4. Linear Algebra Review

STA3142 Statistical Machine Learning

Kibok Lee

Assistant Professor of
Applied Statistics / Statistics and Data Science

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연세대학교
YONSEI UNIVERSITY

Outline

Basic Notation

- By $x \in \mathbb{R}^n$, we denote a vector with n entries.

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}.$$

- By $A \in \mathbb{R}^{m \times n}$, we denote a matrix with m rows and n columns, where the entries of A are real numbers.

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} = \begin{bmatrix} | & | & & | \\ a^1 & a^2 & \cdots & a^n \\ | & | & & | \end{bmatrix} = \begin{bmatrix} — & a_1^\top & — \\ — & a_2^\top & — \\ & \vdots & \\ — & a_m^\top & — \end{bmatrix}.$$

The Identity Matrix

The **identity matrix**, denoted $I \in \mathbb{R}^{n \times n}$, is a square matrix with ones on the diagonal and zeros everywhere else. That is,

$$I = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{bmatrix},$$

or,

$$I_{ij} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}$$

It has the property that for all $A \in \mathbb{R}^{m \times n}$,

$$AI = A = IA.$$

Diagonal matrices

A **diagonal matrix** is a matrix where all non-diagonal elements are 0. This is typically denoted $D = \mathrm{diag}(d_1, d_2, \ldots, d_n)$, with

$$D_{ij} = \begin{cases} d_i & \text{if } i = j, \\ 0 & \text{if } i \neq j. \end{cases}$$

Clearly, $I = \mathrm{diag}(1, 1, \ldots, 1)$.

Outline

Vector-Vector Product

- **inner product** or **dot product**

$$x^\top y \in \mathbb{R} = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \sum_{i=1}^{n} x_i y_i.$$

- **outer product**

$$xy^\top \in \mathbb{R}^{m \times n} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \begin{bmatrix} y_1 & y_2 & \cdots & y_n \end{bmatrix} = \begin{bmatrix} x_1 y_1 & x_1 y_2 & \cdots & x_1 y_n \\ x_2 y_1 & x_2 y_2 & \cdots & x_2 y_n \\ \vdots & \vdots & \ddots & \vdots \\ x_m y_1 & x_m y_2 & \cdots & x_m y_n \end{bmatrix}.$$

Matrix-Vector Product

- If we write A by rows, then we can express Ax as,

$$y = Ax = \begin{bmatrix} — & a_1^\top & — \\ — & a_2^\top & — \\ & \vdots & \\ — & a_m^\top & — \end{bmatrix} x = \begin{bmatrix} a_1^\top x \\ a_2^\top x \\ \vdots \\ a_m^\top x \end{bmatrix}.$$

Matrix-Vector Product

- If we write A by columns, then we have:

$$y = Ax = \begin{bmatrix} | & | & & | \\ a^1 & a^2 & \cdots & a^n \\ | & | & & | \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} | \\ a^1 \\ | \end{bmatrix} x_1 + \begin{bmatrix} | \\ a^2 \\ | \end{bmatrix} x_2 + \cdots + \begin{bmatrix} | \\ a^n \\ | \end{bmatrix} x_n.$$

y is a **linear combination** of the *columns* of A.

Matrix-Vector Product

It is also possible to multiply on the left by a row vector.

- If we write A by columns, then we can express $x^\top A$ as,

$$y^\top = x^\top A = x^\top \begin{bmatrix} | & | & & | \\ a^1 & a^2 & \cdots & a^n \\ | & | & & | \end{bmatrix} = \begin{bmatrix} x^\top a^1 & x^\top a^2 & \cdots & x^\top a^n \end{bmatrix}.$$

Matrix-Vector Product

It is also possible to multiply on the left by a row vector.

- expressing A in terms of rows we have:

$$
\begin{aligned}
y^\top = x^\top A &= \begin{bmatrix} x_1 & x_2 & \cdots & x_m \end{bmatrix} \begin{bmatrix} — & a_1^\top & — \\ — & a_2^\top & — \\ & \vdots & \\ — & a_m^\top & — \end{bmatrix} \\
&= x_1 \begin{bmatrix} — & a_1^\top & — \end{bmatrix} + x_2 \begin{bmatrix} — & a_2^\top & — \end{bmatrix} + \cdots + x_m \begin{bmatrix} — & a_m^\top & — \end{bmatrix}.
\end{aligned}
$$

$y^\top$ is a linear combination of the rows of A.

