MA 1018: Introduction to Scientific Computing
Mathematical Preliminaries

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Review of calculus

- **ε-δ definition of limit:** Let $\varnothing \neq X \subseteq \mathbb{R}$, x_0 be an accumulation point of X, and $f : X \to \mathbb{R}$ be a real-valued function. Then

$$\lim_{x \to x_0} f(x) = L \iff \forall\, \varepsilon > 0,\ \exists\, \delta > 0, \text{ such that if } x \in X \text{ and } 0 < |x - x_0| < \delta \text{ then } |f(x) - L| < \varepsilon.$$

- **Definition (continuity):** $\varnothing \neq X \subseteq \mathbb{R}$, $x_0 \in X$, and $f : X \to \mathbb{R}$.
  - $f(x)$ is said to be continuous at $x = x_0$ if $\lim_{x \to x_0} f(x) = f(x_0)$.
  - f is continuous on X if f is continuous at each number in X.
- **Notation:**

  $C(X) =$ the set of all functions that are continuous on X.

  e.g., $C([a,b]) = C[a,b]$, $C((a,b]) = C(a,b]$, etc.

Sequences

- **Definition:** Let $\{x_n\}_{n=1}^{\infty}$ be an infinite sequence of real (or complex) numbers and $x \in \mathbb{R}$ (or $\mathbb{C}$).

$$\lim_{n\to\infty} x_n = x \iff \forall\, \varepsilon > 0,\ \exists\, N \in \mathbb{N},\ \text{s.t. if } n > N \text{ then } |x_n - x| < \varepsilon.$$

- **Theorem:** $\varnothing \neq X \subseteq \mathbb{R}$, $x_0 \in X$, and $f : X \to \mathbb{R}$.

$$f \text{ is continuous at } x_0 \iff \text{if } \lim_{n\to\infty} x_n = x_0, \text{ then } \lim_{n\to\infty} f(x_n) = f(x_0) = f\big(\lim_{n\to\infty} x_n\big).$$

Smoothness

- **Definition:** Let $\varnothing \neq I \subseteq \mathbb{R}$ be an open interval, $x_0 \in I, f : I \to \mathbb{R}$.
  - If $\lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0}$ exists, then we say f is differentiable at x_0 and $f'(x_0) := \lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0}$ is the derivative of f at x_0.
  - If f is differentiable at each number in I, then we say f is differentiable on I.
- **Alternative definition:** $f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}$.
- **Theorem:** f is differentiable at $x_0 \Longrightarrow f$ is continuous at x_0.
- **Notation:**
  - $C^n(X) =$ the set of all functions that have n continuous derivatives on X.
  - $C^\infty(X) =$ the set of all functions that have derivatives of all orders on X.

    e.g., polynomials, exponential functions, etc., on $X = \mathbb{R}$.

Algorithm (pseudocode)

An algorithm to compute $f'(x)$ at the point $x = 0.5$ with $f(x) = \sin(x)$:

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program numerical differentiation
integer parameter $n \leftarrow 10$
integer i
real $error, h, x, y$
$x \leftarrow 0.5$
$h \leftarrow 1$
for $i = 1$ **to** n **do**
    $h \leftarrow 0.25h$
    $y \leftarrow (\sin(x+h) - \sin(x))/h$
    $error \leftarrow |\cos(x) - y|$
    output $i, h, y, error$
end for
end program

Mean Value Theorem

- **Rolle's Theorem:**
  If f is continuous on $[a,b]$, f' exists on (a,b), and $f(a) = f(b)$, then $\exists\, c \in (a,b)$ s.t. $f'(c) = 0$.
- **Mean Value Theorem:**
  If $f \in C[a,b]$ and f' exists on (a,b), then for $c \in (a,b)$ such that $f'(c) = \frac{f(b)-f(a)}{b-a}$.
- **Generalized Rolle's Theorem:** $f \in C[a,b]$, f is n time differentiable on (a,b). If f is zero at $n+1$ distinct numbers $x_0, x_1, \cdots, x_n \in [a,b]$, then $\exists\, c \in (a,b)$ such that $f^{(n)}(c) = 0$.
- **Extreme Value Theorem:** If $f \in C[a,b]$ then $\exists\, c_1, c_2 \in [a,b]$ such that $f(c_1) \leq f(x) \leq f(c_2)$, $\forall\, x \in [a,b]$.
- **Note:** Extreme Value Theorem + Fermat's Lemma $\Longrightarrow$ Rolle's Theorem $\Longrightarrow$ Mean Value Theorem.

