Computational method and numerical algorithms

Wangtao Lu
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Contact Information

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- Teaching Assistant: Shuying Zheng(**zsyelaine@outlook.com**)

Contents

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Reference Book

Numerical Analysis, 2nd edition, Timothy Sauer, 2012.

Goal: **learn solving mathematical problems by a computer!**
Prerequisite: **Calculus and Linear Algebra.**

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Topics

- Machine arithmetic
- Solving equations
- System of equations: Numerical linear algebra
- Interpolation
- Eigenvalues and singular values
- Numerical differentiation and integration
- Trigonometric Interpolation and the FFT (If time allows)
- ...

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Evaluating and Grading Policies

The final grade will be based on the following components:

- Excercises and Coding assignments: 30%;
- Activities in classes: 10%.
- Final exam (location and date will be noticed in the class): 60%.

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Excercises and Coding Assignments

Each assignment should be written as an report **in English only**, which should include: For coding work:

- the whole code;
- outputs, results and comments.

For excercises:

- complete steps.

Accept only .pdf or .doc files for coding assignments. For writing assignments, handwriting reports are allowed, but you need to take photos of your assignments (make sure they are clear enough) and copy them in your report.

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Messages to TA

Each assignment should be emailed to TA (Miss Shuying Zheng: zsyelaine@outlook.com), and due date will be anounced in class. The subject of your message to TA should include **Your Student ID, your NAME and the Assignment No.** For example, The following subject is accepted:

12345678, Bai Li, Assignment 1

Programming Software

Suggested software: MATLAB. However, C++ or Fortran is also accepted.
A simple tutorial of MATLAB for beginners can be found easily online.

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Cheating and Plagiarism Policy

No cheating is tolerated.
If one is caught cheating on any assignment or the final exam, he/she will automatically receive a "FAIL" on his/her final grade.

Contents

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0.1 Evaluation a polynomial

Problem: What is the best way to evaluate

$$P(x) = 2x^4 + 3x^3 - 3x^2 + 5x - 1,$$

at $x = 3$?

	Method I	Method II	Method III
# of multiplications:			
# of additions:			

0.1 Evaluation a polynomial

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Method I:

$$P(3) = 2*3*3*3*3 + 3*3*3*3 - 3*3*3 + 5*3 - 1.$$

	Method I	Method II	Method III
# of multiplications:	10		
# of additions:	4		

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Method II: Find and store:

$$3*3 = 3^2, \quad 3^2*3 = 3^3, \quad 3^3*3 = 3^4,$$

Then, evaluate

$$P(3) = 2*(3^4) + 3*(3^3) - 3*(3^2) + 5*3 - 1.$$

	Method I	Method II	Method III
# of multiplications:	10	7	
# of additions:	4	4	

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Method III: Nested Multiplication:

$$P(3) = -1 + 3*(5 + 3*(-3 + 3*(3 + 3*2))).$$

	Method I	Method II	Method III
# of multiplications:	10	7	4
# of additions:	4	4	4

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Horner's method

In fact, in nested form,

$$\begin{aligned} P(x) &= 2x^4 + 3x^3 - 3x^2 + 5x - 1 \\ &= -1 + x * (5 + x * ((-3) + x * (3 + x * 2))). \end{aligned}$$

For a general degree n polynomial

$$P(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n.$$

Horner's method: Nested multiplication method rewrites it as

$$P(x) = a_0 + x * (a_1 + x * (a_2 + x * (\cdots (a_{n-1} + a_n * x)))),$$

evaluating the polynomial in multiplications and additions.

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$$P(x) = a_0 + x * (a_1 + x * (a_2 + x * (\cdots (a_{n-1} + a_n * x)))),$$

evaluating the polynomial in n multiplications and n additions.

Horner's method with base points

For a polynomial in the following form:

$$P(x) = a_0 + a_1(x - r_1) + a_2(x - r_1)(x - r_2) + \cdots + a_n(x - r_1)\cdots(x - r_n),$$

with base points: $r_1, \cdots, r_n$.
Horner's method rewrites it, in nested form, as

$$P(x) = a_0 + (x - r_1) * (a_1 + (x - r_2) * (a_2 + \cdots (a_{n-1} + a_n * (x - r_n)))).$$

0.2 How computer stores real numbers?

Stored in binary format using the so-called IEEE Floating Point Standard.
Floating point representations:

$$r = \pm 1.b_1 b_2 b_3 \ldots b_N \times 2^p,$$

where the exponent $p = (p_1 p_2 \ldots p_M)_2$, $b_i, p_j = 0, 1$.

