Mathematical foundations - linear algebra

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Machine Learning

Vector space

Definition (over reals)

A set $\mathcal{X}$ is called a *vector space* over $\mathbb{R}$ if addition and scalar multiplication are defined and satisfy for all $\mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathcal{X}$ and $\lambda, \mu \in \mathbb{R}$:

- Addition:

  associative $\mathbf{x} + (\mathbf{y} + \mathbf{z}) = (\mathbf{x} + \mathbf{y}) + \mathbf{z}$
  commutative $\mathbf{x} + \mathbf{y} = \mathbf{y} + \mathbf{x}$
  identity element $\exists \mathbf{0} \in \mathcal{X} : \mathbf{x} + \mathbf{0} = \mathbf{x}$
  inverse element $\forall \mathbf{x} \in \mathcal{X}\ \exists \mathbf{x}' \in \mathcal{X} : \mathbf{x} + \mathbf{x}' = \mathbf{0}$

- Scalar multiplication:

  distributive over elements $\lambda(\mathbf{x} + \mathbf{y}) = \lambda\mathbf{x} + \lambda\mathbf{y}$
  distributive over scalars $(\lambda + \mu)\mathbf{x} = \lambda\mathbf{x} + \mu\mathbf{x}$
  associative over scalars $\lambda(\mu\mathbf{x}) = (\lambda\mu)\mathbf{x}$
  identity element $\exists 1 \in \mathbb{R} : 1\mathbf{x} = \mathbf{x}$

Properties and operations in vector spaces

subspace Any non-empty subset of $\mathcal{X}$ being itself a vector space (E.g. projection)

linear combination given $\lambda_i \in \mathbb{R}, \mathbf{x}_i \in \mathcal{X}$

$$\sum_{i=1}^{n} \lambda_i \mathbf{x}_i$$

span The span of vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n$ is defined as the set of their linear combinations

$$\left\{ \sum_{i=1}^{n} \lambda_i \mathbf{x}_i, \lambda_i \in \mathbb{R} \right\}$$

Basis in vector space

Linear independency

A set of vectors $\mathbf{x}_i$ is *linearly independent* if none of them can be written as a linear combination of the others

Basis

- A set of vectors $\mathbf{x}_i$ is a *basis* for $\mathcal{X}$ if any element in $\mathcal{X}$ can be *uniquely* written as a linear combination of vectors $\mathbf{x}_i$.
- Necessary condition is that vectors $\mathbf{x}_i$ are linearly independent
- All bases of $\mathcal{X}$ have the same number of elements, called the *dimension* of the vector space.

Linear maps

Definition

Given two vector spaces $\mathcal{X}, \mathcal{Z}$, a function $f : \mathcal{X} \to \mathcal{Z}$ is a *linear map* if for all $\mathbf{x}, \mathbf{y} \in \mathcal{X}$, $\lambda \in \mathbb{R}$:

- $f(\mathbf{x} + \mathbf{y}) = f(\mathbf{x}) + f(\mathbf{y})$
- $f(\lambda \mathbf{x}) = \lambda f(\mathbf{x})$

Linear maps as matrices

A linear map between two finite-dimensional spaces $\mathcal{X}, \mathcal{Z}$ of dimensions n, m can always be written as a matrix:

- Let $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ and $\{\mathbf{z}_1, \ldots, \mathbf{z}_m\}$ be some bases for $\mathcal{X}$ and $\mathcal{Z}$ respectively.
- For any $\mathbf{x} \in \mathcal{X}$ we have:

$$f(\mathbf{x}) = f(\sum_{i=1}^{n} \lambda_i \mathbf{x}_i) = \sum_{i=1}^{n} \lambda_i f(\mathbf{x}_i)$$

$$f(\mathbf{x}_i) = \sum_{j=1}^{m} a_{ji} \mathbf{z}_j$$

$$f(\mathbf{x}) = \sum_{i=1}^{n} \sum_{j=1}^{m} \lambda_i a_{ji} \mathbf{z}_j = \sum_{j=1}^{m} (\sum_{i=1}^{n} \lambda_i a_{ji}) \mathbf{z}_j = \sum_{j=1}^{m} \mu_j \mathbf{z}_j$$

