3. Symmetric eigendecomposition

- eigenvalues and eigenvectors
- symmetric eigendecomposition
- quadratic forms
- low rank matrix approximation

Eigenvalues and eigenvectors

a nonzero vector x is an *eigenvector* of the $n \times n$ matrix A, with *eigenvalue* λ, if

$$Ax = \lambda x$$

- the matrix $\lambda I - A$ is singular and x is a nonzero vector in the nullspace of $\lambda I - A$
- the eigenvalues of A are the roots of the *characteristic polynomial:*

$$\det(\lambda I - A) = \lambda^n + c_{n-1}\lambda^{n-1} + \cdots + c_1\lambda + (-1)^n \det(A) = 0$$

- this immediately shows that every square matrix has at least one eigenvalue
- the roots of the polynomial (and corresponding eigenvectors) may be complex
- *(algebraic) multiplicity* of an eigenvalue is its multiplicity as a root of $\det(\lambda I - A)$
- there are exactly n eigenvalues, counted with their multiplicity
- set of eigenvalues of A is called the *spectrum* of A

Diagonal matrix

$$A = \begin{bmatrix} A_{11} & 0 & \cdots & 0 \\ 0 & A_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & A_{nn} \end{bmatrix}$$

- eigenvalues of A are the diagonal entries $A_{11}, \ldots, A_{nn}$
- the n unit vectors $e_1 = (1, 0, \ldots, 0), \ldots, e_n = (0, \ldots, 0, 1)$ are eigenvectors:

$$Ae_i = A_{ii} e_i$$

- linear combinations of e_i are eigenvectors if the corresponding A_{ii} are equal

Example: $A = \alpha I$ is a scalar multiple of the identity matrix

- one eigenvalue α with multipicity n
- every nonzero vector is an eigenvector

Similarity transformation

two matrices A and B are *similar* if

$$B = T^{-1}AT$$

for some nonsingular matrix T

- the mapping that maps A to $T^{-1}AT$ is called a *similarity transformation*
- similarity transformations preserve eigenvalues:

$$\det(\lambda I - B) = \det(\lambda I - T^{-1}AT) = \det(T^{-1}(\lambda I - A)T) = \det(\lambda I - A)$$

- if x is an eigenvector of A then $y = T^{-1}x$ is an eigenvector of B:

$$By = (T^{-1}AT)(T^{-1}x) = T^{-1}Ax = T^{-1}(\lambda x) = \lambda y$$

of special interest will be *orthogonal* similarity transformations (T is orthogonal)

Diagonalizable matrices

a matrix is *diagonalizable* if it is similar to a diagonal matrix:

$$T^{-1}AT = \Lambda$$

for some nonsingular matrix T

- the diagonal elements of Λ are the eigenvalues of A
- the columns of T are eigenvectors of A:

$$A(Te_i) = T\Lambda e_i = \Lambda_{ii}(Te_i)$$

- the columns of T give a set of n linearly independent eigenvectors

not all square matrices are diagonalizable

Spectral decomposition

suppose A is diagonalizable, with

$$\begin{aligned} A = T\Lambda T^{-1} &= \begin{bmatrix} v_1 & v_2 & \cdots & v_n \end{bmatrix} \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix} \begin{bmatrix} w_1^T \\ w_2^T \\ \vdots \\ w_n^T \end{bmatrix} \\ &= \lambda_1 v_1 w_1^T + \lambda_2 v_2 w_2^T + \cdots + \lambda_n v_n w_n^T \end{aligned}$$

this is a *spectral decomposition* of the linear function $f(x) = Ax$

- elements of $T^{-1}x$ are coefficients of x in the basis of eigenvectors $\{v_1, \ldots, v_n\}$:

$$x = TT^{-1}x = \alpha_1 v_1 + \cdots + \alpha_n v_n \qquad \text{where } \alpha_i = w_i^T x$$

- applied to an eigenvector, $f(v_i) = Av_i = \lambda_i v_i$ is a simple scaling
- by superposition, we find Ax as

$$Ax = \alpha_1 \lambda_1 v_1 + \cdots + \alpha_n \lambda_n v_n = T\Lambda T^{-1} x$$

Exercise

recall from 133A the definition of a *circulant matrix*

$$A = \begin{bmatrix} a_1 & a_n & a_{n-1} & \cdots & a_3 & a_2 \\ a_2 & a_1 & a_n & \cdots & a_4 & a_3 \\ a_3 & a_2 & a_1 & \cdots & a_5 & a_4 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{n-1} & a_{n-2} & a_{n-3} & \cdots & a_1 & a_n \\ a_n & a_{n-1} & a_{n-2} & \cdots & a_2 & a_1 \end{bmatrix}$$

and its factorization

$$A = \frac{1}{n} W \,\mathbf{diag}(Wa) W^H$$

W is the discrete Fourier transform matrix (Wa is the DFT of a) and

$$W^{-1} = \frac{1}{n} W^H$$

what is the spectrum of A?

Outline

- eigenvalues and eigenvectors
- **symmetric eigendecomposition**
- quadratic forms
- low rank matrix approximation

Symmetric eigendecomposition

eigenvalues/vectors of a symmetric matrix have important special properties

- all the eigenvalues are real
- the eigenvectors corresponding to different eigenvalues are orthogonal
- a symmetrix matrix is diagonalizable by an orthogonal similarity transformation:

$$Q^T A Q = \Lambda, \qquad Q^T Q = I$$

in the remainder of the lecture we assume that A is symmetric (and real)

Eigenvalues of a symmetric matrix are real

consider an eigenvalue λ and eigenvector x (possibly complex):

$$Ax = \lambda x, \quad x \neq 0$$

- inner product with x shows that $x^H A x = \lambda x^H x$
- $x^H x = \sum_{i=1}^n |x_i|^2$ is real and positive, and $x^H A x$ is real:

$$x^H A x = \sum_{i=1}^n \sum_{j=1}^n A_{ij} \bar{x}_i x_j = \sum_{i=1}^n A_{ii} |x_i|^2 + 2 \sum_{j<i} A_{ij} \operatorname{Re}(\bar{x}_i x_j)$$