	sign	exponent	mantissa
single precision	1 (bit)	$(M=)8$	$(N=)23$
double precision	1	11	52

For example, in double precision

$$\begin{aligned}9.4 =&(1001.\overline{0110})_2 \\ =&+1.\boxed{0010110011001100110011001100110011001100110011001100} \\ &110\ldots \times 2^3.\end{aligned}$$

Truncation Rule:

- Chopping
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Truncation Rule:

- Chopping
- **Rounding: IEEE Rounding to Nearest Rule.**

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Precision and Error

Machine Epsilon $\varepsilon_{\mathrm{MACH}}$: The distance between 1 and the smallest floating point number greater than 1. In double precision,

$$\varepsilon_{\mathrm{MACH}} = 2^{-52}.$$

fl(x): the IEEE double precision floating point number representation of x, using the rounding to nearest rule.

Absolute error:

$$|x_c - x|,$$

where x_c is a computed version of x.

Relative error:

$$\frac{|x_c - x|}{|x|},$$

when $x \neq 0$.

Relative rounding error: In the IEEE machine arithmetic model,

$$\frac{|fl(x) - x|}{|x|} \leq \frac{1}{2}\varepsilon_{\mathrm{MACH}}.$$

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0.3 Loss of Significance

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Loss of significance can occur in machine arithmetic due to the rounding error, when one subtracts nearly equal numbers.
Example 1. Calculate $\sqrt{9.01} - 3$ on a three-decimal-digit computer.

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Method 1:

$$\sqrt{9.01}-3 \approx 3.00(16662)-3 \approx 0.00(1662).$$

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0.3 Loss of Significance

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Example 1. Calculate $\sqrt{9.01} - 3$ on a three-decimal-digit computer.
Method 1:

$$\sqrt{9.01} - 3 \approx 3.00(16662) - 3 \approx 0.00(1662).$$

Method 2:

$$\sqrt{9.01} - 3 = \frac{(\sqrt{9.01} - 3)(\sqrt{9.01} + 3)}{\sqrt{9.01} + 3} \approx \frac{0.01}{3.00 + 3} \approx 1.67 \times 10^{-3}.$$

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Example 2. Compare

$$E_1 = \frac{1 - \cos x}{\sin^2 x}, E_2 = \frac{1}{1 + \cos x},$$

for x close to 0.

x	E_1	E_2

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1.00000000000000	0.64922320520476	0.64922320520476

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0.00010000000000	0.50000004138685	0.50000000001250

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0.00010000000000	0.50000004138685	0.50000000001250
0.00001000000000	0.50004445029134	0.50000000000013

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0.00000100000000	0.49960036108132	0.50000000000000

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0.00000100000000	0.49960036108132	0.50000000000000
0.00000010000000	0.00000000000000	0.50000000000000

Example 3. The quadratic formula:

$$x_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}.$$

When is this formula unstable numerically?
Trick:

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Example 3. The quadratic formula:

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When is this formula unstable numerically? $ac/(b^2) \approx 0$.
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$$x_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}.$$

When is this formula unstable numerically? $ac/(b^2) \approx 0$.
Trick: Rationalize the numerator.

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Error Analysis

Given two unequal real numbers a and b, we have

$$\text{RELATIVE ERROR} = \left|\frac{[fl(a) - fl(b)] - (a-b)}{a-b}\right| \leq \frac{1}{2}\left|\frac{a+b}{a-b}\right| \varepsilon_{\text{MACH}}.$$

When $b = a + \mathcal{O}(a\varepsilon_{\text{MACH}})$, we have

$$\text{RELATIVE ERROR} \leq \mathcal{O}(1).$$

This indicates that if b and a are nearly equal, then the relative error of the machine arithmetic $fl(b) - fl(a)$ can be **as large as $O(1)$.**

Contents

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Chapter 1: Solving equations

The goal of this chapter: **Finding roots of $f(x) = 0$ by computers!**

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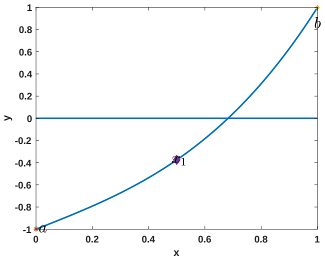
Root: A function $f(x)$ has a root at $x = r$ if $f(r) = 0$.
Theorem: Let f be continuous on $[a, b]$ with $f(a)f(b) < 0$. Then, f **has a root** $r \in (a, b)$.
Searching principle: **Bisect the interval and bracket a root.**



0. $r \in (a, b)$, since $f(a) < 0$ and $f(b) > 0$.