Linear maps as matrices

- Matrix of basis transformation

$$M \in \mathbb{R}^{m \times n} = \begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & \vdots & \vdots \\ a_{m1} & \dots & a_{mn} \end{bmatrix}$$

- Mapping from basis coefficients to basis coefficients

$$M\boldsymbol{\lambda} = \boldsymbol{\mu}$$

Change of Coordinate Matrix

2D example

- let $B = \left\{ \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right\}$ be the standard basis in $\mathbb{R}^2$
- let $B' = \left\{ \begin{bmatrix} 3 \\ 1 \end{bmatrix}, \begin{bmatrix} -2 \\ 1 \end{bmatrix} \right\}$ be an alternative basis
- The change of coordinate matrix from B' to B is:

$$P = \begin{bmatrix} 3 & -2 \\ 1 & 1 \end{bmatrix}$$

- So that:

$$[\mathbf{v}]_B = P \cdot [\mathbf{v}]_{B'} \quad \text{and} \quad [\mathbf{v}]_{B'} = P^{-1} \cdot [\mathbf{v}]_B$$

Note

- For arbitrary B and B', P's columns must be the B' vectors written in terms of the B ones (straightforward here)

Matrix properties

transpose Matrix obtained exchanging rows with columns (indicated with M^T). Properties:

$$(MN)^T = N^T M^T$$

trace Sum of diagonal elements of a matrix

$$tr(M) = \sum_{i=1}^{n} M_{ii}$$

inverse The matrix which multiplied with the original matrix gives the identity

$$MM^{-1} = I$$

rank The rank of an $n \times m$ matrix is the dimension of the space spanned by its columns

Matrix derivatives

$$\frac{\partial M\mathbf{x}}{\partial \mathbf{x}} = M$$
$$\frac{\partial \mathbf{y}^T M\mathbf{x}}{\partial \mathbf{x}} = M^T\mathbf{y}$$
$$\frac{\partial \mathbf{x}^T M\mathbf{x}}{\partial \mathbf{x}} = (M^T + M)\mathbf{x}$$
$$\frac{\partial \mathbf{x}^T M\mathbf{x}}{\partial \mathbf{x}} = 2M\mathbf{x} \quad \text{if M is symmetric}$$
$$\frac{\partial \mathbf{x}^T \mathbf{x}}{\partial \mathbf{x}} = 2\mathbf{x}$$

Note

Results are column vectors. Transpose them if row vectors are needed instead.

Metric structure

Norm

A function $||\cdot|| : \mathcal{X} \to \mathbb{R}_0^+$ is a *norm* if for all $\mathbf{x}, \mathbf{y} \in \mathcal{X}, \lambda \in \mathbb{R}$:

- $||\mathbf{x}+\mathbf{y}|| \leq ||\mathbf{x}|| + ||\mathbf{y}||$
- $||\lambda \mathbf{x}|| = |\lambda| \, ||\mathbf{x}||$
- $||\mathbf{x}|| > 0$ *if* $\mathbf{x} \neq 0$

Metric

A norm defines a metric $d : \mathcal{X} \times \mathcal{X} \to \mathbb{R}_0^+$:

$$d(\mathbf{x}, \mathbf{y}) = ||\mathbf{x} - \mathbf{y}||$$

Note

The concept of norm is stronger than that of metric: not any metric gives rise to a norm

Dot product

Bilinear form

A function $Q : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a *bilinear form* if for all $\mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathcal{X}, \lambda, \mu \in \mathbb{R}$:

- $Q(\lambda\mathbf{x} + \mu\mathbf{y}, \mathbf{z}) = \lambda Q(\mathbf{x}, \mathbf{z}) + \mu Q(\mathbf{y}, \mathbf{z})$
- $Q(\mathbf{x}, \lambda\mathbf{y} + \mu\mathbf{z}) = \lambda Q(\mathbf{x}, \mathbf{y}) + \mu Q(\mathbf{x}, \mathbf{z})$

A bilinear form is *symmetric* if for all $\mathbf{x}, \mathbf{y} \in \mathcal{X}$:

