Scientific Computing: An Introductory Survey Chapter 1 – Scientific Computing

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Outline









Introduction Computational Problems General Strategy

Scientific Computing

- What is *scientific computing*?
 - Design and analysis of algorithms for numerically solving mathematical problems in science and engineering
 - Traditionally called *numerical analysis*
- Distinguishing features of scientific computing
 - Deals with continuous quantities
 - Considers effects of approximations
- Why scientific computing?
 - Simulation of natural phenomena
 - Virtual prototyping of engineering designs



Introduction Computational Problems General Strategy

Well-Posed Problems

- Problem is *well-posed* if solution
 - exists
 - is unique
 - depends continuously on problem data

Otherwise, problem is *ill-posed*

- Even if problem is well posed, solution may still be *sensitive* to input data
- Computational algorithm should not make sensitivity worse

Introduction Computational Problems General Strategy

General Strategy

- Replace difficult problem by easier one having same or closely related solution
 - infinite \rightarrow finite
 - differential \rightarrow algebraic
 - nonlinear \rightarrow linear
 - complicated \rightarrow simple
- Solution obtained may only approximate that of original problem



Sources of Approximation Error Analysis Sensitivity and Conditioning

Sources of Approximation

- Before computation
 - modeling
 - empirical measurements
 - previous computations
- During computation
 - truncation or discretization
 - rounding
- Accuracy of final result reflects all these
- Uncertainty in input may be amplified by problem
- Perturbations during computation may be amplified by algorithm



Sources of Approximation Error Analysis Sensitivity and Conditioning

Example: Approximations

- Computing surface area of Earth using formula $A = 4\pi r^2$ involves several approximations
 - Earth is modeled as sphere, idealizing its true shape
 - Value for radius is based on empirical measurements and previous computations
 - Value for π requires truncating infinite process
 - Values for input data and results of arithmetic operations are rounded in computer

Sources of Approximation Error Analysis Sensitivity and Conditioning

Absolute Error and Relative Error

- Absolute error: approximate value true value
- Relative error:

absolute error true value

- Equivalently, approx value = (true value) \times (1 + rel error)
- True value usually unknown, so we estimate or bound error rather than compute it exactly
- Relative error often taken relative to approximate value, rather than (unknown) true value



 Scientific Computing Approximations
 Sources of Approximation Error Analysis

 Computer Arithmetic
 Sensitivity and Condition

Data Error and Computational Error

- Typical problem: compute value of function $f : \mathbb{R} \to \mathbb{R}$ for given argument
 - x = true value of input
 - f(x) = desired result
 - $\hat{x} = approximate$ (inexact) input
 - $\hat{f} = approximate$ function actually computed
- Total error: $\hat{f}(\hat{x}) f(x) =$

$$\hat{f}(\hat{x}) - f(\hat{x}) + f(\hat{x}) - f(x)$$

computational error + propagated data error

Algorithm has no effect on propagated data error

Truncation Error and Rounding Error

- *Truncation error*: difference between true result (for actual input) and result produced by given algorithm using exact arithmetic
 - Due to approximations such as truncating infinite series or terminating iterative sequence before convergence
- *Rounding error*: difference between result produced by given algorithm using exact arithmetic and result produced by same algorithm using limited precision arithmetic
 - Due to inexact representation of real numbers and arithmetic operations upon them
- Computational error is sum of truncation error and rounding error, but one of these usually dominates

< interactive example >



 Scientific Computing Approximations
 Sources of Approximation

 Computer Arithmetic
 Error Analysis

Example: Finite Difference Approximation

• Error in finite difference approximation

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

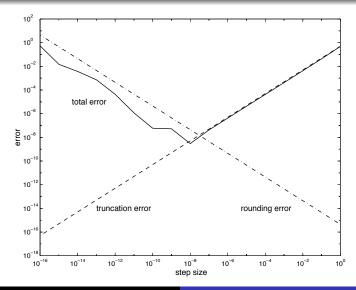
exhibits tradeoff between rounding error and truncation error

- Truncation error bounded by Mh/2, where M bounds |f''(t)| for t near x
- Rounding error bounded by $2\epsilon/h,$ where error in function values bounded by ϵ
- Total error minimized when $h \approx 2\sqrt{\epsilon/M}$
- Error increases for smaller *h* because of rounding error and increases for larger *h* because of truncation error



Scientific Computing Approximations Computer Arithmetic Sensitivity and Conditioning

