データ解析
Rによる多変量解析入門
(3) Rによる線形代数

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行列，ベクトルの操作

行列

$$\boldsymbol{A} = \underbrace{\begin{bmatrix} a_{11} & \cdots & a_{1p} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{n1} & \cdots & a_{np} \end{bmatrix}}_{p} \Bigg\} n$$

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{a}^{(1)} \\ \cdot \\ \cdot \\ \cdot \\ \boldsymbol{a}^{(n)} \end{bmatrix} = [\boldsymbol{a}_1, \ldots, \boldsymbol{a}_p]$$

$\boldsymbol{a}^{(i)}$は行ベクトル，$\boldsymbol{a}_j$は列ベクトル

```
> A <- matrix(1:15,5)  # 5x3行列
```



```
> A
     [,1] [,2] [,3]
[1,]    1    6   11
[2,]    2    7   12
[3,]    3    8   13
[4,]    4    9   14
[5,]    5   10   15
> A[2,]  # 行ベクトルの取り出し
[1]  2  7 12
> A[,2]  # 列ベクトルの取り出し
[1]  6  7  8  9 10
> A[2,,drop=F]  # 行ベクトルの取り出し（1x3行列）
     [,1] [,2] [,3]
[1,]    2    7   12
> A[,2,drop=F]  # 列ベクトルの取り出し（5x1行列）
     [,1]
[1,]    6
[2,]    7
[3,]    8
```

```
[4,]    9
[5,]   10
> A[3:4,2:3]  # 2x2部分行列の取り出し
     [,1] [,2]
[1,]    8   13
[2,]    9   14
> B <- A  # AをBにコピー
> B[2,2] <- -1  # (2,2)要素に-1を代入
> B
     [,1] [,2] [,3]
[1,]    1    6   11
[2,]    2   -1   12
[3,]    3    8   13
[4,]    4    9   14
[5,]    5   10   15
> B[2,] <- 101:103  # 行ベクトルの代入
> B
     [,1] [,2] [,3]
[1,]    1    6   11
```

```
[2,]  101  102  103
[3,]    3    8   13
[4,]    4    9   14
[5,]    5   10   15
> B[,2] <- -1:-5  # 列ベクトルの代入
> B
     [,1] [,2] [,3]
[1,]    1   -1   11
[2,]  101   -2  103
[3,]    3   -3   13
[4,]    4   -4   14
[5,]    5   -5   15
> v <- 1:3 # 3次元ベクトル
> v
[1] 1 2 3
> as.matrix(v) # 3x1行列とみなす
     [,1]
[1,]    1
[2,]    2
[3,]    3
```

行列とベクトルの転置

$$\boldsymbol{A}' = \underbrace{\begin{bmatrix} a_{11} & \cdots & a_{n1} \\ \vdots & & \vdots \\ a_{1p} & \cdots & a_{np} \end{bmatrix}}_{n} \Bigg\} p$$

$$\boldsymbol{v}' = \begin{bmatrix} v_1 \\ \vdots \\ v_n \end{bmatrix}' = [v_1, \ldots, v_n]$$

```
> t(A)
     [,1] [,2] [,3] [,4] [,5]
[1,]    1    2    3    4    5
[2,]    6    7    8    9   10
[3,]   11   12   13   14   15
> t(as.matrix(v))
     [,1] [,2] [,3]
[1,]    1    2    3
```


行列の積

$$\underset{n\times k}{\boldsymbol{A}}\ \underset{k\times m}{\boldsymbol{B}} = \underset{n\times m}{\boldsymbol{C}}$$

$$\underset{n\times k}{\boldsymbol{A}}\ \underset{k\times 1}{\boldsymbol{v}} = \underset{n\times 1}{\boldsymbol{u}}$$

```
> A1 <- matrix(1:6,3)  # 3x2行列
> A1
     [,1] [,2]
[1,]    1    4
[2,]    2    5
[3,]    3    6
> A2 <- matrix(7:14,2)  # 2x4行列
> A2
     [,1] [,2] [,3] [,4]
[1,]    7    9   11   13
```



```
[2,]    8   10   12   14
> A1 %*% A2 -> A3  # 3x4行列
> A3
     [,1] [,2] [,3] [,4]
[1,]   39   49   59   69
[2,]   54   68   82   96
[3,]   69   87  105  123
> v1 <- 1:2  # 2次元ベクトル
> A1 %*% as.matrix(v1)  # 3x2行列  * 2x1行列 = 3x1行列
     [,1]
[1,]    9
[2,]   12
[3,]   15
> A1 %*% v1  # ベクトルは自動的に列ベクトルとみなされる
     [,1]
[1,]    9
[2,]   12
[3,]   15
> v2 <- 1:3
```

```
> as.matrix(v2) %*% A1  # 3x1行列 * 3x2行列  はエラー
Error in as.matrix(v2) %*% A1 : non-conformable arguments
> t(as.matrix(v2)) %*% A1  # 1x3行列 * 3x2行列 = 1x2行列
     [,1] [,2]
[1,]   14   32
> v2 %*% A1  # ベクトルは自動的に行ベクトルとみなされる
     [,1] [,2]
[1,]   14   32
> v2 %*% v2 # 自動的に1x3行列 * 3x1行列とみなされる
     [,1]
[1,]   14
> v2 * v2  # 成分毎に掛け算
[1] 1 4 9
> sum(v2 * v2) # sum()は要素の和を求める関数
[1] 14
> 1:8 * 1:2  # 成分毎に掛け算，短いほうは繰り返し用いられる
[1]  1  4  3  8  5 12  7 16
> rep(1:2,4) # 1:2を4回繰り返す
[1] 1 2 1 2 1 2 1 2
```

```
> 1:8 * rep(1:2,4) # = 1:8 * 1:2
[1]  1  4  3  8  5 12  7 16
> A2 * v1 # やはり成分毎に掛け算，v1は繰り返し用いられている．
     [,1] [,2] [,3] [,4]
[1,]    7    9   11   13
[2,]   16   20   24   28
```

