

SUPPLEMENTAL MATHEMATICAL FACTS

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A.1 Basic logic for proof

[1, p. 60]The negation of

for any $\epsilon > 0$, there exist N > 0, such that for all n > N, we have $|a_n - a| < \epsilon$

is

there exist an $\epsilon > 0$, such that for every N > 0, such that for all n > N, we have $|a_n - a| > \epsilon$.

[1, p. 60]The negation of

for any $\epsilon > 0$, there exist $\delta > 0$, such that for all $|x - x_0| < \delta$, we have $|f(x) - f(x_0)| < \epsilon$

is

there exist an $\epsilon > 0$, such that for every $\delta > 0$, such that for all $|x - x_0| < \delta$, we have $|f(x) - f(x_0)| > \epsilon$.

A.2 Some common limits

Lemma A.2.1 (Stirling approximation). • For positive integer n,

$$ln n! = n ln n - n + O(ln n).$$

•

$$\sqrt{2\pi}n^{n+1/2}e^{-n} \le n! \le en^{n+1/2}e^{-n}, \forall n > 0.$$

Lemma A.2.2 (common limits summary).

•

$$\lim_{n\to\infty}\frac{\ln n}{n}=0.$$

•

$$\lim_{n\to\infty}\frac{x^n}{n!}=0, \forall x\in\mathbb{R}.$$

•

$$\lim_{n\to\infty}\frac{n!}{n^n}=0.$$

•

$$\lim_{n\to\infty} M^{1/n} = 1$$

for any M > 0.

$$\lim_{n\to\infty}\frac{\ln n!}{n}=\infty, \lim_{n\to\infty}(n!)^{1/n}=\infty.$$

Proof. (2)see Lemma 3.6.4 and Lemma 1.4.3.(3)Lemma 1.4.3.(4) Lemma 1.5.1. (5) (a)Use Stirling approximation $\ln n! = n \ln n - n + O(\ln n)$ and $\ln n!/n = n - 1 + O(\ln n/n) \rightarrow \infty$.(b) Note that $(n!)^{1/n} = \exp(\ln(n!)^{1/n}) = \exp(\frac{\ln n!}{n})$. □

Note A.2.1. A helpful and general summary, as $n \to \infty$

$$\ln n \ll n^r (r > 0) \ll a^n (a > 1) \ll n! \ll n^n.$$

Lemma A.2.3 (property of e). Define

$$\lim_{n\to\infty} (1+1/n)^n = e$$

and then

$$\lim_{n\to\infty} (1+x/n)^n = e^x$$

for any real x.

Proof.

$$\lim_{n\to\infty} ((1+x/n)^{n/x})^x = e^x$$

use the fact the $f(y) = y^x$ is continuous, such that function evaluation and limit can be exchanged.

A.3 Common series summation

Lemma A.3.1. [2, p. 1]

•

$$\sum_{k=1}^{n} k = \frac{n(n+1)}{2}$$

•

$$\sum_{k=1}^{n} k^2 = \frac{n(n+1)(2n+1)}{6}$$

•

$$\sum_{k=1}^{n} k^3 = \left[\frac{n(n+1)}{2} \right]^2$$

Lemma A.3.2. [2, p. 1]

Assume $q \neq 1$.

•

$$\sum_{k=1}^{n} aq^{k-1} = a \frac{q^n - 1}{q - 1}$$

•

$$\sum_{k=0}^{n-1} kq^k = \frac{(n-1)q^n}{q-1} + \frac{(q-q^n)}{(q-1)^2}$$

•

$$\sum_{k=0}^{n-1} (n-1-k)q^k = -(n-1)\frac{1}{q-1} - \frac{(q-q^n)}{(q-1)^2}$$

Proof. (3) use (1)(2), we have

$$\sum_{k=0}^{n-1} (n-1-k)q^k = (n-1)\frac{q^n-1}{q-1} - \frac{(n-1)q^n}{q-1} - \frac{(q-q^n)}{(q-1)^2}$$

A.4 Some common spaces

The metric space (\mathbb{R}^n, d_2) is the set \mathbb{R}^n with metric $d_2(x, y) = \sqrt{\sum_{i=1}^n (x_i - y_i)^2}$.

