

Linear Algebra Review

Adapted from CS229 Linear Algebra Review Fall
2022

Outline

- 1 Basic Concepts and Notation
- 2 Matrix Multiplication
- 3 Operations and Properties
- 4 Matrix Calculus

Basic Concepts and Notation

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,

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

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

$$AI = A = IA.$$

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Vector-Vector Product

- *inner product* or *dot product*

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

- *outer product*

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

Matrix-Vector Product

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

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

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 $x^T A$ as,

$$y^T = x^T A = x^T \begin{bmatrix} | & | & & | \\ a^1 & a^2 & \dots & a^n \\ | & | & & | \end{bmatrix} = [x^T a^1 \quad x^T a^2 \quad \dots \quad x^T a^n]$$

Matrix-Matrix Multiplication (different views)

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

$$C = AB = \begin{bmatrix} \text{---} & a_1^T & \text{---} \\ \text{---} & a_2^T & \text{---} \\ & \vdots & \\ \text{---} & a_m^T & \text{---} \end{bmatrix} \begin{bmatrix} | & | & & | \\ b^1 & b^2 & \dots & b^p \\ | & | & & | \end{bmatrix} = \begin{bmatrix} a_1^T b^1 & a_1^T b^2 & \dots & a_1^T b^p \\ a_2^T b^1 & a_2^T b^2 & \dots & a_2^T b^p \\ \vdots & \vdots & \ddots & \vdots \\ a_m^T b^1 & a_m^T b^2 & \dots & a_m^T b^p \end{bmatrix}.$$

Matrix-Matrix Multiplication (different views)

2. As a sum of outer products

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

Matrix-Matrix Multiplication (different views)

4. As a set of vector-matrix products.

$$C = AB = \begin{bmatrix} - & a_1^T & - \\ - & a_2^T & - \\ & \vdots & \\ - & a_m^T & - \end{bmatrix} \quad B = \begin{bmatrix} - & a_1^T B & - \\ - & a_2^T B & - \\ & \vdots & \\ - & a_m^T B & - \end{bmatrix}.$$

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Operations and Properties

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 $A^T \in \mathbb{R}^{n \times m}$, is the $n \times m$ matrix whose entries are given by

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

The following properties of transposes are easily verified:

- $(A^T)^T = A$
- $(AB)^T = B^T A^T$
- $(A + B)^T = A^T + B^T$

Trace

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

$$\text{tr}A = \sum_{i=1}^n A_{ii}.$$

The trace has the following properties:

- For $A \in \mathbb{R}^{n \times n}$, $\text{tr}A = \text{tr}A^T$.
- For $A, B \in \mathbb{R}^{n \times n}$, $\text{tr}(A + B) = \text{tr}A + \text{tr}B$.
- For $A \in \mathbb{R}^{n \times n}$, $t \in \mathbb{R}$, $\text{tr}(tA) = t \text{tr}A$.
- For A, B such that AB is square, $\text{tr}AB = \text{tr}BA$.
- For A, B, C such that ABC is square, $\text{tr}ABC = \text{tr}BCA = \text{tr}CAB$, 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 $f : \mathbb{R}^n \rightarrow \mathbb{R}$ 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,

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

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,

$$\|A\|_F = \sqrt{\sum_{i=1}^m \sum_{j=1}^n A_{ij}^2} = \sqrt{\text{tr}(A^T A)}.$$

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

Linear Independence

A set of vectors $\{x_1, x_2, \dots, x_n\} \subset \mathbb{R}^m$ 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 $\alpha_1, \dots, \alpha_{n-1} \in \mathbb{R}$; otherwise, the vectors are *(linearly) independent*.

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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.
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- 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 $\text{rank}(A)$.

Properties of the Rank

- For $A \in \mathbb{R}^{m \times n}$, $\text{rank}(A) \leq \min(m, n)$. If $\text{rank}(A) = \min(m, n)$, then A is said to be **full rank**.
- For $A \in \mathbb{R}^{m \times n}$, $\text{rank}(A) = \text{rank}(A^T)$.

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- For $A \in \mathbb{R}^{m \times p}$, $B \in \mathbb{R}^{p \times n}$, $\text{rank}(AB) \leq \min(\text{rank}(A), \text{rank}(B))$.

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- For $A, B \in \mathbb{R}^{m \times n}$, $\text{rank}(A + B) \leq \text{rank}(A) + \text{rank}(B)$.

The Inverse of a Square Matrix

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- 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):
 - ▶ $(A^{-1})^{-1} = A$
 - ▶ $(AB)^{-1} = B^{-1}A^{-1}$
 - ▶ $(A^{-1})^T = (A^T)^{-1}$. For this reason this matrix is often denoted A^{-T} .

Orthogonal Matrices

- Two vectors $x, y \in \mathbb{R}^n$ are **orthogonal** if $x^T y = 0$.
- 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**).

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- **Properties:**

- ▶ The inverse of an orthogonal matrix is its transpose.

$$U^T U = I = U U^T.$$

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

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

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

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

Range

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

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- 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,

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

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 $\det : \mathbb{R}^{n \times n} \rightarrow \mathbb{R}$, and is denoted $|A|$ or $\det A$.