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1.1 The bisection method

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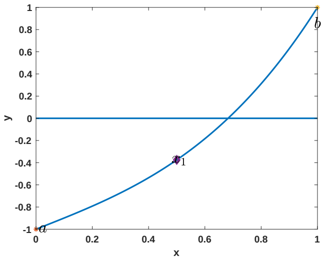

0. $r \in (a, b)$, since $f(a) < 0$ and $f(b) > 0$.
1. Set $x_1 = \frac{a+b}{2}$.
   If $f(x_1) = 0$, then $r = x_1$;
   if $f(x_1) > 0$, then $r \in (a, x_1)$;
   if $f(x_1) < 0$, then $r \in (x_1, b)$.

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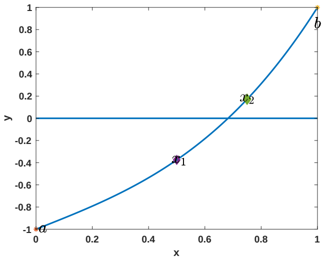

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   If $f(x_2) = 0$, then $r = x_2$;
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   if $f(x_2) < 0$, then $r \in (x_2, b)$.

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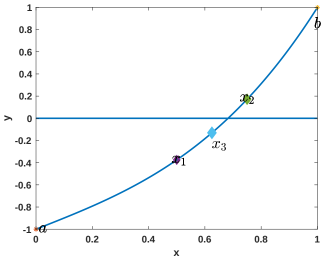

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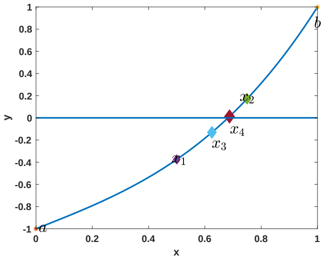

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Pseudocode of Bisection Method

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Bisection Method:
Given initial inverval $[a, b]$ such that $f(a)f(b) < 0$
while $(b-a)/2 > \mathrm{TOL}$
    $c = (a+b)/2$
    if $f(c) = 0$, **stop**, **end**
    if $f(a)f(c) < 0$ $b = c$
    else
        $a = c$
    end
end
The final interval $[a, b]$ contains a root r:

$$r = \frac{a+b}{2} \pm \frac{\mathrm{b} - \mathrm{a}}{2}.$$

Example 1. Find a root of the function $f(x) = x^3 + x - 1$ by using the Bisection Method on the interval [0,1].

i	a_i	$f(a_i)$	c_i	$f(c_i)$	b_i	$f(b_i)$

Example 1. Find a root of the function $f(x) = x^3 + x - 1$ by using the Bisection Method on the interval [0,1].

i	a_i	$f(a_i)$	c_i	$f(c_i)$	b_i	$f(b_i)$
0	0.0000	$-$	0.5000	$-$	1.0000	$+$

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i	a_i	$f(a_i)$	c_i	$f(c_i)$	b_i	$f(b_i)$
0	0.0000	$-$	0.5000	$-$	1.0000	$+$
1	0.5000	$-$	0.7500	$+$	1.0000	$+$

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0	0.0000	$-$	0.5000	$-$	1.0000	$+$
1	0.5000	$-$	0.7500	$+$	1.0000	$+$
2	0.5000	$-$	0.6250	$-$	0.7500	$+$

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3	0.6250	$-$	0.6875	$+$	0.7500	$+$

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2	0.5000	$-$	0.6250	$-$	0.7500	$+$
3	0.6250	$-$	0.6875	$+$	0.7500	$+$
4	0.6250	$-$	0.6562	$-$	0.6875	$+$

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3	0.6250	$-$	0.6875	$+$	0.7500	$+$
4	0.6250	$-$	0.6562	$-$	0.6875	$+$
5	0.6562	$-$	0.6719	$-$	0.6875	$+$

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2	0.5000	$-$	0.6250	$-$	0.7500	$+$
3	0.6250	$-$	0.6875	$+$	0.7500	$+$
4	0.6250	$-$	0.6562	$-$	0.6875	$+$
5	0.6562	$-$	0.6719	$-$	0.6875	$+$
6	0.6719	$-$	0.6797	$-$	0.6875	$+$