[3, p. 122]The metric space l^2 is the set of all infinite sequence of real or complex numbers $\{x_1, x_2, ...\}$ such that $\sum_{i=1} \infty x_i^2 < \infty$, i.e., $\sum_{i=1} \infty x_i^2$ converges. The metric is usually defined as

$$d_2({x_n}, {y_n}) = \sqrt{\sum_{k=1}^{\infty} (x_i - y_i)^2}$$

The metric space l^p , $1 \le p < \infty$, is the set of all infinite sequence of real or complex numbers $\{x_1, x_2, ...\}$ such that $\sum_{i=1}^p \infty |x_i|^p < \infty$, i.e., $\sum_{i=1}^p \infty |x_i|^p$ converges. The metric is usually defined as

$$d_p(\{x_n\}, \{y_n\}) = \sqrt[p]{\sum_{k=1}^{\infty} (x_i - y_i)^p}$$

The metric space l^{∞} , is the set all infinite sequence of real or complex numbers $\{x_1, x_2, ...\}$ such that every x_i is bounded. The metric is defined as

$$d_{\infty}(\lbrace x_n\rbrace, \lbrace y_n\rbrace) = \sup_{n} |x_n - y_n|$$

[4, p. 75]. The metric space $C[a,b]=(C[a,b],d_{\infty})$ denote the set of real-valued (or complex valued) functions defined on the interval [a,b]. The metric d_{∞} is given as

$$d_{\infty}(x,y) = \sup_{t} |x(t) - y(t)|$$

Remark A.4.1. Caution! Sometimes C[a, b] refers to only continuous functions.[5, p. 23]

The metric space $(C[a,b],d_p)$ denote the set of real-valued(or complex valued) functions defined on the interval [a,b]. The metric d_p is given as

$$d_p(x,y) = \left[\int_a^b |x(t) - y(t)|^p dt \right]^{1/p}$$

where $1 \le p < \infty$.[4, p. 75].

The vector space $\mathcal{L}(V, W)$ usually denotes the set of all linear operators from V into W.

- A.4.1 Notations on continuously differentiable functions
 - *C*⁰ refers to continuous function

- *C*¹ refers to functions having continuous first derivatives, also called continuously differentiable functions.
- \bullet C^2 refers to functions having continuous second derivatives
- C^{∞} refers to smooth functions

A.5 Different modes of continuity

Chain of inclusions for functions over a closed and bounded subset of the real line $continuouslyDifferntiable \subseteq LipschitzContinuous \subseteq UniformlyContinuous$

Remark A.5.1.

• Continuously differentiable on a closed interval indicates the derivative is bounded $f' \leq M$, then we have

$$|f(x) - f(y)| = f'(s)|x - y| \le M|x - y|$$

hence Lipschitz continuous.

- f(x) = |x| is Lipschitz continuous but is not differentiable everywhere except at x = 0, therefore it is not continuously differentiable.
- Lipschitz continuous → continuous:

$$|f(x) - f(y)| \le L|x - y| \to 0$$

as
$$|x-y| \to 0$$

Lemma A.5.1 (differentiable implies continuous). *If* f *is differentiable on* [a,b]*, then it is continuous on* [a,b]*.*

Proof:

$$\lim_{y \to x} f(y) - f(x) = \lim_{y \to x} (y - x)(f(y) - f(x))/(y - x) = \lim_{y \to x} (y - x) \lim_{y \to x} (f(y) - f(x))/(y - x) = 0$$

where we have use the property that if two limits exist then they can multiply.[3, p. 42].

Remark A.5.2. This lemma indicates that a function differentiable everywhere will be continous everywhere.

Lemma A.5.2 (differentiable everywhere NOT implies continuously differentiable). A function is differentiable everywhere NOT implies it is continuously differentiable function.

The standard example is

$$f(x) = \begin{cases} x^2 \sin(\frac{1}{x}), & x \neq 0 \\ 0, & x = 0 \end{cases}$$

This function can be differentiated every where and f'(0) = 0, but $\lim_{x\to 0} f'(x)$ does not exist. See link.

A.5.1 continuity vs. uniform continuity

Definition A.5.1. A function $f: X \to Y$ is uniformly continuous if for every $\epsilon > 0$ there exist a $\delta > 0$ such that for every $x, x_0 \in X$,

$$\rho(x, x_0) \le \delta \Rightarrow \rho(f(x), f(x_0)) < \epsilon$$

Theorem A.5.1. [3, p. 154] If f is a continuous function from a compact metric space M_1 into a metric space M_2 , then f is uniformly continuous on M_1 .

Corollary A.5.1.1. [3, p. 154] If f is a continuous real-value function on a closed and bounded subset X of \mathbb{R}^n , then f is uniformly continuous on X.

Example A.5.1. The function $f(x) = x^2$ is continuous but not uniformly continuous on the interval $(0, \infty)$.

Lemma A.5.3 (sufficient condition). *Let* $S = \mathbb{R}$. *if* f *is global Lipschitz continuous, i.e.*

$$|f(x_1) - f(x_2)| < M|x_1 - x_2|$$

 $\forall x_1, x_2 \in S$, then f is uniformly continuous.

Proof:
$$|f(x_1) - f(x_2)| < M|x_1 - x_2| \to 0$$

A.6 Exchanges of limits

A.6.1 Overall remark

Remark A.6.1.

- Usually, the necessary conditions for exchanging limits is difficult to find, therefore only sufficient conditions are given.
- Many operations are in nature taking limits, for example, summing infinite terms is taking limits on partial sums; integrals is taking limits on both summation and partitions; derivative is taking limits on quotient expressions.

