

$$\blacksquare \mathbf{A}\mathbf{V} = \mathbf{U}\mathbf{\Lambda}$$

$$\mathbf{A}'\mathbf{U} = \mathbf{V}\mathbf{\Lambda}$$

$$\blacksquare \mathbf{A}\mathbf{A}' = \mathbf{U}\mathbf{\Lambda}^2\mathbf{U}'$$

\Rightarrow squared singular values of \mathbf{A} are eigenvalues of $\mathbf{A}\mathbf{A}'$ and columns of \mathbf{U} are eigenvectors of $\mathbf{A}\mathbf{A}'$

$$\mathbf{A}'\mathbf{A} = \mathbf{V}\mathbf{\Lambda}^2\mathbf{V}'$$

\Rightarrow squared singular values of \mathbf{A} are eigenvalues of $\mathbf{A}'\mathbf{A}$ and columns of \mathbf{V} are eigenvectors of $\mathbf{A}'\mathbf{A}$

➤ quadratic form

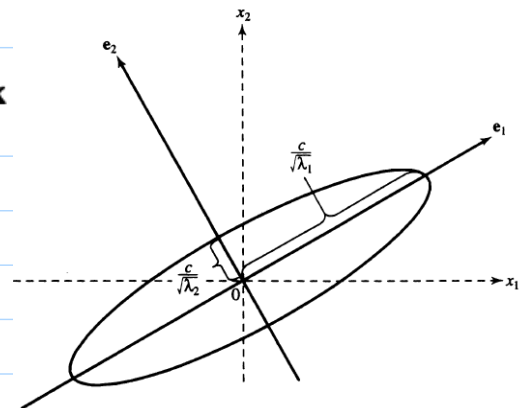
Definition 2A.32. A quadratic form $Q(\mathbf{x})$ in the k variables x_1, x_2, \dots, x_k is $Q(\mathbf{x}) = \mathbf{x}'\mathbf{A}\mathbf{x}$, where $\mathbf{x}' = [x_1, x_2, \dots, x_k]$ and \mathbf{A} is a $k \times k$ symmetric matrix.

$$\mathbf{x}'\mathbf{A}\mathbf{x}$$

$$= \mathbf{x}'(\lambda_1 \mathbf{e}_1 \mathbf{e}_1' + \lambda_2 \mathbf{e}_2 \mathbf{e}_2' + \dots + \lambda_k \mathbf{e}_k \mathbf{e}_k')$$

$$= \lambda_1 (\mathbf{x}'\mathbf{e}_1)(\mathbf{e}_1'\mathbf{x}) + \dots + \lambda_k (\mathbf{x}'\mathbf{e}_k)(\mathbf{e}_k'\mathbf{x})$$

$$= \lambda_1 (\mathbf{x}'\mathbf{e}_1)^2 + \dots + \lambda_p (\mathbf{x}'\mathbf{e}_p)^2$$



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➤ nonnegative definite and positive definite matrix

▪ When a $k \times k$ symmetric matrix \mathbf{A} is such that

$$0 \leq \mathbf{x}'\mathbf{A}\mathbf{x}$$

for all $\mathbf{x}' = [x_1, x_2, \dots, x_k]$, both the matrix \mathbf{A} and the quadratic form are said to be *nonnegative definite*.

▪ When a $k \times k$ symmetric matrix \mathbf{A} is such that

$$0 < \mathbf{x}'\mathbf{A}\mathbf{x}$$

for all vectors $\mathbf{x} \neq \mathbf{0}$, \mathbf{A} or the quadratic form is said to be *positive definite*.

▪ \mathbf{A} is a positive definite matrix if and only if every eigenvalue of \mathbf{A} is positive

\mathbf{A} is a nonnegative definite matrix if and only if all of its eigenvalues are greater than or equal to zero

▪ For nonnegative definite or positive definite matrix

$$\mathbf{x}'\mathbf{A}\mathbf{x} =$$

▪ statistical distance and positive definite matrix

$$(\text{distance})^2 = a_{11}x_1^2 + a_{22}x_2^2 + \dots + a_{pp}x_p^2$$

$$+ 2(a_{12}x_1x_2 + a_{13}x_1x_3 + \dots + a_{p-1,p}x_{p-1}x_p)$$

$$= [x_1, x_2, \dots, x_p] \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1p} \\ a_{21} & a_{22} & \dots & a_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ a_{p1} & a_{p2} & \dots & a_{pp} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_p \end{bmatrix} = \mathbf{x}'\mathbf{A}\mathbf{x}$$

\Rightarrow distance is determined from a positive definite quadratic form $\mathbf{x}'\mathbf{A}\mathbf{x}$.