- $Q(\mathbf{x}, \mathbf{y}) = Q(\mathbf{y}, \mathbf{x})$

Dot product

Dot product

A dot product $\langle \cdot, \cdot \rangle : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a symmetric bilinear form which is *positive semi-definite*:

$$\langle \mathbf{x}, \mathbf{x} \rangle \geq 0 \; \forall \, \mathbf{x} \in \mathcal{X}$$

A *positive definite* dot product satisfies

$$\langle \mathbf{x}, \mathbf{x} \rangle = 0 \textit{ iff } \mathbf{x} = \mathbf{0}$$

Norm

Any dot product defines a corresponding norm via:

$$||\mathbf{x}|| = \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle}$$

Properties of dot product

angle The angle θ between two vectors is defined as:

$$cos\theta = \frac{\langle \mathbf{x}, \mathbf{z} \rangle}{||\mathbf{x}||\ ||\mathbf{z}||}$$

orthogonal Two vectors are *orthogonal* if $\langle \mathbf{x}, \mathbf{y} \rangle = 0$

orthonormal A set of vectors $\{\mathbf{x}_1, \dots, \mathbf{x}_n\}$ is *orthonormal* if

$$\langle \mathbf{x}_i, \mathbf{x}_j \rangle = \delta_{ij}$$

where $\delta_{ij} = 1$ if $i = j, 0$ otherwise.

Note

If $\mathbf{x}$ and $\mathbf{y}$ are n-dimensional column vectors, their dot product is computed as:

$$\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^T \mathbf{y} = \sum_{i=1}^{n} x_i y_i$$

Eigenvalues and eigenvectors

Definition

Given an $n \times n$ matrix M, the real value λ and (non-zero) vector $\mathbf{x}$ are an *eigenvalue* and corresponding *eigenvector* of M if

$$M\mathbf{x} = \lambda\mathbf{x}$$

Cardinality

- An $n \times n$ matrix has n eigenvalues (roots of characteristic polynomial)
- An $n \times n$ matrix can have **less than** n **distinct** eigenvalues
- An $n \times n$ matrix can have **less than** n **linear independent** eigenvectors (also fewer then the number of distinct eigenvalues)

Eigenvalues and eigenvectors

Singular matrices

- A matrix is *singular* if it has a zero eigenvalue

$$M\mathbf{x} = 0\mathbf{x} = \mathbf{0}$$

- A singular matrix has linearly dependent columns:

$$\begin{bmatrix} M_1 & \dots & M_{n-1} & M_n \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_{n-1} \\ x_n \end{bmatrix} = \mathbf{0}$$

Eigenvalues and eigenvectors

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$$M_1 x_1 + \cdots + M_{n-1} x_{n-1} + M_n x_n = 0$$

Singular matrices

- A matrix is *singular* if it has a zero eigenvalue

$$M\mathbf{x} = 0\mathbf{x} = \mathbf{0}$$

- A singular matrix has linearly dependent columns:

$$M_n = M_1 \frac{-x_1}{x_n} + \cdots + M_{n-1} \frac{-x_{n-1}}{x_n}$$

Eigenvalues and eigenvectors

Singular matrices

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$$M\mathbf{x} = 0\mathbf{x} = \mathbf{0}$$

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$$M_n = M_1 \frac{-x_1}{x_n} + \cdots + M_{n-1} \frac{-x_{n-1}}{x_n}$$

Determinant

- The *determinant* $|M|$ of a $n \times n$ matrix M is the product of its eigenvalues
- A matrix is *invertible* if its determinant is not zero (i.e. it is not singular)

Eigenvalues and eigenvectors

Symmetric matrices

Eigenvectors corresponding to distinct eigenvalues are orthogonal:

$$\begin{aligned}
\lambda\langle \mathbf{x}, \mathbf{z}\rangle &= \langle A\mathbf{x}, \mathbf{z}\rangle \\
&= (A\mathbf{x})^T\mathbf{z} \\
&= \mathbf{x}^T A^T \mathbf{z} \\
&= \mathbf{x}^T A\mathbf{z} \\
&= \langle \mathbf{x}, A\mathbf{z}\rangle \\
&= \mu\langle \mathbf{x}, \mathbf{z}\rangle
\end{aligned}$$