特殊なベクトル，行列

$$\mathbf{1}_n = \begin{bmatrix} 1 \\ \cdot \\ \cdot \\ \cdot \\ 1 \end{bmatrix} \Bigg\} n$$

$$\boldsymbol{I}_n = \underbrace{\begin{bmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{bmatrix}}_{n} \Bigg\} n$$


```
> rep(1,5)  # 成分がすべて1の5次元ベクトル
[1] 1 1 1 1 1
> as.matrix(rep(1,5))  # 5x1行列
     [,1]
[1,]    1
[2,]    1
[3,]    1
[4,]    1
[5,]    1
> diag(5)  # 5x5単位行列
     [,1] [,2] [,3] [,4] [,5]
[1,]    1    0    0    0    0
[2,]    0    1    0    0    0
[3,]    0    0    1    0    0
[4,]    0    0    0    1    0
[5,]    0    0    0    0    1
```

対角行列と対角成分

```
> diag(1:5) # 1:5を対角成分とする5x5行列
     [,1] [,2] [,3] [,4] [,5]
[1,]    1    0    0    0    0
[2,]    0    2    0    0    0
[3,]    0    0    3    0    0
[4,]    0    0    0    4    0
[5,]    0    0    0    0    5
> diag(matrix(1:25,5))  # 対角成分の取り出し
[1]  1  7 13 19 25
```


内積と直交性

ベクトルの内積

$$\boldsymbol{a} = \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix}, \quad \boldsymbol{b} = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$$

$$\langle \boldsymbol{a}, \boldsymbol{b} \rangle = \boldsymbol{a}'\boldsymbol{b} = \sum_{i=1}^{n} a_i b_i$$

```
> naiseki <- function(a,b) sum(a*b)
> a <- 1:5
> b <- c(1,2,1,2,1)
> naiseki(a,b)
[1] 21
```


ベクトルの長さ

$$\boldsymbol{a} = \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix}$$

$$\|\boldsymbol{a}\| = \sqrt{\langle \boldsymbol{a}, \boldsymbol{a} \rangle} = \sqrt{\boldsymbol{a}'\boldsymbol{a}} = \left(\sum_{i=1}^{n} a_i a_i \right)^{-\frac{1}{2}}$$

```
> naiseki <- function(a,b=a) sum(a*b)
> naiseki(a,b)
[1] 21
> sqrt(naiseki(a,a))
[1] 7.416198
> sqrt(naiseki(a))
[1] 7.416198
```


ベクトル間の距離

$$\boldsymbol{a} = \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix}, \quad \boldsymbol{b} = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$$

$$d(\boldsymbol{a}, \boldsymbol{b}) = \|\boldsymbol{a} - \boldsymbol{b}\| = \left(\sum_{i=1}^{n} (a_i - b_i)^2 \right)^{-\frac{1}{2}}$$

```
> sqrt(naiseki(a-b))
[1] 4.898979
> (a-b)^2
[1]  0  0  4  4 16
> sqrt(sum((a-b)^2))
[1] 4.898979
```

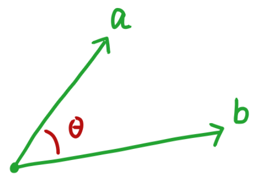
単位ベクトル

$$a = \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix}$$

$$u = \frac{a}{\|a\|}$$

```
> unitvec <- function(a) a/sqrt(sum(a*a))
> unitvec(a)
[1] 0.1348400 0.2696799 0.4045199 0.5393599 0.6741999
> naiseki(unitvec(a))
[1] 1
```


ベクトル間の角度



$$a = \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix}, \quad b = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$$

$$\cos\theta = \langle \frac{a}{\|a\|}, \frac{b}{\|b\|} \rangle = \frac{a'b}{\|a\|\|b\|} = \frac{\sum_{i=1}^n a_i b_i}{\sqrt{\sum_{i=1}^n a_i^2}\sqrt{\sum_{i=1}^n b_i^2}}$$


```
> unitvec(a)
[1] 0.1348400 0.2696799 0.4045199 0.5393599 0.6741999
> unitvec(b)
[1] 0.3015113 0.6030227 0.3015113 0.6030227 0.3015113
> naiseki(unitvec(a),unitvec(b))
[1] 0.8537714
> acos(naiseki(unitvec(a),unitvec(b)))  # ラジアン
[1] 0.5476098
> acos(naiseki(unitvec(a),unitvec(b))) * 180/pi  # 度
[1] 31.37573
```

平均，分散，共分散，相関

平均 $\bar{a} = \frac{1}{n}\sum a_i = \frac{1}{n}1_n' a$

分散 $s_a^2 = \frac{1}{n}\sum(a_i - \bar{a})^2 = \frac{1}{n}\|a - \bar{a}1_n\|^2$

共分散 $s_{ab} = \frac{1}{n}\sum(a_i - \bar{a})(b_i - \bar{b}) = \frac{1}{n}(a - \bar{a}1_n)'(b - \bar{b}1_n)$

相関 $r_{ab} = \frac{s_{ab}}{s_a s_b} = \frac{(a - \bar{a}1_n)'(b - \bar{b}1_n)}{\|a - \bar{a}1_n\|\|b - \bar{b}1_n\|}$

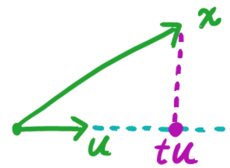
はじめに中心化 $a \leftarrow a - \bar{a}1_n$ **をすると**