A.6.2 exchange limits with infinite summations

Let $\lim_{m\to\infty} \sum_{n=1}^{\infty} f(m,n) = \sum_{n=1}^{\infty} \lim_{m\to\infty} f(m,n)$ Based on dominated convergence, if there is a g(n) such that f(m,n) < g(n), $\forall m$ and $\sum_{n=1}^{\infty} g(n)$ exists, then we can exchange.

To use the dominated convergence theorem in Lebesgue integral, we can define a simple function s_n on $[0, \infty]$ take f(m, n) on the interval [m-1, m). Then the integral of s_n with respect to Legesbue measure on real lime will give the $\int_{[0,\infty)} s_n d\mu = \sum_{m=1}^{\infty} f(m, n)$

Theorem A.6.1. [3, pp. 94, 373]Let $a_{m,n}$ be non-negative and $\sum_{m=0}^{\infty} \sum_{n=0}^{\infty} a_{m,n}$ exists, then

$$\sum_{m}^{\infty} \sum_{n}^{\infty} a_{m,n} = \sum_{n}^{\infty} \sum_{m}^{\infty} a_{m,n}$$

Corollary A.6.1.1. *Let* $a_{m,n}$ *be increasing on both* m, n *and* $\lim_{m\to\infty} \lim_{n\to\infty} a_{m,n}$ *exists, then*

$$\lim_{m\to\infty}\lim_{n\to\infty}a_{m,n}=\lim_{n\to\infty}\lim_{m\to\infty}a_{m,n}$$

Proof: by constructing partial sums.

A.6.3 Exchange limits with integration and differentiation

Theorem A.6.2. [3, p. 249] Let α be a function of bounded variation on [a,b] and let f_n be a sequence of functions in $\mathcal{R}_{\alpha}[a,b]$ which converges uniformly to a function f. Then $f \in \mathcal{R}_{\alpha}[a,b]$ and

$$\lim_{n\to\infty}\int_a^b f_n d\alpha = \int_a^b \lim_{n\to\infty} f d\alpha$$

Theorem A.6.3. [3, p. 249] Let $\{f_n\}$ be a sequence of differentiable functions on (a,b). Suppose that

- f'_n is continuous on (a,b)
- $\{f_n\}$ converges pointwise to f
- $\{f'_n\}$ converges uniformly

then f is differentiable on (a,b) and f'_n converges uniformly to f'.

A.6.4 Exchange differentiation with integration

Theorem A.6.4. Let f(x,y) be continuous on $[a,b] \times [c,d]$. Then

$$\phi(y) = \int_{a}^{b} f(x, y) dx$$

defined above is continuous function on [c,d]

Proof: for any $\epsilon > 0$, there exist δ , such that

$$|\phi(y) - \phi(y')| \le \int_a^b |f(x,y) - f(x,y')| dx \le \epsilon(b-a) \forall |y-y'| < \delta$$

where we have the fact of f(x,y) - f(x,y) is bounded (since continuous function on a compace set is uniformly continuous and will have maximum and minimum) which shows $\phi(y)$ is uniformly continuous.

Theorem A.6.5. Let f and f_y be continuous on $[a,b] \times [c,d]$. Then ϕ is differentiable and

$$\phi_y = \int_a^b f_y(x, y) dx$$

Proof:

$$\frac{\phi(y+h) - \phi(y)}{h} = \frac{1}{h} \int_{a}^{b} f(x, y+h) - f(x, y) dx = \int_{a}^{b} f_{y}(x, z)$$

due to Taylor theorem, where $z \in [y, y + h]$. Then

$$\left| \frac{\phi(y+h) - \phi(y)}{h} - \int_a^b f_y(x,y) dx \right| \le \int_a^b \left| f_y(x,z) - f_y(x,y) \right| dx$$

Because f_y is continuous on compact set, then it is uniformly continuous. Therefore given $\epsilon > 0$, there exists δ such that

$$|f_y(x,y') - f_y(x,y)| < \epsilon/(b-a), \forall |y-y'| < \delta$$

Taking $h < \delta$, we have

$$\left|\frac{\phi(y+h)-\phi(y)}{h}-\int_a^b f_y(x,y)dx\right|<\epsilon.$$

Take the limit on *h* and we get the result.

A.6.5 Exchange limit and function evaluations

Lemma A.6.1. Let $\{x_n\}$ be a sequence with limit x, let f be a continuous function

$$\lim_{n\to\infty} f(x_n) = f(\lim_{n\to\infty} x_n) = f(x)$$

Proof: from the definition of continuous function.