Example: Finite Difference Approximation

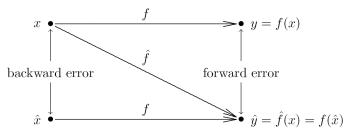


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Forward and Backward Error

- Suppose we want to compute y = f(x), where f: ℝ → ℝ, but obtain approximate value ŷ
- Forward error: $\Delta y = \hat{y} y$
- **Backward error**: $\Delta x = \hat{x} x$, where $f(\hat{x}) = \hat{y}$



 Scientific Computing
 Sources of Approximation

 Approximations
 Error Analysis

 Computer Arithmetic
 Sensitivity and Conditionin

Example: Forward and Backward Error

• As approximation to $y = \sqrt{2}$, $\hat{y} = 1.4$ has absolute forward error

$$|\Delta y| = |\hat{y} - y| = |1.4 - 1.41421\dots| \approx 0.0142$$

or relative forward error of about 1 percent

• Since $\sqrt{1.96} = 1.4$, absolute backward error is

$$|\Delta x| = |\hat{x} - x| = |1.96 - 2| = 0.04$$

or relative backward error of 2 percent

Sources of Approximation Error Analysis Sensitivity and Conditioning

Backward Error Analysis

- Idea: approximate solution is exact solution to modified problem
- How much must original problem change to give result actually obtained?
- How much data error in input would explain *all* error in computed result?
- Approximate solution is good if it is exact solution to *nearby* problem
- Backward error is often easier to estimate than forward error



 Scientific Computing Approximations
 Sources of Approximation

 Computer Arithmetic
 Sensitivity and Conditionin

Example: Backward Error Analysis

• Approximating cosine function $f(x) = \cos(x)$ by truncating Taylor series after two terms gives

$$\hat{y} = \hat{f}(x) = 1 - x^2/2$$

Forward error is given by

$$\Delta y = \hat{y} - y = \hat{f}(x) - f(x) = 1 - x^2/2 - \cos(x)$$

- To determine backward error, need value \hat{x} such that $f(\hat{x}) = \hat{f}(x)$
- For cosine function, $\hat{x} = \arccos(\hat{f}(x)) = \arccos(\hat{y})$

Sources of Approximation Error Analysis Sensitivity and Conditioning

Example, continued

• For x = 1,

$$y = f(1) = \cos(1) \approx 0.5403$$

$$\hat{y} = \hat{f}(1) = 1 - 1^2/2 = 0.5$$

$$\hat{x} = \arccos(\hat{y}) = \arccos(0.5) \approx 1.0472$$

• Forward error: $\Delta y = \hat{y} - y \approx 0.5 - 0.5403 = -0.0403$

• Backward error: $\Delta x = \hat{x} - x \approx 1.0472 - 1 = 0.0472$

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Sensitivity and Conditioning

- Problem is *insensitive*, or *well-conditioned*, if relative change in input causes similar relative change in solution
- Problem is *sensitive*, or *ill-conditioned*, if relative change in solution can be much larger than that in input data
- Condition number:

$$cond = \frac{|\text{relative change in solution}|}{|\text{relative change in input data}|}$$
$$= \frac{|[f(\hat{x}) - f(x)]/f(x)|}{|(\hat{x} - x)/x|} = \frac{|\Delta y/y|}{|\Delta x/x|}$$

• Problem is sensitive, or ill-conditioned, if $cond \gg 1$

Scientific Computing Approximations Computer Arithmetic Sensitivity and Conditioning

Condition Number

• Condition number is *amplification factor* relating relative forward error to relative backward error

 $\begin{vmatrix} relative \\ forward error \end{vmatrix} = cond \times \begin{vmatrix} relative \\ backward error \end{vmatrix}$

 Condition number usually is not known exactly and may vary with input, so rough estimate or upper bound is used for cond, yielding

$$\left| \begin{array}{c|c} \text{relative} \\ \text{forward error} \end{array} \right| \stackrel{\sim}{\approx} \operatorname{cond} \times \left| \begin{array}{c} \text{relative} \\ \text{backward error} \end{array} \right|$$



Scientific Computing Sources of Approximation Approximations Error Analysis Computer Arithmetic Sensitivity and Conditioning

Example: Evaluating Function

• Evaluating function f for approximate input $\hat{x} = x + \Delta x$ instead of true input x gives

Absolute forward error: $f(x + \Delta x) - f(x) \approx f'(x)\Delta x$

Relative forward error:
$$\frac{f(x + \Delta x) - f(x)}{f(x)} \approx \frac{f'(x)\Delta x}{f(x)}$$