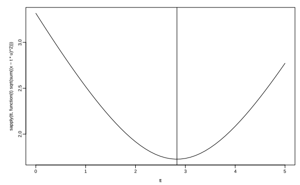
$$\bar{a} = 0, \quad s_a^2 = \frac{1}{n}\|a\|^2, \quad s_{ab} = \frac{1}{n}a'b, \quad r_{ab} = \frac{a'b}{\|a\|\|b\|}$$

c.f. 不偏分散や不偏共分散の分母はnの代わりに$n-1$を用いる

射影

単位ベクトルのつくる直線への射影





$$u = \begin{bmatrix} u_1 \\ \vdots \\ u_n \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

直線への射影： t**を自由に動かして**tu**が**x**へ最も近くなるようにする**

$$\|tu - x\|^2 = \|(tu - uu'x) + (uu'x - x)\|^2$$
$$= (t - u'x)^2 + x'(I_n - uu')x$$

この最小は$t = u'x$**のとき．**x**の**u**への射影は**

$$tu = (u'x)u = uu'x = Px$$

ただし $P = uu'$**は射影行列．なお**$\cos\theta = u'x/\|x\|$**とすれば，**

$$t = \|x\|\cos\theta$$

```
> u <- unitvec(1:5)  # 単位ベクトル
> x <- c(1,2,1,2,1)  # ベクトル
> naiseki(u,x)  # これがt
[1] 2.831639
> sum(u*x) # これでも同じ
[1] 2.831639
> tt <- seq(0,5,0.1) # 0..5
> psinit("20020922-1.eps")
> plot(tt,sapply(tt,function(t) sqrt(sum((x-t*u)^2))),type="l")
> abline(v=naiseki(u,x)) # 最小値をとるt
> dev.off()
> u*sum(u*x)  # xのu方向への射影
[1] 0.3818182 0.7636364 1.1454545 1.5272727 1.9090909
```

```
> naiseki(u,unitvec(x))  # cos(theta)
[1] 0.8537714
> acos(naiseki(u,unitvec(x))) * 180/pi  # 角度
[1] 31.37573
> P <- as.matrix(u) %*% t(as.matrix(u))  # 射影行列
> P
           [,1]       [,2]       [,3]       [,4]      [,5]
[1,] 0.01818182 0.03636364 0.05454545 0.07272727 0.0909091
[2,] 0.03636364 0.07272727 0.10909091 0.14545455 0.1818182
[3,] 0.05454545 0.10909091 0.16363636 0.21818182 0.2727273
[4,] 0.07272727 0.14545455 0.21818182 0.29090909 0.3636364
[5,] 0.09090909 0.18181818 0.27272727 0.36363636 0.4545455
> P %*% x  #  これも射影
          [,1]
[1,] 0.3818182
[2,] 0.7636364
[3,] 1.1454545
[4,] 1.5272727
[5,] 1.9090909
```

ベクトルのつくる直線への射影

$$a = \begin{bmatrix} a_1 \\ \vdots \\ a_n \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

直線への射影： β**を自由に動かして**βa**が**x**へ最も近くなるようにする**

$$u = \frac{a}{\|a\|}$$

とおけば，射影は$uu'x$**である．したがって**

$$\left(\frac{aa'}{\|a\|^2}\right)x = \left(\frac{a'x}{\|a\|^2}\right)a = \beta a$$

```
> a <- 1:5 # 射影方向
> x <- c(1,2,1,2,1)  # ベクトル
> shaei1 <- function(a,x) sum(a*x)/sum(a*a)
> shaei1(a,x)
[1] 0.3818182
> shaei1(a,x) * a
[1] 0.3818182 0.7636364 1.1454545 1.5272727 1.9090909
```

互いに直交する単位ベクトルの張る線形部分空間への射影

$$u_1 = \begin{bmatrix} u_{11} \\ \vdots \\ u_{n1} \end{bmatrix}, \dots, u_p = \begin{bmatrix} u_{1p} \\ \vdots \\ u_{np} \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

$$u_i' u_j = \delta_{ij} = \begin{cases} 1 & i = j \text{のとき} \\ 0 & i \neq j \text{のとき} \end{cases}$$

$$U = [u_1, \dots, u_p], \quad U'U = I_n$$

部分空間への射影： $t = [t_1, \dots, t_p]'$ **を自由に動かして**

$$Ut = t_1 u_1 + \cdots + t_p u_p$$

が x **へ最も近くなるようにする．**

$$\begin{aligned} \|Ut - x\|^2 =& \|(t_1 u_1 - u_1 u_1' x) + \cdots + (t_p u_p - u_p u_p' x) \\ &+ (u_1 u_1' x + \cdots + u_p u_p' x - x)\|^2 \\ =& (t_1 - u_1' x)^2 + \cdots + (t_p - u_p' x)^2 \\ &+ x'(I_n - UU')x \end{aligned}$$