Example 1. Find a root of the function $f(x) = x^3 + x - 1$ by using the Bisection Method on the interval [0,1].

i	a_i	$f(a_i)$	c_i	$f(c_i)$	b_i	$f(b_i)$
0	0.0000	$-$	0.5000	$-$	1.0000	$+$
1	0.5000	$-$	0.7500	$+$	1.0000	$+$
2	0.5000	$-$	0.6250	$-$	0.7500	$+$
3	0.6250	$-$	0.6875	$+$	0.7500	$+$
4	0.6250	$-$	0.6562	$-$	0.6875	$+$
5	0.6562	$-$	0.6719	$-$	0.6875	$+$
6	0.6719	$-$	0.6797	$-$	0.6875	$+$
7	0.6797	$-$	0.6836	$+$	0.6875	$+$

Example 1. Find a root of the function $f(x) = x^3 + x - 1$ by using the Bisection Method on the interval [0,1].

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0	0.0000	$-$	0.5000	$-$	1.0000	$+$
1	0.5000	$-$	0.7500	$+$	1.0000	$+$
2	0.5000	$-$	0.6250	$-$	0.7500	$+$
3	0.6250	$-$	0.6875	$+$	0.7500	$+$
4	0.6250	$-$	0.6562	$-$	0.6875	$+$
5	0.6562	$-$	0.6719	$-$	0.6875	$+$
6	0.6719	$-$	0.6797	$-$	0.6875	$+$
7	0.6797	$-$	0.6836	$+$	0.6875	$+$
8	0.6797	$-$	0.6816	$-$	0.6836	$+$

Example 1. Find a root of the function $f(x) = x^3 + x - 1$ by using the Bisection Method on the interval [0,1].

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2	0.5000	$-$	0.6250	$-$	0.7500	$+$
3	0.6250	$-$	0.6875	$+$	0.7500	$+$
4	0.6250	$-$	0.6562	$-$	0.6875	$+$
5	0.6562	$-$	0.6719	$-$	0.6875	$+$
6	0.6719	$-$	0.6797	$-$	0.6875	$+$
7	0.6797	$-$	0.6836	$+$	0.6875	$+$
8	0.6797	$-$	0.6816	$-$	0.6836	$+$
9	0.6816	$-$	0.6826	$+$	0.6836	$+$

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Example 1. Find a root of the function $f(x) = x^3 + x - 1$ by using the Bisection Method on the interval [0,1].

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2	0.5000	$-$	0.6250	$-$	0.7500	$+$
3	0.6250	$-$	0.6875	$+$	0.7500	$+$
4	0.6250	$-$	0.6562	$-$	0.6875	$+$
5	0.6562	$-$	0.6719	$-$	0.6875	$+$
6	0.6719	$-$	0.6797	$-$	0.6875	$+$
7	0.6797	$-$	0.6836	$+$	0.6875	$+$
8	0.6797	$-$	0.6816	$-$	0.6836	$+$
9	0.6816	$-$	0.6826	$+$	0.6836	$+$

Thus, the solution is bracketed in $[0.6816, 0.6826]$. Its midpoint gives the best guess of r, i.e.,

$$r = 0.6821 \pm 0.0005.$$

Error Analysis

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After n bisection steps, the resulting interval (a_n, b_n) that contains a root has length $\frac{b-a}{2^n}$. Choosing $x_c = \frac{a_n+b_n}{2}$, we see:

$$\text{Solution Error} = |x_c - r| < \frac{b-a}{2^{n+1}},$$

and

$$\text{Function Evaluations} = n + 2.$$

A solution is **correct with p decimal places** if the error is less than 0.5×10^{-p}.

Example 2. Use the Bisection Method to find a root of $f(x) = \cos x - x$ in the interval $[0, 1]$ to within 6 correct places.

Sol. By

$$\frac{1-0}{2^{n+1}} < 0.5 \times 10^{-6},$$

we see that $n > \frac{6}{\log_{10} 2} \approx 19.9$. Therefore, at most 20 steps will give a solution with the desired accuracy.

1.2 Limits of Accuracy

In a double-precision computer, numbers are stored and correct with about 16 decimal digits. However, one cannot expect that problems can be solved with answers that are also correct with 16 decimal digits.