Intermediate Value Theorem

- **Bolzano's Theorem:** If f is a continuous function on $[a, b]$ and $f(a)f(b) < 0$, then $\exists\, c \in (a, b)$ s.t. $f(c) = 0$.
- **Intermediate-Value Theorem:** If f is a continuous function on $[a, b]$ and K is any number between $f(a)$ and $f(b)$, that is, $f(a) < K < f(b)$ or $f(b) < K < f(a)$, then $\exists\, c \in (a, b)$ s.t. $f(c) = K$.
- **Note:** The Least-Upper-Bound Axiom + sign-preserving property $\Longrightarrow$ Bolzano's Theorem $\Longrightarrow$ Intermediate Value Theorem.

Riemann integral

- **Definition:** Let $\{x_0 = a, x_1, x_2, \cdots, x_n = b\}$ be a partition of $[a, b]$ with $\Delta x_i = x_i - x_{i-1}$, $i = 1, 2, \cdots, n$ and $z_i \in [x_{i-1}, x_i]$ is arbitrary chosen. If $\displaystyle\lim_{\max \Delta x_i \to 0} \sum_{i=1}^{n} f(z_i)\Delta x_i$ exists, then

$$\int_a^b f(x)dx := \lim_{\max \Delta x_i \to 0} \sum_{i=1}^{n} f(z_i)\Delta x_i$$

is called the (Riemann) integral of f on $[a, b]$.

- **Lebesgue Theorem:** Let $f : A \subseteq \mathbb{R}^n \to \mathbb{R}$ be a bounded function on a bounded set A.

f is Riemann integrable $\iff$ the set $\{$discontinuous points of $f\}$ is measure zero.

- **Note:** $f \in C[a, b] \Longrightarrow f$ is integrable on $[a, b]$.

equal spaced, $z_i = x_i \Longrightarrow \displaystyle\int_a^b f(x)dx = \lim_{n\to\infty} \frac{b-a}{n} \sum_{i=1}^{n} f(x_i)$.

Weighted Mean Value Theorem for integral

Theorem: If $f \in C[a,b]$, g is Riemann integrable on $[a,b]$ and does not change sign on $[a,b]$. Then $\exists\, c \in (a,b)$ such that

$$\int_a^b f(x)g(x)dx = f(c)\int_a^b g(x)dx.$$

Sketch of the proof:

$\because f \in C[a,b] \quad \therefore \exists\, m, M \in \mathbb{R}$ such that $m \le f(x) \le M, \;\; \forall x \in [a,b]$.

$\$$ $g(x) \ge 0$ on $[a,b]$. Then $\int_a^b mg(x)dx \le \int_a^b f(x)g(x)dx \le \int_a^b Mg(x)dx$.

$\$$ $\int_a^b g(x)dx > 0$, otherwise OK. Then $m \le \frac{\int_a^b f(x)g(x)dx}{\int_a^b g(x)dx} \le M$.

Then the assertion holds by the Intermediate Value Theorem. □

Note: $g(x) \equiv 1$ on $[a,b] \Longrightarrow \int_a^b f(x)dx = f(c)(b-a) \Longrightarrow$
$f(c) := \frac{1}{b-a}\int_a^b f(x)dx$ is called the average value of f on $[a,b]$.