A.7 Useful inequalities

Lemma A.7.1 (arithmetic-geometric mean inequality). For $x_1, ..., X_n \ge 0$, we have

$$(x_1x_2...x_n)^{1/n} \le \sum_{i=1}^n x_i/n.$$

Specifically,

$$\frac{x_1 + x_2}{x} \ge \sqrt{x_1 x_2}$$

Proof. use $y = \ln(x)$ and concavity of $\ln(x)$

A.7.1 Gronwall's inequality

see [6]

A.7.2 Inequality for norms

Lemma A.7.2. [7]For L^p normed space, we have

$$||x||_2 \le ||x||_1$$

where

$$||x||_2 = \left(\int_{-\infty}^{\infty} |f(x)|^2 d\mu(x)\right)^{0.5}$$

and

$$||x||_1 = \int_{-\infty}^{\infty} |f(x)| d\mu(x)$$

Proof: for finite dimensional normed space cases: we need to prove

$$\sqrt{x_1^2 + x_2^2 + \dots + x_n^2} \le |x_1| + |x_2| + \dots + |x_n|$$

By squaring both sides, we can get the result. For continuous case, TODO

Theorem A.7.1. [7]For L^p normed space, we have

$$||x||_q \leq ||x||_q$$

whenever $p \leq q$ where

$$||x||_q = \left(\int_{-\infty}^{\infty} |f(x)|^q d\mu(x)\right)^{1/q}$$

Proof: todo

Remark A.7.1. For complete description on L^p norms, see [7]

A.7.3 Young's inequality for product

Lemma A.7.3. If
$$a, b \ge 0$$
, and $p, q > 1, 1/p + 1/q = 1$, then $ab \le a^p/p + b^q/q$

Proof:

$$\log(a^p/p + b^q/q) \ge \log(a^p)/p + \log(a^q)/q = \log(a) + \log(b) = \log(ab)$$

where we use the fact of log is concave.

Useful properties of matrix **A.8**

A.8.1 Matrix derivatives

Lemma A.8.1 (common matrix derivative in quadratic forms). [8] For $A \in$ $\mathbb{R}^{m \times n}$, $x \in \mathbb{R}^n$, we have:

$$\frac{\partial a^T x}{\partial x} = \frac{\partial x^T a}{\partial x} = a$$
$$\frac{\partial Ax}{\partial x} = A$$
$$\frac{\partial BAx}{\partial x} = BA$$
$$\frac{\partial x^T Ax}{\partial x} = (A + A^T)x$$
$$\frac{\partial x^T Ax}{\partial x} = 2A$$

Lemma A.8.2. If f(x) = g(Ax), $A \in \mathbb{R}^{n \times n}$, $x \in \mathbb{R}^n$ for some differentiable function g(y), then

$$\nabla f = A^T \nabla g$$

In particularly, $a \in \mathbb{R}^n$, then

$$\nabla a^T A x = A^T x$$

A.8.2 Matrix inversion lemma

Lemma A.8.3 (matrix inversion lemma). [9, p. 120]

- $(E FH^{-1}G)^{-1} = E^{-1} + E^{-1}F(H GE^{-1}F)^{-1}GE^{-1}$ $(E FH^{-1}G)^{-1}FH^{-1} = E^{-1}F(H GE^{-1}F)^{-1}$

Proof. (1) can be verified (2) expand the parenthesis using (1).

Corollary A.8.0.1 (matrix inversion of rank one update). Let H = I, $F = \pm u \in \mathbb{R}^n$, and $G = \pm v \in \mathbb{R}^n$, we have

$$(E - uv)^{-1} = E^{-1} - \frac{E^{-1}uv^{T}E^{-1}}{1 + v^{T}E^{-1}u}$$

•

$$(E - uv)^{-1} = E^{-1} + \frac{E^{-1}uv^{T}E^{-1}}{1 - v^{T}E^{-1}u}$$

A.8.3 Block matrix

Lemma A.8.4. Given an $(m \times p)$ matrix A with q row partions and s colun partitions and a $(p \times n)$ matrix B with s row partions and r colun partitions,

$$A = \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1s} \\ A_{21} & A_{22} & \cdots & A_{2s} \\ \vdots & \vdots & \ddots & \vdots \\ A_{q1} & A_{q2} & \cdots & A_{qs} \end{pmatrix}, B = \begin{pmatrix} B_{11} & B_{12} & \cdots & B_{1r} \\ B_{21} & B_{22} & \cdots & B_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ B_{s1} & B_{s2} & \cdots & B_{sr} \end{pmatrix},$$

then the matrix product

$$C = AB$$

can be formed blockwise, giving C as an $(m \times n)$ matrix with q row partitions and r column partitions. In particular,

$$C_{\alpha\beta} = \sum_{\gamma=1}^{s} A_{\alpha\gamma} B_{\gamma\beta}.$$

Lemma A.8.5 (sum of vector product to matrix product). *Consider column vectors* $x_1, x_2, ..., x_N \in \mathbb{R}^d$ *and column vectors* $x_1, x_2, ..., x_N \in \mathbb{R}^d$. *It follows that*

•

$$\sum_{i=1}^{N} x_i^T y_i = X_C^T Y_C,$$

where $X_C \in \mathbb{R}^{Nd}$ is a vector stacking all the $x_1, ..., x_N$ (similarly Y_C).

