  2.18  0.72 1.58    -0.04     1.2

  Shimane Okayama Hiroshima Yamaguchi Tokushima Kagawa Ehime Kochi Fukuoka
Y    0.81    1.23       0.6      0.02      0.24   0.99  0.01 -0.83   -0.12

  Saga Nagasaki Kumamoto Ooita Miyazaki Kagoshima Okinawa
```

```
  Y 0.23    -0.89     0.51 -0.57    -1.76     -0.68   -2.38
> sum(e)
[1] 9.947598e-14
> sum(f1$pred * e)
[1] 3.312767e-12
> mymean1(e)
[1] 2.116510e-15
> mycor1(f1$pred,e)
[1] 1.675907e-15
> ## ピタゴラスの定理
> sum(y^2)
[1] 49980.06
> sum(f1$pred^2)
[1] 49903.54
> sum(e^2)
[1] 76.52033
> sum(f1$pred^2) + sum(e^2) - sum(y^2)
[1] -7.275958e-12
```

重相関係数と残差の関係

まず $y \leftarrow y - \bar{y}$, $\hat{y} \leftarrow \hat{y} - \bar{y}$ と中心化しておくと，

$$R = \frac{y'\hat{y}}{\|y\| \cdot \|\hat{y}\|} = \cos\theta = \frac{\|\hat{y}\|}{\|y\|}$$

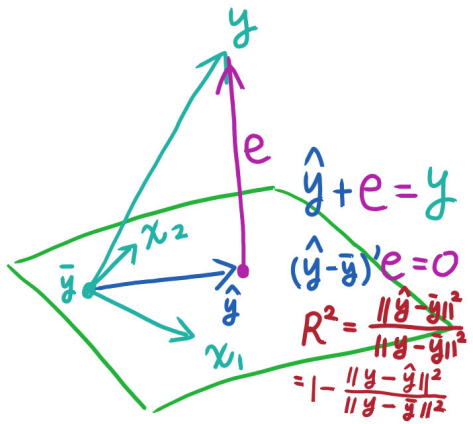
したがって

$$R^2 = (\cos\theta)^2 = \frac{\|\hat{y}\|^2}{\|y\|^2}, \quad 1 - R^2 = (\sin\theta)^2 = \frac{\|e\|^2}{\|y\|^2}$$

($e'\hat{y} = 0$ なので $y'\hat{y} = (\hat{y} + e)'\hat{y} = \|\hat{y}\|^2$ をつかって示しても良い)

中心化していない場合は

$$R^2 = \frac{\|\hat{y} - \bar{y}\|^2}{\|y - \bar{y}\|^2} = 1 - \frac{\|y - \hat{y}\|^2}{\|y - \bar{y}\|^2}$$



$$\|y - \hat{y}\|^2 + \|\hat{y} - \bar{y}\|^2 = \|y - \bar{y}\|^2$$


```
> ### 重相関係数と残差の関係
> e <- y-f1$pred # 残差
> cor(f1$pred,y)^2 # R^2
       [,1]
Y 0.1988971
> sum(f1$pred^2)/sum(y^2) # 中心化しないとダメ
[1] 0.998469
> sum((f1$pred-mymean1(f1$pred))^2)/sum((y-mymean1(y))^2) # R^2
[1] 0.1988971
> myvar1(f1$pred)/myvar1(y) # これでも OK
[1] 0.1988971
> 1-sum(e^2)/sum(y^2) # 中心化しないとダメ
[1] 0.998469
> 1-sum(e^2)/sum((y-mymean1(y))^2) # R^2
[1] 0.1988971
> 1-myvar1(e)/myvar1(y) # これでも OK
[1] 0.1988971
```

部分回帰

部分回帰（Subset Regression）

モデル (k)

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \cdots + \beta_k x_k + \epsilon$$

すなわち

$$\beta_{k+1} = \cdots = \beta_p = 0$$

$$X^{(k)} = \left[1_n, x_1, \ldots, x_k\right], \quad \beta^{(k)} = \begin{bmatrix}\beta_0 \\ \vdots \\ \beta_k\end{bmatrix}$$

$$y = X^{(k)}\beta^{(k)} + \epsilon$$

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

一般に $\hat{\beta}^{(k)}$ と $\hat{\beta}$ の対応する要素は一致しない: $\quad \hat{\beta}_i^{(k)} \neq \hat{\beta}_i$


```
> ### 部分回帰
> t(f1$coef)

    Intercept           X
Y  33.17502 -0.01808129
> t(f2$coef)

    Intercept          x           x^2
Y  32.24523 0.05023272 -0.0005693289
> t(f3$coef)

