Module 10: Differentiation and Integration

Operational math bootcamp

Ichiro Hashimoto

University of Toronto

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Last time

- Eigenvalues and eigenvectors
- Algebraic and geometric multiplicity of eigenvalues
- Matrix diagonalization

Outline

- Matrix decompositions
  - Jordan canonical form
  - Singular value decomposition
  - QR
- Differentiation on $\mathbb{R}$
  - Mean value theorem
  - l'Hôpital's rule
  - Smoothness classes
- Integration on $\mathbb{R}$
  - Riemann sums and Riemann integral
  - Integration rules
  - Drawbacks of Riemann integration

Recall

Definition

Given an operator $A\colon V \to V$ and $\lambda \in \mathbb{F}$, λ is called an *eigenvalue* of A if there exists a non-zero vector $\mathbf{v} \in V \setminus \{\mathbf{0}\}$ such that

$$A\mathbf{v} = \lambda \mathbf{v}.$$

$0 \overset{?}{\neq} v \in \ker(A - \lambda I)$

We call such $\mathbf{v}$ an *eigenvector* of A with eigenvalue λ. We call the set of all eigenvalues of A *spectrum* of A and denote it by $\sigma(A)$.

Recall

- The multiplicity of the root λ in the characteristic polynomial is called the *algebraic multiplicity* of the eigenvalue λ
- The dimension of the eigenspace $\text{null}(A - \lambda I)$ is called the *geometric multiplicity* of the eigenvalue λ.
- An $n \times n$ matrix A is **diagonalizable** if there exists an invertible matrix $S \in M_n(\mathbb{C})$ such that $A = SDS^{-1}$, where D is a diagonal matrix with the eigenvalues of A in the diagonal.
- If $A \in M_n(\mathbb{C})$ has n distinct eigenvalues, then A is diagonalizable.
- A is diagonalizable if and only if for each eigenvalue λ, the geometric multiplicity of λ and the algebraic multiplicity of λ are the same.

Block matrices

Definition

A block matrix is a matrix that can be broken into sections called blocks, which are smaller matrices.

Example

$$\begin{bmatrix} 2 & 1 & 0 & 1 \\ 0 & 2 & 1 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 2 & 1 \end{bmatrix} = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$$

$$A = \begin{pmatrix} 2 & 1 \\ 0 & 2 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}, \quad C = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad D = \begin{pmatrix} 1 & 0 \\ 2 & 1 \end{pmatrix}$$

Definition

A square matrix is called *block diagonal* if it can be written as a block matrix where the main-diagonal blocks are all square matrices and the off-diagonal blocks are all zero.

Example

The matrix

$$\begin{bmatrix} 2 & 1 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 2 & 1 \end{bmatrix}$$

is block diagonal.

Definition

A vector $\mathbf{v}$ is called a *generalized eigenvector* of A corresponding to an eigenvalue λ if there exists $k \geq 1$ such that

$$(A - \lambda I)^k \mathbf{v} = 0.$$

$\iff v \in \ker[(A-\lambda I)^k]$ for some $k \geq 1$.

The set of generalized eigenvectors of an eigenvalue λ (plus $\mathbf{0}$) is called the *generalized eigenspace* of λ.

$\ker(A-\lambda I) \subset \ker(A-\lambda I)^2 \subset \ker(A-\lambda I)^3 \subset \cdots\cdots$

Proposition

The algebraic multiplicity of an eigenvalue λ is the same as the dimension of the corresponding generalized eigenspace.

If we know algebraic multiplicity of λ is 3, then the dimension of space of generalized eigenvectors is 3.

Theorem (Jordan decomposition theorem)

For any operator A there exists a basis such that A is block diagonal with blocks that have eigenvalues on the diagonal and 1s on the upper off-diagonal. In other words, A can be written in the form

$$A = \begin{bmatrix} J_1 & 0 & \dots & 0 \\ 0 & J_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & J_k \end{bmatrix}$$

where the blocks J_i on the main diagonal are Jordan block of the form

eigenvector

$$[\lambda], \begin{bmatrix} \lambda & 1 \\ 0 & \lambda \end{bmatrix}, \begin{bmatrix} \lambda & 1 & 0 \\ 0 & \lambda & 1 \\ 0 & 0 & \lambda \end{bmatrix}, \text{etc.}$$

generalized eigen space has dim. 3.