- therefore $\lambda = (x^H A x)/(x^H x)$ is real
- if x is complex, its real and imaginary part are real eigenvectors (if nonzero):

$$A(x_{\text{re}} + \mathrm{j} x_{\text{im}}) = \lambda(x_{\text{re}} + \mathrm{j} x_{\text{im}}) \qquad \Longrightarrow \qquad A x_{\text{re}} = \lambda x_{\text{re}}, \quad A x_{\text{im}} = \lambda x_{\text{im}}$$

therefore, eigenvectors can be assumed to be real

Orthogonality of eigenvectors

suppose x and y are eigenvectors for different eigenvalues λ, μ:

$$Ax = \lambda x, \qquad Ay = \mu y, \qquad \lambda \neq \mu$$

- take inner products with x, y:

$$\lambda y^T x = y^T A x = x^T A y = \mu x^T y$$

  second equality holds because A is symmetric

- if $\lambda \neq \mu$ this implies that

$$x^T y = 0$$

Eigendecomposition

every real symmetric $n \times n$ matrix A can be factored as

$$A = Q \Lambda Q^T \tag{1}$$

- Q is orthogonal
- $\Lambda = \mathbf{diag}(\lambda_1, \ldots, \lambda_n)$ is diagonal, with real diagonal elements
- A is diagonalizable by an orthogonal similarity transformation: $Q^T A Q = \Lambda$
- the columns of Q are an orthonormal set of n eigenvectors: write $AQ = Q\Lambda$ as

$$\begin{aligned} A \begin{bmatrix} q_1 & q_2 & \cdots & q_n \end{bmatrix} &= \begin{bmatrix} q_1 & q_2 & \cdots & q_n \end{bmatrix} \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix} \\ &= \begin{bmatrix} \lambda_1 q_1 & \lambda_2 q_2 & \cdots & \lambda_n q_n \end{bmatrix} \end{aligned}$$

Proof by induction

- the decomposition (1) obviously exists if $n = 1$
- suppose it exists if $n = m$ and A is an $(m+1) \times (m+1)$ matrix
- A has at least one eigenvalue (page 3.2)
- let λ_1 be any eigenvalue and q_1 a corresponding eigenvector, with $\|q_1\| = 1$
- let V be an $(m+1) \times m$ matrix that makes the matrix $\begin{bmatrix} q_1 & V \end{bmatrix}$ orthogonal:

$$\begin{bmatrix} q_1^T \\ V^T \end{bmatrix} A \begin{bmatrix} q_1 & V \end{bmatrix} = \begin{bmatrix} q_1^T A q_1 & q_1^T A V \\ V^T A q_1 & V^T A V \end{bmatrix} = \begin{bmatrix} \lambda_1 q_1^T q_1 & \lambda_1 q_1^T V \\ \lambda_1 V^T q_1 & V^T A V \end{bmatrix} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & V^T A V \end{bmatrix}$$

- $V^T A V$ is a symmetric $m \times m$ matrix, so by the induction hypothesis,

$$V^T A V = \tilde{Q} \tilde{\Lambda} \tilde{Q}^T \quad \text{for some orthogonal } \tilde{Q} \text{ and diagonal } \tilde{\Lambda}$$

- matrix $Q = \begin{bmatrix} q_1 & V\tilde{Q} \end{bmatrix}$ is orthogonal and defines a similarity that diagonalizes A:

$$Q^T A Q = \begin{bmatrix} q_1^T \\ \tilde{Q}^T V^T \end{bmatrix} A \begin{bmatrix} q_1 & V\tilde{Q} \end{bmatrix} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \tilde{Q}^T V^T A V \tilde{Q} \end{bmatrix} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \tilde{\Lambda} \end{bmatrix}$$

Spectral decomposition

the decomposition (1) expresses A as a sum of rank-one matrices:

$$
\begin{aligned}
A = Q\Lambda Q^T &= \begin{bmatrix} q_1 & q_2 & \cdots & q_n \end{bmatrix} \begin{bmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix} \begin{bmatrix} q_1^T \\ q_2^T \\ \vdots \\ q_n^T \end{bmatrix} \\
&= \sum_{i=1}^{n} \lambda_i q_i q_i^T
\end{aligned}
$$

- the matrix–vector product Ax is decomposed as

$$
Ax = \sum_{i=1}^{n} \lambda_i q_i (q_i^T x)
$$

- $(q_1^T x, \ldots, q_n^T x)$ are coordinates of x in the orthonormal basis $\{q_1, \ldots, q_n\}$
- $(\lambda_1 q_1^T x, \ldots, \lambda_n q_n^T x)$ are coordinates of Ax in the orthonormal basis $\{q_1, \ldots, q_n\}$

Non-uniqueness

some freedom exists in the choice of Λ and Q in the eigendecomposition

$$A = Q\Lambda Q^T = \begin{bmatrix} q_1 & \cdots & q_n \end{bmatrix} \begin{bmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_n \end{bmatrix} \begin{bmatrix} q_1^T \\ \vdots \\ q_n^T \end{bmatrix}$$

Ordering of eigenvalues

diagonal Λ and columns of Q can be permuted; we will assume that

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$$

Choice of eigenvectors

suppose λ_i is an eigenvalue with multiplicity k: $\lambda_i = \lambda_{i+1} = \cdots = \lambda_{i+k-1}$

- nonzero vectors in $\text{span}\{q_i, \ldots, q_{i+k-1}\}$ are eigenvectors with eigenvalue λ_i
- $q_i, \ldots, q_{i+k-1}$ can be replaced with any orthonormal basis of this "eigenspace"