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Forward and Backward Error

Example 1. Use the Bisection Method to find the root of
$f(x) = x^3 - 2x^2 + \frac{4}{3}x - \frac{8}{27}$.
Since $f(0)f(1) < 0$, we see there is a root $r \in (0, 1)$. In fact, $r = 0.6666666\ldots$.
According to the previous root formula, we expect that 20 steps should give 6 precise digits. But running the Bisection code in MATLAB gives:

i	a_i	$f(a_i)$	c_i	$f(c_i)$	b_i	$f(b_i)$
0	0.0000000	$-$	0.5000000	$-$	1.0000000	$+$
2	0.5000000	$-$	0.6250000	$-$	0.7500000	$+$
4	0.6250000	$-$	0.6562500	$-$	0.6875000	$+$
6	0.6562500	$-$	0.6640625	$-$	0.6718750	$+$
8	0.6640625	$-$	0.6660156	$-$	0.6679688	$+$
16	0.6666565	$-$	0.6666641	0	0.6666718	$+$

The Bisection Method Fails to give results with 6 or more accurate digits!
What happens behind this failure?

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Forward and Backward Error

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Since $f(0)f(1) < 0$, we see there is a root $r \in (0, 1)$. In fact, $r = 0.6666666\ldots$.
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2	0.5000000	−	0.6250000	−	0.7500000	+
4	0.6250000	−	0.6562500	−	0.6875000	+
6	0.6562500	−	0.6640625	−	0.6718750	+
8	0.6640625	−	0.6660156	−	0.6679688	+
16	0.6666565	−	0.6666641	0	0.6666718	+

The Bisection Method Fails to give results with 6 or more accurate digits!
What happens behind this failure? Since in double precision, the machine cannot differentiate

$$f(0.6666641) \approx -1.6909 \times 10^{-17}$$

from 0.

Forward and Backward Errors

Assume that r is a root of function $f(x)$. Assume that a root-finding method gives a solution x_a to approximate r. Then,

- **Forward (output) error:** $|r - x_a|$.
- **Backward (input) error:** $f(x_a)$.

$$\boxed{\text{Input : f(x);}} \rightarrow \boxed{\text{Purpose : find r } \textit{such that } \text{f(r)=0;}} \rightarrow \boxed{\text{Output : r.}}$$

Stopping Criteria

Either of the following conditions

- FORWORD ERROR $<$ MAXIMUM TOLERABLE FORWARD ERROR;
- BACKWARD ERROR $<$ MAXIMUM TOLERABLE BACKWARD ERROR;
- RUNNING ITERATION$<$ MAXIMUM TOLERABLE NUMBER OF ITERATIONS,

is satisfied will stop/end the execution of a code.

Sensitivity Analysis

A problem is called **sensitive** if small errors in the input, lead to large errors in the output.

Example 2. Analyze the sensitivity of the problem of finding a root of $f(x) = x^3 - 2x^2 + \frac{4}{3}x - \frac{8}{27}$.

Sol. If a small error ε is involved in the input for a solution x_a, i.e., the backward error

$$|f(x_a)| = \left|(x - \frac{2}{3})^3\right| = \varepsilon,$$

then, we see that the forward error

$$\left|x_a - \frac{2}{3}\right| = \sqrt[3]{\varepsilon}.$$

When ε is as small as the machine epsilon $\varepsilon_{\text{MACH}} \approx 2.22 \times 10^{-16}$, then **the forward error can be as large as 6.1×10^{-6}.** This explains why the bisection method only gives 5 accurate digits.

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Sensitivity Formula

Assume that r is a root of $f(x)$, and $r + \Delta r$ is a root of $f(x) + \varepsilon g(x)$ for $\varepsilon > 0$. Then,

$$\Delta r \approx -\frac{\varepsilon g(r)}{f'(r)},$$

if $\varepsilon << f''(r)$.

Proof. From

$$f(r + \Delta r) + \varepsilon g(r + \Delta r) = 0,$$

and its taylor expansion at r, we get

$$f(r) + \Delta r f'(r) + \varepsilon(g(r) + \Delta r g'(r)) + \mathcal{O}((\Delta r)^2) = 0.$$

Suppose Δr is sufficiently small such that $O((\Delta r)^2) \approx 0$, then directly solving this linear system of Δr yields

$$\Delta r \approx -\frac{f(r) + \varepsilon g(r)}{f'(r) + \varepsilon g'(r)} \approx -\frac{\varepsilon g(r)}{f'(r)}.$$

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Example 3. Estimate the largest root of
$P(x) = (x-1)(x-2)(x-3)(x-4)(x-5)(x-6) - 10^{-6}x^7$.
Sol. Take $f(x) = (x-1)(x-2)\cdots(x-6)$, $g(x) = -x^7$ and $\varepsilon = 10^{-6}$.
According to the sensitivity formula, we get

$$\Delta r \approx -\frac{\varepsilon(-6^7)}{f'(6)} = 2332.8\varepsilon.$$

Thus, we estimates the largest root of $P(x)$ to be

$$r + \Delta r = 6 + \Delta r \approx 6.0023328.$$

Using MATLAB, we can find that the largest root of $P(x) \approx 6.0023268$.