This form is called Jordan canonical form.

Connection to algebraic and geometric multiplicity:

- The algebraic multiplicity of an eigenvalue λ is the number of times λ appears on the diagonal.
- The geometric multiplicity of λ is the number of Jordan blocks associated with λ.

Why is Jordan form useful?

$$N = \begin{pmatrix} 0 & 1 & & 0 \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ 0 & & & 0 \end{pmatrix}$$

$$JCF = D + N$$

$D \downarrow$ diagonal

$N \downarrow$ non-diagonal.

N is "nilpotent", i.e.

$\exists\, k \geq 1$ s.t. $N^k = 0$

Singular value decomposition

$O^T O = O O^T = I_n$

Theorem

Let $A \in M_n(\mathbb{R})$ be a symmetric matrix. Then, there exists an orthogonal matrix $O \in M_n(\mathbb{R})$ such that $A = ODO^T$, where D is a diagonal matrix with the eigenvalues of A in the diagonal. Furthermore, all eigenvalues of A are real.

Note: $A^T A$ is symmetric (AA^T)

That means $A^T A$, AA^T is diagonalizable with orthogonal matrix for any A. (any size is allowed)

Definition

Let A be an $m \times n$ matrix. Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of $A^T A$. Then the *singular values* of A are defined as

$$\sigma_1 = \sqrt{\lambda_1}, \ldots, \sigma_n = \sqrt{\lambda_n}.$$

$A^T A$ is also PSD $\Rightarrow \lambda_i \geq 0$ for $\forall i$.

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Theorem (Singular value decomposition)

If A is an $m \times n$ matrix of rank k, then we can write

no need to be square.

$$A = U\Sigma V^T$$

U, V are orthogonal.

where Σ is an $m \times n$ matrix of the form

diagonal — zero's

$$\begin{bmatrix} D_{k\times k} & 0_{k\times(n-k)} \\ 0_{(m-k)\times k} & 0_{(m-k)\times(n-k)} \end{bmatrix},$$

D is a diagonal matrix with the singular values of A, $\sigma_1, \ldots, \sigma_k$, on the diagonal and U and V are both orthogonal matrices (of size $m \times m$ and $n \times n$, respectively).

Let $U = (u_1 \cdots u_m)$, $V = (v_1 \cdots v_n)$, A takes $v_i \to \sigma_i u_i$

$$A = U\Sigma V^T = \sum_{i=1}^{k} \sigma_i u_i v_i^T$$

Uses of SVD:

- Useful in many statistical application.
- U, V are orthogonal ⟹ computation is easy.

Differences between JCF and SVD:

- SVD can be applied to any size of matrices.

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LU-decomposition

Definition

The LU-decomposition of a square matrix A is the factorization of A into a lower triangular matrix L and an upper triangular matrix U as follows:

$$A = LU.$$

Why is this useful? Consider the linear system $A\mathbf{x} = \mathbf{b}$

$L\underbrace{Ux}_{=y} = b$

First solve $Ly = b \Rightarrow$ easy to solve since L is triangular.

Then solve $Ux = y \Rightarrow$ easy to solve since U is triangular.

Recall: orthonormal basis

Definition

Two vectors $\mathbf{x}, \mathbf{y} \in V$ are called *orthogonal* if $\langle \mathbf{x}, \mathbf{y} \rangle = 0$, denoted $\mathbf{x} \perp \mathbf{y}$. We call them *orthonormal* if additionally the vectors are normalized, i.e. $\|\mathbf{x}\| = \|\mathbf{y}\| = 1$. A basis $\mathbf{x}_1, \ldots, \mathbf{x}_n$ of V is called *orthonormal basis (ONB)*, if the vectors are pairwise orthogonal and normalized.

Starting from a set of linearly independent vectors, we can construct another set of vectors which are orthonormal and span the same space using the **Gram-Schmidt Algorithm**.

QR-decomposition

Definition (QR-decomposition)

The QR-decomposition of an $m \times n$ matrix A with linearly independent column vectors is the factorization of A as follows:

↳ Apply Gram-Schmidt algorithm to these vectors.

$$A = QR,$$

where Q is an $m \times n$ matrix with orthonormal column vectors and R is an $n \times n$ invertible upper triangular matrix.

