CS229 Section: Linear Algebra

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Slides adapted from past CS229 teams

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

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

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

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

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

\[ xy^T \in \mathbb{R}^{m \times n} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix} \begin{bmatrix} y_1 & y_2 & \cdots & y_n \end{bmatrix} = \begin{bmatrix} x_1 y_1 & x_1 y_2 & \cdots & x_1 y_n \\ x_2 y_1 & x_2 y_2 & \cdots & x_2 y_n \\ \vdots & \vdots & \ddots & \vdots \\ x_m y_1 & x_m y_2 & \cdots & x_m y_n \end{bmatrix}. \]
If we write $A$ by rows, then we can express $Ax$ as,

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

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

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

(1)

$y$ is a \textit{linear combination} of the \textit{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,

$$y^T = x^T A = x^T \begin{bmatrix} a^1 & a^2 & \cdots & a^n \end{bmatrix} = \begin{bmatrix} x^T a^1 \\ x^T a^2 \\ \vdots \\ x^T a^n \end{bmatrix}$$
Matrix-Vector Product

It is also possible to multiply on the left by a row vector. Expressing $A$ in terms of rows we have:

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

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

$y^T$ is a linear combination of the rows of $A$. 
Matrix-Matrix Multiplication (different views)

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

\[ C = AB = \begin{bmatrix} a_1^T & \cdots & a_m^T \end{bmatrix} \begin{bmatrix} b_1 \ b_2 \ \ldots \ b_p \end{bmatrix} = \begin{bmatrix} a_1^T b_1 & a_1^T b_2 & \cdots & a_1^T b_p \\ a_2^T b_1 & a_2^T b_2 & \cdots & a_2^T b_p \\ \vdots & \vdots & \ddots & \vdots \\ a_m^T b_1 & a_m^T b_2 & \cdots & a_m^T b_p \end{bmatrix}. \]
Matrix-Matrix Multiplication (different views)

2. As a sum of outer products

\[ C = AB = \sum_{i=1}^{p} a_i b_i^T. \]
3. As a set of matrix-vector products.

\[
C = AB = A \begin{bmatrix} b^1 & b^2 & \cdots & b^n \end{bmatrix} = \begin{bmatrix} Ab^1 & Ab^2 & \cdots & Ab^n \end{bmatrix}.
\]  

(2)

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.

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

- Addition
- Subtraction
- Scalar multiplication
- Matrix multiplication
- Transpose
- Inverse
- Eigenvalues and eigenvectors
- Trace
- Determinant

**Key Properties**

- Commutativity
- Associativity
- Distributivity
- Identity matrix
- Invertibility
- Diagonalizability
- Normal matrices
- Symmetric matrices
- Hermitian matrices

**Important Results**

- **Cayley-Hamilton Theorem**
- **Sylvester's Criterion**
- **Jordan Canonical Form**
- **Lyapunov's Equation**

**Applications**

- **Signal Processing**
- **Computer Graphics**
- **Data Analysis**
- **Optimization**
- **Machine Learning**
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:

- $(A^T)^T = A$
- $(AB)^T = B^T A^T$
- $(A + B)^T = A^T + B^T$
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.
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 $\ell_2$ norm,

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

The $\ell_1$ norm,

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

The $\ell_\infty$ norm,

$$||x||_\infty = \max_i |x_i|.$$
In fact, all three norms presented so far are examples of the family of $\ell_p$ norms, which are parameterized by a real number $p \geq 1$, and defined as

$$\|x\|_p = \left( \sum_{i=1}^{n} |x_i|^p \right)^{1/p}.$$
Norms can also be defined for matrices, such as the Frobenius norm,

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

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 \textit{(linearly) dependent} if one vector belonging to the set \textit{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 \textit{(linearly) independent}. 

Example:

\[
\begin{align*}
x_1 &= \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \\
x_2 &= \begin{pmatrix} 4 \\ 1 \\ 5 \end{pmatrix} \\
x_3 &= \begin{pmatrix} 2 \\ -3 \\ -1 \end{pmatrix}
\end{align*}
\]

are linearly dependent because \( x_3 = -2x_1 + x_2 \).
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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 $\text{rank}(A)$. 
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.
Properties of the Rank

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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

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

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

\[ U^T U = I = UU^T. \]
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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 $\{x_1, x_2, \ldots x_n\}$ is the set of all vectors that can be expressed as a linear combination of $\{x_1, \ldots, x_n\}$. That is,

$$\text{span}(\{x_1, \ldots, x_n\}) = \left\{ v : v = \sum_{i=1}^{n} \alpha_i x_i, \quad \alpha_i \in \mathbb{R} \right\}.$$
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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 \( v \in \text{span}(\{x_1, \ldots, x_n\}) \), such that \( v \) is as close as possible to \( y \), as measured by the Euclidean norm \( \|v - y\|_2 \).

\[
\text{Proj}(y; \{x_1, \ldots, x_n\}) = \arg\min_{v \in \text{span}(\{x_1, \ldots, x_n\})} \|y - v\|_2.
\]
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,

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

$$\text{Proj}(y; A) = \arg\min_{v \in \mathcal{R}(A)} \| v - y \|_2.$$
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:

