Numerical Analysis

SMIE SYSU
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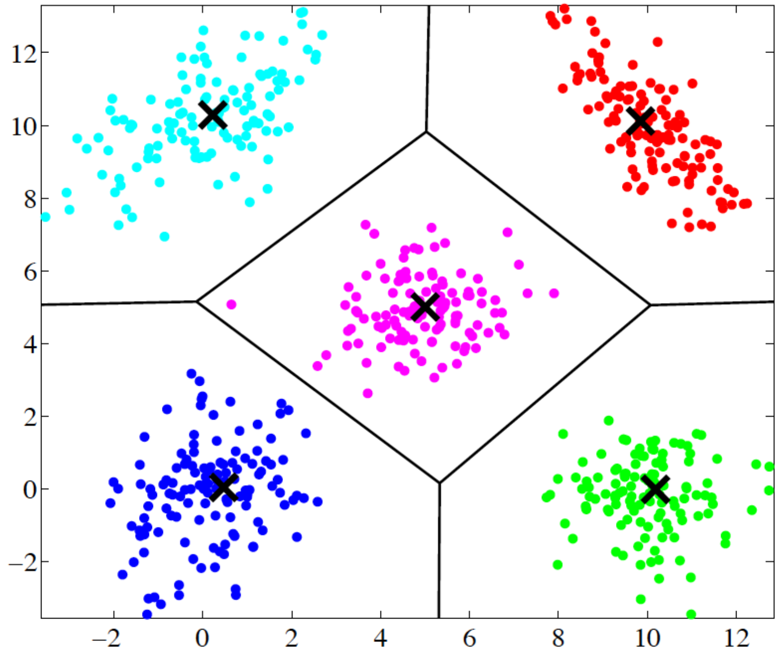
What is Numerical Analysis? S1

We are given a set of data points, each being a vector representing the properties of one object, now we want to find a partition of these data points such that similar data points are partitioned into the same group, and find some number of representative data points (prototypes) that best represent each group. i.e., minimize the following objective function,



$$J^{CCL} = \sum_{n=1}^{N} \|\mathbf{x}_n - \mathbf{w}_{k(n)}\|^2$$

$$\boxed{\text{Find a root of the function } f(x) = x^3 + x - 1}$$

IntroExampleBisect.m

How to solve this problem?

What is Numerical Analysis? S2

- **Goal:** Construct and explore algorithms for solving science and engineering problems.
- **key:** Principles of these algorithms, including convergence, complexity, conditioning, compression, and orthogonality.
- **Prerequisite courses:** Calculus and matrix (linear) algebra.
- **For whom?** Students of engineering, science, mathematics, and computer science, etc.
- **Coding:** Matlab, C/C++.

Outline

- 0 Introduction & Fundamentals
- 1 Solving Equations
- 2 Systems of Equations
- 3 Interpolation
- 4 Least Squares
- 5 Numerical Differentiation and Integration
- 6 Ordinary Differential Equations
- 7 Boundary Value Problems
- 8 Partial Differential Equations
- 9 Random Numbers and Applications
- 10 Trigonometric Interpolation and the FFT
- 11 Compression
- 12 Eigenvalues and Singular Values
- 13 Optimization

Grading

• Class Participation	10%
• Written Assignments	30%
• Coding/Projects	30%
• Final Examination	30%

References

- Numerical Analysis, 2nd Edition, Timothy Sauer
- Numerical Computing with MATLAB, Cleve Moler

About the instructor

- Chang-Dong Wang
- Assistant Professor at SMIE of SYSU.
- PHD in SYSU and Visiting student at University of Illinois at Chicago
- Research interest: Data mining, Big data, Social network.
- Research achievements: Published over 20 papers within 3 years, including 9 SCI indexed papers.
- Honors: Several top honors including 2012 MSRA Fellowship Nomination Award (one of the 27 computer science students in Asia).

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Fundamentals

- Evaluating a polynomial
- Binary numbers (omitted)
- Floating point representation (omitted)
- Loss of significance
- Review of calculus

Evaluating a polynomial S1

- How to evaluate the following polynomial

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

  at x=1/2?