Matrix-Matrix Multiplication (different views)

1. As a set of vector-vector products (dot product)

$$C = AB = \begin{bmatrix} — & a_1^\top & — \\ — & a_2^\top & — \\ & \vdots & \\ — & a_m^\top & — \end{bmatrix} \begin{bmatrix} | & | & & | \\ b^1 & b^2 & \cdots & b^p \\ | & | & & | \end{bmatrix} = \begin{bmatrix} a_1^\top b^1 & a_1^\top b^2 & \cdots & a_1^\top b^p \\ a_2^\top b^1 & a_2^\top b^2 & \cdots & a_2^\top b^p \\ \vdots & \vdots & \ddots & \vdots \\ a_m^\top b^1 & a_m^\top b^2 & \cdots & a_m^\top b^p \end{bmatrix}.$$

Matrix-Matrix Multiplication (different views)

2. As a sum of outer products

$$C = AB = \begin{bmatrix} | & | & & | \\ a^1 & a^2 & \cdots & a^p \\ | & | & & | \end{bmatrix} \begin{bmatrix} — & b_1^\top & — \\ — & b_2^\top & — \\ & \vdots & \\ — & b_p^\top & — \end{bmatrix} = \sum_{i=1}^{p} a^i b_i^\top .$$

Matrix-Matrix Multiplication (different views)

3. As a set of matrix-vector products.

$$C = AB = A \begin{bmatrix} | & | & & | \\ b^1 & b^2 & \cdots & b^p \\ | & | & & | \end{bmatrix} = \begin{bmatrix} | & | & & | \\ Ab^1 & Ab^2 & \cdots & Ab^p \\ | & | & & | \end{bmatrix}.$$

Here the i-th column of C is given by the matrix-vector product with the vector on the right, $c^i = Ab^i$. These matrix-vector products can in turn be interpreted using both viewpoints given in the previous subsection.

Matrix-Matrix Multiplication (different views)

4. As a set of vector-matrix products.

$$C = AB = \begin{bmatrix} — & a_1^\top & — \\ — & a_2^\top & — \\ & \vdots & \\ — & a_m^\top & — \end{bmatrix} B = \begin{bmatrix} — & a_1^\top B & — \\ — & a_2^\top B & — \\ & \vdots & \\ — & a_m^\top B & — \end{bmatrix}.$$

Matrix-Matrix Multiplication (properties)

- Associative: $(AB)C = A(BC)$.
- Distributive: $A(B + C) = AB + AC$.
- In general, *not* commutative; that is, it can be the case that $AB \neq BA$. (For example, if $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{n \times q}$, the matrix product BA does not even exist if *m* and *q* are not equal!)

Outline

The Transpose

The **transpose** of a matrix results from "flipping" the rows and columns. Given a matrix $A \in \mathbb{R}^{m\times n}$, its transpose, written $A^\top \in \mathbb{R}^{n\times m}$, is the $n \times m$ matrix whose entries are given by

$$(A^\top)_{ij} = A_{ji}.$$

The following properties of transposes are easily verified:

- $(A^\top)^\top = A$
- $(AB)^\top = B^\top A^\top$
- $(A+B)^\top = A^\top + B^\top$

Trace

The **trace** of a square matrix $A \in \mathbb{R}^{n \times n}$, denoted $\operatorname{tr}(A)$, is the sum of diagonal elements in the matrix:

$$\operatorname{tr}(A) = \sum_{i=1}^{n} A_{ii}.$$

The trace has the following properties:

- For $A \in \mathbb{R}^{n \times n}, \operatorname{tr}(A) = \operatorname{tr}(A^\top)$.
- For $A, B \in \mathbb{R}^{n \times n},\ \operatorname{tr}(A + B) = \operatorname{tr}(A) + \operatorname{tr}(B)$.
- For $A \in \mathbb{R}^{n \times n},\ t \in \mathbb{R}, \operatorname{tr}(tA) = t \cdot \operatorname{tr}(A)$.
- If AB is square, *i.e.*, $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{n \times m}$, then $\operatorname{tr}(AB) = \operatorname{tr}(BA)$.
- If ABC is square, *i.e.*, $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{n \times p}$, and $C \in \mathbb{R}^{p \times m}$, then $\operatorname{tr}(ABC) = \operatorname{tr}(BCA) = \operatorname{tr}(CAB)$, and so on for the product of more matrices.

Norms

A **norm** of a vector $\|x\|$ is informally a measure of the "length" of the vector.
More formally, a norm is any function $f : \mathbb{R}^n \to \mathbb{R}$ that satisfies 4 properties:

1. For all $x \in \mathbb{R}^n$, $f(x) \geq 0$ (non-negativity).
2. $f(x) = 0$ if and only if $x = 0$ (definiteness).
3. For all $x \in \mathbb{R}^n$, $t \in \mathbb{R}$, $f(tx) = |t| f(x)$ (homogeneity).
4. For all $x, y \in \mathbb{R}^n$, $f(x + y) \leq f(x) + f(y)$ (triangle inequality).