Inverse

a symmetric matrix is invertible if and only if all its eigenvalues are nonzero:

- inverse of $A = Q\Lambda Q^T$ is

$$A^{-1} = (Q\Lambda Q^T)^{-1} = Q\Lambda^{-1}Q^T, \qquad \Lambda^{-1} = \begin{bmatrix} 1/\lambda_1 & 0 & \cdots & 0 \\ 0 & 1/\lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1/\lambda_n \end{bmatrix}$$

- eigenvectors of A^{-1} are the eigenvectors of A
- eigenvalues of A^{-1} are reciprocals of eigenvalues of A

Spectral matrix functions

Integer powers

$$A^k = (Q\Lambda Q^T)^k = Q\Lambda^k Q^T, \qquad \Lambda^k = \mathbf{diag}(\lambda_1^k, \ldots, \lambda_n^k)$$

- negative powers are defined if A is invertible (all eigenvalues are nonzero)
- A^k has the same eigenvectors as A, eigenvalues λ_i^k

Square root

$$A^{1/2} = Q\Lambda^{1/2} Q^T, \qquad \Lambda^{1/2} = \mathbf{diag}(\sqrt{\lambda_1}, \ldots, \sqrt{\lambda_n})$$

- defined if eigenvalues are nonnegative
- a symmetric matrix that satisfies $A^{1/2}A^{1/2} = A$

Other matrix functions: can be defined via power series, for example,

$$\exp(A) = Q \exp(\Lambda) Q^T, \qquad \exp(\Lambda) = \mathbf{diag}(e^{\lambda_1}, \ldots, e^{\lambda_n})$$

Range, nullspace, rank

eigendecomposition with nonzero eigenvalues placed first in Λ:

$$A = Q\Lambda Q^T = \begin{bmatrix} Q_1 & Q_2 \end{bmatrix} \begin{bmatrix} \Lambda_1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} Q_1^T \\ Q_2^T \end{bmatrix} = Q_1 \Lambda_1 Q_1^T$$

diagonal entries of Λ_1 are the nonzero eigenvalues of A

- columns of Q_1 are an orthonormal basis for $\mathrm{range}(A)$
- columns of Q_2 are an orthonormal basis for $\mathrm{null}(A)$
- this is an example of a full-rank factorization (page 1.27): $A = BC$ with

$$B = Q_1, \qquad C = \Lambda_1 Q_1^T$$

- rank of A is the number of nonzero eigenvalues (with their multiplicities)

Pseudo-inverse

we use the same notation as on the previous page

$$A = \begin{bmatrix} Q_1 & Q_2 \end{bmatrix} \begin{bmatrix} \Lambda_1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} Q_1^T \\ Q_2^T \end{bmatrix} = Q_1 \Lambda_1 Q_1^T$$

diagonal entries of Λ_1 are the nonzero eigenvalues of A

- pseudo-inverse follows from page 1.36 with $B = Q_1$ and $C = \Lambda_1 Q_1^T$
- the pseudo-inverse is $A^\dagger = C^\dagger B^\dagger = (Q_1 \Lambda_1^{-1}) Q_1^T$:

$$A^\dagger = Q_1 \Lambda_1^{-1} Q_1^T = \begin{bmatrix} Q_1 & Q_2 \end{bmatrix} \begin{bmatrix} \Lambda_1^{-1} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} Q_1^T \\ Q_2^T \end{bmatrix}$$

- eigenvectors of $A^\dagger$ are the eigenvectors of A
- nonzero eigenvalues of $A^\dagger$ are reciprocals of nonzero eigenvalues of A
- range, nullspace, and rank of $A^\dagger$ are the same as for A

Trace

the *trace* of an $n \times n$ matrix B is the sum of its diagonal elements

$$\operatorname{trace}(B) = \sum_{i=1}^{n} B_{ii}$$

- *transpose:* $\operatorname{trace}(B^T) = \operatorname{trace}(B)$
- *product:* if B is $n \times m$ and C is $m \times n$, then

$$\operatorname{trace}(BC) = \operatorname{trace}(CB) = \sum_{i=1}^{n} \sum_{j=1}^{m} B_{ij} C_{ji}$$

- *eigenvalues:* the trace of a symmetric matrix is the sum of the eigenvalues

$$\operatorname{trace}(Q \Lambda Q^T) = \operatorname{trace}(Q^T Q \Lambda) = \operatorname{trace}(\Lambda) = \sum_{i=1}^{n} \lambda_i$$

Frobenius norm

recall the definition of *Frobenius norm* of an $m \times n$ matrix B:

$$\|B\|_F = \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n} B_{ij}^2} = \sqrt{\operatorname{trace}(B^T B)} = \sqrt{\operatorname{trace}(B B^T)}$$

- this is an example of a *unitarily invariant* norm: if U, V are orthogonal, then

$$\|UBV\|_F = \|B\|_F$$

Proof:

$$\|UBV\|_F^2 = \operatorname{trace}(V^T B^T U^T U B V) = \operatorname{trace}(V V^T B^T B) = \operatorname{trace}(B^T B) = \|B\|_F^2$$

- for a symmetric $n \times n$ matrix with eigenvalues $\lambda_1, \ldots, \lambda_n$,

$$\|A\|_F = \|Q\Lambda Q^T\|_F = \|\Lambda\|_F = \left(\sum_{i=1}^{n} \lambda_i^2\right)^{1/2}$$

2-Norm

recall the definition of *2-norm* or *spectral norm* of an $m \times n$ matrix B:

$$\|B\|_2 = \max_{x \neq 0} \frac{\|Bx\|}{\|x\|}$$

- this norm is also unitarily invariant: if U, V are orthogonal, then

$$\|UBV\|_2 = \|B\|_2$$

Proof:

$$\|UBV\|_2 = \max_{x \neq 0} \frac{\|UBVx\|}{\|x\|} = \max_{y \neq 0} \frac{\|UBy\|}{\|V^T y\|} = \max_{y \neq 0} \frac{\|By\|}{\|y\|} = \|B\|_2$$