Comment. Let the square of the distance from the point $\mathbf{x}' = [x_1, x_2, \dots, x_p]$ to the origin be given by $\mathbf{x}'\mathbf{A}\mathbf{x}$, where \mathbf{A} is a $p \times p$ symmetric positive definite matrix. Then the square of the distance from \mathbf{x} to an arbitrary fixed point $\boldsymbol{\mu}' = [\mu_1, \mu_2, \dots, \mu_p]$ is given by the general expression $(\mathbf{x} - \boldsymbol{\mu})'\mathbf{A}(\mathbf{x} - \boldsymbol{\mu})$.

If $p > 2$, the points $\mathbf{x}' = [x_1, x_2, \dots, x_p]$ a constant distance $c = \sqrt{\mathbf{x}'\mathbf{A}\mathbf{x}}$ from the origin lie on hyperellipsoids $c^2 = \lambda_1(\mathbf{x}'\mathbf{e}_1)^2 + \dots + \lambda_p(\mathbf{x}'\mathbf{e}_p)^2$, whose axes are given by the eigenvectors of \mathbf{A} . The half-length in the direction \mathbf{e}_i is equal to $c/\sqrt{\lambda_i}$, $i = 1, 2, \dots, p$, where $\lambda_1, \lambda_2, \dots, \lambda_p$ are the eigenvalues of \mathbf{A} .

• square-root matrix

➤ Recall: matrix representation of spectral decomposition

Let \mathbf{A} be a $k \times k$ positive definite matrix with the spectral decomposition $\mathbf{A} = \sum_{i=1}^k \lambda_i \mathbf{e}_i \mathbf{e}_i'$

Let the normalized eigenvectors be the columns of another matrix

$$\mathbf{P} = [\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_k]$$

Then

$$\mathbf{A} = \sum_{i=1}^k \lambda_i \mathbf{e}_i \mathbf{e}_i' = \mathbf{P} \boldsymbol{\Lambda} \mathbf{P}'$$

$(k \times k) \quad (k \times 1)(1 \times k) \quad (k \times k)(k \times k)(k \times k)$

where $\mathbf{P}\mathbf{P}' = \mathbf{P}'\mathbf{P} = \mathbf{I}$ and $\boldsymbol{\Lambda} = \begin{bmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_k \end{bmatrix}$ with $\lambda_i > 0$

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➤ inverse

$$\mathbf{A}^{-1} = \mathbf{P}\boldsymbol{\Lambda}^{-1}\mathbf{P}' = \sum_{i=1}^k \frac{1}{\lambda_i} \mathbf{e}_i \mathbf{e}_i'$$

➤ square-root matrix

$$\mathbf{A}^{1/2} = \sum_{i=1}^k \sqrt{\lambda_i} \mathbf{e}_i \mathbf{e}_i' = \mathbf{P}\boldsymbol{\Lambda}^{1/2}\mathbf{P}'$$

▪ some properties

1. $(\mathbf{A}^{1/2})' = \mathbf{A}^{1/2}$ (that is, $\mathbf{A}^{1/2}$ is symmetric).

2. $\mathbf{A}^{1/2}\mathbf{A}^{1/2} = \mathbf{A}$.

3. $(\mathbf{A}^{1/2})^{-1} = \sum_{i=1}^k \frac{1}{\sqrt{\lambda_i}} \mathbf{e}_i \mathbf{e}_i' = \mathbf{P}\boldsymbol{\Lambda}^{-1/2}\mathbf{P}'$, where $\boldsymbol{\Lambda}^{-1/2}$ is a diagonal matrix with $1/\sqrt{\lambda_i}$ as the i th diagonal element.

4. $\mathbf{A}^{1/2}\mathbf{A}^{-1/2} = \mathbf{A}^{-1/2}\mathbf{A}^{1/2} = \mathbf{I}$, and $\mathbf{A}^{-1/2}\mathbf{A}^{-1/2} = \mathbf{A}^{-1}$, where $\mathbf{A}^{-1/2} = (\mathbf{A}^{1/2})^{-1}$.