Examples of Norms

The commonly-used Euclidean or ℓ_2 norm,

$$\|x\|_2 = \sqrt{\sum_{i=1}^{n} x_i^2} = \sqrt{x^\top x}.$$

The ℓ_1 norm,

$$\|x\|_1 = \sum_{i=1}^{n} |x_i|.$$

The ℓ_∞ norm,

$$\|x\|_\infty = \max_i \; |x_i|.$$

Examples of Norms

In fact, all three norms presented so far are examples of the family of ℓ_p norms, which are parameterized by a real number $p \geq 1$, and defined as

$$\|x\|_p = \left(\sum_{i=1}^{n} |x_i|^p \right)^{1/p}.$$

Matrix Norms

Norms can also be defined for matrices, such as the Frobenius norm,

$$\|A\|_F = \sqrt{\sum_{i=1}^{m}\sum_{j=1}^{n} A_{ij}^2} = \sqrt{\operatorname{tr}\left(A^\top A\right)}.$$

Many other norms exist, but they are beyond the scope of this review.

Linear Independence

A set of vectors $\{x_1, x_2, \ldots x_n\} \subset \mathbb{R}^m$ is said to be **(linearly) dependent** if one vector belonging to the set *can* be represented as a linear combination of the remaining vectors; that is, if

$$x_n = \sum_{i=1}^{n-1} \alpha_i x_i$$

for some scalar values $\alpha_1, \cdots, \alpha_{n-1} \in \mathbb{R}$; otherwise, the vectors are **(linearly) independent**.

Example:

$$x_1 = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \quad x_2 = \begin{bmatrix} 4 \\ 1 \\ 5 \end{bmatrix} \quad x_3 = \begin{bmatrix} 2 \\ -3 \\ -1 \end{bmatrix}$$

are linearly dependent because $x_3 = -2x_1 + x_2$.

Rank of a Matrix

- The **column rank** of a matrix $A \in \mathbb{R}^{m \times n}$ is the largest number of columns of A that constitute a linearly independent set.
- The **row rank** is the largest number of rows of A that constitute a linearly independent set.
- For any matrix $A \in \mathbb{R}^{m \times n}$, it turns out that the column rank of A is equal to the row rank of A (prove it yourself!), and so both quantities are referred to collectively as the **rank** of A, denoted as $\mathrm{rank}\,(A)$.

Properties of the Rank

- For $A \in \mathbb{R}^{m \times n}$, $\operatorname{rank}(A) \leq \min(m, n)$. If $\operatorname{rank}(A) = \min(m, n)$, then A is said to be **full rank**.
- For $A \in \mathbb{R}^{m \times n}$, $\operatorname{rank}(A) = \operatorname{rank}(A^\top)$.
- For $A \in \mathbb{R}^{m \times p}, B \in \mathbb{R}^{p \times n}$ $\operatorname{rank}(AB) \leq \min(\operatorname{rank}(A), \operatorname{rank}(B))$.
- For $A, B \in \mathbb{R}^{m \times n}$, $\operatorname{rank}(A + B) \leq \operatorname{rank}(A) + \operatorname{rank}(B)$.

The Inverse of a Square Matrix

- The **inverse** of a square matrix $A \in \mathbb{R}^{n \times n}$ is denoted A^{-1}, and is the unique matrix such that

$$A^{-1}A = I = AA^{-1}.$$

- We say that A is **invertible** or **non-singular** if A^{-1} exists and **non-invertible** or **singular** otherwise.

- In order for a square matrix A to have an inverse A^{-1}, then A must be full rank.

- Properties (Assuming $A, B \in \mathbb{R}^{n \times n}$ are non-singular):
  - $(A^{-1})^{-1} = A$
  - $(AB)^{-1} = B^{-1}A^{-1}$
  - $(A^{-1})^\top = (A^\top)^{-1}$. For this reason this matrix is often denoted $A^{-\top}$.

Orthogonal Matrices

- Two vectors $x, y \in \mathbb{R}^n$ are **orthogonal** if $x^\top y = 0$.
- A vector $x \in \mathbb{R}^n$ is **normalized** if $\|x\|_2 = 1$.
- A square matrix $U \in \mathbb{R}^{n \times n}$ is **orthogonal** if all its columns are orthogonal to each other and are normalized (the columns are then referred to as being **orthonormal**).

- Properties:
  - The inverse of an orthogonal matrix is its transpose.

$$U^\top U = I = UU^\top \text{ or } U^{-1} = U^\top.$$

  - Operating on a vector with an orthogonal matrix will not change its Euclidean norm, *i.e.*,

$$\|Ux\|_2 = \|x\|_2$$

for any $x \in \mathbb{R}^n, U \in \mathbb{R}^{n \times n}$ orthogonal.