- for a symmetric $n \times n$ matrix with eigenvalues $\lambda_1, \ldots, \lambda_n$,

$$\|A\|_2 = \|Q\Lambda Q^T\|_2 = \|\Lambda\|_2 = \max_{i=1,\ldots,n} |\lambda_i| = \max\{\lambda_1, -\lambda_n\}$$

Exercises

Exercise 1

suppose A has eigendecomposition $A = Q\Lambda Q^T$; give an eigendecomposition of

$$A - \alpha I$$

Exercise 2

what are the eigenvalues and eigenvectors of an orthogonal projector

$$A = UU^T \qquad \text{(where } U^TU = I\text{)}$$

Exercise 3

the condition number of a nonsingular matrix is defined as

$$\kappa(A) = \|A\|_2 \|A^{-1}\|_2$$

express the condition number of a symmetric matrix in terms of its eigenvalues

Outline

- eigenvalues and eigenvectors
- symmetric eigendecomposition
- **quadratic forms**
- low rank matrix approximation

Quadratic forms

the eigendecomposition is a useful tool for problems that involve quadratic forms

$$f(x) = x^T A x$$

- substitute $A = Q\Lambda Q^T$ and make an orthogonal change of variables $y = Q^T x$:

$$f(Qy) = y^T \Lambda y = \lambda_1 y_1^2 + \cdots + \lambda_n y_n^2$$

- $y_1, \ldots, y_n$ are coordinates of x in the orthonormal basis of eigenvectors
- the orthogonal change of variables preserves inner products and norms:

$$\|y\|_2 = \|Q^T x\|_2 = \|x\|_2$$

Maximum and minimum value

consider the optimization problems with variable x

$$\begin{array}{ll} \text{maximize} & x^T A x \\ \text{subject to} & x^T x = 1 \end{array} \qquad \begin{array}{ll} \text{minimize} & x^T A x \\ \text{subject to} & x^T x = 1 \end{array}$$

change coordinates to the spectral basis ($y = Q^T x$ and $x = Qy$):

$$\begin{array}{ll} \text{maximize} & \lambda_1 y_1^2 + \cdots + \lambda_n y_n^2 \\ \text{subject to} & y_1^2 + \cdots + y_n^2 = 1 \end{array} \qquad \begin{array}{ll} \text{minimize} & \lambda_1 y_1^2 + \cdots + \lambda_n y_n^2 \\ \text{subject to} & y_1^2 + \cdots + y_n^2 = 1 \end{array}$$

- maximization: $y = (1, 0, \ldots, 0)$ and $x = q_1$ are optimal; maximal value is

$$\max_{\|x\|=1} x^T A x = \max_{\|y\|=1} (\lambda_1 y_1^2 + \cdots + \lambda_n y_n^2) = \lambda_1 = \max_{i=1,\ldots,n} \lambda_i$$

- minimization: $y = (0, 0, \ldots, 1)$ and $x = q_n$ are optimal; minimal value is

$$\min_{\|x\|=1} x^T A x = \min_{\|y\|=1} (\lambda_1 y_1^2 + \cdots + \lambda_n y_n^2) = \lambda_n = \min_{i=1,\ldots,n} \lambda_i$$

Exercises

Exercise 1: find the extreme values of the *Rayleigh quotient* $(x^T Ax)/(x^T x)$, *i.e.*,

$$\max_{x \neq 0} \frac{x^T Ax}{x^T x}, \qquad \min_{x \neq 0} \frac{x^T Ax}{x^T x}$$

Exercise 2: solve the optimization problems

$$\begin{array}{ll} \text{maximize} & x^T Ax \\ \text{subject to} & x^T x \leq 1 \end{array} \qquad \begin{array}{ll} \text{minimize} & x^T Ax \\ \text{subject to} & x^T x \leq 1 \end{array}$$

Exercise 3: show that (for symmetric A)

$$\|A\|_2 = \max_{i=1,\ldots,n} |\lambda_i| = \max_{\|x\|=1} |x^T Ax|$$

Sign of eigenvalues

matrix property	condition on eigenvalues
positive definite	$\lambda_n > 0$
positive semidefinite	$\lambda_n \geq 0$
indefinite	$\lambda_n < 0$ and $\lambda_1 > 0$
negative semidefinite	$\lambda_1 \leq 0$
negative definite	$\lambda_1 < 0$

- λ_1 and λ_n denote the largest and smallest eigenvalues:

$$\lambda_1 = \max_{i=1,\ldots,n} \lambda_i, \qquad \lambda_n = \min_{i=1,\ldots,n} \lambda_i$$

- properties in the table follow from

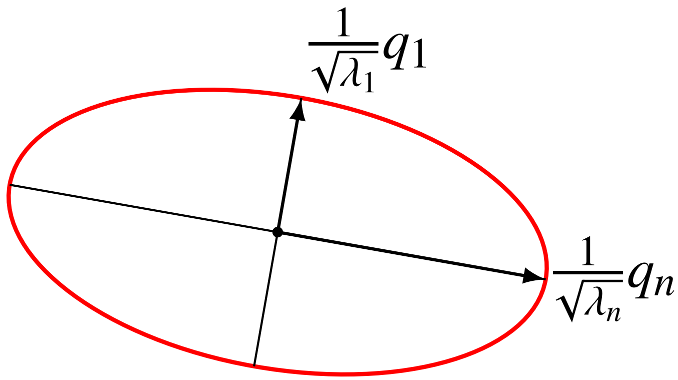
$$\lambda_1 = \max_{\|x\|=1} x^T A x = \max_{x \neq 0} \frac{x^T A x}{x^T x}, \qquad \lambda_n = \min_{\|x\|=1} x^T A x = \min_{x \neq 0} \frac{x^T A x}{x^T x}$$