Taylor's Theorem

Theorem: Let $f \in C^{n+1}[a,b]$ and $x_0 \in [a,b]$. Then for every $x \in [a,b]$, $\exists\ \xi(x)$ between x and x_0 such that

$$f(x) = P_n(x) + R_n(x),$$

where the n-th Taylor polynomial $P_n(x)$ is given by

$$P_n(x) = \sum_{k=0}^{n} \frac{1}{k!} f^{(k)}(x_0)(x - x_0)^k$$

and the remainder (error) term $R_n(x)$ is given by

$$\begin{aligned} R_n(x) &= \frac{1}{n!}\int_{x_0}^{x} (x-t)^n f^{(n+1)}(t)\,dt && \text{(integral form)} \\ &= \frac{1}{(n+1)!} f^{(n+1)}(\xi(x))(x - x_0)^{n+1} && \text{(Lagrange form)} \\ & \quad \text{(by the weighted MVT for integral)} \end{aligned}$$

Some remarks

Assume that $f \in C^\infty[a,b]$.

- $\sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}(x_0)(x-x_0)^k$ is called the Taylor series of f at x_0.

  (when $x_0 = 0$, called the Maclaurin series)

- If $\lim_{n\to\infty} R_n(x) = 0$, then $\lim_{n\to\infty} P_n(x) = f(x)$, i.e.,

$$f(x) = \sum_{k=0}^{\infty} \frac{1}{k!} f^{(k)}(x_0)(x-x_0)^k.$$

Example: Taylor polynomial of $f(x) = \cos(x)$ at $x_0 = 0$

$f'(x) = -\sin(x)$, $f''(x) = -\cos(x)$, $f'''(x) = \sin(x)$, $f^{(4)}(x) = \cos(x)$.

$f(0) = 1$, $f'(0) = 0$, $f''(0) = -1$, $f'''(0) = 0$, $f^{(4)}(0) = 1$.

Case $n = 2$:

$\cos(x) = 1 - \frac{1}{2}x^2 + \frac{1}{6}x^3 \sin(\xi(x))$, where $\xi(x)$ is between 0 and x.

$\cos(0.01) = 0.99995 + 0.1\bar{6} \times 10^{-6} \sin(\xi(x))$, where $0 < \xi(x) < 0.01$.

$|\cos(0.01) - 0.99995| \leq 0.1\bar{6} \times 10^{-6} |\sin(\xi(x))| \leq 0.1\bar{6} \times 10^{-6} \times 0.01$

$= 0.1\bar{6} \times 10^{-8}$, where we use the fact $|\sin(x)| \leq |x|$, $\forall\, x \in \mathbb{R}$.

Case $n = 3$:

$\cos(x) = 1 - \frac{1}{2}x^2 + \frac{1}{24}x^4 \cos(\tilde{\xi}(x))$, where $\tilde{\xi}(x)$ is between 0 and x.

$|\cos(0.01) - 0.99995| \leq \frac{1}{24}(0.01)^4 \times 1 \leq 4.2 \times 10^{-10}$.

Example (cont'd)

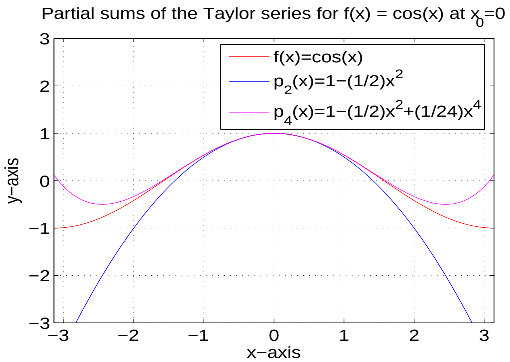
Use the Taylor polynomial to estimate

$$\begin{aligned}\int_0^{0.1}\cos(x)dx &= \int_0^{0.1}(1-\frac{1}{2}x^2)dx + \int_0^{0.1}\frac{1}{24}x^4\cos(\tilde{\xi}(x))dx\\ &= (x-\frac{1}{6}x^3)\Big|_0^{0.1} + \int_0^{0.1}\frac{1}{24}x^4\cos(\tilde{\xi}(x))dx\\ &= 0.0998\bar{3} + \int_0^{0.1}\frac{1}{24}x^4\cos(\tilde{\xi}(x))dx.\end{aligned}$$

$$\begin{aligned}\left|\int_0^{0.1}\cos(x)dx - 0.0998\bar{3}\right| &\le \frac{1}{24}\int_0^{0.1}x^4|\cos(\tilde{\xi}(x))|dx\\ &\le \frac{1}{24}\int_0^{0.1}x^4dx = 8.\bar{3}\times 10^{-8}.\end{aligned}$$

True value is 0.099833416647, actual error for this approximation is 8.3314×10^{-8}.