 $\sum_{i=1}^{N} x_i y_i^T = X_R^T Y_R,$

where $X_R \in \mathbb{R}^{N \times d}$ is a matrix stacking all the $x_1^T, ..., x_N^T$ (similarly Y_R).

Lemma A.8.6 (block matrix inversion formula).

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}^{-1} = \begin{pmatrix} A_{11}^{-1} + B_{12}B_{22}^{-1}B_{21} & -B_{12}B_{22}^{-1} \\ -B_{22}^{-1}B_{21} & B_{22}^{-1} \end{pmatrix}$$
$$= \begin{pmatrix} C_{11}^{-1} & -C_{11}^{-1}C_{12} \\ -C_{21}C_{11}^{-1} & A_{22}^{-1} + C_{21}C_{11}^{-1}C_{12} \end{pmatrix}$$

where

$$B_{22} = A_{22} - A_{21}A_{11}^{-1}A_{12}, B_{12} = A_{11}^{-1}A_{12}, B_{21} = A_{21}A_{11}^{-1}$$

and

$$C_{11} = A_{11} - A_{12}A_{22}^{-1}A_{21}, C_{12} = A_{12}A_{22}^{-1}, C_{21} = A_{22}^{-1}A_{21}$$

A.8.4 Matrix trace

Lemma A.8.7. •
$$||A||_F^2 = Tr(AA^T)$$

Lemma A.8.8 (matrix trace).

- (linearity)Tr(aA + bB) = aTr(A) + bTr(B)
- (commutative) Tr(AB) = Tr(BA)
- (invariance under transposition) $Tr(A) = Tr(A^T)$
- (cyclic rule) Tr(ABCD) = Tr(DABC) = Tr(CDAB) = Tr(BCDA) or Tr(ABC) = Tr(CAB) = Tr(BCA)

Proof. (1)(2)(3) can be proved directly from definition. (4) We can group three elements together and commute with the fourth. For example, we can group (ABC) together and commute with D to prove the first equality.

Corollary A.8.0.2.

- (invariance under similar transformation) $Tr(PAP^{-1}) = Tr(A)$
- $Tr(X^TY) = Tr(XY^T) = Tr(Y^TX) = Tr(XY^T)$

Proof. (1) Use cyclic rule. (2) Use invariance under transposition and commutative rule. \Box

Lemma A.8.9 (common matrix derivative involving matrix trace). [8] Let $A, X, B \in \mathbb{R}^{m \times m}$. We have

$$\frac{\partial Tr(X)}{\partial X} = I$$

$$\frac{\partial Tr(XA)}{\partial X} = \frac{\partial Tr(AX)}{X} = A^{T}$$

$$\frac{\partial Tr(X^{T}A)}{\partial X} = \frac{\partial Tr(AX^{T})}{X} = A$$

$$\frac{\partial Tr(AXB)}{\partial X} = \frac{\partial Tr(BAX)}{X} = A^{T}B^{T}$$

$$\frac{\partial Tr(AX^{T}B)}{\partial X} = \frac{\partial Tr(BAX^{T})}{X} = BA$$

$$\frac{\partial Tr(XX^{T})}{\partial X} = 2X$$

$$\frac{\partial Tr(XX)}{\partial X} = 2X^{T}$$

Additional, we have chain rule given by

$$\frac{\partial Tr(X^TA^TAX)}{\partial X} = \frac{\partial Tr(XX^TA^TA)}{\partial X} = \frac{\partial Tr(XX^TA^TA)}{\partial XX^T} \frac{\partial XX^T}{\partial X} = 2A^TAX.$$

A.8.5 Matrix elementary operator

Lemma A.8.10 (elementary operator matrix). *Left multiply a matrix A by an elementary matrix is equivalent to performing row operation. The elementary operator matrix is given by*

• (Interchange row i and j) For example, exchange row 2 and row 3:

$$R_1 = \begin{bmatrix} 1 & & & \\ & 0 & 1 & \\ & 1 & 0 & \\ & & & 1 \end{bmatrix}$$

• (Multiply row i by s) For example

$$R_2 = \begin{bmatrix} 1 & & & \\ & s & & \\ & & 1 & \\ & & & 1 \end{bmatrix}$$

• (Add s times row i to row j) For example, add s times row 2 to row 3

$$R_3 = \begin{bmatrix} 1 & & & \\ & 1 & 0 & \\ & s & 1 & \\ & & & 1 \end{bmatrix}.$$

Note that $R_3 = R_1 R_2 \neq R_2 R_1$.