• matrix inequalities and maximization

➤ **Cauchy-Schwarz Inequality.** Let \mathbf{b} and \mathbf{d} be any two $p \times 1$ vectors. Then

$$(\mathbf{b}'\mathbf{d})^2 \leq (\mathbf{b}'\mathbf{b})(\mathbf{d}'\mathbf{d})$$

with equality if and only if $\mathbf{b} = c\mathbf{d}$ (or $\mathbf{d} = c\mathbf{b}$) for some constant c .

Extended Cauchy–Schwarz Inequality. Let \mathbf{b} and \mathbf{d} be any two vectors, and let \mathbf{B} be a positive definite matrix. Then

$$(\mathbf{b}'\mathbf{d})^2 \leq (\mathbf{b}'\mathbf{B}\mathbf{b})(\mathbf{d}'\mathbf{B}^{-1}\mathbf{d})$$

with equality if and only if $\mathbf{b} = c\mathbf{B}^{-1}\mathbf{d}$ (or $\mathbf{d} = c\mathbf{B}\mathbf{b}$) for some constant c .

- **Maximization Lemma.** Let \mathbf{B} be positive definite and \mathbf{d} be a given vector. Then, for an arbitrary nonzero vector \mathbf{x} ,

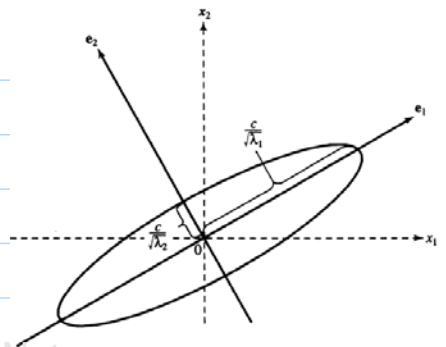
$$\max_{\mathbf{x} \neq \mathbf{0}} \frac{(\mathbf{x}'\mathbf{d})^2}{\mathbf{x}'\mathbf{B}\mathbf{x}} = \mathbf{d}'\mathbf{B}^{-1}\mathbf{d}$$

with the maximum attained when $\mathbf{x} = c\mathbf{B}^{-1}\mathbf{d}$ for any constant $c \neq 0$.

- **Maximization of Quadratic Forms for Points on the Unit Sphere.** Let \mathbf{B} be a positive definite matrix with eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p \geq 0$ and associated normalized eigenvectors $\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_p$. Then

$$\max_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}'\mathbf{B}\mathbf{x}}{\mathbf{x}'\mathbf{x}} = \lambda_1 \quad (\text{attained when } \mathbf{x} = \mathbf{e}_1)$$

$$\min_{\mathbf{x} \neq \mathbf{0}} \frac{\mathbf{x}'\mathbf{B}\mathbf{x}}{\mathbf{x}'\mathbf{x}} = \lambda_p \quad (\text{attained when } \mathbf{x} = \mathbf{e}_p)$$



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Moreover,

$$\max_{\mathbf{x} \perp \mathbf{e}_1, \dots, \mathbf{e}_k} \frac{\mathbf{x}'\mathbf{B}\mathbf{x}}{\mathbf{x}'\mathbf{x}} = \lambda_{k+1} \quad (\text{attained when } \mathbf{x} = \mathbf{e}_{k+1}, k = 1, 2, \dots, p-1)$$

where the symbol \perp is read “is perpendicular to.”

- approximation of a rectangular matrix by a lower-dimensional matrix

- sum of squared differences

$$\sum_{i=1}^m \sum_{j=1}^k (a_{ij} - b_{ij})^2 = \text{tr}[(\mathbf{A} - \mathbf{B})(\mathbf{A} - \mathbf{B})']$$

- **Result 2A.16.** Let \mathbf{A} be an $m \times k$ matrix of real numbers with $m \geq k$ and singular value decomposition $\mathbf{U}\mathbf{\Lambda}\mathbf{V}'$. Let $s < k = \text{rank}(\mathbf{A})$. Then

$$\mathbf{B} = \sum_{i=1}^s \lambda_i \mathbf{u}_i \mathbf{v}_i'$$

is the rank- s least squares approximation to \mathbf{A} . It minimizes

$$\text{tr}[(\mathbf{A} - \mathbf{B})(\mathbf{A} - \mathbf{B})']$$

over all $m \times k$ matrices \mathbf{B} having rank no greater than s . The minimum value, or

error of approximation, is $\sum_{i=s+1}^k \lambda_i^2$.