この最小は $t_1 = u_1' x, \dots, t_p = u_p' x$ **のとき．まとめて** $t = U'x$ **とも書ける．** U **の張る空間への** x **の射影は**

$$Ut = UU'x = Px$$

ただし $P = UU'$ **は射影行列．** $Q = I_n - P$ **は直交補空間への射影行列．**

$$x = Px + Qx$$

と分解すると， $(Px)'(Qx) = 0$ **で直交している．**

$$P'Q = (UU')(I_n - UU') = UU' - UU'UU' = UU' - UU' = 0$$

```
> u1 <- unitvec(c(1,1,1,1))
> u2 <- unitvec(c(1,1,-1,-1))
> u3 <- unitvec(c(1,-1,1,-1))
> U <- cbind(u1,u2,u3)
> U
      u1   u2   u3
[1,] 0.5  0.5  0.5
[2,] 0.5  0.5 -0.5
[3,] 0.5 -0.5  0.5
[4,] 0.5 -0.5 -0.5
> t(U) %*% U  # 正規直交

    u1 u2 u3
  u1  1  0  0
  u2  0  1  0
  u3  0  0  1
> P <- U %*% t(U) # 射影行列
> P
```

```
      [,1]  [,2]  [,3]  [,4]
 [1,]  0.75  0.25  0.25 -0.25
 [2,]  0.25  0.75 -0.25  0.25
 [3,]  0.25 -0.25  0.75  0.25
 [4,] -0.25  0.25  0.25  0.75
> x <- c(1,2,2,2)  # ベクトル
> t(U) %*% x  # tの成分

    [,1]
 u1  3.5
 u2 -0.5
 u3 -0.5
> px <- P %*% x  # 射影
> px

     [,1]
 [1,] 1.25
 [2,] 1.75
 [3,] 1.75
```

```
 [4,] 2.25
> Q <- diag(4) - P # 直交補空間への射影行列
> Q

      [,1]  [,2]  [,3]  [,4]
 [1,]  0.25 -0.25 -0.25  0.25
 [2,] -0.25  0.25  0.25 -0.25
 [3,] -0.25  0.25  0.25 -0.25
 [4,]  0.25 -0.25 -0.25  0.25
> qx <- Q %*% x  # 直交補空間への射影
> qx

      [,1]
 [1,] -0.25
 [2,]  0.25
 [3,]  0.25
 [4,] -0.25
> x - px  # これでも同じ
```

```
      [,1]
 [1,] -0.25
 [2,]  0.25
 [3,]  0.25
 [4,] -0.25
> naiseki(px,qx)  # pxとqxは直交
[1] 0
> t(P) %*% Q  # PとQの張る空間は直交している

     [,1] [,2] [,3] [,4]
 [1,]    0    0    0    0
 [2,]    0    0    0    0
 [3,]    0    0    0    0
 [4,]    0    0    0    0
```

直交変換

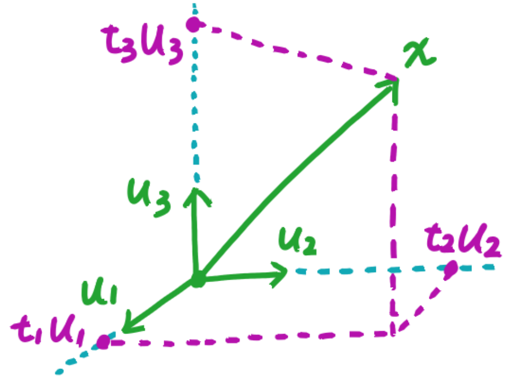
$$u_1 = \begin{bmatrix} u_{11} \\ \vdots \\ u_{n1} \end{bmatrix}, \dots, u_n = \begin{bmatrix} u_{1n} \\ \vdots \\ u_{nn} \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

$$U = [u_1, \dots, u_n], \quad U'U = UU' = I_n$$

$$x = Ut = t_1 u_1 + \cdots + t_n u_n$$

$$t = U'x, \quad t_i = u_i' x$$

$$\begin{aligned} I_n &= u_1 u_1' + \cdots + u_n u_n' \\ &= (u_1 u_1' + \cdots + u_p u_p') + (u_{p+1} u_{p+1}' + \cdots + u_n u_n') \\ &= P + Q \end{aligned}$$




```
> u1 <- unitvec(c(1,1,1,1))
> u2 <- unitvec(c(1,1,-1,-1))
> u3 <- unitvec(c(1,-1,1,-1))
> u4 <- unitvec(c(1,-1,-1,1))
> U <- cbind(u1,u2,u3,u4)
> U
      u1   u2   u3   u4
[1,] 0.5  0.5  0.5  0.5
[2,] 0.5  0.5 -0.5 -0.5
[3,] 0.5 -0.5  0.5 -0.5
[4,] 0.5 -0.5 -0.5  0.5
> t(U) %*% U

    u1 u2 u3 u4
  u1  1  0  0  0
  u2  0  1  0  0
  u3  0  0  1  0
  u4  0  0  0  1
> U %*% t(U)
```

```
      [,1] [,2] [,3] [,4]
 [1,]    1    0    0    0
 [2,]    0    1    0    0
 [3,]    0    0    1    0
 [4,]    0    0    0    1
> x <- c(1,2,2,2)  # ベクトル
> t(U) %*% x

    [,1]
 u1  3.5
 u2 -0.5
 u3 -0.5
 u4 -0.5
> U %*% (t(U) %*% x)

      [,1]
 [1,]    1
 [2,]    2
 [3,]    2
 [4,]    2
> U[,1:3]
      u1   u2   u3
[1,] 0.5  0.5  0.5
[2,] 0.5  0.5 -0.5
[3,] 0.5 -0.5  0.5
[4,] 0.5 -0.5 -0.5
> U[,4,drop=F]
       u4
[1,]  0.5
[2,] -0.5
[3,] -0.5
[4,]  0.5
> P <- U[,1:3] %*% t(U[,1:3])
> P

       [,1]  [,2]  [,3]  [,4]
 [1,]  0.75  0.25  0.25 -0.25
 [2,]  0.25  0.75 -0.25  0.25
 [3,]  0.25 -0.25  0.75  0.25
 [4,] -0.25  0.25  0.25  0.75
> Q <- U[,4,drop=F] %*% t(U[,4,drop=F])
> Q

       [,1]  [,2]  [,3]  [,4]
 [1,]  0.25 -0.25 -0.25  0.25
 [2,] -0.25  0.25  0.25 -0.25
 [3,] -0.25  0.25  0.25 -0.25
 [4,]  0.25 -0.25 -0.25  0.25
> P + Q

      [,1] [,2] [,3] [,4]
 [1,]    1    0    0    0
 [2,]    0    1    0    0
 [3,]    0    0    1    0
 [4,]    0    0    0    1
```