    Intercept         x          x^2          x^3
Y  31.62375 0.1227429 -0.002052218 7.450801e-06
```

直交化とQR分解

- QR分解

$$X = \left[x_0, \ldots, x_p\right], \quad Q = \left[q_0, \ldots, q_p\right], \quad Q'Q = I_{p+1}$$

$$X = QR, \quad r_{ij} = 0, i > j$$

- 回帰係数の変数変換：$\beta \leftrightarrow \gamma$

$$\gamma = R\beta$$

- 回帰モデルも変換される

$$X\beta = (QR)\beta = Q(R\beta) = Q\gamma$$

$$y = X\beta + \epsilon = Q\gamma + \epsilon$$

- 回帰係数の推定

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

$$\hat{\gamma} = (Q'Q)^{-1}Q'y = Q'y$$

$$\hat{\gamma} = R\hat{\beta}, \quad \hat{\beta} = R^{-1}\hat{\gamma}$$

つまりどちらで推定しても互いに変換できる．

- γ をつかう利点: $\gamma_k = r_{kk}\beta_k + \cdots + r_{kp}\beta_p$ に注意すると

$$\gamma_{k+1} = \cdots = \gamma_p = 0 \Leftrightarrow \beta_{k+1} = \cdots = \beta_p = 0$$

部分回帰モデル (k)

$$\hat{\gamma}^{(k)} = Q^{(k)\prime}y = \begin{bmatrix}q_0' \\ \vdots \\ q_k'\end{bmatrix} y, \quad \hat{\gamma}_i^{(k)} = \hat{\gamma}_i$$

- $\hat{\gamma}$ を $\hat{\beta}^{(0)}, \ldots, \hat{\beta}^{(p)}$ に戻すのも容易．

$$\begin{bmatrix}\hat{\beta}_0^{(k)} \\ \vdots \\ \hat{\beta}_k^{(k)} \\ 0\end{bmatrix} = R^{-1}\begin{bmatrix}\hat{\gamma}_0 \\ \vdots \\ \hat{\gamma}_k \\ 0\end{bmatrix}$$

つまり $\hat{\gamma}$ と R^{-1} の計算は一度だけでよい．

- 部分モデルの計算を γ を通して行なうのは，計算量を減らすという目的というだけでなく，むしろ，回帰分析の性質を理論的に調べる際に重要．

