CS229 Section: Linear Algebra

Nandita Bhaskhar

Slides adapted from past CS229 teams

April 1, 2022

Outline

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

Basic Concepts and Notation

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 $D = \mathrm{diag}(d_1, d_2, \ldots, d_n)$, with

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

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

Outline

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

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

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

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

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,

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

Matrix-Vector Product

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

- expressing A in terms of rows we have:

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

$$= x_1 \begin{bmatrix} — & a_1^T & — \end{bmatrix} + x_2 \begin{bmatrix} — & a_2^T & — \end{bmatrix} + \ldots + x_m \begin{bmatrix} — & a_m^T & — \end{bmatrix}$$

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

Matrix-Matrix Multiplication (different views)

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

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

Matrix-Matrix Multiplication (different views)

2. As a sum of outer products

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

Matrix-Matrix Multiplication (different views)

3. As a set of matrix-vector products.

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

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)

4. As a set of vector-matrix products.

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

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

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

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 $\mathrm{tr}A$, is the sum of diagonal elements in the matrix:

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

The trace has the following properties:

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

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

Matrix Norms

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

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

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***.

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***.

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.

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.

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

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 $A \in \mathbb{R}^{m \times n}$, $\text{rank}(A) = \text{rank}(A^T)$.

Properties of the Rank

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

Properties of the Rank

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

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

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.

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.

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):
  - $(A^{-1})^{-1} = A$
  - $(AB)^{-1} = B^{-1}A^{-1}$
  - $(A^{-1})^T = (A^T)^{-1}$. 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***).

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***).

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

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

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***).

- **Properties:**
  - The inverse of an orthogonal matrix is its transpose.
  $$U^T U = I = UU^T.$$
  - 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 $\{x_1, x_2, \ldots x_n\}$ is the set of all vectors that can be expressed as a linear combination of $\{x_1, \ldots, x_n\}$. That is,

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

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,

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

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

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

Range

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

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

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,

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

- 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,

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

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:

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

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

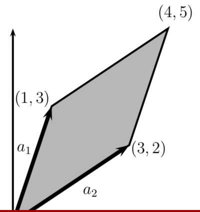
The Determinant: Intuition

For example, consider the 2×2 matrix,

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

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).

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.)

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^T and a_j^T of A, then the determinant of the new matrix is $-|A|$, for example

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^T and a_j^T of A, then the determinant of the new matrix is $-|A|$, for example

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^T and a_j^T of A, then the determinant of the new matrix is $-|A|$, for example

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 ith row and jth column from A.
The general (recursive) formula for the determinant is

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

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:

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

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

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

Quadratic Forms

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

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

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

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

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

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

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

Properties of eigenvalues and eigenvectors

- The trace of a 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,

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

Properties of eigenvalues and eigenvectors

- The trace of a 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.

Properties of eigenvalues and eigenvectors

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

Properties of eigenvalues and eigenvectors

- The trace of a 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:

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

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 $\lambda_1, \ldots, \lambda_n$.

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

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 $\lambda_1, \ldots, \lambda_n$.

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

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

$$A = AUU^T = U\Lambda U^T \tag{4}$$

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

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

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:

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

- 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 $q = AAAx$.

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

"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.)

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

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

Outline

1 Basic Concepts and Notation

2 Matrix Multiplication

3 Operations and Properties

4 Matrix Calculus

Matrix Calculus

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:

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

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

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

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

The Hessian

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

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

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,

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

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 $f(x) = b^T x$ 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 $\partial/(\partial x)\ ax = a$.

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:

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

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:

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

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:

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

Gradients of Quadratic Function

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

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

Hessian of Quadratic Functions

Finally, let's look at the Hessian of the quadratic function $f(x) = x^T Ax$
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 $\nabla_x^2 x^T Ax = 2A$, which should be entirely expected (and again analogous to the single-variable fact that $\partial^2/(\partial x^2)\ ax^2 = 2a$).

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 $A \in \mathbb{R}^{m \times n}$, 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 $\|Ax - b\|_2^2$.

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

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

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

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

- Taking the gradient with respect to x we have:

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

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

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

- Taking the gradient with respect to x we have:

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

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

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