Eigen-decomposition

Raleigh quotient

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

$$\frac{x^T A\mathbf{x}}{\mathbf{x}^T\mathbf{x}} = \lambda\frac{\mathbf{x}^T\mathbf{x}}{\mathbf{x}^T\mathbf{x}} = \lambda$$

Finding eigenvector

1. Maximize eigenvalue:

$$\mathbf{x} = max_{\mathbf{v}}\frac{\mathbf{v}^T A\mathbf{v}}{\mathbf{v}^T\mathbf{v}}$$

2. Normalize eigenvector (solution is invariant to rescaling)

$$\mathbf{x} \leftarrow \frac{\mathbf{x}}{||\mathbf{x}||}$$

Eigen-decomposition

Deflating matrix

$$\tilde{A} = A - \lambda \mathbf{x}\mathbf{x}^T$$

- Deflation turns $\mathbf{x}$ into a zero-eigenvalue eigenvector:

$$\begin{aligned} \tilde{A}\mathbf{x} &= A\mathbf{x} - \lambda \mathbf{x}\mathbf{x}^T\mathbf{x} \quad (\mathbf{x} \text{ is normalized}) \\ &= A\mathbf{x} - \lambda \mathbf{x} = 0 \end{aligned}$$

- Other eigenvalues are unchanged as eigenvectors with distinct eigenvalues are orthogonal (symmetric matrix):

$$\begin{aligned} \tilde{A}\mathbf{z} &= A\mathbf{z} - \lambda \mathbf{x}\mathbf{x}^T\mathbf{z} \quad (\mathbf{x} \text{ and } \mathbf{z} \text{ orthonormal}) \\ \tilde{A}\mathbf{z} &= A\mathbf{z} \end{aligned}$$

Eigen-decomposition

Iterating

- The maximization procedure is repeated on the deflated matrix (until solution is zero)
- Minimization is iterated to get eigenvectors with negative eigevalues
- Eigenvectors with zero eigenvalues are obtained extending the obtained set to an orthonormal basis

Eigen-decomposition

Eigen-decomposition

- Let $V = [\mathbf{v}_1 \dots \mathbf{v}_n]$ be a matrix with orthonormal eigenvectors as columns
- Let Λ be the diagonal matrix of corresponding eigenvalues
- A square simmetric matrix can be *diagonalized* as:

$$V^T A V = \Lambda$$

  proof follows..

Note

- A diagonalized matrix is much simpler to manage and has the same properties as the original one (e.g. same eigen-decomposition)
- E.g. change of coordinate system

Eigen-decomposition

Proof

$$A\,[\mathbf{v}_1 \ldots \mathbf{v}_n] = [\mathbf{v}_1 \ldots \mathbf{v}_n] \begin{bmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{bmatrix}$$

$$AV = V\Lambda$$

$$V^{-1}AV = V^{-1}V\Lambda$$

$$V^{T}AV = \Lambda$$

Note

V is a *unitary* matrix (orthonormal columns), for which:

$$V^{-1} = V^{T}$$

Positive semi-definite matrix

Definition

An $n \times n$ symmetrix matrix M is *positive semi-definite* if all its eigenvalues are non-negative.

Alternative sufficient and necessary conditions

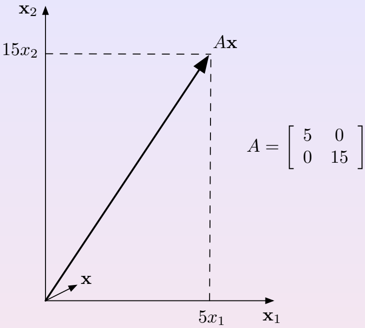
- for all $\mathbf{x} \in \mathbb{R}^n$

$$\mathbf{x}^T M \mathbf{x} \geq 0$$

- there exists a real matrix B s.t.