一次独立なベクトルの張る空間への射影

$$a_1 = \begin{bmatrix} a_{11} \\ \vdots \\ a_{n1} \end{bmatrix}, \dots, a_p = \begin{bmatrix} a_{1p} \\ \vdots \\ a_{np} \end{bmatrix}, \quad x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, \quad \beta = \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_p \end{bmatrix}$$

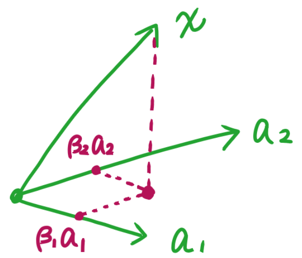
$$A = [a_1, \dots, a_p], \quad P = A(A'A)^{-1}A', \quad PA = A$$

$$\begin{aligned} \|A\beta - x\|^2 &= \|(A\beta - Px) + (Px - x)\|^2 \\ &= \|A\beta - Px\|^2 + \|Px - x\|^2 \\ &= \|A(\beta - (A'A)^{-1}A'x)\|^2 + x'(I_n - P)x \end{aligned}$$

を最小にするには

$$\beta = (A'A)^{-1}A'x, \quad A\beta = Px$$

$P^2 = P$なので$P(I_n - P) = 0$にも注意．つまり$(Px)'(x - Px) = 0$




```
> a1 <- c(1,1,1,1)
> a2 <- c(1,2,3,4)
> A <- cbind(a1,a2)
> A
     a1 a2
[1,]  1  1
[2,]  1  2
[3,]  1  3
[4,]  1  4
> B <- solve(t(A) %*% A) %*% t(A)  # solve() は逆行列
> B

    [,1] [,2]         [,3] [,4]
 a1  1.0  0.5 3.885781e-16 -0.5
 a2 -0.3 -0.1 1.000000e-01  0.3
> x <- c(1,2,2,2)  # ベクトル
> B %*% x  # beta

    [,1]
 a1  1.0
 a2  0.3
> A %*% (B %*% x)  # 射影

      [,1]
 [1,]  1.3
 [2,]  1.6
 [3,]  1.9
 [4,]  2.2
> P <- A %*% B  # 射影行列
> P

      [,1] [,2] [,3] [,4]
 [1,]  0.7  0.4  0.1 -0.2
 [2,]  0.4  0.3  0.2  0.1
 [3,]  0.1  0.2  0.3  0.4
 [4,] -0.2  0.1  0.4  0.7
> P %*% A  # = Aのハズ

     a1 a2
 [1,]  1  1
 [2,]  1  2
 [3,]  1  3
 [4,]  1  4
> P %*% x  #  射影

      [,1]
 [1,]  1.3
 [2,]  1.6
 [3,]  1.9
 [4,]  2.2
> P %*% P

      [,1] [,2] [,3] [,4]
 [1,]  0.7  0.4  0.1 -0.2
 [2,]  0.4  0.3  0.2  0.1
 [3,]  0.1  0.2  0.3  0.4
 [4,] -0.2  0.1  0.4  0.7
> Q <- diag(4) - P
> t(P) %*% Q

              [,1]         [,2]          [,3]          [,4]
 [1,] 1.409988e-15 5.662026e-16 -2.053953e-16 -9.769949e-16
 [2,] 8.437651e-16 3.996818e-16 -1.109613e-17 -4.218868e-16
 [3,] 2.942050e-16 2.109485e-16  1.776465e-16  1.443276e-16
 [4,] -2.553432e-16 2.219904e-17  3.663790e-16  7.105454e-16
> round(t(P) %*% Q,6)

      [,1] [,2] [,3] [,4]
 [1,]    0    0    0    0
 [2,]    0    0    0    0
 [3,]    0    0    0    0
 [4,]    0    0    0    0
> t(P %*% x) %*% (x - P %*% x)

             [,1]
 [1,] 8.704138e-15
> shaei2 <- function(A,x) solve(t(A) %*% A) %*% t(A) %*% x
> shaei2(A,x)

    [,1]
 a1  1.0
 a2  0.3
> A %*% shaei2(A,x)
```

```
      [,1]
[1,]  1.3
[2,]  1.6
[3,]  1.9
[4,]  2.2
> a <- as.matrix(1:5) # 射影方向
> x <- c(1,2,1,2,1)  # ベクトル
> shaei2(a,x)  # 以前にやったshaei1(a,x)と比べよ
          [,1]
[1,] 0.3818182
> a %*% shaei2(a,x)
          [,1]
[1,] 0.3818182
[2,] 0.7636364
[3,] 1.1454545
[4,] 1.5272727
[5,] 1.9090909
```

行列の分解

特異値分解

$$\boldsymbol{A} = \underbrace{\begin{bmatrix} a_{11} & \dots & a_{1p} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ a_{n1} & \dots & a_{np} \end{bmatrix}}_{p} \Bigg\} n\,, \quad n \geq p$$

$$\boldsymbol{U} = \underset{n \times p}{[\boldsymbol{u}_1, \dots, \boldsymbol{u}_p]}\,, \quad \boldsymbol{V} = \underset{p \times p}{[\boldsymbol{v}_1, \dots, \boldsymbol{v}_p]}$$

$$\boldsymbol{U}'\boldsymbol{U} = \boldsymbol{V}'\boldsymbol{V} = \boldsymbol{I}_p$$

$$\boldsymbol{A} = d_1 \boldsymbol{u}_1 \boldsymbol{v}_1' + \dots + d_p \boldsymbol{u}_p \boldsymbol{v}_p'$$

$$d_1 \geq \dots \geq d_p \geq 0$$

特異値$d_1, \dots, d_p$を対角成分にもつ行列Dを使うと

$$\boldsymbol{D} = \begin{bmatrix} d_1 & & 0 \\ & \ddots & \\ 0 & & d_p \end{bmatrix}, \quad \boldsymbol{A} = \boldsymbol{U}\boldsymbol{D}\boldsymbol{V}'$$

