

Mathematics for Machine Learning

— Linear Algebra: Eigenvalues, Eigenvectors, Eigenspaces, Cholesky Decomposition & Diagonalization

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Credits for the resource

- The slides are based on the textbooks:
 - *Marc Peter Deisenroth, A. Aldo Faisal, and Cheng Soon Ong: Mathematics for Machine Learning. Cambridge University Press. 2020.*
 - *Howard Anton, Chris Rorres, Anton Kaul: Elementary Linear Algebra. Wiley. 2019.*
- We could partially refer to the monograph:
Francesco Orabona: A Modern Introduction to Online Learning.
<https://arxiv.org/abs/1912.13213>

- Matrix decomposition or matrix factorization.

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- Three matrix decompositions will be introduced.

Outline

- 1 Eigenvalues & Eigenvectors
- 2 Cholesky Decomposition
- 3 Eigendecomposition & Diagonalization

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Characteristic Polynomial

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For $\lambda \in \mathbb{R}$ and a square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$,

$$\begin{aligned} p_{\mathbf{A}}(\lambda) &:= \det(\mathbf{A} - \lambda \mathbf{I}) \\ &= (-1)^n (\lambda - \lambda_1) \cdots (\lambda - \lambda_n) \\ &= c_0 + c_1 \lambda + \cdots + c_{n-1} \lambda^{n-1} + (-1)^n \lambda^n, \end{aligned}$$

for $c_0, \dots, c_{n-1} \in \mathbb{R}$, is called the **characteristic polynomial** of \mathbf{A} .

Note that

- $c_0 = \det(\mathbf{A})$

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back

Example

Given $\mathbf{A} = \begin{bmatrix} 3 & 0 \\ 8 & -1 \end{bmatrix}$,

$$\det(\mathbf{A} - \lambda \mathbf{I}) = \begin{vmatrix} 3 - \lambda & 0 \\ 8 & -1 - \lambda \end{vmatrix} = (3 - \lambda)(-1 - \lambda).$$

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Given $\mathbf{B} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 4 & -17 & 8 \end{bmatrix}$,

$$\det(\mathbf{B} - \lambda \mathbf{I}) = \begin{vmatrix} -\lambda & 1 & 0 \\ 0 & -\lambda & 1 \\ 4 & -17 & 8 - \lambda \end{vmatrix} = -\lambda^3 + 8\lambda^2 - 17\lambda + 4.$$

Eigenvalue Equation

Eigenvalues & Eigenvectors

Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ be a square matrix. Then

- $\lambda \in \mathbb{R}$ is an **eigenvalue** of \mathbf{A} and
- $\mathbf{x} \in \mathbb{R}^n \setminus \{\mathbf{0}\}$ is the corresponding **eigenvector** of \mathbf{A}

if $\mathbf{Ax} = \lambda\mathbf{x}$.

$$\mathbf{Ax} = \lambda\mathbf{x} \iff (\mathbf{A} - \lambda\mathbf{I})\mathbf{x} = \mathbf{0}$$

Equivalent statements:

- λ is an eigenvalue of $\mathbf{A} \in \mathbb{R}^{n \times n}$.
- There exists an $\mathbf{x} \in \mathbb{R}^n \setminus \{\mathbf{0}\}$ with $\mathbf{Ax} = \lambda \mathbf{x}$ (i.e., $(\mathbf{A} - \lambda \mathbf{I}_n)\mathbf{x} = \mathbf{0}$) that can be solved non-trivially (i.e., $\mathbf{x} \neq \mathbf{0}$).
- $\text{rank}(\mathbf{A} - \lambda \mathbf{I}_n) < n$.
- $\det(\mathbf{A} - \lambda \mathbf{I}_n) = 0$.

Remark

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- Suppose \mathbf{x} is an eigenvector of \mathbf{A} w.r.t. eigenvalue λ , then for any $c \in \mathbb{R} \setminus \mathbf{0}$

$$\mathbf{A}(c\mathbf{x}) = c\mathbf{A}\mathbf{x} = c\lambda\mathbf{x} = \lambda(c\mathbf{x}).$$

Theorems (or Definitions)

Theorem

$\lambda \in \mathbb{R}$ is an eigenvalue of $\mathbf{A} \in \mathbb{R}^{n \times n}$ if and only if λ is a root of the characteristic polynomial $p_{\mathbf{A}}(\lambda)$ of \mathbf{A} .

