Linear Algebra and Calculus Review

Can Li

ChE 597: Computational Optimization Purdue University

Disclaimer

This lecture is like a cheat sheet for linear algebra and calculus. The theorems are given without proof.

It is impossible to memorize the theorems and formulas since they are not intuitive. I would strongly recommend watching the YouTube video by 3Blue1Brown listed in the references to get some geometric intuition.

Matrix and Vector Notation

- 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.
- By $x \in \mathbb{R}^n$, we denote a vector with n entries. By convention, an n-dimensional vector is often thought of as a matrix with n rows and 1 column, known as a *column vector*. If we want to explicitly represent a *row vector*—a matrix with 1 row and n columns—we typically write x^\top
- The *i*-th element of a vector x is denoted x_i:

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

Matrix Notation

• We use the notation a_{ij} (or A_{ij} , $A_{i,j}$, etc.) to denote the entry of A in the i-th row and j-th column:

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}.$$

• We denote the *j*-th column of A by a_i or $A_{::,j}$:

$$A = \begin{bmatrix} | & | & | \\ a_1 & a_2 & \cdots & a_n \\ | & | & | \end{bmatrix}.$$

• We denote the *i*-th row of A by a_i^{\top} or $A_{i,:}$:

$$A = \begin{vmatrix} - & a_{1}^{\top} & - \\ - & a_{2}^{\top} & - \\ & \vdots \\ - & a_{m}^{\top} & - \end{vmatrix}.$$

Matrix Multiplication

The product of two matrices $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{n \times p}$ is the matrix

$$C = AB \in \mathbb{R}^{m \times p}$$
,

where

$$C_{ij} = \sum_{k=1}^{n} A_{ik} B_{kj}.$$

Note that in order for the matrix product to exist, the number of columns in *A* must equal the number of rows in *B*.

$$C = AB = \begin{bmatrix} - & a_1^\top & - \\ - & a_2^\top & - \\ \vdots & & & \\ - & a_m^\top & - \end{bmatrix} \begin{bmatrix} | & | & & & | \\ b_1 & b_2 & \cdots & b_p \\ | & | & & & | \end{bmatrix} = \begin{bmatrix} a_1^\top b_1 & a_1^\top b_2 & \cdots & a_1^\top b_p \\ a_2^\top b_1 & a_2^\top b_2 & \cdots & a_2^\top b_p \\ \vdots & \vdots & \ddots & \vdots \\ a_m^\top b_1 & a_m^\top b_2 & \cdots & a_m^\top b_p \end{bmatrix}$$

Examples: vector products

• Inner product (dot product) of two vectors. Given two vectors $x, y \in \mathbb{R}^n$

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

• Outer product of two vectors. Given vectors $x \in \mathbb{R}^m$, $y \in \mathbb{R}^n$ (not necessarily of the same size), $xy^\top \in \mathbb{R}^{m \times n}$ is called the outer product of the vectors. It is a matrix whose entries are given by $(xy^\top)_{ij} = x_i y_j$, i.e.,

$$xy^{\top} \in \mathbb{R}^{m \times n} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix} \begin{bmatrix} y_1 & y_2 & \cdots & y_n \end{bmatrix} = \begin{bmatrix} x_1y_1 & x_1y_2 & \cdots & x_1y_n \\ x_2y_1 & x_2y_2 & \cdots & x_2y_n \\ \vdots & \vdots & \ddots & \vdots \\ x_my_1 & x_my_2 & \cdots & x_my_n \end{bmatrix}$$

Matrix-Vector Multiplication

Given a matrix $A \in \mathbb{R}^{m \times n}$ and a vector $x \in \mathbb{R}^n$, their product is a vector $y = Ax \in \mathbb{R}^m$.

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

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

Alternatively, let's write A in column form. In this case, we see that:

$$y = Ax = \begin{bmatrix} | & | & & | \\ a_1 & a_2 & \cdots & a_n \\ | & | & & | \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = [a_1] x_1 + [a_2] x_2 + \cdots + [a_n] x_n.$$

In other words, y is a *linear combination* of the *columns* of A, where the coefficients of the linear combination are given by the entries of x.