Error Magnification Factor and Condition Number

Suppose x_c is the root of $f(x) + \varepsilon g(x)$, we define

$$\text{error magnification factor} = \frac{\text{relative forward error}}{\text{relative backward error}}.$$

One derives that

$$\text{error magnification factor} = \left|\frac{\Delta r/r}{\varepsilon g(r)/g(r)}\right| = \left|\frac{g(r)}{rf'(r)}\right|.$$

Notice: $\varepsilon g(x)$ should be a typical representation of the backward error of $f(x)$.
Condition number:

$$\text{Condition number} = \max_g \left|\frac{g(r)}{rf'(r)}\right|.$$

Indicates that we can lose

$$\log_{10} \text{Condition number}$$

digits of the 16 digits of precision, from input to output.

A famous example: Wilkinson's Polynomial

Find a root, nearest to 16, of

$$\begin{aligned} W(x) = & x^{20} - 210x^{19} + 20615x^{18} - 1256850x^{17} + 53327946x^{16} \\ & - 1672280820x^{15} + 40171771630x^{14} - 756111184500x^{13} \\ & + 11310276995381x^{12} - 135585182899530x^{11} \\ & + 1307535010540395x^{10} - 10142299865511450x^{9} \\ & + 63030812099294896x^{8} - 311333643161390640x^{7} \\ & + 1206647803780373360x^{6} - 3599979517947607200x^{5} \\ & + 8037811822645051776x^{4} - 12870931245150988800x^{3} \\ & + 13803759753640704000x^{2} - 8752948036761600000x \\ & + 2432902008176640000 \end{aligned}$$

Using the bisection method or fzero function in MATLAB, gives a very bad result:

$$16.01468030580458$$

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Using the bisection method or fzero function in MATLAB, gives a very bad result:

$$16.01468030580458$$

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Sensitivity analysis

Define $W_\varepsilon(x) = W(x) + \varepsilon g(x)$, where we take

$$g(x) = -1,672,280,820x^{15}.$$

Then, the sensitivity formula for root $r = 16$ gives

$$\Delta r \approx -\frac{\varepsilon g(16)}{W'(16)} \approx 6.1432 \times 10^{13}\varepsilon.$$

Thus, even when $\varepsilon = \pm\varepsilon_{\mathrm{MACH}} \approx \pm 2.2 \times 10^{-16}$, we get

$$\Delta r \approx \pm 0.0136.$$

On the other hand,

$$\text{Condition Number} \geq \left|\frac{g(16)}{16W'(16)}\right| \approx 3.8 \times 10^{12}.$$

We can only get at most $16 - 12 = 4$ accurate digits from input to output.

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A question

Why do we choose $g(x) = -1,672,280,820x^{15}$ for $r = 16$?

$$
\begin{aligned}
W(x) =& x^{20} - 210x^{19} + 20615x^{18} - 1256850x^{17} + 53327946x^{16} \\
& -1672280820x^{15} + 40171771630x^{14} - 756111184500x^{13} \\
& + 11310276995381x^{12} - 135585182899530x^{11} \\
& + 1307535010540395x^{10} - 10142299865511450x^{9} \\
& + 63030812099294896x^{8} - 311333643161390640x^{7} \\
& + 1206647803780373360x^{6} - 3599979517947607200x^{5} \\
& + 8037811822645051776x^{4} - 12870931245150988800x^{3} \\
& + 13803759753640704000x^{2} - 8752948036761600000x \\
& + 2432902008176640000 \\
=& (x-1)(x-2)\cdots(x-20).
\end{aligned}
$$

Ill-conditioned and well-conditioned

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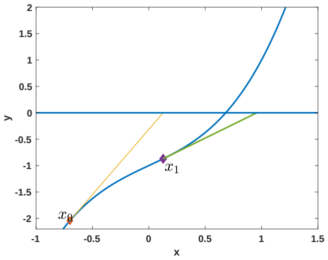
If the condition number of a problem is:

- near or even greater than 10^{16}, we say that the problem is ill-conditioned;
- near 1, we say that the problem is well-conditioned.