Lemma A.8.11 (elementary operator matrix). Right multiply a matrix A by an elementary matrix is equivalent to performing row operation. The elementary operator matrix is given by

• (Interchange column i and j) For example, exchange row 2 and row 3:

$$C_1 = \begin{bmatrix} 1 & & & \\ & 0 & 1 & \\ & 1 & 0 & \\ & & & 1 \end{bmatrix}$$

• (Multiply column i by s) For example

$$C_2 = \begin{bmatrix} 1 & & & \\ & s & & \\ & & 1 & \\ & & & 1 \end{bmatrix}$$

• (Add s times column i to column j) For example, add s times column 2 to column 3

$$C_3 = \begin{bmatrix} 1 & & & \\ & 1 & s & \\ & & 1 & \\ & & & 1 \end{bmatrix}.$$

Note that $C_3 = C_1C_2 \neq C_2C_1$.

A.8.6 Matrix determinant

Lemma A.8.12 (properties of determinant).

- All elementary operator matrix has determinant 1.
- For matrix $A \in \mathbb{R}^{n \times n}$,

$$det(kA) = k^n det(A)$$
.

- det(AB) = det(A)det(B).
- All elementary operation on a matrix will not change its determinant.

A.9 Numerical integration

Definition A.9.1 (Newton-Cotes Formula). Suppose we want to evaluate $\int_a^b f(x)dx$. We can evaluate f(x) at n+1 equally spacing points $x_i = a + i(b-a)/n$, and then we approximate f(x) by n degree of Lagrange polynomial and do the integral. Specifically, we have

$$\int_{a}^{b} f(x)dx \approx \int_{a}^{b} L(x)dx = \int_{a}^{b} \left(\sum_{i=0}^{n} f(x_{i})l_{i}(x)\right) = \sum_{i=1}^{n} f(x_{i}) \int_{a}^{b} l_{i}(x)dx = \sum_{i=1}^{n} f(x_{i})w_{i}$$

where L is the Lagrange polynomial of degree n, and $l_i(x)$, i = 0, ..., n is the (n+1) Lagrange polynomial basis, given as Lemma 3.5.2.

Example A.9.1. Consider we use degree 1 Lagrange polynomial to approximate f(x), then

$$L(x) = f(a)\frac{x-a}{b-a} + f(b)\frac{x-b}{a-b}$$

where $l_0(x) = \frac{x-a}{b-a}$ and $l_1(x) = \frac{x-b}{a-b}$. Then

$$w_0 = \int_a^b l_0(x) dx = \frac{1}{2}, w_1 = \int_a^b l_1(x) dx = \frac{1}{2}.$$

Table A.9.1: Closed Newton-Cotes Formula

Notation: $\int_a^b f(x)dx$, $f_i = f(x_i)$, $x_i = a + i(b-a)/n$						
Degree	Name	Formula	Error term			
1	Trapezoid rule	$\frac{b-a}{2}(f_0+f_1)$	$-\frac{(b-a)^3}{12}f^{(2)}(\eta)$			
2	Simpson's rule	$\frac{b-a}{6}(f_0+4f_1+f_2)$	$-\frac{(b-a)^5}{2880}f^{(4)}(\eta)$			
3	Simpson's 3/8 rule	$\frac{b-a}{8}(f_0+3f_1+3f_2+f_3)$	$-\frac{(b-a)^3}{6480}f^{(5)}(\eta)$			

Remark A.9.1 (Error analysis). For detailed error analysis, see [10, p. 252].

Remark A.9.2 (how to use). Usually, given the integral $\int_a^b f(x)dx$, we will first divide into smaller intervals and do the numerical integral on each interval and add them up. For example

$$\int_{a}^{b} f(x)dx = \int_{a}^{a+h} f(x)dx + \int_{a+h}^{a+2h} f(x)dx... + \int_{b-h}^{b} f(x)dx.$$

Lemma A.9.1 (Trapezoid rule and the error bound). Given the integral $\int_a^b f(x)dx$, we have

$$\int_{a}^{b} f(x)dx \approx \frac{b-a}{n} \left(\frac{f(a)}{2} + \sum_{k=1}^{n-1} \left(f(a+k\frac{b-a}{n})\right) + \frac{f(b)}{2}\right)$$

where we divide b-a into n subintervals, and we do the Trapezoid rule on each subinterval. And the error bound is

$$\frac{(b-a)^3}{12n^2} \max_{x \in [a,b]} f^{(2)}(x)$$

Proof. Note that on each subinterval, the error is $-\frac{(b-a/n)^3}{12}f^{(2)}(\eta)$. Sum up n terms, and we have upper bound

$$\frac{(b-a)^3}{12n^3} n \max_{x \in [a,b]} f^{(2)}(x)$$

Lemma A.9.2 (Midpoint rule and the error bound). Given the integral $\int_a^b f(x)dx$, we have

$$\int_{a}^{b} f(x)dx \approx \frac{b-a}{n} \left(\sum_{k=1}^{n} \left(f(a + (k-0.5) \frac{b-a}{n}) \right) \right)$$

where we divide b - a into n subintervals, and we do the Trapezoid rule on each subinterval. And the error bound is

$$\frac{(b-a)^3}{n^2}K$$

A.9.1 Gaussian quadrature

$$\int_{a}^{b} w(x)f(x)dx \approx \sum_{i=1}^{n} w_{i}f(x_{i})$$

which is exact when f is a polynomial.