One obtains the factorization by applying the Gram-Schmidt algorithm to the columns of A. Let $\mathbf{u}_1, \ldots, \mathbf{u}_n$ be the column vectors of A. Let $\mathbf{q}_1, \ldots, \mathbf{q}_n$ be the orthonormal vectors obtained by applying Gram Schmidt. Then one can write:

$$\begin{aligned}
\mathbf{u}_1 &= \langle \mathbf{u}_1, \mathbf{q}_1 \rangle \mathbf{q}_1 + \langle \mathbf{u}_2, \mathbf{q}_2 \rangle \mathbf{q}_2 + \ldots + \langle \mathbf{u}_n, \mathbf{q}_n \rangle \mathbf{q}_n \\
\mathbf{u}_2 &= \langle \mathbf{u}_2, \mathbf{q}_2 \rangle \mathbf{q}_2 + \ldots + \langle \mathbf{u}_n, \mathbf{q}_n \rangle \mathbf{q}_n \\
&\vdots \\
\mathbf{u}_n &= \langle \mathbf{u}_n, \mathbf{q}_n \rangle \mathbf{q}_n
\end{aligned}$$

Thus the orthonormal vectors obtained using Gram-Schmidt form the columns of Q, while R is the terms needed to go between the columns of A and thsoe of Q, i.e.

$$R = \begin{bmatrix} \langle \mathbf{u}_1, \mathbf{q}_1 \rangle & \langle \mathbf{u}_2, \mathbf{q}_2 \rangle & \ldots & \langle \mathbf{u}_n, \mathbf{q}_n \rangle \\ 0 & \langle \mathbf{u}_2, \mathbf{q}_2 \rangle & \ldots & \langle \mathbf{u}_n, \mathbf{q}_n \rangle \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & \langle \mathbf{u}_n, \mathbf{q}_n \rangle \end{bmatrix}.$$

Why use QR-decomposition?

$$Ax = b$$

$$QRx = b$$

Q: orthogonal matrix

R: triangular

First solve

$$Qy = b$$

$$\Rightarrow y = Q^T b$$

$Q^{-1} = Q^T$ since Q is orthogonal.

Then solve

$$Rx = y.$$

R: triangular

Differentiation

Derivative

Recall the definition of the derivative:

Definition

A function $f : (a, b) \to \mathbb{R}$ is *differentiable* at $x \in (a, b)$ if

$$L := \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

exists. L is the *derivative* of f at x, denoted $L = f'(x)$. If f is differentiable at every $x \in (a, b)$, we say f is *differentiable*.

Proposition

The following are key rules for differentiation:

1. If f is differentiable at x, then it is continuous at x.
2. The derivative of a constant function is zero.
3. If f and g are differentiable at x, then so is $f+g$ with $(f+g)'(x) = f'(x) + g'(x)$.
4. Product rule: If f and g are differentiable at x, then so is fg with
$$(fg)'(x) = f'(x)g(x) + f(x)g'(x).$$
5. Quotient rule: If f and g are differentiable at x and $g(x) \neq 0$, then so is f/g with
$$(f/g)'(x) = \frac{f'(x)g(x) - f(x)g'(x)}{g^2(x)}.$$
6. Chain rule: If f is differentiable at x and g is differentiable at $f(x)$, then so is $g \circ f$ with
$$(g \circ f)'(x) = g'(f(x))f'(x).$$

Next we recall a theorem we proved in greater generality when we discussed compactness in the topology section:

Theorem (Extreme value theorem)

If $f : [a, b] \to \mathbb{R}$ is continuous, then f attains a maximum and a minimum, i.e. there exists $c, d \in [a, b]$ such that

$$f(c) \leq f(x) \leq f(d) \quad \forall x \in [a, b].$$

This theorem is used to prove the following important result:

Theorem (Mean value theorem)

If f is continuous on $[a, b]$ and differentiable on (a, b), then there exists $c \in (a, b)$ such that

$$f(b) - f(a) = f'(c)(b - a).$$

Lemma

If $f : (a, b) \to \mathbb{R}$ is differentiable on (a, b) and achieves a (local) maximum or (local) minimum at $c \in (a, b)$, then $f'(c) = 0$.

