Linear Algebra Review

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Outline

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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.

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

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,

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

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

$$AI = A = IA$$

.

Diagonal Matrices

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

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

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

Outline

Vector-Vector Product

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

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

- ***outer product***

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

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

If we write A by columns, then we have,

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

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 $x^T A$ as,

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

Matrix-Vector Product

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

- Expressing A in terms of rows we have:

$$y^T = x^T A = \begin{bmatrix} x_1 & x_2 & \dots & x_m \end{bmatrix} \begin{bmatrix} — & a_1^T & — \\ — & a_2^T & — \\ & \vdots & \\ — & a_m^T & — \end{bmatrix}$$

$$= x_1 \begin{bmatrix} — & a_1^T & — \end{bmatrix} + \dots + x_m \begin{bmatrix} — & a_m^T & — \end{bmatrix}$$

y^T is a linear combination of the rows of A

Matrix-Matrix Multiplication (different views)

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

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

Matrix-Matrix Multiplication (different views)

- As a sum of outer products

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

Matrix-Matrix Multiplication (different views)

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$$C = AB = A \begin{bmatrix} | & & | \\ b^1 & \dots & b^n \\ | & & | \end{bmatrix} = \begin{bmatrix} | & & | \\ Ab^1 & \dots & Ab^n \\ | & & | \end{bmatrix}$$

Here the ith 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)

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

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

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

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

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

Matrix Norms

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

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

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

Linear Independence

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

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

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

Rank of a Matrix

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- 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 $rank(A)$.

Properties of the Rank

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

The Inverse of a Square Matrix

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- 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:**
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  - 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 $\{x_1,\ x_2,\ldots,x_n\}$. That is,

$$span(\{x_1,\ x_2,\ldots,x_n\}) = \left\{v:\ \ v = \sum_{i=1}^{n}\alpha_i x_i,\quad \alpha_i \in \mathbb{R}\right\}$$

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- The **projection** of a vector $y \in \mathbb{R}^m$ onto the span of $\{x_1,\ldots,x_n\}$ is the vector $v \in span(\{x_1,\ x_2,\ldots,x_n\})$, such that v is as close as possible to y, as measured by the Euclidean norm $\|v - y\|_2$.

$$Proj(y;\ \{x_1,\ x_2,\ldots,x_n\}) = argmin_{v\in span(\{x_1,\ x_2,\ldots,x_n\})}\|y - v\|_2$$

Span and Projection

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

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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,

$$Proj(y;\ A) = argmin_{v \in \mathcal{R}(A)} \|v - y\|_2$$

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 $\det : \mathbb{R}^{n\times n} \to \mathbb{R}$, 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:

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

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

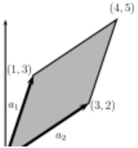
The Determinant: Intuition

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:

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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 $A \in \mathbb{R}^{n \times n}$, $\det(A) = \det\left(A^T\right)$
- For $A,\ B \in \mathbb{R}^{n \times n}$, $\det(AB) = \det(A)\det(B)$
- For $A \in \mathbb{R}^{n \times n}$, $\det(A) = 0$ 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, $\det\left(A^{-1}\right) = \frac{1}{\det(A)}$

The Determinant: Formula

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

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

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^TAx is called a **quadratic form.** Written explicitly, we see that

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

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

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

Positive Semidefinite Matrices

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

- **Positive definite** (PD), denoted $A \succ 0$ if 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 all non-zero vectors $x \in \mathbb{R}^n$, $x^T A x < 0$
- **Negative semidefinite** (NSD), denoted $A \preceq 0$ if 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 $(\lambda; x)$ 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.,

$$\det(\lambda I - A) = 0$$

We can now use the previous definition of the determinant to expand this expression $\det(\lambda I - A) = 0$ 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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- Suppose A is non-singular with eigenvalue λ and an associated eigenvector x. Then $\frac{1}{\lambda}$ is eigenvalue of A^{-1} with an associated eigenvector x, i.e., $A^{-1}x = (\frac{1}{\lambda})x$