```
> ### 直交化とQR分解
> xx <- cbind(1,x,x^2,x^3)
> dimnames(xx)[[2]] <- c(1,"x","x^2","x^3")
> Q <- qr.Q(qr(xx))
> R <- qr.R(qr(xx))
> cbind(xx,Q)
          1   x    x^2     x^3
Hokkaido  1 145 21025 3048625 -0.145865 -0.46469866  0.58635783  0.54555490
Aomori    1 119 14161 1685159 -0.145865 -0.35684268  0.16893012 -0.16646877
Iwate     1 110 12100 1331000 -0.145865 -0.31950791  0.05955370 -0.25620527
Miyagi    1  73  5329  389017 -0.145865 -0.16602055 -0.20035745 -0.12673425
Akita     1 112 12544 1404928 -0.145865 -0.32780453  0.08229878 -0.24191600
Yamagata  1  97  9409  912673 -0.145865 -0.26557992 -0.06654976 -0.28255814
Fukushima 1  69  4761  328509 -0.145865 -0.14942732 -0.21017241 -0.08803184
Ibaraki   1  10   100    1000 -0.145865  0.09532280  0.05944675 -0.01420506
Tochigi   1  13   169    2197 -0.145865  0.08287788  0.02700782  0.03316958
Gumma     1   8    64     512 -0.145865  0.10361942  0.08218756 -0.05056613
Saitama   1   9    81     729 -0.145865  0.09947111  0.07070567 -0.03189642
Chiba     1   4    16      64 -0.145865  0.12021265  0.13034481 -0.13536963
Tokyo     1   7    49     343 -0.145865  0.10776772  0.09389241 -0.07023124
Kanagawa  1   7    49     343 -0.145865  0.10776772  0.09389241 -0.07023124
Niigata   1  74  5476  405224 -0.145865 -0.17016885 -0.19734628 -0.13616848
Toyama    1  50  2500  125000 -0.145865 -0.07060948 -0.20807451  0.08707592
Ishikawa  1  50  2500  125000 -0.145865 -0.07060948 -0.20807451  0.08707592
Fukui     1  48  2304  110592 -0.145865 -0.06231287 -0.20317131  0.10168360
Yamanashi 1  13   169    2197 -0.145865  0.08287788  0.02700782  0.03316958
Nagano    1  71  5041  357911 -0.145865 -0.15772393 -0.20571087 -0.10754201
Gifu      1  25   625   15625 -0.145865  0.03309820 -0.08268060  0.14536604
Shizuoka  1   5    25     125 -0.145865  0.11606434  0.11797104 -0.11261593
Aichi     1  18   324    5832 -0.145865  0.06213635 -0.02259767  0.09415285
Mie       1  20   400    8000 -0.145865  0.05383973 -0.04087907  0.11265321
Shiga     1  39  1521   59319 -0.145865 -0.02497810 -0.17006988  0.14995720
Kyoto     1  37  1369   50653 -0.145865 -0.01668149 -0.16026134  0.15599117
Osaka     1  14   196    2744 -0.145865  0.07872957  0.01664078  0.04711818
Hyogo     1  22   484   10648 -0.145865  0.04554312 -0.05826859  0.12799090
Nara      1  25   625   15625 -0.145865  0.03309820 -0.08268060  0.14536604
Wakayama  1  13   169    2197 -0.145865  0.08287788  0.02700782  0.03316958
Tottori   1  43  1849   79507 -0.145865 -0.04157133 -0.18701133  0.13242784
Shimane   1  38  1444   54872 -0.145865 -0.02082980 -0.16527710  0.15321596
Okayama   1  17   289    4913 -0.145865  0.06628465 -0.01312251  0.08367402
Hiroshima 1  21   441    9261 -0.145865  0.04969142 -0.04968532  0.12070886
Yamaguchi 1  22   484   10648 -0.145865  0.04554312 -0.05826859  0.12799090
Tokushima 1  12   144    1728 -0.145865  0.08702619  0.03759783  0.01831088
Kagawa    1   9    81     729 -0.145865  0.09947111  0.07070567 -0.03189642
Ehime     1  10   100    1000 -0.145865  0.09532280  0.05944675 -0.01420506
Kochi     1   8    64     512 -0.145865  0.10361942  0.08218756 -0.05056613
Fukuoka   1  14   196    2744 -0.145865  0.07872957  0.01664078  0.04711818
Saga      1  17   289    4913 -0.145865  0.06628465 -0.01312251  0.08367402
Nagasaki  1  10   100    1000 -0.145865  0.09532280  0.05944675 -0.01420506
Kumamoto  1  10   100    1000 -0.145865  0.09532280  0.05944675 -0.01420506
Ooita     1   6    36     216 -0.145865  0.11191603  0.10582024 -0.09090882
Miyazaki  1   1     1       1 -0.145865  0.13265757  0.16880393 -0.21008090
Kagoshima 1   5    25     125 -0.145865  0.11606434  0.11797104 -0.11261593
Okinawa   1   0     0       0 -0.145865  0.13680587  0.18206958 -0.23719159
> R
                1         x         x^2         x^3
Hokkaido -6.855655 -226.0907 -15932.541 -1542516.5
Aomori    0.000000 -241.0622 -28925.150 -3410817.3
Iwate     0.000000    0.0000   8969.815  1785209.7
Miyagi    0.000000    0.0000      0.000   351663.8
> ir <- solve(R)
> ir
          [,1]          [,2]          [,3]          [,4]
1   -0.145865  0.136805874  0.1820695765 -2.371916e-01
x    0.000000 -0.004148307 -0.0133771326  2.767379e-02
x^2  0.000000  0.000000000  0.0001114850 -5.659501e-04
x^3  0.000000  0.000000000  0.0000000000  2.843625e-06
> g3 <- t(Q) %*% y # gamma
> t(g3)
          [,1]     [,2]      [,3]     [,4]
[1,] -223.3485 4.358715 -5.106775 2.620177
> t(ir %*% g3)  # betaに等しいハズ

             1         x          x^2          x^3
  [1,] 31.62375 0.1227429 -0.002052218 7.450801e-06
> t(f3$coef) # beta

    Intercept         x          x^2          x^3
  Y  31.62375 0.1227429 -0.002052218 7.450801e-06
> t(ir[1:2,1:2] %*% g3[1:2]) # gamma (1次)

             1          x
  [1,] 33.17502 -0.01808129
> t(f1$coef)

    Intercept           X
  Y  33.17502 -0.01808129
> t(ir[1:3,1:3] %*% g3[1:3]) # gamma (2次)

             1          x          x^2
  [1,] 32.24523 0.05023272 -0.0005693289
> t(f2$coef)