1.3 Newton's method

Problem: find a root r of a smooth function $f(x)$, for a given initial guess x_0.
Searching principle: to find the next guess x_1, we draw a line at $(x_0, f(x_0))$ that should be tangent to the curve $y = f(x)$, then the intersection point of this line with x-axis is the next guess, that is supposed to be closer to root r.



1. Find the tangent line of $y = f(x)$ at $x = x_0$, and find the intersection point x_1;

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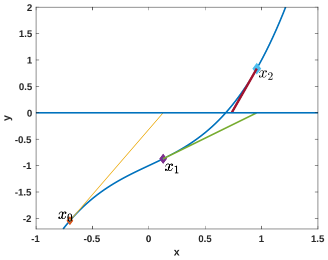

1. Find the tangent line of $y = f(x)$ at $x = x_0$, and find the intersection point x_1;
2. Find the tangent line of $y = f(x)$ at $x = x_1$, and find the intersection point x_2;

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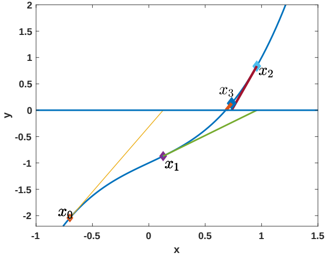

1. Find the tangent line of $y = f(x)$ at $x = x_0$, and find the intersection point x_1;
2. Find the tangent line of $y = f(x)$ at $x = x_1$, and find the intersection point x_2;
3. Find the tangent line of $y = f(x)$ at $x = x_2$, and find the intersection point x_3;

...

Algebraic Formula for Newton's Method

Clearly, the tangent line of $f(x)$ at $x = x_0$ is

$$y - f(x_0) = f'(x_0)(x - x_0).$$

Let $y = 0$, we get its intersection point at x-axis,

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}.$$

Repeating the above procedure, we expect the resulting sequence $\{x_n\}_{n=1}^{\infty}$converges to r. In summary:

Newton's Method

$$\begin{aligned} x_0 &= \text{initial guess}, \\ x_{n+1} &= x_n - \tfrac{f(x_n)}{f'(x_n)}, \ \textbf{for } i = 1, 2, \ldots. \end{aligned}$$

Example 1. Find a root of $x^3 + x - 1 = 0$.
Sol. Newton's Method formula gives

$$x_{n+1} = x_n - \frac{x_n^3 + x_n - 1}{3x_n^2 + 1}.$$

For a given initial guess $x_0 = -0.7$, we get the following table.

n	x_n	$e_n = \|x_n - r\|$	e_n/e_{n-1}^2
0	-0.70000000	1.38232780	—
1	0.12712551	0.55520230	0.2906
2	0.95767812	0.27535032	0.8933
3	0.73482779	0.05249999	0.6924
4	0.68 459177	0.00226397	0.8214
5	0.6823 3217	0.00000437	0.8527
6	0.68232780	0.00000000	0.8541
7	0.68232780	0.00000000	—

Quadratic convergence of Newton's method

Quadratic convergence: Let e_n be the error after step n of an iterative method. The iteration is quadratically convergent if

$$M = \lim_{n\to\infty} \frac{e_{n+1}}{e_n^2} < \infty.$$

Theorem: Let f be twice continuously differentiable and f(r)=0. If $f'(r) \neq 0$, then Newton's Method is locally and quadratically convergent to r. The error e_n at step n satisfies

$$\lim_{n\to\infty} \frac{e_{n+1}}{e_n^2} = \left| \frac{f''(r)}{2f'(r)} \right|.$$

Proof. Here, "locally" indicates that x_0, the initial guess, should be close enough to r. Taylor's theorem indicates that

$$0 = f(r) = f(x_n) + (r - x_n)f'(x_n) + \frac{(r - x_n)^2}{2} f''(c_n),$$

for $c_n \in (x_n, r)$. Divided by $f'(x_n)$ and with some rearranging,

$$x_{n+1} - r = x_n - \frac{f'(x_n)}{f(x_n)} - r = \frac{(r - x_n)^2}{2f'(x_n)} f''(c_n).$$