Span and Projection

- The **span** of a set of vectors $\{x_1, x_2, \ldots, x_n\}$ is the set of all vectors that can be expressed as a linear combination of $\{x_1, \ldots, x_n\}$. That is,

$$\operatorname{span}(\{x_1, \ldots, x_n\}) = \left\{ v : v = \sum_{i=1}^{n} \alpha_i x_i,\ \ \alpha_i \in \mathbb{R} \right\}.$$

- The **projection** of a vector $y \in \mathbb{R}^m$ onto the span of $\{x_1, \ldots x_n\}$ is the vector $v \in \operatorname{span}(\{x_1, \ldots, x_n\})$, such that v is as close as possible to y, as measured by the Euclidean norm $\|v - y\|_2$.

$$\operatorname{Proj}(y; \{x_1, \ldots x_n\}) = \operatorname{argmin}_{v \in \operatorname{span}(\{x_1, \ldots, x_n\})} \|y - v\|_2.$$

Range

- The **range** or the column space of a matrix $A \in \mathbb{R}^{m \times n}$, denoted $\mathcal{R}(A)$, is the span of the columns of A. In other words,

$$\mathcal{R}(A) = \{v \in \mathbb{R}^m : v = Ax, x \in \mathbb{R}^n\}.$$

- Assuming A is full rank and $n < m$, the projection of a vector $y \in \mathbb{R}^m$ onto the range of A is given by,

$$\mathrm{Proj}(y; A) = \mathrm{argmin}_{v \in \mathcal{R}(A)} \|y - v\|_2.$$

Null Space

The **nullspace** of a matrix $A \in \mathbb{R}^{m \times n}$, denoted $\mathcal{N}(A)$ is the set of all vectors that equal 0 when multiplied by A, *i.e.*,

$$\mathcal{N}(A) = \{x \in \mathbb{R}^n : Ax = 0\}.$$

The Determinant

The **determinant** of a square matrix $A \in \mathbb{R}^{n\times n}$, is a function $\det : \mathbb{R}^{n\times n} \to \mathbb{R}$, and is denoted $|A|$ or $\det(A)$.
Given a matrix

$$\begin{bmatrix} - & a_1^\top & - \\ - & a_2^\top & - \\ & \vdots & \\ - & a_n^\top & - \end{bmatrix},$$

consider the set of points $S \subset \mathbb{R}^n$ as follows:

$$S = \{v \in \mathbb{R}^n : v = \sum_{i=1}^{n} \alpha_i a_i \text{ where } 0 \leq \alpha_i \leq 1, i = 1, \ldots, n\}.$$

The absolute value of the determinant of A is a measure of the "volume" of the set S.

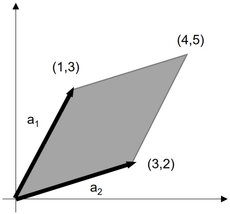
The Determinant: Intuition

For example, consider the 2×2 matrix,

$$A = \begin{bmatrix} 1 & 3 \\ 3 & 2 \end{bmatrix}.$$

Here, the rows of the matrix are

$$a_1 = \begin{bmatrix} 1 \\ 3 \end{bmatrix}, a_2 = \begin{bmatrix} 3 \\ 2 \end{bmatrix}.$$



The Determinant: Properties

Algebraically, the determinant satisfies the following three properties:

1. The determinant of the identity is 1, $|I| = 1$. (Geometrically, the volume of a unit hypercube is 1).
2. Given a matrix $A \in \mathbb{R}^{n \times n}$, if we multiply a single row in A by a scalar $t \in \mathbb{R}$, then the determinant of the new matrix is $t|A|$, (Geometrically, multiplying one of the sides of the set S by a factor t causes the volume to increase by a factor t.)
3. If we exchange any two rows $a_i^\top$ and $a_j^\top$ of A, then the determinant of the new matrix is $-|A|$.

In case you are wondering, it is not immediately obvious that a function satisfying the above three properties exists. In fact, though, such a function does exist, and is unique (which we will not prove here).

The Determinant: Properties

- For $A \in \mathbb{R}^{n\times n}$, $|A| = |A^\top|$.
- For $A, B \in \mathbb{R}^{n\times n}$, $|AB| = |A||B|$.
- For $A \in \mathbb{R}^{n\times n}$, $|A| = 0$ if and only if A is singular (*i.e.*, non-invertible). (If A is singular then it does not have full rank, and hence its columns are linearly dependent. In this case, the set S corresponds to a "flat sheet" within the n-dimensional space and hence has zero volume.).
- For $A \in \mathbb{R}^{n\times n}$ and A non-singular, $|A^{-1}| = 1/|A|$.