特異値のうち0でないものの個数rが行列Aのランク（階数）である．

$$d_1 \geq \dots \geq d_r > d_{r+1} = \dots = d_p = 0$$

$$\begin{aligned} \boldsymbol{A} &= d_1 \boldsymbol{u}_1 \boldsymbol{v}_1' + \dots + d_r \boldsymbol{u}_r \boldsymbol{v}_r' \\ &= [\boldsymbol{u}_1, \dots, \boldsymbol{u}_r] \mathrm{diag}(d_1, \dots, d_r) [\boldsymbol{v}_1, \dots, \boldsymbol{v}_r]' \end{aligned}$$

```
> A <- matrix(1:15,5)  # 5x3行列
> A
     [,1] [,2] [,3]
[1,]    1    6   11
[2,]    2    7   12
[3,]    3    8   13
[4,]    4    9   14
[5,]    5   10   15
> s <- svd(A)  # 特異値分解
> s
$d
[1] 35.127223  2.465397  0.000000

$u
           [,1]        [,2]       [,3]
[1,] -0.3545571 -0.68868664  0.3656475
[2,] -0.3986964 -0.37555453 -0.3101123
[3,] -0.4428357 -0.06242242  0.0736526
[4,] -0.4869750  0.25070970 -0.6795585
[5,] -0.5311143  0.56384181  0.5503706

$v
           [,1]       [,2]       [,3]
[1,] -0.2016649  0.8903171  0.4082483
[2,] -0.5168305  0.2573316 -0.8164966
[3,] -0.8319961 -0.3756539  0.4082483
> round(t(s$u) %*% s$u,10) # U'U = I
     [,1] [,2] [,3]
[1,]    1    0    0
[2,]    0    1    0
[3,]    0    0    1
> round(t(s$v) %*% s$v,10)  # V'V = I
     [,1] [,2] [,3]
[1,]    1    0    0
[2,]    0    1    0
[3,]    0    0    1
> s$u %*% diag(s$d) %*% t(s$v) # A = U D V'
     [,1] [,2] [,3]
[1,]    1    6   11
[2,]    2    7   12
[3,]    3    8   13
[4,]    4    9   14
[5,]    5   10   15
> s$u[,1:2] %*% diag(s$d[1:2]) %*% t(s$v[,1:2])  # r=2個だけ正の特異値
     [,1] [,2] [,3]
[1,]    1    6   11
[2,]    2    7   12
[3,]    3    8   13
[4,]    4    9   14
[5,]    5   10   15
```

スペクトル分解

$$\begin{aligned} \boldsymbol{G} &= \boldsymbol{U}\boldsymbol{D}\boldsymbol{U}' \\ &= d_1 \boldsymbol{u}_1 \boldsymbol{u}_1' + \dots + d_n \boldsymbol{u}_n \boldsymbol{u}_n' \end{aligned}$$