Condition number: $\operatorname{cond} \approx \left|\frac{f'(x)\Delta x/f(x)}{\Delta x/x}\right| = \left|\frac{xf'(x)}{f(x)}\right|$

• Relative error in function value can be much larger or smaller than that in input, depending on particular *f* and *x*

Sources of Approximation Error Analysis Sensitivity and Conditioning

Example: Sensitivity

- Tangent function is sensitive for arguments near $\pi/2$
 - $\tan(1.57079) \approx 1.58058 \times 10^5$
 - $\tan(1.57078) \approx 6.12490 \times 10^4$
- Relative change in output is quarter million times greater than relative change in input

• For x = 1.57079, cond $\approx 2.48275 \times 10^5$

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Stability

- Algorithm is *stable* if result produced is relatively insensitive to perturbations *during* computation
- Stability of algorithms is analogous to conditioning of problems
- From point of view of backward error analysis, algorithm is stable if result produced is exact solution to nearby problem
- For stable algorithm, effect of computational error is no worse than effect of small data error in input

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- Accuracy: closeness of computed solution to true solution of problem
- Stability alone does not guarantee accurate results
- Accuracy depends on conditioning of problem as well as stability of algorithm
- Inaccuracy can result from applying stable algorithm to ill-conditioned problem or unstable algorithm to well-conditioned problem
- Applying stable algorithm to well-conditioned problem yields accurate solution



Floating-Point Numbers Floating-Point Arithmetic

Floating-Point Numbers

- Floating-point number system is characterized by four integers
 - $\begin{array}{ll} \beta & \mbox{base or radix} \\ p & \mbox{precision} \\ [L,U] & \mbox{exponent range} \end{array}$
- Number x is represented as

$$x = \pm \left(d_0 + \frac{d_1}{\beta} + \frac{d_2}{\beta^2} + \dots + \frac{d_{p-1}}{\beta^{p-1}} \right) \beta^E$$

where $0 \le d_i \le \beta - 1$, $i = 0, \dots, p - 1$, and $L \le E \le U$

Floating-Point Numbers Floating-Point Arithmetic

Floating-Point Numbers, continued

- Portions of floating-poing number designated as follows
 - exponent: E
 - mantissa: $d_0d_1\cdots d_{p-1}$
 - fraction: $d_1 d_2 \cdots d_{p-1}$
- Sign, exponent, and mantissa are stored in separate fixed-width *fields* of each floating-point *word*



Floating-Point Numbers Floating-Point Arithmetic

Typical Floating-Point Systems

Parameters for typical floating-point systems					
system	β	p	L	U	
IEEE SP	2	24	-126	127	
IEEE DP	2	53	-1022	1023	
Cray	2	48	-16383	16384	
HP calculator	10	12	-499	499	
IBM mainframe	16	6	-64	63	

- Most modern computers use binary ($\beta = 2$) arithmetic
- IEEE floating-point systems are now almost universal in digital computers



Floating-Point Numbers Floating-Point Arithmetic

Normalization

- Floating-point system is *normalized* if leading digit d₀ is always nonzero unless number represented is zero
- In normalized systems, mantissa m of nonzero floating-point number always satisfies $1 \le m < \beta$
- Reasons for normalization
 - representation of each number unique
 - no digits wasted on leading zeros
 - leading bit need not be stored (in binary system)



Properties of Floating-Point Systems

- Floating-point number system is finite and discrete
- Total number of normalized floating-point numbers is

$$2(\beta - 1)\beta^{p-1}(U - L + 1) + 1$$

- Smallest positive normalized number: $UFL = \beta^L$
- Largest floating-point number: $OFL = \beta^{U+1}(1 \beta^{-p})$
- Floating-point numbers equally spaced only between successive powers of β
- Not all real numbers exactly representable; those that are are called *machine numbers*





• Tick marks indicate all 25 numbers in floating-point system having $\beta = 2$, p = 3, L = -1, and U = 1

• OFL =
$$(1.11)_2 \times 2^1 = (3.5)_{10}$$

• UFL =
$$(1.00)_2 \times 2^{-1} = (0.5)_{10}$$

 At sufficiently high magnification, all normalized floating-point systems look grainy and unequally spaced