Partial sums of the Taylor series for $f(x) = \cos(x)$ at $x_0 = 0$



Note: A Taylor series converges rapidly near the point of expansion and slowly (or not at all) at more remote points.

Taylor's Theorem in two variables

If $f \in C^{n+1}([a,b] \times [c,d])$, then for (x,y), $(x+h, y+k) \in [a,b] \times [c,d]$ we have

$$f(x+h, y+k) = \sum_{i=0}^{n} \frac{1}{i!} (h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y})^i f(x,y) + R_n(h,k),$$

where

$$R_n(h,k) = \frac{1}{(n+1)!} \left(h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y} \right)^{n+1} f(x+\theta h, y+\theta k)$$

for some $0 < \theta < 1$.

Example: First few terms in the Taylor formula for $f(x,y) = \cos(xy)$:

Taylor's formula with $n = 1$ is

$$\cos\big((x+h)(y+k)\big) = \cos(xy) - hy\sin(xy) - kx\sin(xy) + R_1(h,k),$$
$$R_1(h,k) = \cdots .$$

How about $n = 2$?

Big O notation for sequences

- **Definition:** Suppose that $\lim_{n\to\infty} \beta_n = 0$ and $\lim_{n\to\infty} \alpha_n = \alpha$. If $\exists\, K > 0$ and $n_0 \in \mathbb{N}$ such that $|\alpha_n - \alpha| \leq K|\beta_n - 0|$ for all $n \geq n_0$, then we say that $\{\alpha_n\}$ converges to α with rate of convergence $O(\beta_n)$ and write $\alpha_n = \alpha + O(\beta_n)$.
- **Examples:**

$$\alpha_n = 1 + \frac{n+1}{n^2} \implies \lim_{n\to\infty} \alpha_n = \alpha = 1.$$

$$\widetilde{\alpha}_n = 2 + \frac{n+3}{n^3} \implies \lim_{n\to\infty} \widetilde{\alpha}_n = \widetilde{\alpha} = 2.$$

Let $\beta_n = \frac{1}{n}$ and $\widetilde{\beta}_n = \frac{1}{n^2}$. Then $\lim_{n\to\infty} \beta_n = 0 = \lim_{n\to\infty} \widetilde{\beta}_n$.

$$\implies |\alpha_n - 1| = \frac{n+1}{n^2} \leq \frac{n+n}{n^2} = 2\frac{1}{n} = 2|\beta_n - 0|$$

$$\text{and } |\widetilde{\alpha}_n - 2| = \frac{n+3}{n^3} \leq \frac{n+3n}{n^3} = 4\frac{1}{n^2} = 4|\widetilde{\beta}_n - 0|.$$

$$\implies \alpha_n = 1 + O\left(\frac{1}{n}\right) \text{ and } \widetilde{\alpha}_n = 2 + O\left(\frac{1}{n^2}\right).$$

Big O notation for functions

- **Definition:** Suppose that $\lim_{h \to 0} G(h) = 0$ and $\lim_{h \to 0} F(h) = L$. If $\exists\, K > 0$ and small $h_0 > 0$ such that $|F(h) - L| \le K|G(h) - 0|$ for all $|h| \le h_0$, then we say that $F(h)$ converges to L with rate of convergence $O(G(h))$ and write $F(h) = L + O(G(h))$.
- **Example:**

$$\cos(h) = 1 - \frac{1}{2}h^2 + \frac{1}{24}h^4 \cos(\xi(h)),\ \xi(h) \text{ is between 0 and } h.$$

$$\because \left|\cos(h) + \frac{1}{2}h^2 - 1\right| = \left|\frac{1}{24}\cos(\xi(h))\right| h^4 \le \frac{1}{24}h^4 \text{ for all } h.$$

$$\therefore \cos(h) + \frac{1}{2}h^2 = 1 + O(h^4).$$