

Mathematics for Computer Science

Linear Algebra (Part 2)

Spectral Decomposition

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Thanks to Andrei Krokhin and William Moses for use of slides.

Outline

- 1 Plan for Today
- 2 Orthogonal Matrices
- 3 Orthogonal Diagonalisation
- 4 Spectral Decomposition of Symmetric Matrices
- 5 Wrapping Things Up

Contents for Today's Lecture

- Orthogonal matrices: definition, properties, and characterisations
- Orthogonal diagonalisation: a characterisation and an algorithm
- Spectral decomposition

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Before we continue, reminder of earlier learned concepts.

Reminder from Earlier Lectures

- **Orthonormal** = consisting of unit vectors, which are pairwise orthogonal
- Every finite-dimensional inner product space V has an **orthonormal basis**, which can be constructed from any basis of V via the Gram-Schmidt process.
- For any column vectors \mathbf{u} and \mathbf{v} in \mathbb{R}^n with Euclidean inner product, we have

$$\langle \mathbf{u}, \mathbf{v} \rangle = \mathbf{u}^T \mathbf{v}.$$

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Orthogonal Matrices: Definition

Definition

A square matrix Q is called **orthogonal** if $Q^T = Q^{-1}$ (equivalently, $Q^T Q = I$).

Example: Rotation and reflection matrices in \mathbb{R}^2 are orthogonal. Easy to check:

$$\begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}^{-1} = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix}$$

$$\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}^{-1} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

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Example: All permutation matrices are orthogonal.

Rows and Columns in Orthogonal Matrices

Theorem

For any $n \times n$ matrix Q , the following are equivalent:

- ① *Q is orthogonal.*
- ② *The rows of Q form an orthonormal basis in \mathbb{R}^n (with the Euclidean inner product).*
- ③ *The columns of Q form an orthonormal basis in \mathbb{R}^n (with the Euclidean inner product).*

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Proof.

We prove $(1) \Leftrightarrow (3)$, the proof of $(1) \Leftrightarrow (2)$ is similar.

If $Q = [\mathbf{u}_1 | \dots | \mathbf{u}_n]$ then each entry (i, j) in the product $Q^T Q$ is $\langle \mathbf{u}_i, \mathbf{u}_j \rangle$.

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Hence, $Q^T Q = I$ iff we have $\langle \mathbf{u}_i, \mathbf{u}_j \rangle = 0$ for all $i \neq j$ and $\langle \mathbf{u}_i, \mathbf{u}_i \rangle = 1$ for all i , which holds iff the set $\{\mathbf{u}_1, \dots, \mathbf{u}_n\}$ is orthonormal.

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Any orthonormal set with n vectors in \mathbb{R}^n is a basis. □

Properties of Orthogonal Matrices

Theorem

- ① *The transpose of an orthogonal matrix is also orthogonal.*
- ② *The inverse of an orthogonal matrix is also orthogonal.*
- ③ *A product of orthogonal matrices is also orthogonal.*
- ④ *If Q is orthogonal then $\det(Q) = 1$ or $\det(Q) = -1$.*

All four proofs are easy (one-line) exercises.

Orthogonal Matrices as Linear Operators

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For any $n \times n$ matrix Q , the following are equivalent:

- ❶ *Q is orthogonal.*
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- ❸ *$\langle Q\mathbf{x}, Q\mathbf{y} \rangle = \langle \mathbf{x}, \mathbf{y} \rangle$ for all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$.*

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Proof

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$$2 = \|\mathbf{e}_i + \mathbf{e}_i\|^2 = \|Q(\mathbf{e}_i + \mathbf{e}_i)\|^2 = \|Q\mathbf{e}_i + Q\mathbf{e}_i\|^2 = \langle Q\mathbf{e}_i + Q\mathbf{e}_i, Q\mathbf{e}_i + Q\mathbf{e}_i \rangle =$$

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Orthogonal Diagonalisation

Let A and B be $n \times n$ matrices. **Recall:**

- A and B are similar if there is an invertible matrix P such that $P^{-1}AP = B$.
- If B above can be chosen to be diagonal then we say that A is diagonalisable and that P diagonalises A .
- We proved: A is diagonalisable iff it has n linearly independent eigenvectors.