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Algebraic Multiplicity

Suppose that matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ has an eigenvalue λ_i . The **algebraic multiplicity** of λ_i is the number of times the root appears in the characteristic polynomial.

- Denoted by $\text{am}(\lambda_i)$

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Theorems (or Definitions)

Eigenspace

For $\mathbf{A} \in \mathbb{R}^{n \times n}$, the set of all eigenvectors of \mathbf{A} associated with the eigenvalue λ spans the **eigenspace** of \mathbf{A} (denoted by E_λ).

Geometric Multiplicity

$\dim(E_\lambda)$ is called the **geometric multiplicity** of λ .

- Denoted by $\text{gm}(\lambda)$.

Eigenspectrum (Spectrum)

The set of all eigenvalues of \mathbf{A} is called the **eigenspectrum** (or spectrum) of \mathbf{A} .

Relation b/w $\text{am}(\lambda)$ & $\text{gm}(\lambda)$

Geometric multiplicity \leq Algebraic multiplicity

Given $\mathbf{A} \in \mathbb{R}^{n \times n}$ and assume that λ is a eigenvalue of \mathbf{A} , then

$$\text{gm}(\lambda) \leq \text{am}(\lambda).$$

- Assume that $\dim(E_\lambda) = k \leq n$ and let $\{\mathbf{v}_1, \dots, \mathbf{v}_k\}$ is a basis of E_λ such that $\mathbf{v}_1, \dots, \mathbf{v}_k$ are eigenvectors w.r.t. λ .

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- $\exists \mathbf{v}_{k+1}, \dots, \mathbf{v}_n$ such that $\{\mathbf{v}_1, \dots, \mathbf{v}_n\}$ is a basis of \mathbb{R}^n .

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- $\exists \mathbf{v}_{k+1}, \dots, \mathbf{v}_n$ such that $\{\mathbf{v}_1, \dots, \mathbf{v}_n\}$ is a basis of \mathbb{R}^n .
- Denote by $\mathbf{P} = [\mathbf{U} \ \mathbf{V}]$ for $\mathbf{U} = [\mathbf{v}_1 \cdots \mathbf{v}_k]$ and $\mathbf{V} = [\mathbf{v}_{k+1} \cdots \mathbf{v}_n]$ (note: \mathbf{P} is invertible).

Relation b/w $\text{am}(\lambda)$ & $\text{gm}(\lambda)$ (contd.)

- $\because \mathbf{P}$ is invertible \Rightarrow Let $\mathbf{P}^{-1} = \begin{bmatrix} \mathbf{X} \\ \mathbf{Y} \end{bmatrix}$, where $\mathbf{X} \in \mathbb{R}^{k \times n}$ and $\mathbf{Y} \in \mathbb{R}^{(n-k) \times n}$.

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- $\because P$ is invertible \Rightarrow Let $P^{-1} = \begin{bmatrix} X \\ Y \end{bmatrix}$, where $X \in \mathbb{R}^{k \times n}$ and $Y \in \mathbb{R}^{(n-k) \times n}$.
- Then,

$$\begin{bmatrix} I_k & O \\ O & I_{n-k} \end{bmatrix} = P^{-1}P = \begin{bmatrix} X \\ Y \end{bmatrix} [U \ V] = \begin{bmatrix} XU & XV \\ YU & YV \end{bmatrix}$$

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- Then,

$$\begin{bmatrix} \mathbf{I}_k & \mathbf{O} \\ \mathbf{O} & \mathbf{I}_{n-k} \end{bmatrix} = \mathbf{P}^{-1}\mathbf{P} = \begin{bmatrix} \mathbf{X} \\ \mathbf{Y} \end{bmatrix} [\mathbf{U} \ \mathbf{V}] = \begin{bmatrix} \mathbf{XU} & \mathbf{XV} \\ \mathbf{YU} & \mathbf{YV} \end{bmatrix}$$

- Note that $\mathbf{AU} = \mathbf{A}[\mathbf{v}_1 \cdots \mathbf{v}_k] = [\mathbf{Av}_1 \cdots \mathbf{Av}_k] = [\lambda \mathbf{v}_1 \cdots \lambda \mathbf{v}_k] = \lambda \mathbf{U}$.

