Computational Data Mining

Fatemeh Mansoori

$Q\Lambda Q^{\mathrm{T}}$

- starts with a symmetric matrix S
- Symmetric matrix S $\quad S^T = S$ $\qquad$ All $S_{ij} = S_{ji}$
- Orthogonal square matrix Q $\quad Q^{\mathrm{T}} = Q^{-1}$
- Every real symmetric matrix S
    - has n orthonormal eigenvectors q_1 to q_n.
    - When multiplied by S the eigenvectors keep the same direction. They are just rescaled by the number λ

$$\boxed{\textbf{Eigenvector } q \textbf{ and eigenvalue } \boldsymbol{\lambda} \qquad S\boldsymbol{q} = \lambda \boldsymbol{q}}$$

$$\boldsymbol{SQ} = S\begin{bmatrix} \boldsymbol{q}_1 & \dots & \boldsymbol{q}_n \end{bmatrix} = \begin{bmatrix} \lambda_1\boldsymbol{q}_1 & \dots & \lambda_n\boldsymbol{q}_n \end{bmatrix} = \begin{bmatrix} \boldsymbol{q}_1 & \dots & \boldsymbol{q}_n \end{bmatrix}\begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} = \boldsymbol{Q\Lambda}$$

Multiply $SQ = Q\Lambda$ by $Q^{-1} = Q^{\mathrm{T}}$ to get $\boldsymbol{S = Q\Lambda Q^{\mathrm{T}}}$ = a symmetric matrix

eigenvalue λ_k and each eigenvector $\boldsymbol{q}_k$ contribute a rank one piece $\lambda_k\boldsymbol{q}_k\boldsymbol{q}_k^{\mathrm{T}}$ to S.

Rank one pieces $\quad S = (Q\Lambda)Q^{\mathrm{T}} = (\lambda_1\boldsymbol{q}_1)\boldsymbol{q}_1^{\mathrm{T}} + (\lambda_2\boldsymbol{q}_2)\boldsymbol{q}_2^{\mathrm{T}} + \cdots + (\lambda_n\boldsymbol{q}_n)\boldsymbol{q}_n^{\mathrm{T}}$

Symmetric Positive Definite Matrices

- Symmetric matrices $S = S^T$
- All *n* eigenvalues of a symmetric matrix *S* are real numbers
- n eigenvectors *q* can be chosen orthogonal (perpendicular to each other)
  - identity matrix $S = I$ is an extreme case
  - All eigenvalues are equals 1

The eigenvector matrix for S has $Q^{\mathrm{T}}Q = I$

Spectral Theorem **Every real symmetric matrix has the form $S = Q\Lambda Q^{\mathrm{T}}$.**

A positive definite matrix has all positive eigenvalues.

- We would like to check for positive eigenvalues without computing them

Tests to identify positive definite symmetric matrix

- **All the leading determinants $D_1, D_2, \ldots, D_n$ of S are positive**
- **All the pivots of S are positive** (in elimination)
- Energy test :

$$\boxed{\textbf{S is positive definite if the energy } x^{\mathrm{T}} S x \textbf{ is positive for all vectors } x \neq 0}$$

$S = I$ is positive definite: All $\lambda_i = 1$. The energy is $x^{\mathrm{T}} I x = x^{\mathrm{T}} x$, positive

- $S = A^{\mathrm{T}} A$ **for a matrix A with independent columns**

Determinant Test

$$S = \begin{bmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & -1 & 2 & -1 \\ & & -1 & 2 \end{bmatrix} \quad \text{has} \quad \begin{array}{l} \text{1st determinant } D_1 = \mathbf{2} \\ \text{2nd determinant } D_2 = \mathbf{3} \\ \text{3rd determinant } D_3 = \mathbf{4} \\ \text{4th determinant } D_4 = \mathbf{5} \end{array}$$

Pivot test

The kth pivot equals the ratio $\frac{D_k}{D_{k-1}}$ of the leading determinants (sizes k and $k-1$)

$$d_k = \frac{det(A_k)}{det(A_{k-1})}$$

A_k is the upper left $k \times k$ submatrix.

pivots are all positive when the leading determinants are all positive.

Example - Is the following matrix positive definite?

$$\begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}$$

Question

- Show for the matrix S = $\begin{bmatrix} 2 & 4 \\ 4 & 9 \end{bmatrix}$ the energy is positive

Energy test

- Show that if $x^T Sx$ is positive for every vector then S is positive definitive matrix (x is the eigen vector of S)

If $Sx = \lambda x$ then $x^T Sx = \lambda x^T x$. So $\lambda > 0$ leads to $x^T Sx > 0$.

If $x^T Sx > 0$ for the eigenvectors of S, then $x^T Sx > 0$ for every nonzero vector x.

Every x is a combination $c_1 x_1 + \cdots + c_n x_n$ of the eigenvectors.