$$M = B^T B$$

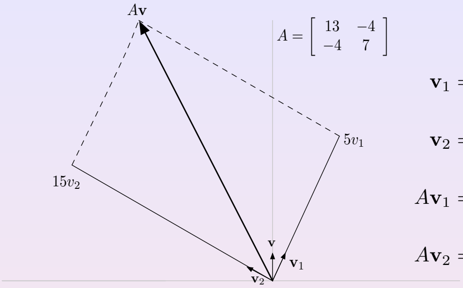
Understanding eigendecomposition



Scaling transformation in standard basis

- let $\mathbf{x}_1 = [1, 0], \mathbf{x}_2 = [0, 1]$ be the standard orthonormal basis in $\mathbb{R}^2$
- let $\mathbf{x} = [x_1, x_2]$ be an arbitrary vector in $\mathbb{R}^2$
- A linear transformation is a *scaling* transformation if it only stretches $\mathbf{x}$ along its directions

Understanding eigendecomposition



$$\mathbf{v}_1 = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

$$\mathbf{v}_2 = \begin{bmatrix} -2 \\ 1 \end{bmatrix}$$

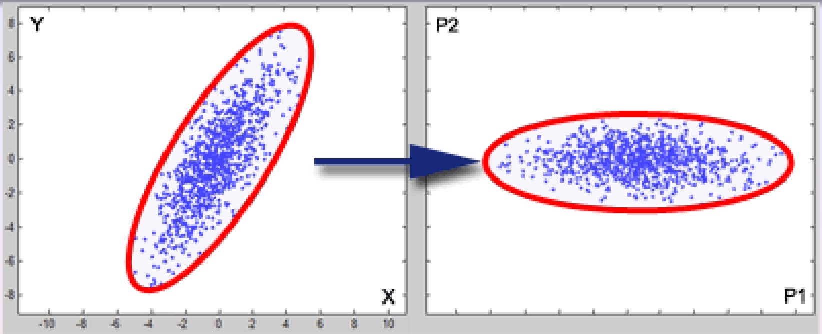
$$A\mathbf{v}_1 = \begin{bmatrix} 13-8 \\ -4+14 \end{bmatrix} = \begin{bmatrix} 5 \\ 10 \end{bmatrix} = 5\mathbf{v}_1$$

$$A\mathbf{v}_2 = \begin{bmatrix} -26-4 \\ 8+7 \end{bmatrix} = \begin{bmatrix} -30 \\ 15 \end{bmatrix} = 15\mathbf{v}_2$$

Scaling transformation in eigenbasis

- let A be a non-scaling linear transformation in $\mathbb{R}^2$.
- let $\{\mathbf{v}_1, \mathbf{v}_2\}$ be an *eigenbasis* for A.
- By representing vectors in $\mathbb{R}^2$ in terms of the $\{\mathbf{v}_1, \mathbf{v}_2\}$ basis (instead of the standard $\{\mathbf{x}_1, \mathbf{x}_2\}$), A becomes a *scaling* transformation

Principal Component Analysis (PCA)



Description

- Let X be a data matrix with correlated coordinates.
- PCA is a linear transformation mapping data to a system of *uncorrelated* coordinates.
- It corresponds to fitting an *ellipsoid* to the data, whose axes are the coordinates of the new space.

Principal Component Analysis (PCA)

Procedure (1)

Given a dataset $X \in \mathbb{R}^{n\times d}$ in d dimensions.

1. Compute the mean of the data (X_i is ith row vector of X):

$$\bar{\mathbf{x}} = \frac{1}{n}\sum_{i=1}^{n} X_i$$

2. Center the data into the origin:

$$X - \begin{bmatrix} \bar{\mathbf{x}} \\ \vdots \\ \bar{\mathbf{x}} \end{bmatrix}$$

3. Compute the data covariance: $C = \frac{1}{n}X^T X$

Principal Component Analysis (PCA)

Procedure (2)

4 Compute the (orthonormal) eigendecomposition of C:

$$V^T C V = \Lambda$$

5 Use it as the new coordinate system:

$$\mathbf{x}' = V^{-1}\mathbf{x} = V^T\mathbf{x}$$

($V^{-1} = V^T$ as V is unitary)

Warning

- It assumes linear correlations (and Gaussian distributions)

Principal Component Analysis (PCA)

Dimensionality reduction

- Each eigenvalue corresponds to the amount of variance in that direction
- Select only the *k* eigenvectors with largest eigenvalues for dimensionality reduction (e.g. visualization)

Procedure

1. $W = [\mathbf{v}_1, \ldots, \mathbf{v}_k]$
2. $\mathbf{x}' = W^T \mathbf{x}$