Numerical Methods

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***Definition* 1** (Numerical Methods)**.** Numerical Methods are algorithmic approaches to numerically solve mathematical problems. We use it often when it is hard/difficult/impossible to solve analytically.

1 Taylor series

Given a function $f : \mathbb{R} \to \mathbb{R}$ (that is hard to evaluate for some $x \in \mathbb{R}$), but f and $f^{(n)}$ are known for a value c, which is close to x. Can we use this information to approximate $f(x)$?

We know values for $\cos^{(n)}(0)$.

$$\begin{cases} f(0) = \cos(0) = 1 \\ f'(0) = -\sin(0) = 0 \\ f''(0) = -\cos(0) = -1 \end{cases} \qquad \text{for } c = 0$$

Can we get $\cos(0.1)$ from this?

***Definition* 1** (Taylor series)**.** Let $f : \mathbb{R} \to \mathbb{R}$, differentiable infinitely many times at $c \in \mathbb{R}$. So we have $f^{(k)}(c),\ k = 1, 2, \ldots$. Then the Taylor series of f at c is:

$$f(x) \approx f(c) + \frac{f(c)}{1!}(x-c)^1 + \frac{f''(c)}{2!}(x-c)^2 + \cdots = \sum_{k=0}^{\infty} \frac{f^{(k)}}{k!}(x-c)^k$$

Remark. Taylor series is a power series.

Remark. For $c = 0$ also known as Maclaurin series

Remark. A power series has an interval/radius of convergence. You can only evaluate the series if $x \in$ interval of convergence.

Example 1. What is the Taylor series for $f(x) = e^x$ at $c = 0$? We have $f^{(k)}(x) = e^x$, so $f^{(k)}(0) = 1$. Thus:

$$\sum_{k=0}^{\infty} \frac{1}{k!} x^k$$

and the radius of convergence is ∞.

I.e. for any $x \in \mathbb{R}$:

$$e^x = \sum_{k=0}^{\infty} \frac{x^k}{k!}$$

For an algorithm we need a finite amount of terms. For example,

$$e^x \approx \frac{1}{0!}x^0 + \frac{1}{1!}x^1 + \frac{1}{2!}x^2 = 1 + x + \frac{x^2}{2}$$

This is a polynomial!

Example 2. Let's calculate Taylor series of a polynomial.

$$f(x) = 4x^2 + 5x + 7,\ c = 2$$
$$f(2) = 33,\ f'(2) = 8x + 5\Big|_{x=2} = 21,\ f''(2) = 8$$

Taylor series:

$$33 + 21(x-2) + \frac{8}{2}(x-2)^2 = 4x^2 + 5x + 7 = f(x)$$

Taylor series of a polynomial is itself.

Theorem 1 (Taylor theorem)**.** Let $f \in C^{n+1}([a,b])$ (i.e. f is $(n+1)$-times continuously differentiable). Then for any $x \in [a,b]$ we have that

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(c)}{k!}(x-c)^k + \frac{f^{(n+1)}(\xi_x)}{(n+1)!}(x-c)^{n+1}$$

where ξ_x is a point that depends on x and which is between c and x.

The first sum is called *truncated Taylor series*, the remainder is called *the error*.

Example. For $n = 0$:

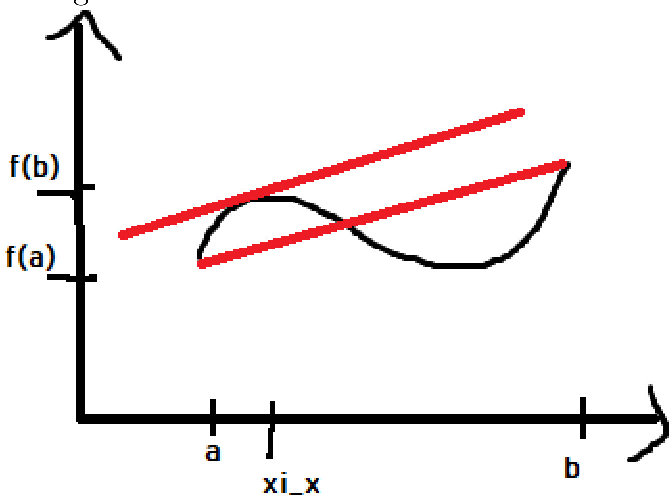
$$f(x) = f(c) + f'(\xi_x)(x-c)$$

Choose $c = a$, $x = b$:

$$f(b) = f(a) + f'(\xi_x)(b-a) \iff f'(\xi_x) = \frac{f(b)-f(a)}{b-a}$$

This is the mean value theorem!