Proof of Mean Value Theorem:

l'Hôpital's rule

Theorem (l'Hôpital's rule)

If f, g *are differentiable on* (a, b)*, where* a, b *may be* $\pm\infty$*, and* $\lim_{x\to b} f(x) = 0 = \lim_{x\to b} g(x)$*, or both limits equal* $\pm\infty$*, then*

$$\lim_{x\to b} \frac{f'(x)}{g'(x)} = L$$

implies

$$\lim_{x\to b} \frac{f(x)}{g(x)} = L$$

Example

$$\lim_{x \to 0} \frac{5^x - 2^x}{x^2 - x} = \lim_{x \to 0} \frac{e^{x\ln 5} - e^{x \ln 2}}{x^2 - x} = \lim_{x \to 0} \frac{\ln 5 \cdot e^{x\ln 5} - \ln 2 \cdot e^{x \ln 2}}{2x - 1}$$

$$= \frac{\ln 5 - \ln 2}{-1} = \ln \frac{2}{5}$$

$$\lim_{x \to -\infty} xe^x = \lim_{t \to \infty} \frac{-t}{e^t} = -\lim_{t \to \infty} \frac{1}{e^t} = 0$$

$x = -t$

Higher order derivatives

Definition

We define higher-order derivatives inductively as $f^{(r)}(x) = (f^{(r-1)})'(x)$. If $f^{(r)}$ exists (at x), we say that f is r^{th}-order differentiable (at x).

Definition

If $f^{(r)}$ exists for all $r \in \mathbb{N}$ and for all $x \in (a, b)$, then we say f is infinitely differentiable or *smooth*. We denote this $f \in C^{\infty}((a, b))$.

If $f \in C^k$ that means f is continuously differentiable at least k times.

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Smoothness classes

Definition

If f is differentiable and its derivative $f'(x)$ is continuous, we say that f is *continuously differentiable*, and that $f \in C^1$. If $f^{(r)}$ exists and is continuous, we say that $f \in C^r$. If f is continuous, we say $f \in C^0$.

Since differentiability implies continuity, we have $C^\infty \subset \cdots \subset C^2 \subset C^1 \subset C^0$.

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Example

- The function $f(x) = |x|$ is C^0 but not C^1.
- The function $f(x) = x|x|$ is C^1 but not C^2.
- $f(x) = e^x$ and $f(x) = x$ are smooth functions, i.e., in C^∞.

Integration

Riemann integration

Definition (Riemann sum)

Let $f : [a, b] \to \mathbb{R}$ be a function. We call a set of points $P = \{x_0, \dots, x_n\} \subseteq [a, b]$ a *partition* of $[a, b]$ if the following holds

$$a = x_0 \leq x_1 \leq \dots \leq x_{n-1} \leq x_n = b.$$

We call the largest sub-interval of the partition P the *mesh* of P, denoted $|P|$, i.e.

$$|P| = \max_{i=1,\dots,n} (x_i - x_{i-1}).$$

Definition continued (Riemann sum)

Given a partition $P = \{x_0, \ldots, x_n\} \subseteq [a, b]$ of $[a, b]$ and a set of points $T = \{t_1, \ldots, t_n\} \subseteq [a, b]$ such that $t_i \in [x_{i-1}, x_i]$ for $i = 1, \ldots, n$, we define the *Riemann sum* $R(f, P, T)$ corresponding to f, P, T as

$$R(f, P, T) = \sum_{i=1}^{n} f(t_i)(x_i - x_{i-1}) := \sum_{i=1}^{n} f(t_i)\Delta x_i,$$

where we used $\Delta x_i = x_i - x_{i-1}$.

The idea is to define the Riemann integral as the "limit" of the Riemann sums over all partition such that their mesh is becoming arbitrarily small:

Definition (Riemann integrable)

A function $f : [a, b] \to \mathbb{R}$ is called *Riemann integrable* if there exists $I \in \mathbb{R}$ such that for all $\epsilon > 0$, there exists a $\delta > 0$ such that for any partition $P = \{x_0, \ldots, x_n\}$ of $[a, b]$ with $|P| < \delta$ and set of points $T = \{t_1, \ldots, t_n\} \subseteq [a, b]$ such that $t_i \in [x_{i-1}, x_i]$ for $i = 1, \ldots, n$ we have $|R(f, P, T) - I| < \epsilon$.
We say that I is the Riemann integral of f, denoted $I = \int_a^b f(x)\mathrm{d}x$.