Ellipsoids

if A is positive definite, the set

$$\mathcal{E} = \{x \mid x^T A x \leq 1\}$$

is an ellipsoid with center at the origin



after the orthogonal change of coordinates $y = Q^T x$ the set is described by

$$\lambda_1 y_1^2 + \cdots + \lambda_n y_n^2 \leq 1$$

this shows that:

- eigenvectors of A give the principal axes
- the width along the principal axis determined by q_i is $2/\sqrt{\lambda_i}$

Exercise

give an interpretation of $\mathrm{trace}(A^{-1})$ as a measure of the size of the ellipsoid

$$\mathcal{E} = \{x \mid x^T A x \leq 1\}$$

Max–min characterization of eigenvalues

as an extension of the maximization problem on page 3.24, consider

$$\begin{array}{ll} \text{maximize} & \lambda_{\min}(X^T A X) \\ \text{subject to} & X^T X = I \end{array} \qquad (2)$$

the variable X is an $n \times k$ matrix, for some given value of k between 1 and n

- $\lambda_{\min}(X^T A X)$ denotes the smallest eigenvalue of the $k \times k$ matrix $X^T A X$
- for $k = 1$ this is the problem on page 3.24: $\lambda_{\min}(x^T A x) = x^T A x$

Solution: from the eigendecomposition $A = Q \Lambda Q^T = \sum_{i=1}^{n} \lambda_i q_i q_i^T$

- the optimal value of (2) is the kth eigenvalue λ_k of A
- an optimal choice for X is formed from the first k columns of Q:

$$X = \begin{bmatrix} q_1 & q_2 & \cdots & q_k \end{bmatrix}$$

this is known as the *Courant–Fischer min–max theorem*

Proof of the max–min characteriation

we make a change of variables $Y = Q^T X$:

$$\begin{array}{ll} \text{maximize} & \lambda_{\min}(Y^T \Lambda Y) \\ \text{subject to} & Y^T Y = I \end{array}$$

we also partition Λ as

$$\Lambda = \begin{bmatrix} \Lambda_1 & 0 \\ 0 & \Lambda_2 \end{bmatrix}, \qquad \Lambda_1 = \begin{bmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_k \end{bmatrix}, \qquad \Lambda_2 = \begin{bmatrix} \lambda_{k+1} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_n \end{bmatrix}$$

we show that the matrix $\hat{Y} = \begin{bmatrix} I \\ 0 \end{bmatrix}$ is optimal

- for this matrix

$$\hat{Y}^T \Lambda \hat{Y} = \begin{bmatrix} I \\ 0 \end{bmatrix}^T \begin{bmatrix} \Lambda_1 & 0 \\ 0 & \Lambda_2 \end{bmatrix} \begin{bmatrix} I \\ 0 \end{bmatrix} = \Lambda_1, \quad \lambda_{\min}(\hat{Y}^T \Lambda \hat{Y}) = \lambda_{\min}(\Lambda_1) = \lambda_k$$

- on the next page we show that $\lambda_{\min}(Y^T \Lambda Y) \leq \lambda_k$ if Y is $n \times k$ with $Y^T Y = I$

Proof of the max–min characteriation

- on page 3.24, we have seen that

$$\lambda_{\min}(Y^T \Lambda Y) = \min_{\|u\|=1} u^T (Y^T \Lambda Y) u$$

- if Y has k columns, there exists $v \neq 0$ such that Yv has $k-1$ leading zeros:

$$Yv = \begin{bmatrix} Y_{11} & \cdots & Y_{1k} \\ \vdots & & \vdots \\ Y_{k-1,1} & \cdots & Y_{k-1,k} \\ Y_{k1} & \cdots & Y_{kk} \\ \vdots & & \vdots \\ Y_{n1} & \cdots & Y_{nk} \end{bmatrix} \begin{bmatrix} v_1 \\ \vdots \\ v_k \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ y_k \\ \vdots \\ y_n \end{bmatrix}$$

- if $Y^T Y = I$ and we normalize v, then $\|Yv\| = \|v\| = 1$ and

$$(Yv)^T \Lambda (Yv) = \lambda_k y_k^2 + \cdots + \lambda_n y_n^2 \leq \lambda_k (y_k^2 + \cdots + y_n^2) = \lambda_k$$

- this shows that

$$\lambda_{\min}(Y^T \Lambda Y) = \min_{\|u\|=1} u^T (Y^T \Lambda Y) u \leq v^T (Y^T \Lambda Y) v \leq \lambda_k$$

Min–max characterization of eigenvalues

the minimization problem on page 3.24 can be extended in a similar way:

$$\begin{array}{ll} \text{minimize} & \lambda_{\max}(X^T A X) \\ \text{subject to} & X^T X = I \end{array} \qquad (3)$$

the variable X is an $n \times k$ matrix

- $\lambda_{\max}(X^T A X)$ denotes the largest eigenvalue of the $k \times k$ matrix $X^T A X$
- for $k = 1$ this is the minimization problem on page 3.24: $\lambda_{\max}(x^T A x) = x^T A x$

Solution: from the eigenvalue decomposition $A = Q \Lambda Q^T = \sum_{i=1}^n \lambda_i q_i q_i^T$

- the optimal value of (3) is eigenvalue λ_{n-k+1} of A
- an optimal choice of X is formed from the last k columns of Q:

$$X = \begin{bmatrix} q_{n-k+1} & \cdots & q_{n-1} & q_n \end{bmatrix}$$

this follows from the max–min characterization on page 3.29 applied to $-A$

Exercises

Exercise 1: suppose B is an $m \times m$ principal submatrix of A, for example,

$$B = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1m} \\ A_{21} & A_{22} & \cdots & A_{2m} \\ \vdots & \vdots & & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mm} \end{bmatrix}, \tag{4}$$

and denote the m eigenvalues of B by $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_m$

show that

$$\mu_1 \leq \lambda_1, \qquad \mu_2 \leq \lambda_2, \qquad \ldots, \qquad \mu_m \leq \lambda_m$$