Figure 1: Mean value theorem illustration

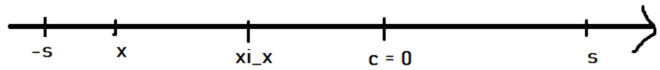


Definition 2. We say that the Taylor series *represents* the function f at x if the Taylor series converges at that point, i.e. the remainder tends to zero as $n \to \infty$.

Example 1. Back to e^x: $f(x) = e^x$, $c = 0$, ξ_x is between c and x.

$$e^x = \sum_{k=0}^{n} \frac{x^k}{k!} + \frac{e^{\xi_x}}{(n+1)!}x^{n+1}$$

For any $x \in \mathbb{R}$ we find $s \in \mathbb{R}_0^+$ ($\mathbb{R}_0^+$ are all real, positive numbers including 0) so that $|x| \leqslant s$, and $|\xi_x| \leqslant s$ because ξ_x is between c and x.



Because e^x is monotone increasing, we have $e^{\xi_x} \leqslant e^s$, thus

$$\lim_{n\to\infty}\left|\frac{e^{\xi^x}}{(n+1)!}x^{n+1}\right| \leqslant \lim_{n\to\infty}\left|\frac{e^s}{(n+1)!}\right|s^{n+1} = e^s \lim_{n\to\infty}\frac{s^{n+1}}{(n+1)!} = 0$$

Because $(n+1)!$ will grow faster than any power of $s \implies \lim_{n\to\infty}\left|\frac{e^{\xi_x}}{(n+1)!}x^{n+1}\right| = 0$.

Thus e^x is *represented* by its Taylor series.

Example 2.

$$\begin{aligned}
&f(x) = \log(1+x),\ c = 0\\
&f'(x) = \frac{1}{1+x} = (1+x)^{-1}\\
&f''(x) = -(1+x)^{-2}\\
&f'''(x) = +2(1+x)^{-3}\\
&f^{(k)}(x) = (-1)^{k+1}(k-1)!\frac{1}{(1+x)^k}
\end{aligned}$$

So $f^{(k)}(0) = (-1)^{k-1}(k-1)!$ for $k \geqslant 1$, $f(0) = \log(1) = 0$.

Taylor series:

$$\begin{aligned}
f(x) &= \sum_{k=1}^{n}\frac{(-1)^{k-1}}{k}x^k + \frac{(-1)^k}{n+1}\frac{1}{(1+\xi_x)^{n+1}}\cdot x^{n+1} \quad \left(\frac{n!}{(n+1)!} = \frac{1}{n+1}\right)\\
E_n(x) &= \frac{(-1)^k}{n+1}\frac{1}{(1+\xi_x)^{n+1}}\cdot x^{n+1} \text{ — the remainder}
\end{aligned}$$

Question: for which x does $\lim_{n\to\infty} E_n(x) = 0$?

$$\lim_{n\to\infty} E_n(x) = \lim_{n\to\infty}\frac{(-1)^n}{n+1}\left(\frac{x}{\xi_x+1}\right)^{n+1} \text{ for } \xi_x \in (c,x)\ (c=0)$$

Such a limit converges to 0, if the fraction is less than 1.

$$0 < \frac{x}{\xi_x+1} < 1 \iff x < \xi_x + 1 \iff x - \xi_x < 1 \text{ with } \xi_x \in (0,x) \iff x \leqslant 1$$

Consequence. $\lim_{n\to\infty} E_n(x) = 0$ if $0 < x \leqslant 1$. This means that the Taylor series represents $\log(x+1)$ for $x \in [0,1]$. We can extend this to show $x \in (-1,1]$.

Example 3. Let's compute $\cos(0.1)$. Let's approximate it with Taylor series with $c = 0$ (around zero).

$$\cos(x) = 1 - \frac{x^2}{2} + \frac{x^4}{4!} - \frac{x^6}{6!} \pm \cdots + \text{remainder}$$

Consequence.

$$\left|\cos(x) - \sum_{k=0}^{n}(-1)^k \frac{x^{2k}}{(2k!)}\right| = \left|(-1)^{n+1}\cos(\xi_x)\frac{x^{2(n+1)}}{\big(2(n+1)\big)!}\right| \leqslant \frac{0.1^{2(n+1)}}{2(n+1)!} \underset{n\to\infty}{\longrightarrow} 0$$

n	Taylor polynomial	$\lvert error\rvert \leqslant$
0	1	$\frac{(0.1)^2}{2} = 0.0005$
1	0.995	$\frac{0.0001}{24}$
2	0.99500416	$\frac{0.000001}{6!}$

Error depends on choice of $|x-c|$ and n.