Properties of Matrix Multiplication

Matrix multiplication is associative:

$$(AB)C = A(BC).$$

Matrix multiplication is distributive:

$$A(B+C)=AB+AC.$$

 Matrix multiplication is, 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!

The Transpose and Symmetric Matrices

The Transpose:

- The transpose of a matrix $A \in \mathbb{R}^{m \times n}$, written $A^{\top} \in \mathbb{R}^{n \times m}$, is defined as $(A^{\top})_{ij} = A_{ji}$.
- Properties:

$$(A^{\top})^{\top} = A, \quad (AB)^{\top} = B^{\top}A^{\top}, \quad (A+B)^{\top} = A^{\top} + B^{\top}.$$

Symmetric Matrices:

- A square matrix $A \in \mathbb{R}^{n \times n}$ is:
 - *Symmetric* if $A = A^{\top}$.
 - Anti-symmetric if $A = -A^{\top}$.
- Any square matrix can be decomposed as:

$$A = \frac{1}{2}(A + A^{T}) + \frac{1}{2}(A - A^{T}),$$

where the first term is symmetric and the second is anti-symmetric.

The Trace of a Matrix

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

$$trA = \sum_{i=1}^{n} A_{ii}.$$

Properties of the Trace:

- For $A \in \mathbb{R}^{n \times n}$, $\operatorname{tr} A = \operatorname{tr} A^{\top}$.
- For $A, B \in \mathbb{R}^{n \times n}$, tr(A + B) = trA + trB.
- For $A \in \mathbb{R}^{n \times n}$, $t \in \mathbb{R}$, tr(tA) = t tr A.
- For A, B such that AB is square, tr(AB) = tr(BA).
- For A, B, C such that ABC is square,
 tr(ABC) = tr(BCA) = tr(CAB), and so on for products of more matrices.

Norms of Vectors and Matrices

Definition of a Norm: A *norm* measures the "length" of a vector. Commonly used norms include:

• Euclidean or ℓ_2 norm:

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

Note: $||x||_2^2 = x^T x$.

• ℓ_1 norm:

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

• ℓ_{∞} norm:

$$||x||_{\infty} = \max_i |x_i|.$$

• ℓ_p norm:

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

Norms of Vectors and Matrices

More formally, a norm is any function $f: \mathbb{R}^n \to \mathbb{R}$ that satisfies 4 properties:

- 1. For all $x \in \mathbb{R}^n$, $f(x) \ge 0$ (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 $x, y \in \mathbb{R}^n$, $f(x+y) \le f(x) + f(y)$ (triangle inequality).

Matrix Norm: The Frobenius norm is defined as:

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

The 2-norm (spectral norm) of a matrix $A \in \mathbb{R}^{m \times n}$ is defined as:

$$\|A\|_2 = \sqrt{\lambda_{\mathsf{max}}(A^\top A)}$$

where $\lambda_{\max}(A^{\top}A)$ denotes the largest eigenvalue of the matrix $A^{\top}A$.

Linear Independence and Dependence

A set of vectors $\{x_1, x_2, \dots, x_n\} \subset \mathbb{R}^m$ is:

- **Linearly independent** if no vector can be represented as a linear combination of the remaining vectors.
- Linearly dependent if one vector can be expressed as a linear combination of the others:

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

for some scalars $\alpha_1, \ldots, \alpha_{n-1} \in \mathbb{R}$. zero vector is always linearly dependent on others.

Example: The vectors

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

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

Rank of a Matrix

Definition:

- The *column rank* of a matrix $A \in \mathbb{R}^{m \times n}$ is the size of the largest subset of linearly independent columns.
- The row rank is the size of the largest subset of linearly independent rows.
- For any matrix $A \in \mathbb{R}^{m \times n}$, the column rank equals the row rank, collectively referred to as the rank of A, denoted as rank(A).