($\lambda_1, \ldots, \lambda_m$ are the first m eigenvalues of A)

Exercise 2: consider the matrix B in (4) with $m = n - 1$; show that

$$\lambda_1 \geq \mu_1 \geq \lambda_2 \geq \mu_2 \geq \cdots \geq \lambda_{n-1} \geq \mu_{n-1} \geq \lambda_n$$

this is known as the eigenvalue *interlacing theorem*

Eigendecomposition of covariance matrix

- suppose x is a random n-vector with mean μ, covariance matrix Σ
- Σ is positive semidefinite with eigendecomposition

$$\Sigma = \mathbf{E}((x - \mu)(x - \mu)^T) = Q\Lambda Q^T$$

define a random n-vector $y = Q^T(x - \mu)$

- y has zero mean and covariance matrix Λ:

$$\mathbf{E}(yy^T) = Q^T\,\mathbf{E}((x - \mu)(x - \mu)^T)Q = Q^T\Sigma Q = \Lambda$$

- components of y are uncorrelated and have variances $\mathbf{E}(y_i^2) = \lambda_i$
- x is decomposed in uncorrelated components with decreasing variance:

$$\mathbf{E}(y_1^2) \geq \mathbf{E}(y_2^2) \geq \cdots \geq \mathbf{E}(y_n^2)$$

the transformation is known as the *Karhunen–Loève* or *Hotelling* transform

Multivariate normal distribution

multivariate normal (Gaussian) probability density function

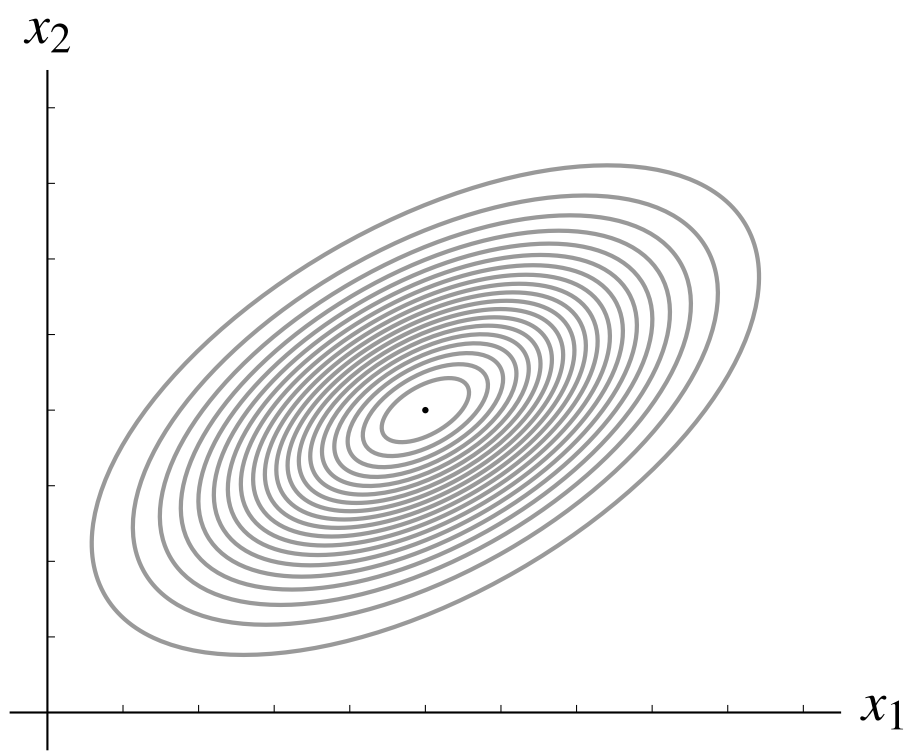
$$p(x) = \frac{1}{(2\pi)^{n/2}\sqrt{\det \Sigma}} e^{-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)}$$

contour lines of density function for

$$\Sigma = \frac{1}{4} \begin{bmatrix} 7 & \sqrt{3} \\ \sqrt{3} & 5 \end{bmatrix}, \quad \mu = \begin{bmatrix} 5 \\ 4 \end{bmatrix}$$

eigenvalues of Σ are $\lambda_1 = 2$, $\lambda_2 = 1$,

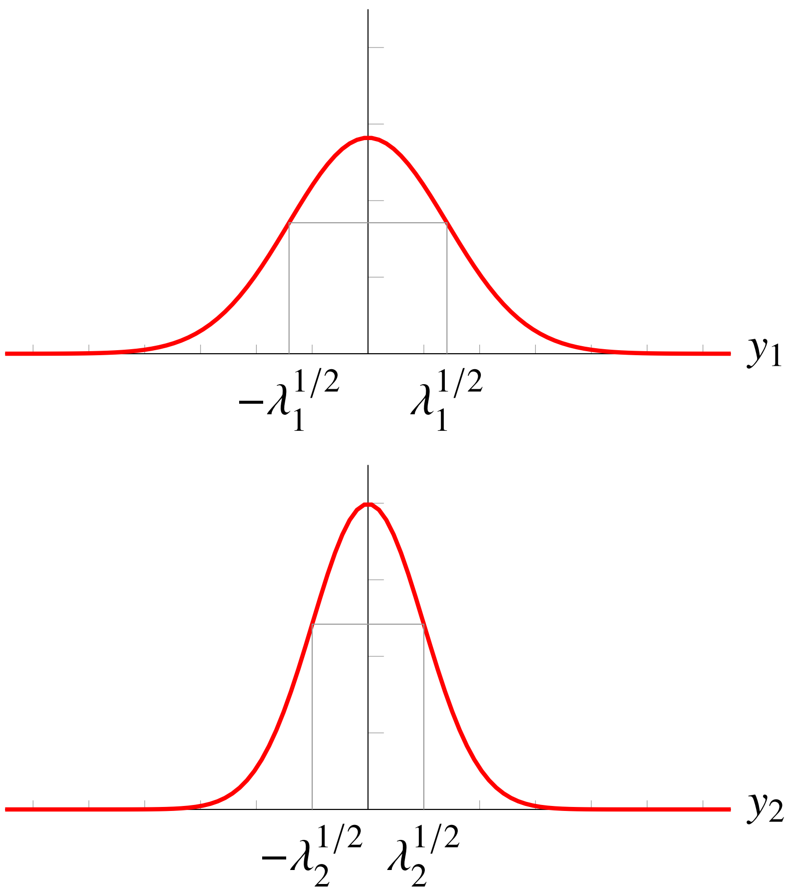
$$q_1 = \begin{bmatrix} \sqrt{3}/2 \\ 1/2 \end{bmatrix}, \quad q_2 = \begin{bmatrix} 1/2 \\ -\sqrt{3}/2 \end{bmatrix}$$