Example 4. Compute $\log(2)$ using $f(x) = \log(x+1)$

$$\log(2) = 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \frac{1}{5} - \frac{1}{6} + \dots$$

Keeping 8 terms (until $n = 8$) we get $\log(2) \approx 0.63452$, the actual solution is $\log(2) = 0.693147$. Not so accurate. Can we improve?

We can use Taylor series of $\log\big(\frac{1+x}{1-x}\big)$ instead, since $\log\big(\frac{1+x}{1-x}\big) = \log(1+x) - \log(1-x)$. We choose $x = \frac{1}{3}$ instead of $x = 1$. Since x is closer to zero, both of the logarithms converge quicker.

$$\left(\log\Big(\frac{1+1/3}{1-1/3}\Big) = \log(2)\right)$$

We then get

$$\log(2) = 2\cdot\left(\frac{1}{3} + \frac{1}{3^3\cdot 5} + \dots\right)$$

We only need 4 terms to get $\log 2 \approx 0.69313$.

Theorem 2 (Reformulation of Taylor's theorem)**.** $f \in \mathrm{C}^{n+1}([a,b])$. We change c to x and the old x to $x+h$ from previous version $\implies$ get for $x,\ x+h \in [a,b]$:

$$f(x+h) = \sum_{k=0}^{n}\frac{f^{(k)}(x)}{k!}h^k + \frac{f^{(n+1)}(\xi_x)}{(n+1)!}h^{n+1} \text{ where } \xi_x \in (x, x+h),\ h > 0$$

We can write error term as

$$f(x+h) - \sum_{k=0}^{n}\frac{f^{(k)}(x)}{k!}h^k = \mathcal{O}(h^{n+1})$$

Remark. Let's recall what the $\mathcal{O}$-notation means. $a(h) = \mathcal{O}\big(b(h)\big)$ if $\exists c > 0$ such that $\frac{a(j)}{b(j)} \leqslant c$ as $h \to 0$. So, for $n = 1$ the error decreases with h^2 (quadratic convergence).
$n = 2$: error decreases cubically, i.e. h^3, etc.

Summary of Taylor series:

- Problem: Evaluate $f(x)$ with a given error bound.
- Required: $f \in \mathrm{C}^{n+1}$, values of derivatives $f^{(k)}(a)$.
- Check interval of convergence: does Taylor series expansion work?
- Estimate the maximum error for n terms of the Taylor polynomial.
- Choose n, such that the error bound is low enough.
- Evaluate the Taylor polynomial.

2 Number representation

2.1 Errors

There are different error types:

1. An error in data (partly due to roundoff).
2. Roundoff errors (during computation). For example, multiplication increases the amount of needed significant digits, and we can't store them all on a computer.
3. Truncation error, that is inherent to numeric methods. For example, if we take a finite number of terms in our Taylor series.

Definition 1. Let $\tilde{a}$ be an approximation of a. Then $|\tilde{a} - a|$ is the *absolute error*, and $\left|\frac{\tilde{a}-a}{a}\right|$ is the *relative error*. The *error bound* is the magnitude of admissable error.

Example. 0.00123 with error $0.000004 = 0.4 \cdot 10^{-5}$. The error is below $\frac{1}{2} \cdot 10^{-t}$ with $t = 5$, so there's 5 correct digits and 3 significant digits (the number of non-leading zeros).

Example. 0.00123 with error $0.000006 = 0.06 \cdot 10^{-4} > \frac{1}{2} \cdot 10^{-5}$. Only has 2 significant digits, because we have to round the error up.

Theorem 1. In addition/subtraction the bounds for absolute errors are added, in multiplication/division the relative errors are added.

Example. Solve $x^2 - 56x + 1 = 0$:

$$x = 28 - \sqrt{783} \approx 28 - 27.982 \text{ (5 significant digits)} = 0.018 \pm \frac{1}{2} \cdot 10^{-3}$$

We end up with 2 significant digits in the answer, despite that we used to have 5. That's why computers use floating point numbers, as leading zeros are bad.

