12.
Matrix factorization theorem (spectral decomposition)

Twierdzenie 1 *Each positive definite and symmetrical matrix* $\mathbf{M}$ *can be expressed in the form*

$$\mathbf{M} = \mathbf{P}\mathbf{P}^T$$

where $\mathbf{P}$ *is nonsingular matrix (called "root of* $\mathbf{M}$*").*

Proof

let

$$\begin{aligned} w_i \text{ – eigenvalues of } M, \qquad i &= 1, 2, ..., s \\ \lambda_i \text{ – eigenvectors of } M, \qquad i &= 1, 2, ..., s \end{aligned}$$

obviously

$$Mw_i = \lambda_i w_i$$

introducing

$$W = [w_1, w_2, ..., w_s] \text{ and } \Lambda = diag(\lambda_i) = \begin{bmatrix} \lambda_1 & 0 & .. & 0 \\ 0 & \lambda_2 & 0 & .. \\ .. & 0 & .. & 0 \\ 0 & .. & 0 & \lambda_s \end{bmatrix}$$

since M is symmetrical

$$\begin{aligned} &\lambda_i \text{ – real} \\ &w_i \text{ – mutually orthogonal} \end{aligned}$$

and since $M > 0$

$$\lambda_i > 0 \text{ for each } i = 1, 2, ..., s$$

conclusion

$$\begin{aligned} W &\text{ – orthogonal} \\ W^T W &= I \Longrightarrow W^{-1} = W^T \end{aligned}$$

hence

$$\begin{aligned} MW &= W\Lambda \\ M &= W\Lambda W^{-1} = W\Lambda W^T \text{ (spectral decomposition)} \end{aligned}$$

introducing

$$\Lambda = \Lambda^{1/2}\Lambda^{1/2}, \text{ where } \Lambda^{1/2} = diag(\sqrt{\lambda_i}) = \begin{bmatrix} \sqrt{\lambda_1} & 0 & .. & 0 \\ 0 & \sqrt{\lambda_2} & 0 & .. \\ .. & 0 & .. & 0 \\ 0 & .. & 0 & \sqrt{\lambda_s} \end{bmatrix}$$

we get

$$W\Lambda W^T = W\Lambda^{1/2}\left(W\Lambda^{1/2}\right)^T$$

stąd

$$M = PP^T, \text{ where } P = W\Lambda^{1/2} \blacksquare$$

1. Cholesky LU decomposition

$$\begin{aligned} Ma &= b \\ M \text{ -- positive } (M &> 0), \text{ symmetrical } (M^T = M) \end{aligned}$$

Cholesky

$$M = LDL^T$$

where

$$\begin{aligned} L \text{ -- lower triangular matrix, i.e. for } i &< j \text{ it hold that } L[i,j] = 0 \\ D \text{ -- diagonal, } D &= diag(d_i),\ d_i > 0 \end{aligned}$$

hence

$$\begin{aligned} M &= LD^{1/2}D^{1/2}L^T \\ \text{where } D^{1/2} &= diag(\sqrt{d_i}) \end{aligned}$$

for

$$\overline{L} = LD^{1/2}$$

we get

$$\begin{aligned} M &= \overline{L}\overline{L}^T \\ & \overline{L} \text{ -- lower triangular} \\ & \overline{L}^T \text{ -- upper triangular} \\ \det M &= \det \overline{L}\overline{L}^T = \det \overline{L} \det \overline{L}^T > 0 \end{aligned}$$

Procedure

$$\overline{L}\overline{L}^T a = b$$

Stage 1.

for $\alpha = \overline{L}^T a$ solve "external" problem

$$\overline{L}\alpha = b$$

since $\det \overline{L} > 0$ diagonal elements of $\overline{L}$ are nonzero, the solution exists and is unique

Stage 2.

α_N – given (computed in Stage 1)

solve "internal" problem

$$\overline{L}^T a = \alpha_N$$

since $\det \overline{L}^T > 0$ ....