- How many additions and multiplications are required?

Evaluating a polynomial S2

- Method 1: evaluate it directly.

$$P\left(\frac{1}{2}\right) = 2 * \frac{1}{2} * \frac{1}{2} * \frac{1}{2} * \frac{1}{2} + 3 * \frac{1}{2} * \frac{1}{2} * \frac{1}{2} - 3 * \frac{1}{2} * \frac{1}{2} + 5 * \frac{1}{2} - 1 = \frac{5}{4}$$

4 additions + 10 multiplications.

- Method 2: first compute $(1/2)^4$

$$\frac{1}{2} * \frac{1}{2} = \left(\frac{1}{2}\right)^2 \qquad \left(\frac{1}{2}\right)^2 * \frac{1}{2} = \left(\frac{1}{2}\right)^3 \qquad \left(\frac{1}{2}\right)^3 * \frac{1}{2} = \left(\frac{1}{2}\right)^4$$

then add them up

$$P\left(\frac{1}{2}\right) = 2 * \left(\frac{1}{2}\right)^4 + 3 * \left(\frac{1}{2}\right)^3 - 3 * \left(\frac{1}{2}\right)^2 + 5 * \frac{1}{2} - 1 = \frac{5}{4}$$

4 additions + 7 multiplications.

Evaluating a polynomial S3

- Method 3: Nested Multiplication. Rewrite the polynomial so that it can be evaluated from the inside out:

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

4 additions + 4 multiplications.

- General form of nested multiplication

$$
c_1 + (x - r_1)(c_2 + (x - r_2)(c_3 + (x - r_3)(c_4 + (x - r_4)(c_5))))
$$

we call r_1, r_2, r_3, and r_4 the **base points**

Evaluating a polynomial S4

- Compare three methods by running 10^6 times.

EvaluatePolynomia.m

- Evaluating time for direct method (i.e. method 1) is 0.29622
- Evaluating time for method 2 is 0.28913
- Evaluating time for nest is 0.27764

- If in the program, there are plenty of polynomial to be evaluated, computational time is the key.

Evaluating a polynomial S5

- First, computers are very fast at doing very simple things. Running 10^6 times within 0.2 second.
- Second, it is important to do even simple tasks as efficiently as possible, since they may be executed many times.
- Third, the best way may not be the obvious way.

Evaluating a polynomial S6

- EXAMPLE

Find an efficient method for evaluating the polynomial

$$P(x) = 4x^5 + 7x^8 - 3x^{11} + 2x^{14}$$

Factor x^5 out of each term, and then x^3.

$$\begin{aligned} P(x) &= x^5(4 + 7x^3 - 3x^6 + 2x^9) \\ &= x^5 * (4 + x^3 * (7 + x^3 * (-3 + x^3 * (2)))) \end{aligned}$$

Coding assignment (page 5, Computer problem 2):

Use `nest.m` to evaluate $P(x) = 1 - x + x^2 - x^3 + \cdots + x^{98} - x^{99}$ at $x = 1.00001$. Find a simpler, equivalent expression, and use it to estimate the error of the nested multiplication.

Loss of significance S1

- Assume that through considerable effort, as part of a long calculation, we have determined two numbers correct to seven significant digits, and now need to subtract them:

$$\begin{array}{r} 123.4567 \\ -\ 123.4566 \\ \hline 000.0001 \end{array}$$

- The subtraction problem began with two input numbers that we knew to seven-digit accuracy, and ended with a result that has only one-digit accuracy.