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Which indicates that

$$e_{n+1} = \frac{e_n^2}{2}\left|\frac{f''(c_n)}{f'(x_n)}\right| = e_n\left|\frac{e_n}{2f'(x_n)}f''(c_n)\right|.$$

Thus, if $e_0 = |x_0 - r|$ is quite small such that $q = |\frac{e_0}{2f'(x_0)}f''(c_0)| < 1$, then

$$e_{n+1} < e_n q < \cdots < e_0 q^{n+1},$$

which indicates that $\lim_{n\to\infty} e_n = 0$, or equivalently, $\lim_{n\to\infty} x_n = r$. On the other hand,

$$\lim_{n\to\infty}\frac{e_{n+1}}{e_n^2} = \lim_{n\to\infty}\left|\frac{f''(c_n)}{2f'(x_n)}\right| = \left|\frac{f''(r)}{2f'(r)}\right|.$$

Revisiting **Example 1.**Find a root of $x^3 + x - 1 = 0$.

Sol. Newton's Method formula gives

$$x_{n+1} = x_n - \frac{x_n^3 + x_n - 1}{3x_n^2 + 1}.$$

For a given initial guess $x_0 = -0.7$, we get the following table.

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5	0.6823 3217	0.00000437	0.8527
6	0.68232780	0.00000000	0.8541
7	0.68232780	0.00000000	–

Rate:

$$\lim_{n\to\infty} \lvert e_n/e_{n-1}^2 \rvert = \lvert f''(0.68232780)/2f'(0.68232780) \rvert \approx 0.85.$$

Counter Examples: $f'(r) = 0$

Example 2. Find a root of $f(x) = x^2$ using $x_0 = 1$ Newton's Method Formula:

$$x_{n+1} = x_n - x_n^2/(2x_n) = x_n/2.$$

n	x_n	$e_n = \|x_n - r\|$	e_n/e_{n-1}^2
0	1.0000	1.0000	−
1	0.5000	0.5000	0.5
2	0.2500	0.2500	1
3	0.1250	0.1250	2
4	0.0625	0.0625	4
...	...	...	...

In fact, it shows only linear convergence in the sense that $\lim_{n\to\infty} \frac{e_n}{e_{n-1}} = 1/2$.

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Counter Examples: x_0 is far away from r

Example 3. Apply Newton's Method to $f(x) = 4x^4 - 6x^2 - 11/4$ with intial guess $x_0 = 1/2$. Newton's Method Formula:

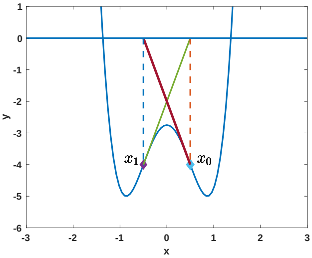
$$x_{n+1} = x_n - \frac{4x_n^4 - 6x_n^2 - \frac{11}{4}}{16x^3 - 12x}.$$

Directly calculation shows that

$$x_{2n+1} = x_{2n-1} = \cdots = x_1 = -1/2,$$

while

$$x_{2n} = x_{2n-2} = \cdots = x_0 = 1/2.$$



1.4 Root-Finding without Derivatives

Newton's method fails when function $f(x)$ is not differentiable. What can we do to find a root of $f(x)$?

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Secant Method

Suppose $f'(x)$ at x_0 is hard to evaluate or even unavailable, then

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)},$$

cannot be used! An alternative way is to find a quantity to approximate $f'(x_0)$. Supppose we choose another x_1 that is different from x_0, then

$$\frac{f(x_1) - f(x_0)}{x_1 - x_0},$$

is a good approximation to $f'(x_0)$ or $f'(x_1)$.
The above idea motivates the development of the **Secant Method**:
Secant Method

$$x_0, x_1 = \text{initial guess}$$

$$x_{n+1} = x_n - \frac{f(x_n)}{\frac{f(x_n)-f(x_{n-1})}{x_n - x_{n-1}}}, \quad \text{for} \quad n = 1, 2, 3, \ldots$$

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Assignment 1

Assignment I:
Page 5, 0.1, Computer Problems: 1.
P19, 0.4 Computer Problems: 1.
P30, 1.1 Computer Problems: 2.
P51, 1.3 Computer Problems: 3.
P59, 1.4 Computer Problems: 1.
P66, 1.5, Computer Problems: 1.
Totally, there are 6 computer problems.
Due date: Sep. 30, 2019.

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