すべて$n \times n$行列．Gは対称行列，Uは直交行列，Dは対角行列．

$$\boldsymbol{G}\boldsymbol{u}_i = d_i \boldsymbol{u}_i$$

なので$\boldsymbol{u}_1, \dots, \boldsymbol{u}_n$は$G$の固有ベクトル，$d_1, \dots, d_n$は固有値．

```
> A <- matrix(rnorm(16),4)  # 乱数をつかって行列を生成
> G <- A + t(A)  # 対称行列
> G
           [,1]       [,2]       [,3]       [,4]
[1,]  1.0199805 -1.6726827  1.7611183 -0.8899458
[2,] -1.6726827  2.7472534  0.8150037 -1.5039038
[3,]  1.7611183  0.8150037 -1.4539209 -0.5922849
[4,] -0.8899458 -1.5039038 -0.5922849 -2.1581990
```



```
> e <- eigen(G,sym=T)  # 対称行列の固有値，固有ベクトル
> e
$values
[1]  3.890266  1.946350 -2.498974 -3.182528

$vectors
             [,1]       [,2]        [,3]       [,4]
[1,]  0.464939132  0.7167020  0.23912371  0.4615081
[2,] -0.872833764  0.3248162  0.02187801  0.3635615
[3,]  0.003675264  0.5096684 -0.76134993 -0.4007130
[4,]  0.148254229 -0.3479523 -0.60223541  0.7030380

> t(e$vec) %*% e$vec  # 直交行列
              [,1]          [,2]          [,3]          [,4]
[1,]  1.000000e+00  2.822822e-16 -1.313172e-16  1.542074e-16
[2,]  2.822822e-16  1.000000e+00 -1.367450e-16  2.432679e-17
[3,] -1.313172e-16 -1.367450e-16  1.000000e+00 -7.887571e-18
[4,]  1.542074e-16  2.432679e-17 -7.887571e-18  1.000000e+00
> e$vec %*% diag(e$val) %*% t(e$vec) # スペクトル分解
```

```
          [,1]       [,2]       [,3]       [,4]
[1,]  1.0199805 -1.6726827  1.7611183 -0.8899458
[2,] -1.6726827  2.7472534  0.8150037 -1.5039038
[3,]  1.7611183  0.8150037 -1.4539209 -0.5922849
[4,] -0.8899458 -1.5039038 -0.5922849 -2.1581990
> naiseki(e$vec %*% diag(e$val) %*% t(e$vec) - G) # Gに等しい
[1] 9.01027e-30
> s <- svd(G)  # 特異値分解でも同じ  （ただしベクトルの符号に注意）
> s
$d
[1] 3.890266 3.182528 2.498974 1.946350

$u
            [,1]       [,2]        [,3]       [,4]
[1,]  0.464939132 -0.4615081 -0.23912371  0.7167020
[2,] -0.872833764 -0.3635615 -0.02187801  0.3248162
[3,]  0.003675264  0.4007130  0.76134993  0.5096684
[4,]  0.148254229 -0.7030380  0.60223541 -0.3479523
```

```
$v
            [,1]       [,2]        [,3]       [,4]
[1,]  0.464939132  0.4615081  0.23912371  0.7167020
[2,] -0.872833764  0.3635615  0.02187801  0.3248162
[3,]  0.003675264 -0.4007130 -0.76134993  0.5096684
[4,]  0.148254229  0.7030380 -0.60223541 -0.3479523

> naiseki(s$u[,1] - s$v[,1])  # u1 =  v1
[1] 6.480773e-32
> naiseki(s$u[,2] + s$v[,2])  # u2 = -v2
[1] 6.594384e-31
> naiseki(s$u[,3] + s$v[,3])  # u3 = -v3
[1] 4.632945e-31
> naiseki(s$u[,4] - s$v[,4])  # u4 =  v4
[1] 6.779273e-31
> e$vec # 特異値分解のU,Vと比べよ
            [,1]       [,2]        [,3]       [,4]
[1,]  0.464939132  0.7167020  0.23912371  0.4615081
[2,] -0.872833764  0.3248162  0.02187801  0.3635615
```

```
[3,]  0.003675264  0.5096684 -0.76134993 -0.4007130
[4,]  0.148254229 -0.3479523 -0.60223541  0.7030380
> naiseki(s$u[,1] - e$vec[,1]) # u1 =  vec1
[1] 5.502171e-31
> naiseki(s$u[,2] + e$vec[,4]) # u2 = -vec4
[1] 2.249486e-31
> naiseki(s$u[,3] + e$vec[,3]) # u3 = -vec3
[1] 2.690524e-31
> naiseki(s$u[,4] - e$vec[,2]) # u4 =  vec2
[1] 5.793197e-31
```

平方根分解

対称行列Gの固有値がすべて非負のとき，Gの平方根分解は

$$G = BB'$$

任意の直交行列Vを用いてBVも平方根分解

$$G = (BV)(BV)'$$

である．Gのスペクトル分解

$$G = UDU' = d_1 u_1 u_1' + \cdots + d_n u_n u_n'$$

よりBとして

$$G^{1/2} = U\mathrm{diag}(\sqrt{d_1}, \ldots, \sqrt{d_n})U' = \sqrt{d_1} u_1 u_1' + \cdots + \sqrt{d_n} u_n u_n'$$

を選べる．


```
> A <- matrix(1:8,4)
> A
     [,1] [,2]
[1,]    1    5
[2,]    2    6
[3,]    3    7
[4,]    4    8
> G <- t(A) %*% A  # 非負定行列
> G
     [,1] [,2]
[1,]   30   70
[2,]   70  174
> e <- eigen(G)
> e
$values
[1] 202.419122   1.580878

$vectors
          [,1]       [,2]
```

```
[1,] 0.3761682  0.9265514
[2,] 0.9265514 -0.3761682

> B <- e$vec %*% diag(sqrt(e$val)) %*% t(e$vec) # 平方根
> B
         [,1]     [,2]
[1,] 3.092629  4.52058
[2,] 4.520580 12.39211
> B %*% t(B)  # 平方根分解
     [,1] [,2]
[1,]   30   70
[2,]   70  174
```

QR分解

$$\underset{n\times p}{A} = \underset{n\times p}{Q}\ \underset{p\times p}{R}$$

$$Q'Q = I_p, \quad R\text{は上三角行列}$$

```
> A <- matrix(1:8,4)
> A
     [,1] [,2]
[1,]    1    5
[2,]    2    6
[3,]    3    7
[4,]    4    8
> q <- qr(A)
> Q <- qr.Q(q)
> Q
           [,1]          [,2]
```



```
[1,] -0.1825742 -8.164966e-01
[2,] -0.3651484 -4.082483e-01
[3,] -0.5477226 -6.163689e-17
[4,] -0.7302967  4.082483e-01
> t(Q) %*% Q
              [,1]          [,2]
[1,]  1.000000e-00 -6.776264e-18
[2,] -6.776264e-18  1.000000e-00
> R <- qr.R(q)
> R
          [,1]       [,2]
[1,] -5.477226 -12.780193
[2,]  0.000000  -3.265986
> Q %*% R
     [,1] [,2]
[1,]    1    5
[2,]    2    6
[3,]    3    7
[4,]    4    8
```

直交化とQR分解

$$A = [a_1, \ldots, a_p], \quad Q = [q_1, \ldots, q_p]$$

グラムシュミットの直交化

$$b_i = a_i - \sum_{j=1}^{i-1} q_j q_j' a_i, \quad q_i = \frac{b_i}{\|b_i\|};$$

$$a_i = \sum_{j=1}^{i} q_j r_{ji}, \quad A = QR$$

$$q_k' b_i = q_k' a_i - \sum_{j=1}^{i-1} (q_k' q_j)(q_j' a_i) = 0,\ k < i$$

$$Q'Q = I_{p+1}$$

実際にはハウスホルダー法で求めることが多い

コレスキー分解

$$G = R'R$$

Gは$n \times n$対称行列で固有値がすべて非負，Rは上三角行列．

```
> G <- t(A) %*% A
> G
     [,1] [,2]
[1,]   30   70
[2,]   70  174
> R <- chol(G)
> R
         [,1]      [,2]
[1,] 5.477226 12.780193
[2,] 0.000000  3.265986
> t(R) %*% R
     [,1] [,2]
[1,]   30   70
[2,]   70  174
```