The Determinant: Formula

Let $A \in \mathbb{R}^{n\times n}$, $A_{-i,-j} \in \mathbb{R}^{(n-1)\times(n-1)}$ be the matrix that results from deleting the ith row and jth column from A.
The general (recursive) formula for the determinant is

$$
\begin{aligned}
|A| &= \sum_{i=1}^{n} (-1)^{i+j} a_{ij} \; |A_{-i,-j}| \text{ (for any } j \in 1, \ldots, n) \\
&= \sum_{j=1}^{n} (-1)^{i+j} a_{ij} \; |A_{-i,-j}| \text{ (for any } i \in 1, \ldots, n)
\end{aligned}
$$

with the initial case that $|A| = a_{11}$ for $A \in \mathbb{R}^{1\times 1}$. If we were to expand this formula completely for $A \in \mathbb{R}^{n\times n}$, there would be a total of $n!$ (n factorial) different terms. For this reason, we hardly ever explicitly write the complete equation of the determinant for matrices bigger than 3×3.

The Determinant: Examples

However, the equations for determinants of matrices up to size 3×3 are fairly common, and it is good to know them:

$$\left|[a_{11}]\right| = a_{11}$$

$$\left|\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}\right| = a_{11}a_{22} - a_{12}a_{21}$$

$$\left|\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}\right| = a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32}$$

$$- a_{11}a_{23}a_{32} - a_{12}a_{21}a_{33} - a_{13}a_{22}a_{31}$$

Quadratic Forms

Given a square matrix $A \in \mathbb{R}^{n\times n}$ and a vector $x \in \mathbb{R}^n$, the scalar value $x^\top Ax$ is called a **quadratic form**. Written explicitly, we see that

$$x^\top Ax = \sum_{i=1}^{n} x_i(Ax)_i = \sum_{i=1}^{n} x_i \left(\sum_{j=1}^{n} A_{ij}x_j \right) = \sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}x_ix_j.$$

We often implicitly assume that the matrices appearing in a quadratic form are symmetric.

$$x^\top Ax = (x^\top Ax)^\top = x^\top A^\top x = x^\top \left(\frac{1}{2}A + \frac{1}{2}A^\top \right) x.$$

Quadratic Forms

A symmetric matrix $A \in \mathbb{S}^n$ is:

- **positive definite** (PD), denoted $A \succ 0$ if for all non-zero vectors $x \in \mathbb{R}^n$, $x^\top Ax > 0$.
- **positive semidefinite** (PSD), denoted $A \succeq 0$ if for all vectors $x \in \mathbb{R}^n$, $x^\top Ax \geq 0$.
- **negative definite** (ND), denoted $A \prec 0$ if for all non-zero vectors $x \in \mathbb{R}^n$, $x^\top Ax < 0$.
- **negative semidefinite** (NSD), denoted $A \preceq 0$ if for all vectors $x \in \mathbb{R}^n$, $x^\top Ax \leq 0$.
- **indefinite**, if it is neither positive semidefinite nor negative semidefinite
  – *i.e.*, if there exists $x_1, x_2 \in \mathbb{R}^n$ such that $x_1^\top Ax_1 > 0$ and $x_2^\top Ax_2 < 0$.

Positive Semidefinite Matrices

- One important property of positive definite and negative definite matrices is that they are always full rank, and hence, invertible.
- Given any matrix $A \in \mathbb{R}^{m \times n}$ (not necessarily symmetric or even square), the matrix $G = A^\top A$ (sometimes called a **Gram matrix**) is always positive semidefinite. Further, if $m \geq n$ and A is full rank, then $G = A^\top A$ is positive definite.

Eigenvalues and Eigenvectors

Given a square matrix $A \in \mathbb{R}^{n \times n}$, we say that $\lambda \in \mathbb{C}$ is an **eigenvalue** of A and $x \in \mathbb{C}^n$ is the corresponding **eigenvector** if

$$Ax = \lambda x, \;\; x \neq 0.$$

Intuitively, this definition means that multiplying A by the vector x results in a new vector that points in the same direction as x, but scaled by a factor λ.

Eigenvalues and Eigenvectors

We can rewrite the equation above to state that (λ, x) is an eigenvalue-eigenvector pair of A if,

$$(\lambda I - A)x = 0, \;\; x \neq 0.$$

But $(\lambda I - A)x = 0$ has a non-zero solution to x if and only if $(\lambda I - A)$ has a non-empty nullspace, which is only the case if $(\lambda I - A)$ is singular, *i.e.*,

$$|(\lambda I - A)| = 0.$$

We can now use the previous definition of the determinant to expand this expression $|(\lambda I - A)|$ into a (very large) polynomial in λ, where λ will have degree n. It's often called the **characteristic polynomial** of the matrix A.