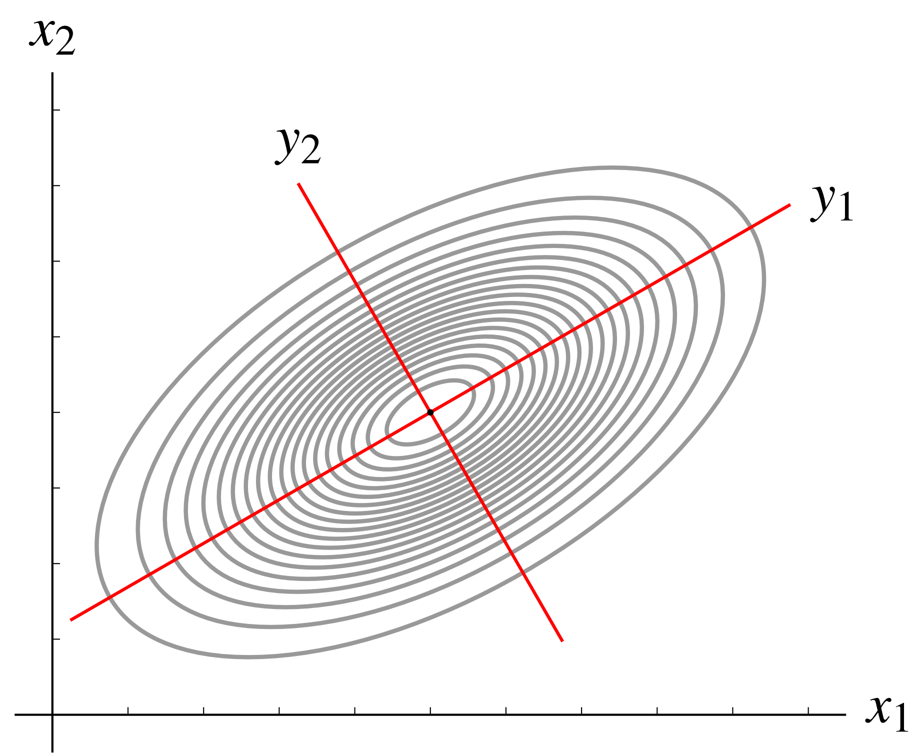


Multivariate normal distribution

the decorrelated and de-meaned variables $y = Q^T(x - \mu)$ have distribution

$$\tilde{p}(y) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi\lambda_i}} \exp(-\frac{y_i^2}{2\lambda_i})$$





Joint diagonalization of two matrices

- a symmetric matrix A is diagonalized by an orthogonal similarity:

$$Q^T A Q = \Lambda$$

- as an extension, if A, B are symmetric and B is positive definite, then

$$S^T A S = D, \qquad S^T B S = I$$

  for some nonsingular S and diagonal D

Algorithm: S and D can be computed is as follows

- Cholesky factorization $B = R^T R$, with R upper triangular and nonsingular
- eigendecomposition $R^{-T} A R^{-1} = Q D Q^T$, with D diagonal, Q orthogonal
- define $S = R^{-1} Q$:

$$S^T A S = Q^T R^{-T} A R^{-1} Q = \Lambda, \qquad S^T B S = Q^T R^{-T} B R^{-1} Q = Q^T Q = I$$

Optimization problems with two quadratic forms

as an extension of the maximization problem on page 3.24, consider

$$\begin{array}{ll} \text{maximize} & x^T A x \\ \text{subject to} & x^T B x = 1 \end{array}$$

where A, B are symmetric and B is positive definite

- compute nonsingular S that diagonalizes A, B:

$$S^T A S = D, \qquad S^T B S = I$$

- make change of variables $x = Sy$:

$$\begin{array}{ll} \text{maximize} & y^T D y \\ \text{subject to} & y^T y = 1 \end{array}$$

- if diagonal elements of D are sorted as $D_{11} \geq \cdots \geq D_{nn}$, solution is

$$y = e_1 = (1, 0, \ldots, 0), \qquad x = Se_1, \qquad x^T A x = D_{11}$$

Outline

- eigenvalues and eigenvectors
- symmetric eigendecomposition
- quadratic forms
- **low rank matrix approximation**