Properties of the Rank:

- $rank(A) \le min(m, n)$. If rank(A) = min(m, n), then A is full rank.
- $\operatorname{rank}(A) = \operatorname{rank}(A^T)$.
- For $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{n \times p}$:

$$rank(AB) \leq min(rank(A), rank(B)).$$

• $rank(A + B) \le rank(A) + rank(B)$.

The Inverse of a Matrix

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

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

Key Points:

- Not all matrices have inverses. Non-square matrices, for example, do not have inverses.
- A square matrix A is *invertible* or *non-singular* if A^{-1} exists; otherwise, it is *non-invertible* or *singular*.
- For A to have an inverse, it must be full rank.

Properties of the Inverse:

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

Application: For a linear system Ax = b, if A is invertible, the solution is $x = A^{-1}b$.

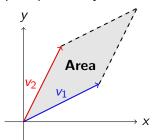
Matrix Determinant and Geometric Intuition

The determinant of a square matrix $A = [a_{ij}] \in \mathbb{R}^{n \times n}$, denoted det(A), is a scalar value that encodes properties of the linear transformation represented by A.

For a 2 × 2 matrix:

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \quad \det(A) = ad - bc$$

- The determinant represents the **signed area** of the parallelogram spanned by the column vectors of *A*.
- In higher dimensions $(n \times n)$, it represents the **signed volume** of the parallelepiped spanned by the columns.

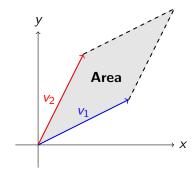


Matrix Determinant and Geometric Intuition

Key Properties:

- det(A) = 0: The transformation collapses space (columns are linearly dependent).
- det(A) > 0: Orientation is preserved.
- det(A) < 0: Orientation is reversed.

Visual Example (2D):



Determinant Formula and Adjoint Method for Inverse

Determinant Formula for an $n \times n$ **Matrix:**

For $A = [a_{ij}] \in \mathbb{R}^{n \times n}$, the determinant is given by:

$$\det(A) = \sum_{j=1}^n (-1)^{1+j} a_{1j} \det(A_{\setminus 1,\setminus j})$$

where $A_{\backslash 1,\backslash j}$ is the $(n-1)\times (n-1)$ matrix obtained by removing the 1st row and j-th column of A.

Adjoint Method to Calculate A^{-1} :

 The adjoint matrix of A, denoted adj(A), is the transpose of the cofactor matrix:

$$\operatorname{adj}(A)_{ij} = (-1)^{i+j} \operatorname{det}(A_{\setminus i,\setminus j}).$$

• If $det(A) \neq 0$, the inverse of A is:

$$A^{-1} = rac{1}{\det(A)} \operatorname{adj}(A)$$

Vector Spaces of Matrix $A \in \mathbb{R}^{m \times n}$

- Column (Range) Space (Col(A), Range(A))
 - Set of all linear combinations of the column vectors of A.
 - Subspace of \mathbb{R}^m . $\{Ax \mid \forall x \in \mathbb{R}^n\}$
 - Dimension equals the rank of A.

Row Space (Row(A))

- Set of all linear combinations of the row vectors of A.
- Subspace of \mathbb{R}^n . $\{A^Ty \mid \forall y \in \mathbb{R}^m\}$
- Dimension equals the rank of A.
- For $A \in \mathcal{S}^n$ (symmetric matrix), Col(A) = Row(A).

Null Space (Null(A))

- Set of all vectors x such that Ax = 0.
- Subspace of \mathbb{R}^n .
- Dimension equals the *n*-rank(A).

Orthogonal Properties

• The row space and null space of A are orthogonal complements in \mathbb{R}^n .

$$\{w: w = u + v, u \in \text{Row}(A), v \in \text{Null}(A)\} = \mathbb{R}^m \text{ and } \text{Row}(A) \cap \text{Null}(A) = \emptyset$$

• The column space and the left null space (null space of A^T) are orthogonal complements in \mathbb{R}^m .