Properties of eigenvalues and eigenvectors

- The trace of A is equal to the sum of its eigenvalues,

$$\mathrm{tr}(A) = \sum_{i=1}^{n} \lambda_i.$$

- The determinant of A is equal to the product of its eigenvalues,

$$|A| = \prod_{i=1}^{n} \lambda_i.$$

- The rank of A is equal to the number of non-zero eigenvalues of A.
- Suppose A is non-singular with eigenvalue λ and an associated eigenvector x. Then $1/\lambda$ is an eigenvalue of A^{-1} with an associated eigenvector x, *i.e.*, $A^{-1}x = (1/\lambda)x$.
- The eigenvalues of a diagonal matrix $D = \mathrm{diag}(d_1, \ldots, d_n)$ are just the diagonal entries $d_1, \ldots, d_n$.

Eigenvalues and Eigenvectors of Symmetric Matrices

Throughout this section, let's assume that A is a symmetric real matrix (*i.e.*, $A^\top = A$). We have the following properties:

1. All eigenvalues of A are real numbers. We denote them by $\lambda_1, \ldots, \lambda_n$.
2. There exists a set of eigenvectors $u_1, \ldots, u_n$ such that (i) for all i, u_i is an eigenvector with eigenvalue λ_i and (ii) $u_1, \ldots, u_n$ are unit vectors and orthogonal to each other.

New Representation for Symmetric Matrices

- Let U be the orthonormal matrix that contains u_i's as columns:

$$U = \begin{bmatrix} | & | & & | \\ u_1 & u_2 & \cdots & u_n \\ | & | & & | \end{bmatrix}.$$

- Let $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$ be the diagonal matrix that contains $\lambda_1, \ldots, \lambda_n$.

$$AU = \begin{bmatrix} | & | & & | \\ Au_1 & Au_2 & \cdots & Au_n \\ | & | & & | \end{bmatrix} = \begin{bmatrix} | & | & & | \\ \lambda_1 u_1 & \lambda_1 u_2 & \cdots & \lambda_1 u_n \\ | & | & & | \end{bmatrix} = U\,\mathrm{diag}(\lambda_1, \ldots, \lambda_n) = U\Lambda.$$

- Recalling that orthonormal matrix U satisfies that $UU^\top = I$, we can diagonalize matrix A:

$$A = AUU^\top = U\Lambda U^\top.$$

Background: representing vector w.r.t. another basis

- Any orthonormal matrix $U = \begin{bmatrix} | & | & & | \\ u_1 & u_2 & \cdots & u_n \\ | & | & & | \end{bmatrix}$ defines a new basis of $\mathbb{R}^n$.
- For any vector $x \in \mathbb{R}^n$ can be represented as a linear combination of $u_1, \ldots, u_n$ with coefficient $\hat{x_1}, \ldots, \hat{x_n}$:

$$x = \hat{x_1} u_1 + \cdots + \hat{x_n} u_n = U\hat{x}$$

- Indeed, such $\hat{x}$ uniquely exists

$$x = U\hat{x} \Longleftrightarrow U^\top x = \hat{x}$$

In other words, the vector $\hat{x} = U^\top x$ can serve as another representation of the vector x w.r.t. the basis defined by U.

"Diagonalizing" matrix-vector multiplication

- Left-multiplying matrix A can be viewed as left-multiplying a diagonal matrix w.r.t. the basis of the eigenvectors.
  - Suppose x is a vector and $\hat{x}$ is its representation w.r.t. to the basis of U.
  - Let $z = Ax$ be the matrix-vector product.
  - The representation z w.r.t. the basis of U:

$$\hat{z} = U^\top z = U^\top Ax = U^\top U \Lambda U^\top x = \Lambda \hat{x} = \begin{bmatrix} \lambda_1 \hat{x_1} \\ \lambda_2 \hat{x_2} \\ \vdots \\ \lambda_n \hat{x_n} \end{bmatrix}$$

- We see that left-multiplying matrix A in the original space is equivalent to left-multiplying the diagonal matrix Λ w.r.t. the new basis, which is merely scaling each coordinate by the corresponding eigenvalue.

“Diagonalizing” matrix-vector multiplication

Under the new basis, multiplying a matrix multiple times becomes much simpler as well. For example, suppose $q = AAAx$.

$$\hat{q} = U^\top q = U^\top AAAx = U^\top U\Lambda U^\top U\Lambda U^\top U\Lambda U^\top x = \Lambda^3 \hat{x} = \begin{bmatrix} \lambda_1^3 \hat{x}_1 \\ \lambda_2^3 \hat{x}_2 \\ \vdots \\ \lambda_n^3 \hat{x}_n \end{bmatrix}$$

"Diagonalizing" quadratic form

As a directly corollary, the quadratic form $x^\top Ax$ can also be simplified under the new basis

$$x^\top Ax = x^\top U\Lambda U^\top x = \hat{x}^\top \Lambda \hat{x} = \sum_{i=1}^{n} \lambda_i \hat{x}_i{}^2$$

(Recall that with the old representation, $x^\top Ax = \sum_{i=1,j=1}^{n} x_i x_j A_{ij}$ involves a sum of n^2 terms instead of n terms in the equation above.)