Relation b/w $\text{am}(\lambda)$ & $\text{gm}(\lambda)$ (contd.)

$$P^{-1}AP = \begin{bmatrix} X \\ Y \end{bmatrix} A[U \ V] = \begin{bmatrix} XAU & XAV \\ YAU & YAV \end{bmatrix}$$

Relation b/w $\text{am}(\lambda)$ & $\text{gm}(\lambda)$ (contd.)

$$\begin{aligned} P^{-1}AP &= \begin{bmatrix} X \\ Y \end{bmatrix} A \begin{bmatrix} U & V \end{bmatrix} = \begin{bmatrix} XAU & XAV \\ YAU & YAV \end{bmatrix} \\ &= \begin{bmatrix} \lambda XU & XAV \\ \lambda YU & YAV \end{bmatrix} = \begin{bmatrix} \lambda I_k & XAV \\ \mathbf{0} & YAV \end{bmatrix} \end{aligned}$$

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 \end{aligned}$$

$$\det(P^{-1}AP - zI) = \det \begin{bmatrix} \lambda I_k - zI_k & XAV \\ \mathbf{0} & YAV - zI_{n-k} \end{bmatrix}$$

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 \det(P^{-1}AP - zI) &= \det \begin{bmatrix} \lambda I_k - zI_k & XAV \\ \mathbf{O} & YAV - zI_{n-k} \end{bmatrix} \\
 &= (\lambda - z)^k \det(YAV - zI_{n-k}).
 \end{aligned}$$

- Note: $\det(A - zI) = \det(P^{-1}AP - zI)$.

Remark

$$\begin{aligned}P^{-1}AP - zI &= P^{-1}AP - zP^{-1}P \\&= P^{-1}AP - P^{-1}(zI)P \\&= P^{-1}(A - zI)P.\end{aligned}$$

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Therefore,

$$\det(\mathbf{A} - z\mathbf{I}) = \det(\mathbf{P}^{-1}\mathbf{A}\mathbf{P} - z\mathbf{I}).$$

The Case of the Identity Matrix

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For $I_n \in \mathbb{R}^{n \times n}$,

- what is $p_I(\lambda)$?
- What are its eigenvalues and the associated eigenvectors?
- What are the eigenspaces?

Useful Properties (1/4)

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- Symmetric, positive definite matrices always have positive, real eigenvalues.
 - $\mathbf{x}^\top \mathbf{Ax} = \mathbf{x}^\top \lambda \mathbf{x} = \lambda \|\mathbf{x}\|^2 > 0$.

Useful Properties (2/4)

Theorem (4.13)

The eigenvectors $\mathbf{x}_1, \dots, \mathbf{x}_n$ of a matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ with n distinct eigenvalues $\lambda_1, \dots, \lambda_n$ are linearly independent.

Theorem (4.14)

Given a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$, we can always obtain a symmetric, positive semidefinite matrix $\mathbf{S} \in \mathbb{R}^{n \times n}$ by defining

$$\mathbf{S} := \mathbf{A}^\top \mathbf{A}.$$

If $\text{rank}(\mathbf{A}) = n$, then $\mathbf{S} := \mathbf{A}^\top \mathbf{A}$ is symmetric, positive definite.

Useful Properties (3/4)

Theorem

If \mathbf{A} is symmetric, then eigenvectors to different eigenvalues are orthogonal.

Proof.

- Assume that $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$ and $\mathbf{A}\mathbf{w} = \mu\mathbf{w}$ for two eigenvectors $\mathbf{v}, \mathbf{w} \in V$ corresponding to eigenvalues λ and μ such that $\lambda \neq \mu$.
- $$\begin{aligned}\lambda\langle\mathbf{v}, \mathbf{w}\rangle &= \langle\lambda\mathbf{v}, \mathbf{w}\rangle = \langle\mathbf{A}\mathbf{v}, \mathbf{w}\rangle = (\mathbf{A}\mathbf{v})^\top \mathbf{w} = \mathbf{v}^\top \mathbf{A}^\top \mathbf{w} = \langle\mathbf{v}, \mathbf{A}^\top \mathbf{w}\rangle \\ &= \langle\mathbf{v}, \mathbf{A}\mathbf{w}\rangle = \langle\mathbf{v}, \mu\mathbf{w}\rangle = \mu\langle\mathbf{v}, \mathbf{w}\rangle.\end{aligned}$$

The equalities hold only if $\langle\mathbf{v}, \mathbf{w}\rangle = 0$.