Loss of significance S2

- EXAMPLE Calculate $\sqrt{9.01} - 3$ on a three-decimal-digit computer
- Since $\sqrt{9.01} \approx 3.0016662$, by storing this intermediate result to three significant digits, we get 3. 00. Subtracting 3. 00, we get a final answer of 0. 00.
- Another way $$\sqrt{9.01} - 3 = \frac{(\sqrt{9.01} - 3)(\sqrt{9.01} + 3)}{\sqrt{9.01} + 3}$$
$$= \frac{9.01 - 3^2}{\sqrt{9.01} + 3}$$
$$= \frac{0.01}{3.00 + 3} = \frac{.01}{6} = 0.00167 \approx 1.67 \times 10^{-3}$$

Loss of significance S3

- EXAMPLE compare the calculation of the expressions for a range of input numbers x

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

$$\text{and} \quad E_2 = \frac{1}{1 + \cos x}$$

$$\sin^2 x + \cos^2 x = 1$$

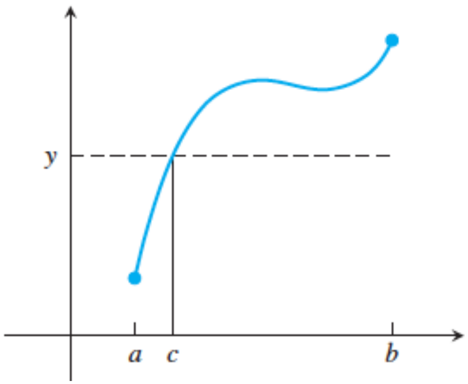
x	E_1	E_2
1.00000000000000	0.64922320520476	0.64922320520476
0.10000000000000	0.50125208628858	0.50125208628857
0.01000000000000	0.50001250020848	0.50001250020834
0.00100000000000	0.50000012499219	0.50000012500002
0.00010000000000	0.49999999862793	0.50000000125000
0.00001000000000	0.50000004138685	0.50000000001250
0.00000100000000	0.50004445029134	0.50000000000013
0.00000010000000	0.49960036108132	0.50000000000000
0.00000001000000	0.00000000000000	0.50000000000000
0.00000000100000	0.00000000000000	0.50000000000000
0.00000000010000	0.00000000000000	0.50000000000000
0.00000000001000	0.00000000000000	0.50000000000000
0.00000000000100	0.00000000000000	0.50000000000000

Coding assignment (page 19, Computer problem 4):

Evaluate the quantity $\sqrt{c^2 + d} - c$ to four correct significant digits, where $c = 246886422468$ and $d = 13579$.

Review of Calculus S1

(Intermediate Value Theorem) Let f be a continuous function on the interval $[a, b]$. Then f realizes every value between $f(a)$ and $f(b)$. More precisely, if y is a number between $f(a)$ and $f(b)$, then there exists a number c with $a \le c \le b$ such that $f(c) = y$. ■



There exist numbers c between a and b such that: (a) f(c) = y, for any given y between f(a) and f(b) by the Intermediate Value Theorem.

- EXAMPLE:

Show that $f(x) = x^2 - 3$ on the interval $[1, 3]$ must take on the values 0 and 1.

Because $f(1) = -2$ and $f(3) = 6$, all values between -2 and 6, including 0 and 1, must be taken on by f. For example, setting $c = \sqrt{3}$, note that $f(c) = f(\sqrt{3}) = 0$, and secondly, $f(2) = 1$. ◀

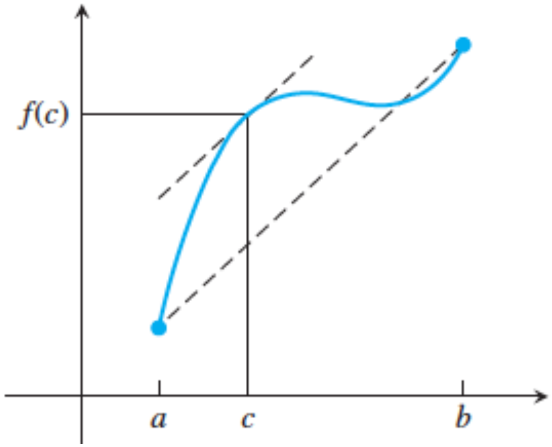
Review of Calculus S2

(Continuous Limits) Let f be a continuous function in a neighborhood of x_0, and assume $\lim_{n\to\infty} x_n = x_0$. Then

$$\lim_{n\to\infty} f(x_n) = f\left(\lim_{n\to\infty} x_n\right) = f(x_0). \qquad \blacksquare$$

In other words, limits may be brought inside continuous functions.