Eigenvalues and Eigenvectors: Definition and Calculation

Definition: For a square matrix $A \in \mathbb{R}^{n \times n}$, a scalar $\lambda \in \mathbb{R}$ and a nonzero vector $v \in \mathbb{R}^n$ are called an **eigenvalue** and **eigenvector**, respectively, if:

$$Av = \lambda v$$

How to Calculate: 1. Solve the **characteristic equation**:

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

This yields the eigenvalues λ .

2. For each eigenvalue λ , solve the system of linear equations:

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

to find the corresponding eigenvectors v.

Example: Let $A = \begin{bmatrix} 4 & 1 \\ 2 & 3 \end{bmatrix}$:

• Solve $det(A - \lambda I) = 0$:

$$\det\left(\begin{bmatrix} 4-\lambda & 1\\ 2 & 3-\lambda \end{bmatrix}\right) = 0$$

Properties of Eigenvalues and Eigenvectors

- For a matrix $A \in \mathbb{R}^{n \times n}$:
 - The sum of the eigenvalues equals the trace of A:

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

• The product of the eigenvalues equals the determinant of *A*:

$$\prod_{i=1}^n \lambda_i = \det(A)$$

• Eigenvectors corresponding to distinct eigenvalues are linearly independent.

PSD, PD, NSD, and ND Symmetric Matrices

Symmetric Matrix $A \in \mathbb{R}^{n \times n}$: $A = A^{\top}$. Notation: $A \in \mathbb{S}^n$

• Positive Semidefinite (PSD): A is PSD if:

$$x^{\top}Ax > 0$$
 for all $x \in \mathbb{R}^n$

All eigenvalues of A are $\lambda_i \geq 0$.

• Positive Definite (PD): A is PD if:

$$x^{\top}Ax > 0$$
 for all nonzero $x \in \mathbb{R}^n$

All eigenvalues of A are $\lambda_i > 0$.

• Negative Semidefinite (NSD): A is NSD if:

$$x^{\top} A x < 0$$
 for all $x \in \mathbb{R}^n$

All eigenvalues of A are $\lambda_i \leq 0$.

• **Negative Definite (ND)**: A is ND if:

$$x^{\top}Ax < 0$$
 for all nonzero $x \in \mathbb{R}^n$

All eigenvalues of A are $\lambda_i < 0$.

 A matrix is indefinite if it has both positive and negative eigenvalues.

Eigenvalue Decomposition (EVD)

Definition: For a symmetric matrix $A \in \mathbb{R}^{n \times n}$, the **eigenvalue decomposition** is:

$$A = Q \Lambda Q^{\top} = \sum_{i=1}^{n} \lambda_i \, q_i \, q_i^{\top}$$

where:

- $Q = \begin{bmatrix} q_1 & q_2 & \dots & q_n \end{bmatrix}$ is an orthogonal matrix $(QQ^T = I)$ containing the eigenvectors of A.
- Λ is a diagonal matrix with the eigenvalues of A as its entries:

$$\Lambda = \operatorname{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$$

Key Properties:

- A is symmetric \implies all eigenvalues are real.
- A is PSD \implies all $\lambda_i \geq 0$.

Notation for Functions

$$f: A \rightarrow B$$

f is a function on the set dom $f \subseteq A$ into the set B; in particular, we can have dom f as a proper subset of the set A.

- $f: \mathbb{R}^n \to \mathbb{R}^m$ means that f maps (some) n-vectors into m-vectors; it does not mean that f(x) is defined for all $x \in \mathbb{R}^n$.
- f(x) = log(x). $f: \mathbb{R}^+ \to \mathbb{R}$

Continuity of Functions

A function $f: \mathbb{R}^n \to \mathbb{R}$ is *continuous* at $x \in \text{dom } f$ if for all $\epsilon > 0$ there exists a δ such that

$$\forall y \in \text{dom } f$$
, $||y - x||_2 \le \delta \implies ||f(y) - f(x)||_2 \le \epsilon$.

Continuity can be described in terms of limits: whenever the sequence $x_1, x_2,...$ in dom f converges to a point $x \in \text{dom } f$, the sequence $f(x_1), f(x_2),...$ converges to f(x), i.e.,

$$\lim_{i\to\infty} f(x_i) = f\left(\lim_{i\to\infty} x_i\right).$$

A function *f* is *continuous* if it is continuous at every point in its domain.