Useful Properties (4/4)

Theorem (4.15; Spectral Theorem)

If $\mathbf{A} \in \mathbb{R}^{n \times n}$ is symmetric, then there exists an orthonormal basis, consisting of eigenvectors of \mathbf{A} , of the corresponding vector space V , and each eigenvalue is real.

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Theorem (4.16)

For a matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$, we have $\det(\mathbf{A}) = \prod_{i=1}^n \lambda_i$, where λ_i 's are the eigenvalues of \mathbf{A} .

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Theorem (4.17)

For a matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$, we have $\text{tr}(\mathbf{A}) = \sum_{i=1}^n \lambda_i$, where λ_i 's are the eigenvalues of \mathbf{A} recall?.

A Practical Example

- Google uses the eigenvector corresponding to the maximal eigenvalue of a matrix \mathbf{A} to determine the rank of a page for search.
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- Compute the weight (importance) $x_i \geq 0$ for a website a_i and get \mathbf{x} .
 - The number of pages pointing to a_i .
- A transition matrix \mathbf{A} (prob.): modeling the navigation behavior of a user.
- **Goal:** $\mathbf{x}, \mathbf{Ax}, \mathbf{A}^2\mathbf{x}, \dots, \mathbf{x}^*$

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- **Goal:** $\mathbf{x}, \mathbf{Ax}, \mathbf{A}^2\mathbf{x}, \dots, \mathbf{x}^* \Rightarrow \mathbf{Ax}^* = \mathbf{x}^* \Rightarrow$ Turning to probabilities (normalization).

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Cholesky Decomposition

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A symmetric, positive definite matrix \mathbf{A} can be factorized into a product $\mathbf{A} = \mathbf{L}\mathbf{L}^\top$, where \mathbf{L} is a lower-triangular matrix with positive diagonal elements.

$$\begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{bmatrix} = \begin{bmatrix} \text{red triangle} \\ \text{red triangle} \\ \text{red triangle} \end{bmatrix} \begin{bmatrix} \text{green triangle} \\ \text{green triangle} \\ \text{green triangle} \end{bmatrix}$$

Example of Cholesky Factorization

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{21} & a_{31} \\ a_{21} & a_{22} & a_{32} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \mathbf{L}\mathbf{L}^T = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} l_{11} & l_{21} & l_{31} \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{bmatrix}.$$

We have

$$\mathbf{A} = \begin{bmatrix} l_{11}^2 & l_{21}l_{11} & l_{31}l_{11} \\ l_{21}l_{11} & l_{21}^2 + l_{22}^2 & l_{31}l_{21} + l_{32}l_{22} \\ l_{31}l_{11} & l_{31}l_{21} + l_{32}l_{22} & l_{31}^2 + l_{32}^2 + l_{33}^2 \end{bmatrix}$$

Finally, solve l_{11}, \dots, l_{33} .

Motivations of Using Cholesky Decomposition

- Symmetric positive definite matrices require frequent manipulation.
 - E.g., Covariance matrix of a multivariate Gaussian variable.
 - The Cholesky factorization of the covariance matrix allows us to **generate samples from a Gaussian distribution**.
- Computing gradients in deep stochastic models such as variational auto-encoder (VAE).

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- Computing gradients in deep stochastic models such as variational auto-encoder (VAE).
- Compute determinants efficiently.
 - $\det(\mathbf{A}) = \det(\mathbf{L}) \det(\mathbf{L}^\top) = \det(\mathbf{L})^2$.
 - Note: $\det(\mathbf{L})$ can be computed efficiently (\because triangular).

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$$\mathbf{D} = \begin{bmatrix} c_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & c_n \end{bmatrix}.$$

- **Question:** What are the determinant, cubic, and inverse of \mathbf{D} ?

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Two matrices \mathbf{A} and $\mathbf{B} \in \mathbb{R}^{n \times n}$ are **similar** if there exists an invertible matrix $\mathbf{S} \in \mathbb{R}^{n \times n}$ such that $\mathbf{A} = \mathbf{S}^{-1}\mathbf{B}\mathbf{S}$.

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Diagonalizable

A matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ is **diagonalizable** if it is *similar* to a *diagonal* matrix..

- $\exists \mathbf{D} \in \mathbb{R}^{n \times n}$, such that $\mathbf{D} = \mathbf{P}^{-1}\mathbf{A}\mathbf{P}$.