(Mean Value Theorem) Let f be a continuously differentiable function on the interval $[a, b]$. Then there exists a number c between a and b such that $f'(c) = (f(b) - f(a))/(b - a)$. $\blacksquare$



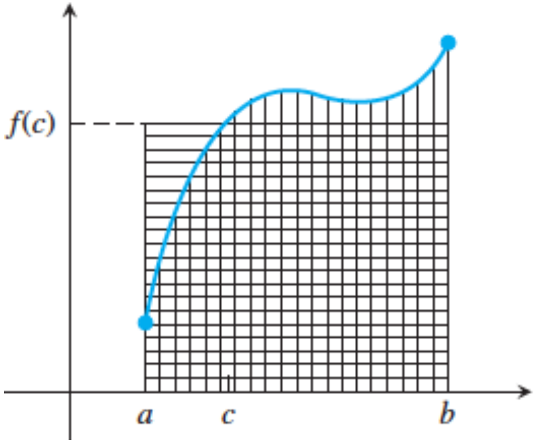
The instantaneous slope of f at c equals
(f**(**b**)** – f**(**a**))/(**b – a**)** by the Mean Value Theorem.

Review of Calculus S3

(Rolle's Theorem) Let f be a continuously differentiable function on the interval $[a, b]$, and assume that $f(a) = f(b)$. Then there exists a number c between a and b such that $f'(c) = 0$. ■

(Mean Value Theorem for Integrals) Let f be a continuous function on the interval $[a, b]$, and let g be an integrable function that does not change sign on $[a, b]$. Then there exists a number c between a and b such that

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

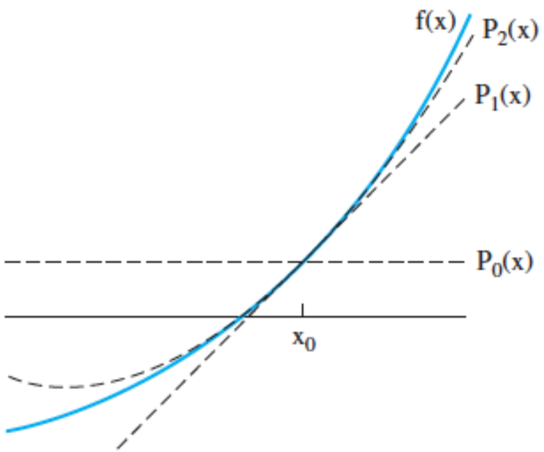


The vertically shaded region is equal in area to the horizontally shaded region, by the Mean Value Theorem for Integrals, shown in the special case **g(x)** = 1.

Review of Calculus S4

(Taylor's Theorem with Remainder) Let x and x_0 be real numbers, and let f be $k+1$ times continuously differentiable on the interval between x and x_0. Then there exists a number c between x and x_0 such that

$$f(x) = f(x_0) + f'(x_0)(x-x_0) + \frac{f''(x_0)}{2!}(x-x_0)^2 + \frac{f'''(x_0)}{3!}(x-x_0)^3 + \cdots$$
$$+ \frac{f^{(k)}(x_0)}{k!}(x-x_0)^k + \frac{f^{(k+1)}(c)}{(k+1)!}(x-x_0)^{k+1}.$$



The function f (x), denoted by the solid curve, is approximated successively better near x0 by the degree 0 Taylor polynomial (horizontal dashed line), the degree 1 Taylor polynomial (slanted dashed line), and the degree 2 Taylor polynomial (dashed parabola). The difference between f (x) and its approximation at x is the Taylor remainder.

Review of Calculus S5

Written assignment (page 22, Exercises 2, 4):

Find c satisfying the Mean Value Theorem for $f(x)$ on the interval $[0, 1]$. (a) $f(x) = e^x$ (b) $f(x) = x^2$ (c) $f(x) = 1/(x + 1)$

Find the Taylor polynomial of degree 2 about the point $x = 0$ for the following functions: (a) $f(x) = e^{x^2}$ (b) $f(x) = \cos 5x$ (c) $f(x) = 1/(x + 1)$