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- The eigenvalues of a diagonal matrix $D = diag(d_1, \ldots, d_n)$ 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., $A^T = A$). 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:

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

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

$$AU = \begin{bmatrix} | & & | \\ Au_1 & \dots & Au_n \\ | & & | \end{bmatrix} = \begin{bmatrix} | & & | \\ \lambda_1 u_1 & \dots & \lambda_n u_n \\ | & & | \end{bmatrix} = U\, diag(\lambda_1, \dots, \lambda$$

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- Recalling that orthonormal matrix U satisfies that $UU^T = 1$, we can diagonalize matrix A:

$$A = AUU^T = U\Lambda U^T$$

Representing vector w.r.t. another basis

- Any orthonormal matrix $U = \begin{bmatrix} | & & | \\ u_1 & \dots & u_n \\ | & & | \end{bmatrix}$ defines a new basis of $\mathbb{R}^n$
- For any vector $x \in \mathbb{R}^n$ can be represented as a linear combination of $u_1, \dots, u_n$ with coefficient $\hat{x}_1, \dots, \hat{x}_n$:

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

- 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 basic 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:

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

- 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 $q = AAAx$

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

"Diagonalizing" quadratic form

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

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

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

Definiteness and Sign of Eigenvalues

1. If all $\lambda_i > 0$, then the matrix A is positive definite because $x^T Ax = \sum_{i=1}^{n} \lambda_i \hat{x}_i^2 > 0$ for any $\hat{x} \neq 0$
2. If all $\lambda_i \geq 0$, it is positive semidefinite because $x^T Ax = \sum_{i=1}^{n} \lambda_i \hat{x}_i^2 \geq 0$ for all $\hat{x}$.
3. Likewise, if all $\lambda_i < 0$ or $\lambda_i \leq 0$, then A is negative definite or negative semidefinite.
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 $x^T Ax = \sum_{i=1}^{n} \lambda_i \hat{x}_i^2 > 0$. Similarly we can let $\hat{x}$ satisfy $\hat{x}_j = 1$ and $\hat{x}_k = 0$, $\forall k \neq j$, then $x^T Ax = \sum_{i=1}^{n} \lambda_i \hat{x}_i^2 < 0$

The Gradient

Suppose that $f\colon\ \mathbb{R}^{m\times n} \to \mathbb{R}$ 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:

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

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

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

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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 $t \in \mathbb{R}$, $\nabla_x(tf(x)) = t\nabla_x(f(x))$

The Hessian

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

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

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

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Note that the Hessian is always symmetric, since

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

Gradients of Linear Functions

For $x \in \mathbb{R}^n$, let $f(x) = b^T x$ 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 $\nabla_x b^T x = b$. 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 $f(x) = x^T Ax$ 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_{jk} x_j x_k + A_{kk} x_k^2 \right] \\
&= \sum_{i \neq k} A_{ik} x_i + \sum_{j \neq k} A_{jk} x_j + 2A_{kk} x_k
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Hessian of Quadratic Function

Finally, let's look at the Hessian of the quadratic function
$f(x) = x^T A x$
In this case,

$$\frac{\partial^2 f(x)}{\partial x_k \partial x_\ell} = \frac{\partial}{\partial x_k}\left[\frac{\partial f(x)}{\partial x_\ell}\right] = \frac{\partial}{\partial x_k}\left[2\sum_{i=1}^{n} A_{\ell i} x_i\right] = 2A_{\ell k} = 2A_{k\ell}$$

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

Recap

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

Matrix Calculus Example: Least Squares

- Given a full rank matrix $A \in \mathbb{R}^{n\times m}$, 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 $\|Ax - b\|_2^2$

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- Using the fact that $\|x\|_2^2 = x^T x$, we have

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

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

$$x = (A^T A)^{-1} A^T b$$

Outline