Remark A.9.3. In Newton-Cotes formulas, we fix nodes and try to find suitable weights; in Gaussian quadrature, we use a weighted sum of function values at specified points within the domain of integration.

A.10 Vector calculus

Lemma A.10.1 (divergence theorem).

$$\iiint\limits_{V} (\nabla \cdot \mathbf{F}) dV = \iint\limits_{S(V)} \mathbf{F} \cdot \hat{\mathbf{n}} dS$$

$$\iiint\limits_{V} (\nabla \times \mathbf{F}) dV = \iint\limits_{S(V)} \hat{\mathbf{n}} \times \mathbf{F} dS$$

$$\iiint\limits_{V} (\nabla f) dV = \iint\limits_{S(V)} \hat{\mathbf{n}} f dS$$

Lemma A.10.2 (Lapacian product rule). *Given functions* $u : \mathbb{R}^n \to \mathbb{R}$ *and* $v : \mathbb{R}^n \to \mathbb{R}$ *, we have*

$$\nabla^2(uv) = u\nabla v + 2\nabla u \cdot \nabla v + v\nabla^2 u.$$

Proof. Directly use product rule.

A.11 Numerical linear algebra computation complexity

Note A.11.1. [11, p. 606]

- For a $m \times n$ matrix multiplying a n dimensional vector, mn.
- For a $n \times n$ matrix multiplying a $n \times n$ matrix, n^3 (without optimization).
- For a $n \times n$ matrix, LU decomposition $2n^3/3$ (for symmetric matrix $n^3/3$).
- For a $m \times n$ matrix, Cholesky decomposition $4m^2n/3$ (for square matrix $4n^3/3$).
- For a $m \times n$ matrix, QR decomposition $4m^2n/3$ (for square matrix $4n^3/3$).

Note A.11.2 (solving triangular linear system). Let L be a $n \times n$ lower triangle matrix, the forward substitution algorithm for solving

$$Ly = d$$
,

is given by

```
y(1) = d(1) / L(1,1); for i=2:n y(i) = (d(i) - L(i,1:i-1)* y(1:i-1))/L(i,i) end
```

This algorithm has complexity of $O(n^2)$.

Let U be a $n \times n$ upper triangle matrix, the backward substitution algorithm for solving

$$Ux = d$$

is given by

```
x(n) = d(n)/U(n,n);
for i = n - 1: -1:1
x(i) = (d(i) - U(i,i + 1:n)*x(i + 1:n) )/U(i,i)
end
```

This algorithm has complexity of $O(n^2)$.

Distributions A.12

Lemma A.12.1. [12, p. 579] Let K be an externally given parameter. We have

$$\int_{-\infty}^{\infty} \delta(x)dx = 1, x\delta(x) = 0, \int_{-\infty}^{\infty} f(x)\delta(x - K)dx = f(K).$$

- $\delta(g(x)) = \sum_i \frac{\delta(x-x_i)}{|g'(x_i)|}$, where x_i , i = 1, 2, ... are the zeros of the function g(x).
- $\delta(\lambda x) = \frac{\delta(x)}{|\lambda|}$, $\delta(x K) = \delta(K x)$. (step function definition)

$$H(x) \triangleq \frac{d}{dx} \max\{x, 0\}, H(x - A) \triangleq \frac{d}{dx} \max\{x - A, 0\}$$

 $\bullet H(x-K) + H(K-x) = 1.$

$$\frac{dH(x-K)}{dx} = \delta(x-K), \frac{dH(K-x)}{dx} = -\delta(x-K).$$

Proof. Use
$$H(x - K) + H(K - x) = 1$$
 to prove $\frac{dH(K - x)}{dx}$.

A.13 Common integrals

Lemma A.13.1.

$$\int_0^\infty e^{-ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}}, \int_{-\infty}^\infty e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$$

$$\int_0^\infty x e^{-ax^2} dx = \frac{1}{2a'} \int_{-\infty}^\infty x e^{-ax^2} dx = 0$$

$$\int_0^\infty x^2 e^{-ax^2} dx = \frac{1}{4a} \sqrt{\frac{\pi}{a}}$$

$$\int_0^\infty x^n e^{-ax} dx = \frac{n!}{a^{n+1}}$$

$$\int_0^\infty x^m e^{-ax^2} = \frac{\Gamma((m+1)/2)}{2a^{(m+1)/2}}$$

A.14 Nonlinear root finding

A.14.1 Bisection method

Methodology A.14.1.