一般逆行列と射影

一般逆行列

$$AA^{+}A = A$$

とくにムーア＝ペンローズ逆行列は特異値分解を用いて次のように書ける

$$A = UDV', \quad A^{+} = VD^{+}U'$$

$$d_1 \geq \cdots \geq d_r > d_{r+1} = \cdots = d_p = 0$$

$$D = \mathrm{diag}(d_1, \ldots, d_r, 0, \ldots, 0)$$

$$D^{+} = \mathrm{diag}(1/d_1, \ldots, 1/d_r, 0, \ldots, 0)$$

$$DD^{+} = D^{+}D = \mathrm{diag}(1, \ldots, 1, 0, \ldots, 0)$$

$$AA^{+} = UDD^{+}U' = u_1u_1' + \cdots + u_ru_r'$$

$$A^{+}A = VD^{+}DV' = v_1v_1' + \cdots + v_rv_r'$$


```
> A <- matrix(1:15,5)  # 5x3行列
> s <- svd(A) # 特異値分解
> s$d #  特異値
[1] 35.127223  2.465397  0.000000
> ginvd <- function(d,tol=1e-7) {  # D+を求める関数
+   a <- d>tol
+   d[a] <- 1/d[a]
+   d[!a] <- 0
+   d
+ }
> ginvd(s$d)
[1] 0.02846795 0.40561424 0.00000000
> B <- s$v %*% diag(ginvd(s$d)) %*% t(s$u)  # Aの一般逆行列
> B
            [,1]        [,2]          [,3]        [,4]        [,5]
[1,] -0.24666667 -0.13333333 -2.000000e-02  0.09333333  0.20666667
[2,] -0.06666667 -0.03333333 -1.013136e-17  0.03333333  0.06666667
[3,]  0.11333333  0.06666667  2.000000e-02 -0.02666667 -0.07333333
> ginva <- function(A) {
+    s <- svd(A)
+    s$v %*% diag(ginvd(s$d)) %*% t(s$u)
+ }
> ginva(A)
            [,1]        [,2]          [,3]        [,4]        [,5]
[1,] -0.24666667 -0.13333333 -2.000000e-02  0.09333333  0.20666667
[2,] -0.06666667 -0.03333333 -1.013136e-17  0.03333333  0.06666667
[3,]  0.11333333  0.06666667  2.000000e-02 -0.02666667 -0.07333333
> A %*% B %*% A  # Aに等しい
     [,1] [,2] [,3]
[1,]    1    6   11
[2,]    2    7   12
[3,]    3    8   13
[4,]    4    9   14
[5,]    5   10   15
> round(A %*% B,10)  # Aの張る空間への射影行列
     [,1] [,2] [,3] [,4] [,5]
[1,]  0.6  0.4  0.2  0.0 -0.2
[2,]  0.4  0.3  0.2  0.1  0.0
[3,]  0.2  0.2  0.2  0.2  0.2
[4,]  0.0  0.1  0.2  0.3  0.4
[5,] -0.2  0.0  0.2  0.4  0.6
> round(B %*% A,10)  # A'の張る空間への射影行列
          [,1]      [,2]       [,3]
[1,]  0.8333333 0.3333333 -0.1666667
[2,]  0.3333333 0.3333333  0.3333333
[3,] -0.1666667 0.3333333  0.8333333
```

一般逆行列（$r = p$の場合）

$$(A'A)^{-1}A' = (VD^2V')^{-1}VDU'$$
$$= VD^{-2}DU' = VD^{-1}U'$$
$$= A^{+}$$

$$AA^{+} = A(A'A)^{-1}A', \quad A^{+}A = I_p$$

$$\beta = A^{+}x, \quad P = AA^{+}$$

```
> a1 <- c(1,1,1,1)
> a2 <- c(1,2,3,4)
> A <- cbind(a1,a2)
> A
     a1 a2
[1,]  1  1
[2,]  1  2
[3,]  1  3
[4,]  1  4
> round(solve(t(A) %*% A) %*% t(A),10)

     [,1] [,2] [,3] [,4]
  a1  1.0  0.5  0.0 -0.5
  a2 -0.3 -0.1  0.1  0.3
> round(ginva(A),10)
     [,1] [,2] [,3] [,4]
[1,]  1.0  0.5  0.0 -0.5
[2,] -0.3 -0.1  0.1  0.3
> round(ginva(A) %*% A,10)

       a1 a2
  [1,]  1  0
  [2,]  0  1
> round(A %*% ginva(A),10)
     [,1] [,2] [,3] [,4]
  [1,]  0.7  0.4  0.1 -0.2
  [2,]  0.4  0.3  0.2  0.1
  [3,]  0.1  0.2  0.3  0.4
  [4,] -0.2  0.1  0.4  0.7
```

第３回 課題

1．一般逆行列 A^+ を計算する関数`geninv`を作れ．ただし，最大特異値との比が`tol`(デフォルト値 10^{-7}) 以下の特異値はゼロとみなす．

```
geninv <- function(A,tol=1e-7) {
ここでAの一般逆行列を計算
}
```

2．次の二つの行列について一般逆行列を計算し，数値計算の誤差を除いて $AA^+A - A = 0$ となることを確かめよ．

```
A1 <- matrix(1:15,5)
A2 <- matrix(rnorm(15),5)
```

3．上記の二つの行列について A^+A を計算し，もし単位行列でない場合はその理由を述べよ．