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

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 $2 \times 2$ matrix,

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

(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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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 $t$.)
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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
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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

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

$$= \sum_{j=1}^{n} (-1)^{i+j} a_{ij} |A_{\setminus i, \setminus j}| \quad \text{(for any } i \in 1, \ldots, n)$$

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 $3 \times 3$. 
The Determinant: Examples

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

\[
\begin{vmatrix} a_{11} \end{vmatrix} = a_{11}
\]

\[
\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}a_{22} - a_{12}a_{21}
\]

\[
\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32} - a_{11}a_{23}a_{32} - a_{12}a_{21}a_{33} - a_{13}a_{22}a_{31}
\]
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 \( x^T A x \) is called a quadratic form. Written explicitly, we see that

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

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 $A \in S^n$ is:

- **positive definite** (PD), denoted $A \succ 0$ if for all non-zero vectors $x \in \mathbb{R}^n$, $x^T Ax > 0$.

- **positive semidefinite** (PSD), denoted $A \succeq 0$ if for all vectors $x^T Ax \geq 0$.

- **negative definite** (ND), denoted $A \prec 0$ if for all non-zero $x \in \mathbb{R}^n$, $x^T Ax < 0$.

- **negative semidefinite** (NSD), denoted $A \preceq 0$ if for all $x \in \mathbb{R}^n$, $x^T Ax \leq 0$.

- **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 $x_1^T Ax_1 > 0$ and $x_2^T Ax_2 < 0$. 
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.
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 $\lambda$. 
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.,

\[
|\lambda I - A| = 0.
\]

We can now use the previous definition of the determinant to expand this expression \(|\lambda I - A|\) into a (very large) polynomial in \(\lambda\), where \(\lambda\) 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,

$$\text{tr}A = \sum_{i=1}^{n} \lambda_i.$$
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- The determinant of $A$ is equal to the product of its eigenvalues,

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

Suppose $A$ is non-singular with eigenvalue $\lambda$ 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 $D = \text{diag}(d_1, \ldots, d_n)$ are just the diagonal entries $d_1, \ldots, d_n$. 
Properties of eigenvalues and eigenvectors

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Properties of eigenvalues and eigenvectors

- The trace of a $A$ is equal to the sum of its eigenvalues,
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- The eigenvalues of a diagonal matrix $D = \text{diag}(d_1, \ldots d_n)$ are just the diagonal entries $d_1, \ldots d_n$. 
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 $\lambda_i$ 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 $\Lambda = \text{diag}(\lambda_1, \ldots, \lambda_n)$ be the diagonal matrix that contains $\lambda_1, \ldots, \lambda_n$.

$$AU = \begin{bmatrix} Au_1 & Au_2 & \cdots & Au_n \end{bmatrix} = \begin{bmatrix} \lambda_1 u_1 & \lambda_2 u_2 & \cdots & \lambda_n u_n \end{bmatrix} = U\text{diag}(\lambda_1, \ldots, \lambda_n) = U\Lambda$$
New Representation for Symmetric Matrices

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

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

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

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 $U$:

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

- We see that left-multiplying matrix $A$ in the original space is equivalent to left-multiplying the diagonal matrix $\Lambda$ 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 \( q = AAX \).

\[
\hat{q} = U^T q = U^T AAX = U^T UU^T UU^T UU^T x = \Lambda^3 \hat{x} = \begin{bmatrix}
\lambda_1^3 \hat{x}_1 \\
\lambda_2^3 \hat{x}_2 \\
\vdots \\
\lambda_n^3 \hat{x}_n
\end{bmatrix}
\]
“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 $t \in \mathbb{R}$, $\nabla_x (t \cdot f(x)) = t \nabla_x f(x).$
The Hessian

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

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

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 \( f(x) = x^T A x \) 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:

\[
\frac{\partial f(x)}{\partial x_k} = \frac{\partial}{\partial x_k} \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j
\]
Gradients of Quadratic Function

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

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

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

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

$$= \frac{\partial}{\partial x_k} \left[ \sum_{i \neq k} \sum_{j \neq k} A_{ij} x_i x_j + \sum_{i \neq k} A_{ik} x_i x_k + \sum_{j \neq k} A_{kj} x_k x_j + A_{kk} x_k^2 \right]$$

$$= \sum_{i \neq k} A_{ik} x_i + \sum_{j \neq k} A_{kj} x_j + 2A_{kk} x_k$$
Gradients of Quadratic Function

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

\[
\begin{align*}
    f(x) &= \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j.
\end{align*}
\]

To take the partial derivative, we’ll consider the terms including \( x_k \) and \( x_k^2 \) factors separately:

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

- $\nabla_x b^T x = b$
- $\nabla_x^2 b^T x = 0$
- $\nabla_x x^T Ax = 2Ax$ (if $A$ symmetric)
- $\nabla_x^2 x^T Ax = 2A$ (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 $b \not\in \mathcal{R}(A)$, 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 

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

Taking the gradient with respect to $x$ we have:

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

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

$$
x = (A^T A)^{-1} A^T b
$$
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- Using the fact that $\|x\|_2^2 = x^T x$, we have

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

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

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