- sample mean, covariance, and correlation as matrix operation

- sample mean

$$\bar{\mathbf{x}} = \begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \\ \vdots \\ \bar{x}_p \end{bmatrix} = \begin{bmatrix} \frac{\mathbf{y}'_1 \mathbf{1}}{n} \\ \frac{\mathbf{y}'_2 \mathbf{1}}{n} \\ \vdots \\ \frac{\mathbf{y}'_p \mathbf{1}}{n} \end{bmatrix} = \frac{1}{n} \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{22} & \cdots & x_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{p1} & x_{p2} & \cdots & x_{pn} \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} = \frac{1}{n} \mathbf{X}' \mathbf{1}$$

- sample covariance matrix

$$\mathbf{1} \bar{\mathbf{x}}' = \frac{1}{n} \mathbf{1}' \mathbf{X} = \begin{bmatrix} \bar{x}_1 & \bar{x}_2 & \cdots & \bar{x}_p \\ \bar{x}_1 & \bar{x}_2 & \cdots & \bar{x}_p \\ \vdots & \vdots & \ddots & \vdots \\ \bar{x}_1 & \bar{x}_2 & \cdots & \bar{x}_p \end{bmatrix}$$

$$\mathbf{X} - \frac{1}{n} \mathbf{1}' \mathbf{X} = \begin{bmatrix} x_{11} - \bar{x}_1 & x_{12} - \bar{x}_2 & \cdots & x_{1p} - \bar{x}_p \\ x_{21} - \bar{x}_1 & x_{22} - \bar{x}_2 & \cdots & x_{2p} - \bar{x}_p \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} - \bar{x}_1 & x_{n2} - \bar{x}_2 & \cdots & x_{np} - \bar{x}_p \end{bmatrix}$$

$$n \mathbf{S}_n = \left(\mathbf{X} - \frac{1}{n} \mathbf{1}' \mathbf{X} \right)' \left(\mathbf{X} - \frac{1}{n} \mathbf{1}' \mathbf{X} \right) = \mathbf{X}' \left(\mathbf{I} - \frac{1}{n} \mathbf{1}' \mathbf{1} \right) \mathbf{X}$$

$$\text{since } \left(\mathbf{I} - \frac{1}{n} \mathbf{1}' \mathbf{1} \right)' \left(\mathbf{I} - \frac{1}{n} \mathbf{1}' \mathbf{1} \right) = \mathbf{I} - \frac{1}{n} \mathbf{1}' \mathbf{1} - \frac{1}{n} \mathbf{1}' \mathbf{1} + \frac{1}{n^2} \mathbf{1}' \mathbf{1}' \mathbf{1} \mathbf{1}' = \mathbf{I} - \frac{1}{n} \mathbf{1}' \mathbf{1}$$

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- sample correlation matrix

$$\mathbf{D}^{1/2}_{(p \times p)} = \begin{bmatrix} \sqrt{s_{11}} & 0 & \cdots & 0 \\ 0 & \sqrt{s_{22}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \sqrt{s_{pp}} \end{bmatrix} \quad \mathbf{D}^{-1/2}_{(p \times p)} = \begin{bmatrix} \frac{1}{\sqrt{s_{11}}} & 0 & \cdots & 0 \\ 0 & \frac{1}{\sqrt{s_{22}}} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{\sqrt{s_{pp}}} \end{bmatrix}$$

Since

$$\mathbf{S}_n = \begin{bmatrix} s_{11} & s_{12} & \cdots & s_{1p} \\ \vdots & \vdots & \ddots & \vdots \\ s_{1p} & s_{2p} & \cdots & s_{pp} \end{bmatrix}$$

$$\mathbf{R} = \begin{bmatrix} \frac{s_{11}}{\sqrt{s_{11}} \sqrt{s_{11}}} & \frac{s_{12}}{\sqrt{s_{11}} \sqrt{s_{22}}} & \cdots & \frac{s_{1p}}{\sqrt{s_{11}} \sqrt{s_{pp}}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{s_{1p}}{\sqrt{s_{11}} \sqrt{s_{pp}}} & \frac{s_{2p}}{\sqrt{s_{22}} \sqrt{s_{pp}}} & \cdots & \frac{s_{pp}}{\sqrt{s_{pp}} \sqrt{s_{pp}}} \end{bmatrix} = \mathbf{D}^{-1/2} \mathbf{S}_n \mathbf{D}^{-1/2}$$