Low-rank matrix approximation

- low rank is a useful matrix property in many applications
- low rank is not a robust property (easily destroyed by noise or estimation error)
- most matrices in practice have full rank
- often the full-rank matrix is close to being low rank
- computing low-rank approximations is an important problem in linear algebra

on the next pages we discuss this for positive semidefinite matrices

Rank-r approximation of positive semidefinite matrix

let A be a positive semidefinite matrix with $\operatorname{rank}(A) > r$ and eigendecomposition

$$A = Q\Lambda Q^T = \sum_{i=1}^{n} \lambda_i q_i q_i^T, \qquad \lambda_1 \geq \cdots \geq \lambda_n \geq 0, \quad \lambda_{r+1} > 0$$

the best rank-r approximation is the sum of the first r terms in the decomposition:

$$B = \sum_{i=1}^{r} \lambda_i q_i q_i^T$$

- B is the best approximation for the Frobenius norm: for every C with rank r,

$$\|A - C\|_F \geq \|A - B\|_F = \left(\sum_{i=r+1}^{n} \lambda_i^2 \right)^{1/2}$$

- B is also the best approximation for the 2-norm: for every C with rank r,

$$\|A - C\|_2 \geq \|A - B\|_2 = \lambda_{r+1}$$

Rank-r approximation in Frobenius norm

the approximation problem in Frobenius norm is a nonlinear least squares problem

$$\text{minimize} \quad \|A - XX^T\|_F^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} \left(A_{ij} - \sum_{k=1}^{r} X_{ik} X_{jk} \right)^2$$

- we parametrize B as $B = XX^T$ with X of size $n \times r$, and optimize over X
- this can be written in the standard nonlinear least squares form

$$\text{minimize} \quad g(x) = \|f(x)\|^2$$

  with vector x containing the elements of X and $f(x)$ the elements of $A - XX^T$
- the first order (necessary but not sufficient) optimality conditions are

$$\nabla g(x) = 2Df(x)^T f(x) = 0$$

- the first order optimality conditions will be derived on page 3.41; they are

$$4(A - XX^T)X = 0$$

Solution of first order optimality conditions

$$AX = X(X^T X)$$

- define eigendecomposition $X^T X = UDU^T$ (U orthogonal $r \times r$, D diagonal)
- use $Y = XU$ and D as variables:

$$AY = YD, \qquad Y^T Y = D$$

- the r diagonal elements of D must be eigenvalues of A
- the r columns of Y are corresponding orthogonal eigenvectors
- the columns of Y are normalized to have norm $\sqrt{D_{ii}}$

we conclude that the solutions of the first order optimality conditions satisfy

$$XX^T = YY^T = \sum_{i \in I} \lambda_i q_i q_i^T$$

where I is a subset of r elements of $\{1, 2, \ldots, n\}$

Optimal solution

among the solutions of the 1st order conditions we choose the one that minimizes

$$\|A - XX^T\|_F$$

- the squared error in the approximation is

$$\begin{aligned}
\|A - XX^T\|_F^2 &= \|A - \sum_{i \in I} \lambda_i q_i q_i^T\|_F^2 \\
&= \|\sum_{i \notin I} \lambda_i q_i q_i^T\|_F^2 \\
&= \sum_{i \notin I} \lambda_i^2
\end{aligned}$$

- the optimal choice for I is $I = \{1, 2, \ldots, r\}$:

$$XX^T = \sum_{i=1}^{r} \lambda_i q_i q_i^T, \qquad \|A - XX^T\|_F^2 = \sum_{i=r+1}^{n} \lambda_i^2$$

First order optimality

to derive the first order optimality conditions for

$$\text{minimize} \quad \|A - XX^T\|_F^2$$

we substitute $X + \delta X$, with arbitrary small δX, and linearize:

$$\begin{aligned}
&\|A - (X + \delta X)(X + \delta X)^T\|_F^2 \\
&\quad = \quad \|A - XX^T + \delta X\, X^T + X\, \delta X^T + \delta X\, \delta X^T\|_F^2 \\
&\quad \approx \quad \|A - XX^T + \delta X\, X^T + X\, \delta X^T\|_F^2 \\
&\quad = \quad \operatorname{trace}\left((A - XX^T + \delta X\, X^T + X\, \delta X^T)(A - XX^T + \delta X\, X^T + X\, \delta X^T)\right) \\
&\quad \approx \quad \operatorname{trace}\left((A - XX^T)(A - XX^T)\right) + 2\operatorname{trace}\left((\delta X\, X^T + X\, \delta X^T)(A - XX^T)\right) \\
&\quad = \quad \|A - XX^T\|_F^2 + 4\operatorname{trace}\left(\delta X^T (A - XX^T) X\right)
\end{aligned}$$

X is a stationary point if the second term is zero for all δX:

$$4(A - XX^T)X = 0$$

Rank-r approximation in 2-norm

the same matrix B is also the best approximation in 2-norm: if C has rank r, then

$$\|A - C\|_2 \geq \|A - B\|_2$$

the right-hand side is

$$\begin{aligned}
\|A - B\|_2 &= \|\sum_{i=1}^{n} \lambda_i q_i q_i^T - \sum_{i=1}^{r} \lambda_i q_i q_i^T\|_2 \\
&= \|\sum_{i=r+1}^{n} \lambda_i q_i q_i^T\|_2 \\
&= \lambda_{r+1}
\end{aligned}$$

on the next page we show that $\|A - C\|_2 \geq \lambda_{r+1}$ if C has rank r

Proof

- if $\mathrm{rank}(C) = r$, the nullspace of C has dimension $n - r$
- define an $n \times (n-r)$ matrix V with orthonormal columns that span $\mathrm{null}(C)$
- we use the min–max theorem on page 3.32 to bound $\|A - C\|_2$:

$$
\begin{aligned}
\|A - C\|_2 &= \max_{\|x\|=1} |x^T(A-C)x| && \text{(page 3.25)} \\
&\geq \max_{\|x\|=1} x^T(A-C)x \\
&\geq \max_{\|y\|=1} y^T V^T (A-C) V y && (\|Vy\| = \|y\|) \\
&= \max_{\|y\|=1} y^T V^T A V y && (V^T C V = 0) \\
&= \lambda_{\max}(V^T A V) \\
&\geq \lambda_{r+1} && \text{(page 3.32 with } k = n - r\text{)}
\end{aligned}
$$