Advantages

1) reduced complexity

2) better accuracy

$$\begin{aligned} \det M &= \left(\det \overline{L}\right)^2 \\ \det \overline{L} &= \sqrt{\det M} \end{aligned}$$

hence for $0 < \det M < 1$

$$\det \overline{L} = \det \overline{L}^T > \det M$$

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2. Householder reflections

Definicja 1 *Macierzą odbicia Householdera nazywamy macierz postaci*

$$P = I - 2ww^T$$

gdzie $\|w\| = 1$*, tj.* $w^T w = 1$*.*

Interpretacja

$$Pw = (I - 2ww^T)w = w - 2ww^T w = w - 2w = -w$$

Własności:
(i) $P = P^T$ (symetria)
(ii) $P^T P = PP^T = I$ (ortogonalność)
(iii) dla każdego wektora x istnieje macierz P_j, taka że

$$P_j x = \pm \|x\| e_j, \text{ gdzie } e_j \text{ jest } j\text{-tym wersorem } e_j = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$$

(iiii) dla ciągu macierzy Householdera $P_1, P_2, ..., P_s$ przekształcenie złożenia

$$\Psi = P_s \cdot P_{s-1} \cdot ... \cdot P_2 \cdot P_1$$

jest macierzą ortogonalną, tj.

$$\Psi^T \Psi = I$$

Dowody

(i) oczywiste – różnica macierzy symetrycznych jest symetryczna

(ii)

$$PP^T = (I - 2ww^T)(I - 2ww^T) = I - 2ww^T - 2ww^T + 4ww^Tww^T = I - 4ww^T + 4ww^T = I$$

(iii)

$$\begin{aligned} & x \text{ – dowolny wektor} \\ u_j &= x \pm \|x\|\, e_j \\ P_j &= I - \frac{u_j u_j^T}{H_j}, \text{ gdzie } H_j = \frac{1}{2}\|u_j\|^2 = \frac{1}{2}u_j^T u_j \end{aligned}$$

macierz P_j jest macierzą Householdera, ponieważ

$$P_j = I - 2\frac{u_j}{\|u_j\|}\frac{u_j^T}{\|u_j\|} \text{ (wektory o długości 1)}$$

$$\begin{aligned} P_j x &= (I - \frac{u_j u_j^T}{H_j})x = x - u_j \frac{2u_j^T x}{u_j^T u_j} = x - u_j \frac{2(x \pm \|x\|\, e_j)^T x}{(x \pm \|x\|\, e_j)^T (x \pm \|x\|\, e_j)} = \\ &= \ldots = x - u_j = x - x \pm \|x\|\, e_j = \pm \|x\|\, e_j \end{aligned}$$

(iiii)

$$\Psi^T \Psi = P_1^T P_2^T \ldots P_{s-1}^T \underbrace{P_s^T P_s} P_{s-1} \ldots P_2 P_1 = I$$

Lemat 1 *Dla każdej macierzy $X_{N\times s}$ istnieje taki ciąg macierzy Householdera $\{\widetilde{P}_1, \widetilde{P}_2, ..., \widetilde{P}_s\}$, że przekształcenie*

$$\Psi = \widetilde{P}_s \widetilde{P}_{s-1}, ... \widetilde{P}_2 \widetilde{P}_1$$

ma własność

$$\Psi X_{N\times s} = \begin{bmatrix} R \\ 0 \end{bmatrix}$$

gdzie R jest macierzą trójkątną górną o rozmiarach $s \times s$.

Twierdzenie 2 *Oszacowanie NK jest równoważne rozwiązaniu układu równań*

$$Ra = \eta_R$$

gdzie η_R jest wektorem zawierającym s pierwszych elementów wektora ΨY_N.

Rozwiązanie tego układu równań istnieje i jest jednoznaczne. Pytanie dotyczy samego oszacowania NK.

Dowód

$$\begin{aligned}
Q(a) &= \|X_N a - Y_N\|_e^2 \rightarrow \min_a \\
Q(a) &= (X_N a - Y_N)^T (X_N a - Y_N) = \\
&= (X_N a - Y_N)^T \Psi^T \Psi (X_N a - Y_N) = \\
&= [\Psi(X_N a - Y_N)]^T [\Psi(X_N a - Y_N)] = \\
&= [\Psi X_N a - \Psi Y_N]^T [\Psi X_N a - \Psi Y_N] = \\
&= [\begin{bmatrix} R \\ 0 \end{bmatrix} a - \begin{bmatrix} \eta_R \\ \eta_z \end{bmatrix}]^T [\begin{bmatrix} R \\ 0 \end{bmatrix} a - \begin{bmatrix} \eta_R \\ \eta_z \end{bmatrix}] = \\
&= \begin{bmatrix} Ra - \eta_R \\ -\eta_z \end{bmatrix}^T \begin{bmatrix} Ra - \eta_R \\ -\eta_z \end{bmatrix} = (Ra - \eta_R)^T (Ra - \eta_R) + \eta_z^T \eta_z = \\
&= \|Ra - \eta_R\|_e^2 + \|\eta_z\|_e^2 \rightarrow \min_a
\end{aligned}$$

zatem

$$Q(a) \rightarrow \min_a \Rightarrow Ra = \eta_R$$