The definiteness of the matrix A depends entirely on the sign of its eigenvalues

1. If all $\lambda_i > 0$, then the matrix A is positive definite because $x^\top A x = \sum_{i=1}^{n} \lambda_i \hat{x_i}^2 > 0$ for any $\hat{x} \neq 0$. [1]
2. If all $\lambda_i \geq 0$, it is positive semidefinite because $x^\top A x = \sum_{i=1}^{n} \lambda_i \hat{x_i}^2 \geq 0$ for all $\hat{x}$.
3. Likewise, if all $\lambda_i < 0$ or $\lambda_i \leq 0$, then A is negative definite or negative semidefinite, respectively.
4. Finally, if A has both positive and negative eigenvalues, say $\lambda_i > 0$ and $\lambda_j < 0$, then it is indefinite. This is because if we let $\hat{x}$ satisfy $\hat{x_i} = 1$ and $\hat{x_k} = 0, \forall k \neq i$, then $x^\top A x = \sum_{i=1}^{n} \lambda_i \hat{x_i}^2 > 0$. Similarly we can let $\hat{x}$ satisfy $\hat{x_j} = 1$ and $\hat{x_k} = 0, \forall k \neq j$, then $x^\top A x = \sum_{i=1}^{n} \lambda_i \hat{x_i}^2 < 0$.

[1] Note that $\hat{x} \neq 0 \iff x \neq 0$

Outline

The Gradient

Suppose that $f : \mathbb{R}^{m\times n} \to \mathbb{R}$ is a function that takes as input a matrix A of size $m \times n$ and returns a real value. Then the **gradient** of f (with respect to $A \in \mathbb{R}^{m\times n}$) is the matrix of partial derivatives, defined as:

$$\nabla_A f(A) = \begin{bmatrix} \frac{\partial f(A)}{\partial A_{11}} & \frac{\partial f(A)}{\partial A_{12}} & \cdots & \frac{\partial f(A)}{\partial A_{1n}} \\ \frac{\partial f(A)}{\partial A_{21}} & \frac{\partial f(A)}{\partial A_{22}} & \cdots & \frac{\partial f(A)}{\partial A_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f(A)}{\partial A_{m1}} & \frac{\partial f(A)}{\partial A_{m2}} & \cdots & \frac{\partial f(A)}{\partial A_{mn}} \end{bmatrix} \in \mathbb{R}^{m\times n},$$

i.e., an $m \times n$ matrix with

$$(\nabla_A f(A))_{ij} = \frac{\partial f(A)}{\partial A_{ij}}.$$

The Gradient

Note that the size of $\nabla_A f(A)$ is always the same as the size of A. So if, in particular, A is just a vector $x \in \mathbb{R}^n$,

$$\nabla_x f(x) = \begin{bmatrix} \frac{\partial f(x)}{\partial x_1} \\ \frac{\partial f(x)}{\partial x_2} \\ \vdots \\ \frac{\partial f(x)}{\partial x_n} \end{bmatrix}.$$

It follows directly from the equivalent properties of partial derivatives that:

- $\nabla_x (f(x) + g(x)) = \nabla_x f(x) + \nabla_x g(x)$.
- For $t \in \mathbb{R}, \nabla_x (t \cdot f(x)) = t \nabla_x f(x)$

The Hessian

Suppose that $f : \mathbb{R}^n \to \mathbb{R}$ is a function that takes a vector in $\mathbb{R}$ and returns a real number. Then the **Hessian** matrix with respect to x, written $\nabla_x^2 f(x)$ or simply as H is the $n \times n$ matrix of partial derivatives,

$$\nabla_x^2 f(x) = \begin{bmatrix} \frac{\partial^2 f(x)}{\partial x_1^2} & \frac{\partial^2 f(x)}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f(x)}{\partial x_2 \partial x_1} & \frac{\partial^2 f(x)}{\partial x_2^2} & \cdots & \frac{\partial^2 f(x)}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f(x)}{\partial x_n \partial x_1} & \frac{\partial^2 f(x)}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f(x)}{\partial x_n^2} \end{bmatrix} \in \mathbb{R}^{n \times n}.$$

In other words, $\nabla_x^2 f(x) \in \mathbb{R}^{m \times n}$, with

$$(\nabla_x^2 f(x))_{ij} = \frac{\partial^2 f(x)}{\partial x_i \partial x_j}.$$

The Hessian

Suppose that $f : \mathbb{R}^n \to \mathbb{R}$ is a function that takes a vector in $\mathbb{R}$ and returns a real number. Then the **Hessian** matrix with respect to x, written $\nabla_x^2 f(x)$ or simply as H is the $n \times n$ matrix of partial derivatives,