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If, in addition, P **can be chosen to be orthogonal** then we say, respectively, that

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Question: Which matrices are orthogonally diagonalisable?

The Spectral Theorem

Theorem (Spectral theorem)

For any $n \times n$ matrix A , the following are equivalent:

- ① *A is orthogonally diagonalisable,
i.e., $A = QDQ^T$ for some orthogonal matrix Q and some diagonal matrix D .*
- ② *A has an orthonormal set of n eigenvectors.*
- ③ *A is symmetric.*

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$(3) \Rightarrow (1)$ Proof is omitted. □

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$$\begin{aligned}\lambda_1 \langle \mathbf{u}_1, \mathbf{u}_2 \rangle &= \langle \lambda_1 \mathbf{u}_1, \mathbf{u}_2 \rangle = \langle A\mathbf{u}_1, \mathbf{u}_2 \rangle = (A\mathbf{u}_1)^T \mathbf{u}_2 = \\ \mathbf{u}_1^T A^T \mathbf{u}_2 &= \mathbf{u}_1^T A \mathbf{u}_2 = \langle \mathbf{u}_1, A\mathbf{u}_2 \rangle = \langle \mathbf{u}_1, \lambda_2 \mathbf{u}_2 \rangle = \lambda_2 \langle \mathbf{u}_1, \mathbf{u}_2 \rangle.\end{aligned}$$

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Since $(\lambda_1 - \lambda_2) \langle \mathbf{u}_1, \mathbf{u}_2 \rangle = 0$ and $\lambda_1 \neq \lambda_2$, we get $\langle \mathbf{u}_1, \mathbf{u}_2 \rangle = 0$, as required. □

How to Orthogonally Diagonalise a Symmetric Matrix

Algorithm (assuming A is symmetric):

Step 1. Find the eigenvalues and a basis in each eigenspace of A .

Step 2. Apply Gram-Schmidt to each basis to obtain an orthonormal basis for each eigenspace.

Step 3. Form the matrix Q whose columns are the vectors found in Step 2. Q will orthogonally diagonalise A and the diagonal of $D = Q^T A Q$ contains the eigenvalues of A in the same order as eigenvectors in Q .

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Remarks:

- Steps 1 and 3 were also part of the (general) diagonalisation algorithm.
- The columns of Q will form an orthonormal set because eigenvectors from different eigenspaces are orthogonal (and the rest is guaranteed by Step 2).
- This algorithm applies only to symmetric matrices and always returns a diagonalisation, unlike the general diagonalisation algorithm (which applies to arbitrary square matrices and can return “not diagonalisable”).

Example

Orthogonally diagonalise $A = \begin{pmatrix} 4 & 2 & 2 \\ 2 & 4 & 2 \\ 2 & 2 & 4 \end{pmatrix}$.

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Step 1. Find the eigenvalues of A : $\lambda_1 = 2$ and $\lambda_2 = 8$.

Find bases for the eigenspaces: $\{\mathbf{u}_1 = (-1, 1, 0), \mathbf{u}_2 = (-1, 0, 1)\}$ for $\lambda_1 = 2$ and $\{\mathbf{u}_3 = (1, 1, 1)\}$ for $\lambda_2 = 8$.

Step 2. Apply Gram-Schmidt to $\{\mathbf{u}_1, \mathbf{u}_2\}$ to get an orthonormal basis for $\text{span}(\mathbf{u}_1, \mathbf{u}_2)$: $\mathbf{v}_1 = (-1/\sqrt{2}, 1/\sqrt{2}, 0)$ and $\mathbf{v}_2 = (-1/\sqrt{6}, -1/\sqrt{6}, 2/\sqrt{6})$.

Apply G-S to (i.e., normalise) $\mathbf{u}_3 = (1, 1, 1)$ to get $\mathbf{v}_3 = (1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$.