< interactive example >

Floating-Point Numbers Floating-Point Arithmetic

Rounding Rules

- If real number x is not exactly representable, then it is approximated by "nearby" floating-point number fl(x)
- This process is called *rounding*, and error introduced is called *rounding error*
- Two commonly used rounding rules
 - *chop* : truncate base- β expansion of x after (p-1)st digit; also called *round toward zero*
 - round to nearest: fl(x) is nearest floating-point number to x, using floating-point number whose last stored digit is even in case of tie; also called *round to even*
- Round to nearest is most accurate, and is default rounding rule in IEEE systems

< interactive example >



Floating-Point Numbers Floating-Point Arithmetic

Machine Precision

- Accuracy of floating-point system characterized by *unit* roundoff (or machine precision or machine epsilon) denoted by ϵ_{mach}
 - With rounding by chopping, $\epsilon_{\rm mach} = \beta^{1-p}$
 - With rounding to nearest, $\epsilon_{\rm mach} = \frac{1}{2}\beta^{1-p}$
- Alternative definition is smallest number ϵ such that $\mathrm{fl}(1+\epsilon)>1$
- Maximum relative error in representing real number *x* within range of floating-point system is given by

$$\left|\frac{\mathrm{fl}(x) - x}{x}\right| \le \epsilon_{\mathrm{mach}}$$

Floating-Point Numbers Floating-Point Arithmetic

Machine Precision, continued

For toy system illustrated earlier

- $\epsilon_{\rm mach} = (0.01)_2 = (0.25)_{10}$ with rounding by chopping
- $\epsilon_{\text{mach}} = (0.001)_2 = (0.125)_{10}$ with rounding to nearest
- For IEEE floating-point systems
 - $\epsilon_{\rm mach} = 2^{-24} \approx 10^{-7}$ in single precision
 - $\epsilon_{\rm mach} = 2^{-53} \approx 10^{-16}$ in double precision
- So IEEE single and double precision systems have about 7 and 16 decimal digits of precision, respectively

Floating-Point Numbers Floating-Point Arithmetic

Machine Precision, continued

- Though both are "small," unit roundoff ϵ_{mach} should not be confused with underflow level UFL
- Unit roundoff ϵ_{mach} is determined by number of digits in *mantissa* of floating-point system, whereas underflow level UFL is determined by number of digits in *exponent* field
- In all practical floating-point systems,

 $0 < \text{UFL} < \epsilon_{\text{mach}} < \text{OFL}$



Subnormals and Gradual Underflow

- Normalization causes gap around zero in floating-point system
- If leading digits are allowed to be zero, but only when exponent is at its minimum value, then gap is "filled in" by additional *subnormal* or *denormalized* floating-point numbers



- Subnormals extend range of magnitudes representable, but have less precision than normalized numbers, and unit roundoff is no smaller
- Augmented system exhibits gradual underflow

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Exceptional Values

- IEEE floating-point standard provides special values to indicate two exceptional situations
 - Inf, which stands for "infinity," results from dividing a finite number by zero, such as 1/0
 - NaN, which stands for "not a number," results from undefined or indeterminate operations such as $0/0,\,0*{\tt Inf},$ or ${\tt Inf/Inf}$
- Inf and NaN are implemented in IEEE arithmetic through special reserved values of exponent field

Floating-Point Numbers Floating-Point Arithmetic

Floating-Point Arithmetic

- Addition or subtraction: Shifting of mantissa to make exponents match may cause loss of some digits of smaller number, possibly all of them
- *Multiplication*: Product of two *p*-digit mantissas contains up to 2*p* digits, so result may not be representable
- *Division*: Quotient of two p-digit mantissas may contain more than p digits, such as nonterminating binary expansion of 1/10
- Result of floating-point arithmetic operation may differ from result of corresponding real arithmetic operation on same operands

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Example: Floating-Point Arithmetic

- Assume $\beta = 10$, p = 6
- Let $x = 1.92403 \times 10^2$, $y = 6.35782 \times 10^{-1}$
- Floating-point addition gives $x + y = 1.93039 \times 10^2$, assuming rounding to nearest
- Last two digits of y do not affect result, and with even smaller exponent, y could have had no effect on result
- Floating-point multiplication gives $x * y = 1.22326 \times 10^2$, which discards half of digits of true product

Floating-Point Numbers Floating-Point Arithmetic

Floating-Point Arithmetic, continued

- Real result may also fail to be representable because its exponent is beyond available range
- Overflow is usually more serious than underflow because there is *no* good approximation to arbitrarily large magnitudes in floating-point system, whereas zero is often reasonable approximation for arbitrarily small magnitudes
- On many computer systems overflow is fatal, but an underflow may be silently set to zero