Derivative and Differentiable Functions

Derivative: Let $f: \mathbb{R}^n \to \mathbb{R}^m$. We say f is **differentiable at** x if there exists a linear map $Df(x): \mathbb{R}^n \to \mathbb{R}^m$ such that:

$$\lim_{h\to 0} \frac{\|f(x+h) - f(x) - Df(x)h\|}{\|h\|} = 0.$$

Differentiable Functions: A function f is differentiable on an open set U if it is differentiable at every point in U. Differentiability \implies continuity.

Gradient (for scalar functions): If $f: \mathbb{R}^n \to \mathbb{R}$, then the gradient of f at x is:

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

It satisfies: $Df(x)h = \nabla f(x)^{\top}h$.

Gradient Interpretation and C^1 Functions

Interpretation of the Gradient: - The gradient points in the direction of maximum increase of f. - Its magnitude $\|\nabla f(x)\|$ represents the rate of change.

 C^1 Functions: A function $f: \mathbb{R}^n \to \mathbb{R}^m$ is C^1 on an open set U if:

- 1. *f* is differentiable on *U*.
- 2. The map $x \mapsto Df(x)$ (or each partial derivative) is continuous on U.

For scalar functions $f: \mathbb{R}^n \to \mathbb{R}$, this means:

$$f \in C^1(U) \iff \frac{\partial f}{\partial x_i}(x)$$
 exists and is continuous for all *i*.

 C^1 functions are also called smooth functions.

Hessian Matrix

Definition: The **Hessian matrix** of a twice-differentiable scalar function $f: \mathbb{R}^n \to \mathbb{R}$ at a point $x \in \mathbb{R}^n$ is the $n \times n$ matrix of second-order partial derivatives:

$$H_f(x) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}.$$

Properties:

- $H_f(x)$ is symmetric if f is twice continuously differentiable $(f \in C^2)$.
- The Hessian provides information about the curvature of f.

Taylor Series Expansion (Second Order)

Definition: Let $f: \mathbb{R}^n \to \mathbb{R}$ be a twice-differentiable function. The **Taylor series expansion up to the second order** around a point $x \in \mathbb{R}^n$ is given by:

$$f(x+h) \approx f(x) + \nabla f(x)^{\top} h + \frac{1}{2} h^{\top} H_f(x) h,$$

where:

- $\nabla f(x)$ is the gradient of f at x,
- $H_f(x)$ is the Hessian matrix of f at x,
- h = x' x is the displacement vector.

Interpretation:

- The first term, f(x), represents the function value at x.
- The second term, $\nabla f(x)^{\top} h$, is the linear approximation (gradient contribution).
- The third term, $\frac{1}{2}h^{\top}H_f(x)h$, accounts for the curvature (second-order effects).

Peano and Lagrange Remainders in Taylor Series

For a twice-differentiable function $f: \mathbb{R}^n \to \mathbb{R}$, the second-order Taylor expansion of f at x for a small increment h is:

$$f(x+h) = f(x) + \nabla f(x)^{\top} h + \frac{1}{2} h^{\top} H_f(x) h + R_2(x,h),$$

where $H_f(x)$ is the Hessian of f at x and $R_2(x,h)$ is the remainder.

1. Peano Form:

$$R_2(x,h) = o(\|h\|^2)$$
 as $\|h\| \to 0$.

This means $R_2(x, h)$ goes to zero faster than $||h||^2$.

2. Lagrange Form: There exists $\theta \in (0,1)$ such that

$$f(x+h) = f(x) + \nabla f(x)^{\top} h + \frac{1}{2} h^{\top} H_f(x+\theta h) h.$$

Equivalently,

$$R_2(x,h) = \frac{1}{2} h^{\top} [H_f(x+\theta h) - H_f(x)] h.$$

Key Insight: - The *Peano form* expresses how R_2 vanishes asymptotically. - The *Lagrange form* gives a pointwise representation of R_2 via the Hessian at an intermediate point.