- (Goal): We want to find a $x^* \in \mathbb{R}$ such that $f(x^*) = 0$.
- (*Initial input*): *Initial guess of* l_0 *and* r_0 *such that*

$$f(l_0) < 0, f(r_0) > 0$$
; or $f(l_0) > 0, f(r_0) < 0$.

- Repeat (i) is the iteration index:
 - Let $m = \frac{r_i + l_i}{2}$.
 - If $f(l_i) f(m) < 0$, then $l_{i+1} = l_i, r_{i+1} = m$.
 - If $f(l_i) f(m) > 0$ (then we must have $f(r_i) f(m) < 0$), then $l_{i+1} = m, r_{i+1} = r_i$.
 - If $f(l_i) f(m) = 0$, then m is the root.

A.14.2 Newton method

Methodology A.14.2.

- (Goal): We want to find a $x^* \in \mathbb{R}$ such that $f(x^*) = 0$. f is assumed to be differentiable.
- (*Initial input*): Initial guess of x_0 .
- *Repeat*(*i* is the iteration index):
 - Let $x_{i+1} = x_i \frac{f(x_i)}{f'(x_i)}$.
 - If $f(x_{i+1}) = 0$, then x_{i+1} is the root.

A.14.3 Secant method

Methodology A.14.3 (Secant method).

- (Goal): We want to find a $x^* \in \mathbb{R}$ such that $f(x^*) = 0$. f is assumed to be differentiable.
- (*Initial input*): Initial guess of x_0 , x_1 .
- *Repeat*(*i* is the iteration index):

- Let
$$x_{i+1} = x_i - f(x_i) \frac{x_i - x_{i-1}}{f(x_i) - f(x_{i-1})}$$
 .
$$- \text{If } f(x_{i+1}) = 0 \text{, then } x_{i+1} \text{ is the root.}$$

Remark A.14.1 (derivation). Starting with initial guesses x_0 , x_1 , we construct a first order approximation of f(x) via

$$y = \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_1) + f(x_1).$$

And we solve the root for the first-order approximation problem via

$$\frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_1) + f(x_1) = 0 \implies x_2 = x_1 - f(x_1) \frac{x_1 - x_0}{f(x_1) - f(x_0)}.$$

Then we continue the process with x_1, x_2 .

Remark A.14.2 (convergence property).

- There is no guarantee on the global convergence to the root of f.
- Only when the initial values x_0 and x_1 are sufficiently close to the root, the iterates x_n will converge to the root.

A.15 Interpolation

A.15.1 cubic interpolation

Definition A.15.1 (the cubic spine line functional form). [13]

- Suppose $x_1, x_2, ..., x_n$ and $y_1, y_2, ..., y_n$ are known.
- A cubic spine line is given by

$$y(x) = a_i + b_i(x - x_i) + c_i(x - x_i)^2 + d_i(x - x_i)^3, x_i \le x \le x_{i+1}, i = 1, 2, ..., n - 1.$$

- There are 4n 4 unknowns.
- Note that

$$y'(x) = b_i + 2c_i (x - x_i) + 3d_i (x - x_i)^2, x_i < x < x_{i+1}$$

$$y''(x) = 2c_i + 6d_i (x - x_i), x_i < x < x_{i+1}$$

$$y'''(x) = 6d_i x_i < x < x_{i+1}$$

Definition A.15.2 (natural cubic spline condition). [13] Let $h_i = x_{i+1} - x_i$

- (spline line passing data points): for i = 1, 2, ..., n 1, $a_i = y_i$; $a_{n-1} + b_{n-1}h_{n-1} + c_{n-1}h_{n-1}^2 + d_{n-1}h_{n-1}^3 = y_n$.
- (interpolating function is continuous); that is,

$$\lim_{x \to x_i - y} y(x) = \lim_{x \to x_i + y} y(x) \implies a_i + b_i h_i + c_i h_i^2 + d_i h_i^3 = a_{i+1}, \forall i = 1, 2, ..., n-2.$$

• (interpolating function is differentiable); note that the interpolating function is differentiable on interval, therefore we require that,

$$\lim_{x \to x_i -} y'(x) = \lim_{x \to x_i +} y'(x) \implies b_i + 2c_i h_i + 3d_i h_i^2 = b_{i+1}, \forall i = 1, 2, ..., n-2$$

:

• (interpolating function is twice differentiable and the second derivative at each endpoint is o); that is,

$$\lim_{x \to x_{i-}} y''(x) = \lim_{x \to x_{i+}} y''(x) \implies c_i + 3d_i h_i = c_{i+1}, \forall i = 1, 2, ..., n-2,$$

and
$$y''(x_1+) = y''(x_n-) = 0$$
.

• these 4n - 4 equations will solve the 4n - 4 unknowns.

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