Given a matrix

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

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

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

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

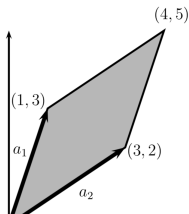
The Determinant: Intuition

For example, consider the 2×2 matrix,

$$A = \begin{bmatrix} 1 & 3 \\ 3 & 2 \end{bmatrix} \quad (3)$$

Here, the rows of the matrix are

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



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).

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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 $A \in \mathbb{R}^{n \times n}$, $|A| = |A^T|$.
- 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 $A \in \mathbb{R}^{n \times n}$, $A_{\setminus i, \setminus j} \in \mathbb{R}^{(n-1) \times (n-1)}$ be the *matrix* that results from deleting the i th row and j th column from A .

The general (recursive) formula for the determinant is

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

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:

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

Quadratic Forms

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

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

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

$$x^T A x = (x^T A x)^T = x^T A^T x = x^T \left(\frac{1}{2} A + \frac{1}{2} A^T \right) x,$$

Positive Semidefinite Matrices

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

- **positive definite** (PD), denoted $A \succ 0$ if for all non-zero vectors $x \in \mathbb{R}^n$, $x^T A x > 0$.
- **positive semidefinite** (PSD), denoted $A \succeq 0$ if for all vectors $x^T A x \geq 0$.
- **negative definite** (ND), denoted $A \prec 0$ if for all non-zero $x \in \mathbb{R}^n$, $x^T A x < 0$.
- **negative semidefinite** (NSD), denoted $A \preceq 0$) if for all $x \in \mathbb{R}^n$, $x^T A x \leq 0$.
- **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 $x_1^T A x_1 > 0$ and $x_2^T A x_2 < 0$.

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 $G = A^T A$ (sometimes called a ***Gram matrix***) is always positive semidefinite. Further, if $m \geq n$ and A is full rank, then $G = A^T A$ 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

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

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,

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

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

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- The rank of A is equal to the number of non-zero eigenvalues of A .

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$$\text{tr}A = \sum_{i=1}^n \lambda_i.$$

- 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., $A^{-1}x = (1/\lambda)x$.

Properties of eigenvalues and eigenvectors

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

$$\text{tr}A = \sum_{i=1}^n \lambda_i.$$

- 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 $D = \text{diag}(d_1, \dots, d_n)$ are just the diagonal entries d_1, \dots, d_n .

Eigenvalues and Eigenvectors of Symmetric Matrices

Throughout this section, let's assume that A is a symmetric real matrix (i.e., $A^T = A$). We have the following properties:

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

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

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

$$AU = \begin{bmatrix} | & | & \cdots & | \\ Au_1 & Au_2 & \cdots & Au_n \\ | & | & \cdots & | \end{bmatrix} = \begin{bmatrix} | & | & \cdots & | \\ \lambda_1 u_1 & \lambda_2 u_2 & \cdots & \lambda_n u_n \\ | & | & \cdots & | \end{bmatrix} = U \text{diag}(\lambda_1, \dots, \lambda_n) = U\Lambda$$

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

$$A = AUU^T = U\Lambda U^T \quad (4)$$

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

- Any orthonormal matrix $U = \begin{bmatrix} | & | & \cdots & | \\ u_1 & u_2 & \cdots & u_n \\ | & | & \cdots & | \end{bmatrix}$ 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, \dots, u_n with coefficient $\hat{x}_1, \dots, \hat{x}_n$:

$$x = \hat{x}_1 u_1 + \cdots + \hat{x}_n u_n = U \hat{x}$$

- Indeed, such \hat{x} uniquely exists

$$x = U \hat{x} \Leftrightarrow U^T x = \hat{x}$$

In other words, the vector $\hat{x} = U^T x$ 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 :

$$\hat{z} = U^T z = U^T A x = U^T U \Lambda U^T x = \Lambda \hat{x} = \begin{bmatrix} \lambda_1 \hat{x}_1 \\ \lambda_2 \hat{x}_2 \\ \vdots \\ \lambda_n \hat{x}_n \end{bmatrix}$$

- 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 $q = AAAx$.

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

Outline

- 1 Basic Concepts and Notation
- 2 Matrix Multiplication
- 3 Operations and Properties
- 4 Matrix Calculus

Matrix Calculus

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 $x \in \mathbb{R}^n$,

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

The Hessian

Suppose that $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is a function that takes a vector in \mathbb{R}^n 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,

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

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

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

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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 Quadratic Function

Now consider the quadratic function $f(x) = x^T A x$ 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:

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

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Gradients of Quadratic Function

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

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

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

Recap

- $\nabla_x b^T x = b$
- $\nabla_x^2 b^T x = 0$
- $\nabla_x x^T A x = 2Ax$ (if A symmetric)
- $\nabla_x^2 x^T A x = 2A$ (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 $\|x\|_2^2 = x^T x$, we have

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

- Taking the gradient with respect to x we have:

$$\begin{aligned}\nabla_x(x^T A^T A x - 2b^T A x + b^T b) &= \nabla_x x^T A^T A x - \nabla_x 2b^T A x + \nabla_x b^T b \\ &= 2A^T A x - 2A^T b\end{aligned}$$