  - S is symmetric then the eigenvectors could be chosen orthogonal

- in physics the energy of a system in state x is represented as $x^T Sx$ so this is frequently called the energy-based definition of a positive definite matrix

Question

- Prove that If S_1 and S_2 are symmetric positive definite, so is $S_1 + S_2$

- If S is symmetric positive definite, does Q^TSQ is symmetric and if yes does it positive definite ?
  - Show with energy test
  - Show with similar matrix

Test : $S = A^T A$

- Show that matrix S is positive definite if and only if it can be written as $S = A^T A$

Why columns of A must be independent in this test 3

$$S = A^{\mathrm{T}} A \qquad \textbf{Energy} = x^{\mathrm{T}} S x = x^{\mathrm{T}} A^{\mathrm{T}} A x = (Ax)^{\mathrm{T}} (Ax) = ||Ax||^2.$$

- The energy is the length squared of the vector Ax
- This energy is positive provided Ax is not the zero vector
  - the columns of A must be independent

$$S = A^{\mathrm{T}} A = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{bmatrix} = \begin{bmatrix} 2 & 3 & 4 \\ 3 & 5 & 7 \\ 4 & 7 & 10 \end{bmatrix} \text{ is } \textbf{not} \text{ positive definite.}$$

Semi definite

$$S = A^{\mathrm{T}}A = \begin{bmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{bmatrix} = \begin{bmatrix} 2 & 3 & 4 \\ 3 & 5 & 7 \\ 4 & 7 & 10 \end{bmatrix} \text{ is } \textbf{not} \text{ positive definite.}$$

This A has column $1 +$ column $3 = 2$ (column 2). Then $\boldsymbol{x} = (1, -2, 1)$ has zero energy. It is an eigenvector of $A^{\mathrm{T}}A$ with $\lambda = 0$. Then $S = A^{\mathrm{T}}A$ is only positive semidefinite.

Equation (2) says that $A^{\mathrm{T}}A$ is at least *semidefinite*, because $\boldsymbol{x}^{\mathrm{T}}S\boldsymbol{x} = ||A\boldsymbol{x}||^2$ is never negative. ***Semidefinite allows energy / eigenvalues / determinants / pivots of S to be zero.***

connect these two tests (2 and 3) to the S= A^TA

- *elimination = triangular factorization (S = LU).*
- *L* has had 1 's on the diagonal and *U* contained the pivots

$$\begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix} = \begin{bmatrix} 1 & & \\ -\frac{1}{2} & 1 & \\ 0 & -\frac{2}{3} & 1 \end{bmatrix} \begin{bmatrix} 2 & -1 & 0 \\ & \frac{3}{2} & -1 \\ & & \frac{4}{3} \end{bmatrix} \qquad \boldsymbol{S = LU} \quad (3)$$

$$\begin{array}{c}\text{pull out} \\ \text{the pivots} \\ \text{in } D\end{array} = \begin{bmatrix} 1 & & \\ -\frac{1}{2} & 1 & \\ 0 & -\frac{2}{3} & 1 \end{bmatrix} \begin{bmatrix} \mathbf{2} & & \\ & \mathbf{\frac{3}{2}} & \\ & & \mathbf{\frac{4}{3}} \end{bmatrix} \begin{bmatrix} 1 & -\frac{1}{2} & 0 \\ & 1 & -\frac{2}{3} \\ & & 1 \end{bmatrix} = \boldsymbol{LDL^{\mathrm{T}}} \quad (4)$$

$$\begin{array}{c}\textbf{share those pivots} \\ \textbf{between } \boldsymbol{A^{\mathrm{T}}} \textbf{ and } \boldsymbol{A}\end{array} = \begin{bmatrix} \sqrt{2} & & \\ -\sqrt{\frac{1}{2}} & \sqrt{\frac{3}{2}} & \\ 0 & -\sqrt{\frac{2}{3}} & \sqrt{\frac{4}{3}} \end{bmatrix} \begin{bmatrix} \sqrt{2} & -\sqrt{\frac{1}{2}} & 0 \\ & \sqrt{\frac{3}{2}} & -\sqrt{\frac{2}{3}} \\ & & \sqrt{\frac{4}{3}} \end{bmatrix} = \boldsymbol{A^{\mathrm{T}}A} \quad (5)$$

Test $S = A^T A$

- Two Special Choices for A

1 If $S = Q\Lambda Q^{\mathrm{T}}$, take square roots of those eigenvalues. Then $A = Q\sqrt{\Lambda}Q^{\mathrm{T}} = A^{\mathrm{T}}$.

2 If $S = LU = LDL^{\mathrm{T}}$ with positive pivots in D, then $S = (L\sqrt{D})(\sqrt{D}L^{\mathrm{T}})$.

Elimination factors every positive definite S into $A^{\mathrm{T}}A$ (A is upper triangular)

This is the Cholesky factorization $S = A^{\mathrm{T}}A$ with $\sqrt{\text{pivots}}$ on the main diagonal of A.

(Cholesky Decomposition)**.** *A symmetric, positive definite matrix* A *can be factorized into a product* $A = LL^T$, *where* L *is a lowertriangular matrix with positive diagonal elements*

For which numbers b and c are these matrices positive definite?

$$S = \begin{bmatrix} 1 & b \\ b & 9 \end{bmatrix} \qquad S = \begin{bmatrix} 2 & 4 \\ 4 & c \end{bmatrix} \qquad S = \begin{bmatrix} c & b \\ b & c \end{bmatrix}.$$

Which symmetric matrices S are also orthogonal? Then $S^{\mathrm{T}} = S$ and $S^{\mathrm{T}} = S^{-1}$.

(a) Show how symmetry and orthogonality lead to $S^2 = I$.

(b) What are the possible eigenvalues of S? Describe all possible Λ.

If S is symmetric, show that $A^{\mathrm{T}}SA$ is also symmetric

- Show that if S is SPD then $A^T SA$ is SPD