Mean Value Theorem

Let $f: U \subseteq \mathbb{R}^n \to \mathbb{R}$ be a function such that:

- f is **continuous** on the line segment joining x to y (i.e., on $\{x + t(y x) : t \in [0, 1]\}$),
- f is **differentiable** in the interior of that segment (i.e., for $t \in (0,1)$).

Then there exists some $\theta \in (0,1)$ such that

$$f(y) - f(x) = \nabla f(x + \theta (y - x))^{\top} (y - x).$$

- The directional derivative of f at some point on the segment from x to y (in the direction y-x) matches the average rate of change $\frac{f(y)-f(x)}{||y-x||}$.
- Geometrically, $\nabla f(\dots)$ at this point captures how f changes most rapidly, and it aligns with the increment y x.
- MVT can be seen as a corollary or special case of the Lagrange form of the first-order Taylor remainder.

Jacobian Matrix

Let $f: \mathbb{R}^n \to \mathbb{R}^m$ be a differentiable vector-valued function:

$$f(x) = \begin{bmatrix} f_1(x_1, x_2, \dots, x_n) \\ f_2(x_1, x_2, \dots, x_n) \\ \vdots \\ f_m(x_1, x_2, \dots, x_n) \end{bmatrix}.$$

The **Jacobian matrix** of f at $x \in \mathbb{R}^n$ is the $m \times n$ matrix of partial derivatives:

$$J_{\mathbf{f}}(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \cdots & \frac{\partial f}{\partial x_n} \end{bmatrix} = \begin{bmatrix} \nabla^{\top} f_1 \\ \vdots \\ \nabla^{\top} f_m \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

- $J_f(x) \in \mathbb{R}^{m \times n}$, where m is the number of outputs, and n is the number of inputs.
- Each row corresponds to the gradient of a component function $f_i(x)$.
- If m = n, and $J_f(x)$ is invertible, f is locally invertible near x.

Chain Rule

Scalar form: If y = f(g(x)), where $g : \mathbb{R} \to \mathbb{R}$ and $f : \mathbb{R} \to \mathbb{R}$, then:

$$\frac{dy}{dx} = f'(g(x)) \cdot g'(x).$$

Matrix Form: If $f: \mathbb{R}^m \to \mathbb{R}^p$ and $g: \mathbb{R}^n \to \mathbb{R}^m$, then for F(x) = f(g(x)),

$$J_F(x) = J_f(g(x)) J_g(x)$$

where $J_g(x) \in \mathbb{R}^{m \times n}$ and $J_f(g(x)) \in \mathbb{R}^{p \times m}$.

Chain Rule for Second Derivative

A general chain rule for the second derivative is cumbersome in most cases, so we state it only for some special cases that we will need.

Composition with Scalar Function: Suppose $f: \mathbb{R}^n \to \mathbb{R}$, $g: \mathbb{R} \to \mathbb{R}$, and h(x) = g(f(x)). By computing the partial derivatives, we get:

$$\nabla^2 h(x) = g'(f(x))\nabla^2 f(x) + g''(f(x))\nabla f(x)\nabla f(x)^T$$

Composition with Affine Function: Suppose $f: \mathbb{R}^n \to \mathbb{R}$, $A \in \mathbb{R}^{n \times m}$, and $b \in \mathbb{R}^n$. Define $g: \mathbb{R}^m \to \mathbb{R}$ by g(x) = f(Ax + b). Then:

$$\nabla^2 g(x) = A^T \nabla^2 f(Ax + b) A.$$

References

- Boyd, S. P., & Vandenberghe, L. (2004). Convex optimization. Cambridge university press. Appendix A.
- Linear algebra review notes by Zico Kolter.
 https://www.cs.cmu.edu/~zkolter/course/linalg/index.html
- YouTube videos review of linear algebra and calculus by 3Blue1Brown.
 - https://www.youtube.com/@3blue1brown/courses **Strongly recommend!** Provides geometric intuition.