Definition 2 (Error propagation)**.** If $y(x)$ is smooth, than the derivative $|y(x)'|$ can be interpreted as the sensitivity of $y(x)$ to errors in x. We can generalize this to functions of multiple variables:

$$|\Delta y| \leqslant \sum \left|\frac{\partial y}{\partial x_i}\right| \cdot |\Delta x_i|, \text{ where } \Delta y = \tilde{y} - y,\ \Delta x_i = \tilde{x_i} - x_i$$

This is an empirical inequality that is only valid for small Δx_i. It is used a lot in physics.

2.2 Base representation

Definition 3 (Base representation)**.** Every number $x \in \mathbb{N}$ can be written in the following form as a unique expansion with respect to the base b, where $b \in \mathbb{N} \setminus \{1\}$:

$$x = a_0 b^0 + a_1 b^1 + a_2 b^2 + \cdots + a_n b_n = \sum_{i=0}^{n} a_i b^i$$
$$a \in \mathbb{N}_0,\ a_i < b,\ a_i \in \{0, \ldots, b-1\}$$

Here b is called the *base*, a_i are called the *digits*. Humans usually use base 10. But, for example, computers can use base 2.

For a real number $x \in \mathbb{R}$ we can write:

$$x = \sum_{i=0}^{n} a_i b^i + \sum_{i=1}^{\infty} a_{-i} b^{-i}$$

Example. $b = 2: \; 1011 = 1 \cdot 2^0 + 1 \cdot 2^1 + 0 \cdot 2^2 + 1 \cdot 2^3 = (11)_{10}$

There are different algorithms that convert number systems.

2.3 Euclid's algorithm

Euclid's algorithm converts $(x)_{10}$ to $(y)_b$.

1. Input $(x)_{10}$.
2. Determine the smallest n, such that $x < b^{n+1}$.
3. For $i = n$ to 0 do:

$$\begin{aligned} a_i &\coloneqq x \text{ div } b^i \text{ (integer division)} \\ x &\coloneqq x \text{ mod } b^i \text{ (the remainder)} \end{aligned}$$

4. Output result $a_n a_{n-1} a_{n-2} \ldots a_0 = (y)_b$.

Example. 1. $(x)_{10} = (13)_{10} \to (y)_2$

2. $n = 3$ since $13 < 2^4$.
3.

$$\begin{aligned} i = 3: \; & a_3 = 13 \text{ div } 2^3 = 1, \; x = 13 \text{ mod } 2^3 = 5 \\ i = 2: \; & a_2 = 5 \text{ div } 2^2 = 1, \; x = 5 \text{ mod } 2^2 = 1 \\ i = 1: \; & a_1 = 1 \text{ div } 2^1 = 0, \; x = 1 \text{ mod } 2^1 = 1 \\ i = 0: \; & a_0 = 1 \text{ div } 2^0 = 1, \; x = 1 \text{ mod } 2^0 = 0 \end{aligned}$$

4. Output: $(1101)_2 = (13)_{10}$.

Two problems of the Euclid's algorithm:

1. Step 2 is inefficient
2. Division by large numbers can be problematic.

2.4 Horner's scheme

Horner's scheme is a more efficient algorithm. The idea is to represent the number as follows:

$$(a_n a_{n-1} \ldots a_0)_b = a_0 + b\big(a_1 + b(a_2 + b(a_3 + \cdots + b(a_n))) \ldots\big)$$

The algorithm is the following:

1. Input $(x)_{10}$.
2. $i \coloneqq 0$.

3. While $x > 0$ do:

$$a_i := x \bmod b$$
$$x := x \operatorname{div} b$$
$$i := i + 1$$

4. Output result $a_n a_{n-1} a_{n-2} \dots a_0 = (y)_b$.

Remark. The algorithm is very similar to the Euclid's algorithm — the difference is that we execute it in reverse. We no longer have divisions by large numbers, and thus it runs faster.