Eigenvectors & Diagonalization

- Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ and $\lambda_1, \dots, \lambda_n$ be a set of scalars.
- Let $\mathbf{p}_1, \dots, \mathbf{p}_n$ be a set of vectors in \mathbb{R}^n .
- Let $\mathbf{D} \in \mathbb{R}^{n \times n}$ be a diagonal matrix with diagonal entries $\lambda_1, \dots, \lambda_n$.

We can show that

$$\mathbf{A}\mathbf{P} = \mathbf{P}\mathbf{D}.$$

if and only if $\lambda_1, \dots, \lambda_n$ are the eigenvalues of \mathbf{A} and $\mathbf{p}_1, \dots, \mathbf{p}_n$ are the corresponding eigenvectors of \mathbf{A} .

Proof of the Claim

We can see that

$$\mathbf{AP} = \mathbf{A}[\mathbf{p}_1, \dots, \mathbf{p}_n] = [\mathbf{A}\mathbf{p}_1, \dots, \mathbf{A}\mathbf{p}_n],$$

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and

$$\mathbf{P}\mathbf{D} = [\mathbf{p}_1, \dots, \mathbf{p}_n] \begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix} = [\lambda_1 \mathbf{p}_1, \dots, \lambda_n \mathbf{p}_n].$$

Thus,

$$\mathbf{A}\mathbf{p}_1 = \lambda_1 \mathbf{p}_1$$

$$\vdots$$

$$\mathbf{A}\mathbf{p}_n = \lambda_n \mathbf{p}_n$$

Therefore, the columns of \mathbf{P} are eigenvectors of \mathbf{A} .

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$$\alpha_1(\lambda_1 - \lambda_n) \mathbf{p}_1 + \alpha_2(\lambda_2 - \lambda_n) \mathbf{p}_2 + \dots + \alpha_{n-1}(\lambda_{n-1} - \lambda_n) \mathbf{p}_{n-1} = \mathbf{0}.$$

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- $\therefore \alpha_1 = \alpha_2 = \dots = \alpha_n = 0$.

Eigendecomposition

Theorem [Eigendecomposition]

A square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ can be factored into

$$\mathbf{A} = \mathbf{P}\mathbf{D}\mathbf{P}^{-1},$$

where $\mathbf{P} \in \mathbb{R}^{n \times n}$ and \mathbf{D} is a diagonal matrix whose diagonal entries are the eigenvalues of \mathbf{A}

if and only if

the eigenvectors of \mathbf{A} form a basis of \mathbb{R}^n .

Put it concisely

Theorem

For a square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$, the following statements are equivalent:

- \mathbf{A} is diagonalizable.
- \mathbf{A} has n linearly independent eigenvectors.

Remark

The spectral theorem tells us that:

We can find an orthonormal basis of the corresponding vector space consisting of eigenvectors of a symmetric matrix $\mathbf{S} \in \mathbb{R}^{n \times n}$.

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Theorem

A symmetric matrix $\mathbf{S} \in \mathbb{R}^{n \times n}$ can be always diagonalized.

Example

Compute the eigendecomposition of $\mathbf{A} = \frac{1}{2} \begin{bmatrix} 5 & -2 \\ -2 & 5 \end{bmatrix}$.

- 1 Compute the eigenvalues and eigenvectors.

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Set $\lambda_1 = \frac{7}{2}, \lambda_2 = \frac{3}{2}$.

- 2 Solving $\mathbf{A}\mathbf{p}_1 = \frac{7}{2}\mathbf{p}_1$ and $\mathbf{A}\mathbf{p}_2 = \frac{3}{2}\mathbf{p}_2$.

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$$\mathbf{p}_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \quad \mathbf{p}_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

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★ Note that $\{\mathbf{p}_1, \mathbf{p}_2\}$ forms an **orthonormal basis**

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Finally we obtain $\mathbf{A} = \mathbf{P}\mathbf{D}\mathbf{P}^{-1}$.

Remark On the Efficiency

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Another Application: Using Maclaurin Series

Maclaurin Series

A Maclaurin Series expansion of $f(x)$ is

$$f(x) = f(0) + f'(0)x + \frac{f''(0)}{2!}x^2 + \frac{f^{(3)}(0)}{3!}x^3 + \cdots + \frac{f^{(n)}(0)}{n!}x^n + \cdots$$

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Discussions