If f is Riemann integrable, then I is unique.

Let $\mathcal{R}([a, b])$ denote the set of functions that are Riemann integrable on $[a, b]$.

Theorem

Riemann integration is linear, i.e. if $f, g \in \mathcal{R}([a, b])$ and $c \in \mathbb{R}$, then $f + cg \in \mathcal{R}([a, b])$.

Sketch of proof

$$R(f, P, T) \to I_1$$

$$R(g, P, T) \to I_2$$

Linearity is immediate for Riemann sum:

$$R(f + cg, P, T) = R(f, P, T) + cR(g, P, T)$$

$$\longrightarrow I_1 + cI_2.$$

Proposition (Rules for integration on $[a, b]$)

1. The constant function $f(x) = c$ is integrable and its integral is $c(b - a)$.
2. If f is Riemann integrable, then it is bounded.
3. If $f, g \in \mathcal{R}([a, b])$ and $f(x) \leq g(x)$ for all $x \in [a, b]$, then
$$\int_a^b f(x)dx \leq \int_a^b g(x)dx.$$
4. If $f \in \mathcal{R}([a, b])$ and $g : [c, d] \to [a, b]$ is a continuously differentiable bijection with $g' > 0$, then
$$\int_a^b f(y)dy = \int_c^d f(g(x))g'(x)dx.$$
change of variables
5. If $f, g : [a, b] \to \mathbb{R}$ are differentiable and $f', g' \in \mathcal{R}([a, b])$, then
$$\int_a^b f(x)g'(x)dx = f(b)g(b) - f(a)g(a) - \int_a^b f'(x)g(x)dx.$$

Theorem (Fundamental Theorem of Calculus)

First part:

If $f : [a, b] \to \mathbb{R}$ is Riemann integrable then its indefinite integral

$$F(x) = \int_a^x f(t)dt$$

is a continuous function of x. In addition, the derivative of F exists and $F'(x) = f(x)$ at all $x \in [a, b]$ where f is continuous.

Second part:

Let $f : [a, b] \to \mathbb{R}$ and let F be a continuous function on $[a, b]$ with antiderivative f on (a, b), i.e. $F'(x) = f(x)$. Then if F is Riemann integrable on $[a, b]$,

$$\int_a^b f(x)dx = F(b) - F(a).$$

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Drawbacks of the Riemann integral

- Riemann integration has many nice properies, but it also has some drawbacks
- To see this, we first introduce a nice alternative characterization of Riemann integrability
- Instead of looking at all the Riemann sums, we can restrict our attention to two special forms of the sum

Definition

Given a function $f\colon [a,b] \to \mathbb{R}$ and a partition $P = \{x_0, \ldots, x_n\}$ of $[a,b]$, we define the *lower* and *upper sum* of f via

$$L(f,P) = \sum_{i=1}^{n} m_i \Delta x_i, \qquad U(f,P) = \sum_{i=1}^{n} M_i \Delta x_i,$$

where $m_i = \inf\{f(t)\colon t \in [x_{i-1}, x_i]\}$ and $M_i = \sup\{f(t)\colon t \in [x_{i-1}, x_i]\}$. We define the *lower* and *upper integral* of f to be

$$\underline{I} = \sup_P L(f,P), \qquad \overline{I} = \inf_P U(f,P).$$

Since f is defined on a compact set, it will be bounded and hence the lower and upper integral exist and are finite.

One can think of the lower and upper integral as lower and upper bounds for the Riemann integral.

Theorem

Let $f : [a, b] \to \mathbb{R}$ be a function. Then f is Riemann integrable if and only if $\underline{I} = \overline{I}$ and we have $\underline{I} = \overline{I} = I$.

A function that is not Riemann integrable

$$f : [0,1] \to \mathbb{R} : x \mapsto \begin{cases} 0 & \text{if } x \in \mathbb{Q}, \\ 1 & \text{otherwise.} \end{cases}$$

countable

$|\mathbb{Q}| < |[0,1] \setminus \mathbb{Q}| = |\mathbb{R}|$

uncountable

So, f should be treated as $f \equiv 1$ (constant function)

Is this function Riemann integrable? Should it be integrable?

Not Riemann integrable since

$L(f, P) = 0$, $U(f, P) = 1$

Thus, $\underline{I} = 0$, $\overline{I} = 1$.

The End

References

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