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Note that the Hessian is always symmetric, since

$$\frac{\partial^2 f(x)}{\partial x_i \partial x_j} = \frac{\partial^2 f(x)}{\partial x_j \partial x_i}.$$

Gradients of Linear Functions

For $x \in \mathbb{R}^n$, let $f(x) = b^\top x$ for some known vector $b \in \mathbb{R}^n$. Then

$$f(x) = \sum_{i=1}^{n} b_i x_i.$$

So

$$\frac{\partial f(x)}{\partial x_k} = \frac{\partial}{\partial x_k} \sum_{i=1}^{n} b_i x_i = b_k.$$

From this, we can easily see that $\nabla_x b^\top x = b$. This should be compared to the analogous situation in single variable calculus, where $\frac{\partial}{\partial x} ax = a$.

Gradients of Quadratic Function

Now consider the quadratic function $f(x) = x^\top Ax$ for $A \in \mathbb{S}^n$. Remember that

$$f(x) = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j.$$

To take the partial derivative, we'll consider the terms including x_k and x_k^2 factors separately:

$$\begin{aligned}
\frac{\partial f(x)}{\partial x_k} &= \frac{\partial}{\partial x_k} \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j \\
&= \frac{\partial}{\partial x_k} \left[\sum_{i \neq k} \sum_{j \neq k} A_{ij} x_i x_j + \sum_{i \neq k} A_{ik} x_i x_k + \sum_{j \neq k} A_{kj} x_k x_j + A_{kk} x_k^2 \right] \\
&= \sum_{i \neq k} A_{ik} x_i + \sum_{j \neq k} A_{kj} x_j + 2 A_{kk} x_k
\end{aligned}$$

Gradients of Quadratic Function

Now consider the quadratic function $f(x) = x^\top Ax$ for $A \in \mathbb{S}^n$. Remember that

$$f(x) = \sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}x_ix_j.$$

To take the partial derivative, we'll consider the terms including x_k and x_k^2 factors separately:

$$\begin{aligned}\frac{\partial f(x)}{\partial x_k} &= \frac{\partial}{\partial x_k}\sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}x_ix_j \\ &= \sum_{i\neq k} A_{ik}x_i + \sum_{j\neq k} A_{kj}x_j + 2A_{kk}x_k \\ &= \sum_{i=1} A_{ik}x_i + \sum_{j=1} A_{kj}x_j = 2\sum_{i=1}^{n} A_{ki}x_i.\end{aligned}$$

Hessian of Quadratic Functions

Finally, let's look at the Hessian of the quadratic function $f(x) = x^\top Ax$
In this case,

$$\frac{\partial^2 f(x)}{\partial x_k \partial x_l} = \frac{\partial}{\partial x_k}\left[\frac{\partial f(x)}{\partial x_l}\right] = \frac{\partial}{\partial x_k}\left[2\sum_{i=1}^{n} A_{li}x_i\right] = 2A_{lk} = 2A_{kl}$$

Therefore, it should be clear that $\nabla_x^2 x^\top Ax = 2A$, which should be entirely expected (and again analogous to the single-variable fact that $\frac{\partial^2}{\partial x^2}ax^2 = 2a$).

Recap

- $\nabla_x b^\top x = b$
- $\nabla_x^2 b^\top x = 0$
- $\nabla_x x^\top A x = 2Ax$ (if A symmetric)
- $\nabla_x^2 x^\top A x = 2A$ (if A symmetric)

Matrix Calculus Example: Least Squares

- Given a full rank matrix $A \in \mathbb{R}^{m \times n}$, and a vector $b \in \mathbb{R}^m$ such that $b \notin \mathcal{R}(A)$, we want to find a vector x such that Ax is as close as possible to b, as measured by the square of the Euclidean norm $\|Ax - b\|_2^2$.
- Using the fact that $\|x\|_2^2 = x^\top x$, we have

$$\|Ax - b\|_2^2 = (Ax - b)^\top (Ax - b) = x^\top A^\top Ax - 2b^\top Ax + b^\top b.$$

- Taking the gradient with respect to x we have:

$$\begin{aligned} \nabla_x (x^\top A^\top Ax - 2b^\top Ax + b^\top b) &= \nabla_x x^\top A^\top Ax - \nabla 2b^\top Ax + \nabla b^\top b \\ &= 2A^\top Ax - 2A^\top b. \end{aligned}$$

- Setting this last expression equal to zero and solving for x gives the normal equations

$$x = (A^\top A)^{-1} A^\top b.$$