    Intercept          x          x^2
  Y  32.24523 0.05023272 -0.0005693289
```

平方和の分解

$$\hat{\boldsymbol{y}} = \boldsymbol{Q}\hat{\boldsymbol{\gamma}} = \hat{\gamma}_0\boldsymbol{q}_0 + \cdots + \hat{\gamma}_p\boldsymbol{q}_p$$

$$\|\hat{\boldsymbol{y}}\|^2 = \|\hat{\gamma}_0\boldsymbol{q}_0\|^2 + \cdots + \|\hat{\gamma}_p\boldsymbol{q}_p\|^2 = \hat{\gamma}_0^2 + \cdots + \hat{\gamma}_p^2$$

$$\boldsymbol{q}_0 = \frac{1}{\sqrt{n}}\mathbf{1}_n, \quad \hat{\gamma}_0 = \sqrt{n}\,\bar{y}$$

モデル(k)

$$\|\boldsymbol{Q}^{(k)}\hat{\boldsymbol{\gamma}}^{(k)} - \bar{y}\mathbf{1}_n\|^2 = \hat{\gamma}_1^2 + \cdots + \hat{\gamma}_k^2$$

$$R^2 = \frac{\hat{\gamma}_1^2 + \cdots + \hat{\gamma}_k^2}{\|\boldsymbol{y} - \bar{y}\mathbf{1}_n\|^2}$$

$$\|\boldsymbol{e}\|^2 = \|\boldsymbol{y}\|^2 - \hat{\gamma}_0^2 - \cdots - \hat{\gamma}_k^2 = \|\boldsymbol{y} - \bar{y}\mathbf{1}_n\|^2 - \hat{\gamma}_1^2 - \cdots - \hat{\gamma}_k^2$$


```
> ### 平方和の分解
> sum((f1$pred-mean(f1$pred))^2) # 予測値の平方和 (1次)
[1] 18.99839
> sum(g3[2]^2) # g[2]^2
[1] 18.99839
> sum((f2$pred-mean(f2$pred))^2) # 予測値の平方和 (2次)
[1] 45.07754
> sum(g3[2:3]^2) # g[2]^2+g[3]^2
[1] 45.07754
> sum((f3$pred-mean(f3$pred))^2) # 予測値の平方和 (3次)
[1] 51.94287
> sum(g3[2:4]^2) # g[2]^2+g[3]^2+g[4]^2
[1] 51.94287
> cor(f1$pred,y)^2 # R^2 (1次)
       [,1]
Y 0.1988971
> sum(g3[2]^2)/sum((y-mean(y))^2)
[1] 0.1988971
> cor(f2$pred,y)^2 # R^2 (2次)
       [,1]
Y 0.4719236
> sum(g3[2:3]^2)/sum((y-mean(y))^2)
[1] 0.4719236
> cor(f3$pred,y)^2 # R^2 (3次)
       [,1]
Y 0.5437978
> sum(g3[2:4]^2)/sum((y-mean(y))^2)
[1] 0.5437978
```

練習問題

2-1. 直線当てはめ（単回帰）の関数kaiki1を作れ.

```
kaiki1 <- function(x,y) {
# x,yは同じ長さの実数ベクトル
# y = coef[1] + coef[2]*x + residの形の単回帰分析を行う
# 以下のcoef, pred, residを計算する
#   coef(係数)は2次元ベクトル
#   resid(残差)はyと同じ長さのベクトル
#   pred(予測値) = coef[1] + coef[2]*xはyと同じ長さのベクトル
# 次の行は結果をリストとして返す.
return(coef,pred,resid)
}
```

2-2. 重回帰分析の関数kaiki2を作れ.

```
kaiki2 <- function(x,y) {
# xはn * p次元の行列
# yは長さnのベクトル
```

```
# y = coef[1] + coef[2]*x[,1] + ... + coef[p+1]*x[,p] + resid
#  の形の重回帰分析を行う
# 以下のcoef, pred, residを計算する
#   coef(係数)はp+1次元ベクトル
#   resid(残差)はyと同じ長さのベクトル
#   pred(予測値)はyと同じ長さのベクトル
# 次の行は結果をリストとして返す.
return(coef,pred,resid)
}
```

2-3. kaiki2の返す値から決定係数R^2を計算する関数ketteikeisuを作れ.

```
ketteikeisu <- function(kout) {
# kout$predは予測値, kout$residは残差
# これらから重相関係数の二乗を計算しrsqに代入
return(rsq)
}
```

2-4. kaiki2, ketteikeisuを使い, X2000$xから適当な項目を選んで重回帰分析する. 係数$\beta$と決定係数$R^2$を計算する. myfunc20020919.Rにあるmylsfitをつかって同じ分析をして, 結果が同じになるかどうか確認する.

2-5. 上で得られた結果について, predをx軸, yをy軸とするプロットをする. x軸=y軸となる直線を描く(abline(0,1)をつかう). さらに県名を使ったプロットをする. myfunc20020919.Rのmyplot関数を参考にせよ. プロットはmyfunc20020919.Rにあるpsinit関数などを使いepsファイルとして出力し, それをプリンタで印刷する.

```
psinit("ファイル名") # これ以後のプロットの結果をファイルにeps形式で書き出す
ここでプロットをおこなう...
dev.off() # ファイルをクローズする
```