General remarks:

- A number with simple representation in one base may be complicated to represent in another base. For example, $(0.1)_{10} = (0.0001100110011\dots)_2$.
- Base 2 is called *binary*, base 8 is *octal*, base 16 is *hexadecimal*.
- To convert from a base b to base 10 we can just perform the following computation:

$$(42)_8 = 4 \cdot 8^1 + 2 \cdot 8^0 = (34)_{10}$$

- Conversion 2 and 8. $8 = 2^3$: three consecutive bits represent one octal digit, e.g.

$$(551.624)_8 = (101101001.110010100)_2$$

- Conversion 2 and $16 = 2^4$: just four bits to one hexadecimal digit.
- Horner's scheme algorithm does not need estimate of n and does not divide by large numbers.
- It is applicable to real numbers, but one needs a critireon to stop if the representation with the new base is infinite.
- On computers we only have finite precision (the number of digits/bits).

2.5 Floating point representation

***Definition* 4.** Normalized floating point representation with respect to a base b stores any number x as follows:

$$x = 0.a_1 a_2 \dots a_k \cdot b^n \text{ where } a_i \in \{0, 1, \dots, b-1\}$$

a_i are called *digits*, k is called *precision*, n is called *exponent*, $a_1 \dots a_k$ is called *mantissa*, $a_1 \neq 0$ is called *normalization*, which makes the representation unique.

Remark. Leading zeros are essentially a waste of space. That's why floating points are useful when you add/subtract/divide numbers — as you're able to move the decimal point.

Example 1. Base 10: $32.213 = 0.32213 \cdot 10^2$.

Base 2: $x = \pm 0.b_1 b_2 \dots b_k \cdot 2^n$ We need another bit to define the sign of the number.

Example 2. For *single precision* floating-point numbers: 4 bytes = 32 bits.

- 1 bit sign mantissa.

- 1 bit sign exponent.
- 7 bits for exponent (integer).
- 23 bits for mantissa (24 effectively, since the first digit is always 1).

7 bits allow for the largest exponent of 127, i.e. $2^127 \approx 10^38$. Anything above that is infinity. So, we have the range of $10^{-38} < |x| < 10^38$.

Since $2^{-24} \approx 10^{-7}$, we can represent 7 significant digits.

We can have a better representation, e.g. with *double precision* (8 bytes).

Issues with floating-point numbers:

- Adding numbers is not commutative, i.e. $x + y$ does not necessarily equal to $y + x$.
- It's not associative, i.e. $(x + y) + z$ does not necessarily equal to $x + (y + z)$. You usually try to add small numbers together first, in hopes that they will become big enough to become significant.

Example 1. Take $x = y = 0.00000033$, $z = 0.00000034$, $w = 1.00000000$. We compute $x + y + z + w$, and in that order we get 1.000001. Reversed order gets 1.000000 with base 10. Why is that? That's because we only have 7 significant digits.

Example 2.

$$\sum_{1}^{10^7} 1 + 10^7 = 1 + \cdots + 1 + 10^7$$

The order of summation will make a difference. You will either get 10^7 or $2 \cdot 10^7$, because $1 + 1 = 2$, but $1 + 10^7 = 10^7$ due to roundoff.

Consequence. Avoid adding numbers of different order of magnitude. Add numbers in increasing order of their size.

Example 3. Compute $x - \sin x$ for x close to 0, e.g. $x = 1/15$. Assume $k = 10$ precision.

$$\begin{aligned} x &= 0.6666666667 \cdot 10^{-1} \\ \sin x &= 0.6661729492 \cdot 10^{-1} \\ x - \sin x &= 0.0004937175 \cdot 10^{-1} = 0.4937175\underline{000} \cdot 10^{-4} \end{aligned}$$

Notice the three zeros at the end — that is a sign of a precision loss (unless the number actually ends with zeros).

Consequence. Avoid subtracting number of similar size, because it leads to a loss of precision.

A potential solution in this case would be to use Taylor series expanison:

$$\begin{aligned} \sin x &= x - \frac{x^3}{3!} + \frac{x^5}{5!} - \ldots \\ x - \sin x &= +\frac{x^3}{3!} - \frac{x^5}{5!} + \ldots \end{aligned}$$

Using 3 terms we get: $0.4937174328 \cdot 10^{-4}$. The error of the Taylor series with 3 terms will be $\leqslant 10^{-13}$ (which is needed for "full" precision for $0. \cdots \cdot 10^{-4}$).

Theorem 2. Let x, y be two normalized floating point numbers with $x > y > 9$ and base $b = 2$. If there exist $p, q \in \mathbb{N}_0$ such that

$$2^{-p} \leqslant 1 - \frac{y}{x} \leqslant 2^{-q}$$

Then at most p and at least q significant bits are lost.