Step 3. Form the matrix Q . We have

$$Q = \begin{pmatrix} -1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{3} \\ 1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{3} \\ 0 & 2/\sqrt{6} & 1/\sqrt{3} \end{pmatrix} \quad \text{and} \quad Q^T A Q = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 8 \end{pmatrix}$$

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$$\begin{aligned} A = QDQ^T &= (\mathbf{u}_1 | \dots | \mathbf{u}_n) \begin{pmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_n \end{pmatrix} \begin{pmatrix} \mathbf{u}_1^T \\ \mathbf{u}_2^T \\ \vdots \\ \mathbf{u}_n^T \end{pmatrix} = \\ &(\lambda_1 \mathbf{u}_1 | \dots | \lambda_n \mathbf{u}_n) \begin{pmatrix} \mathbf{u}_1^T \\ \mathbf{u}_2^T \\ \vdots \\ \mathbf{u}_n^T \end{pmatrix} = \lambda_1 \mathbf{u}_1 \mathbf{u}_1^T + \lambda_2 \mathbf{u}_2 \mathbf{u}_2^T + \dots + \lambda_n \mathbf{u}_n \mathbf{u}_n^T. \end{aligned}$$

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$$A = QDQ^T = (\mathbf{u}_1 | \dots | \mathbf{u}_n) \begin{pmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_n \end{pmatrix} \begin{pmatrix} \mathbf{u}_1^T \\ \mathbf{u}_2^T \\ \vdots \\ \mathbf{u}_n^T \end{pmatrix} =$$
$$(\lambda_1 \mathbf{u}_1 | \dots | \lambda_n \mathbf{u}_n) \begin{pmatrix} \mathbf{u}_1^T \\ \mathbf{u}_2^T \\ \vdots \\ \mathbf{u}_n^T \end{pmatrix} = \lambda_1 \mathbf{u}_1 \mathbf{u}_1^T + \lambda_2 \mathbf{u}_2 \mathbf{u}_2^T + \dots + \lambda_n \mathbf{u}_n \mathbf{u}_n^T.$$

Theorem (Spectral Decomposition)

Let A be a symmetric $n \times n$ matrix. With the \mathbf{u}_i 's and the λ_i 's as above,

$$A = \lambda_1 \mathbf{u}_1 \mathbf{u}_1^T + \lambda_2 \mathbf{u}_2 \mathbf{u}_2^T + \dots + \lambda_n \mathbf{u}_n \mathbf{u}_n^T.$$

Geometric Interpretation of Spectral Decomposition

Consider the matrix transformation T_A corresponding to a symmetric matrix A :

$$T_A(\mathbf{x}) = A\mathbf{x} = (\lambda_1 \mathbf{u}_1 \mathbf{u}_1^T + \lambda_2 \mathbf{u}_2 \mathbf{u}_2^T + \dots + \lambda_n \mathbf{u}_n \mathbf{u}_n^T) \mathbf{x}.$$

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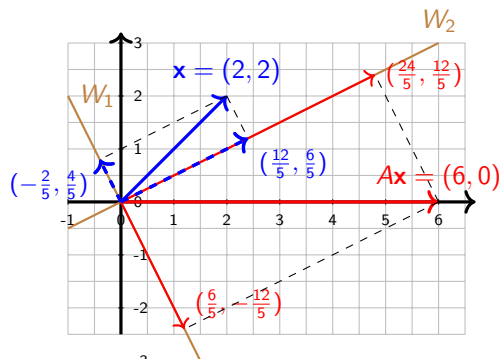
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$$A = \begin{pmatrix} 1 & 2 \\ 2 & -2 \end{pmatrix}$$

$$\lambda_1 = -3, \quad \lambda_2 = 2$$

$$\mathbf{u}_1 = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 \\ -2 \end{pmatrix}, \quad \mathbf{u}_2 = \frac{1}{\sqrt{5}} \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$

Outline

- 1 Plan for Today
- 2 Orthogonal Matrices
- 3 Orthogonal Diagonalisation
- 4 Spectral Decomposition of Symmetric Matrices
- 5 Wrapping Things Up

Wrapping Things Up

Today:

- Orthogonal matrices, their characterisations and properties
- Spectral theorem: Orthogonally diagonalisable = symmetric
- Eigen-properties of symmetric matrices
- Spectral decomposition for symmetric matrices

The End