Floating-Point Numbers Floating-Point Arithmetic

Example: Summing Series

Infinite series

$$\sum_{n=1}^{\infty} \frac{1}{n}$$

has finite sum in floating-point arithmetic even though real series is divergent

- Possible explanations
 - Partial sum eventually overflows
 - 1/n eventually underflows
 - Partial sum ceases to change once 1/n becomes negligible relative to partial sum

$$\frac{1}{n} < \epsilon_{\text{mach}} \sum_{k=1}^{n-1} \frac{1}{k}$$

Floating-Point Arithmetic, continued

- Ideally, x f lop y = fl(x op y), i.e., floating-point arithmetic operations produce correctly rounded results
- Computers satisfying IEEE floating-point standard achieve this ideal as long as *x* op *y* is within range of floating-point system
- But some familiar laws of real arithmetic are not necessarily valid in floating-point system
- Floating-point addition and multiplication are commutative but *not* associative
- Example: if ϵ is positive floating-point number slightly smaller than ϵ_{mach} , then $(1 + \epsilon) + \epsilon = 1$, but $1 + (\epsilon + \epsilon) > 1$



Floating-Point Numbers Floating-Point Arithmetic

Cancellation

- Subtraction between two *p*-digit numbers having same sign and similar magnitudes yields result with *fewer* than *p* digits, so it is usually exactly representable
- Reason is that leading digits of two numbers *cancel* (i.e., their difference is zero)
- For example,

 $1.92403 \times 10^2 - 1.92275 \times 10^2 = 1.28000 \times 10^{-1}$

which is correct, and exactly representable, but has only three significant digits

Floating-Point Numbers Floating-Point Arithmetic

Cancellation, continued

- Despite exactness of result, cancellation often implies serious loss of information
- Operands are often uncertain due to rounding or other previous errors, so relative uncertainty in difference may be large
- Example: if ϵ is positive floating-point number slightly smaller than ϵ_{mach} , then $(1 + \epsilon) (1 \epsilon) = 1 1 = 0$ in floating-point arithmetic, which is correct for actual operands of final subtraction, but true result of overall computation, 2ϵ , has been completely lost
- Subtraction itself is not at fault: it merely signals loss of information that had already occurred



Floating-Point Numbers Floating-Point Arithmetic

Cancellation, continued

- Digits lost to cancellation are most significant, leading digits, whereas digits lost in rounding are least significant, trailing digits
- Because of this effect, it is generally bad idea to compute any small quantity as difference of large quantities, since rounding error is likely to dominate result
- For example, summing alternating series, such as

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots$$

for x < 0, may give disastrous results due to catastrophic cancellation



Floating-Point Numbers Floating-Point Arithmetic

Example: Cancellation

Total energy of helium atom is sum of kinetic and potential energies, which are computed separately and have opposite signs, so suffer cancellation

Year	Kinetic	Potential	Total
1971	13.0	-14.0	-1.0
1977	12.76	-14.02	-1.26
1980	12.22	-14.35	-2.13
1985	12.28	-14.65	-2.37
1988	12.40	-14.84	-2.44

Although computed values for kinetic and potential energies changed by only 6% or less, resulting estimate for total energy changed by 144%

Floating-Point Numbers Floating-Point Arithmetic

Example: Quadratic Formula

• Two solutions of quadratic equation $ax^2 + bx + c = 0$ are given by

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

- Naive use of formula can suffer overflow, or underflow, or severe cancellation
- Rescaling coefficients avoids overflow or harmful underflow
- Cancellation between -b and square root can be avoided by computing one root using alternative formula

$$x = \frac{2c}{-b \mp \sqrt{b^2 - 4ac}}$$

 Cancellation inside square root cannot be easily avoided without using higher precision

< interactive example >

Floating-Point Numbers Floating-Point Arithmetic

Example: Standard Deviation

• Mean and standard deviation of sequence x_i , i = 1, ..., n, are given by

$$\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$$
 and $\sigma = \left[\frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})^2\right]^{\frac{1}{2}}$

• Mathematically equivalent formula

$$\sigma = \left[\frac{1}{n-1}\left(\sum_{i=1}^{n} x_i^2 - n\bar{x}^2\right)\right]^{\frac{1}{2}}$$

avoids making two passes through data

 Single cancellation at end of one-pass formula is more damaging numerically than all cancellations in two-pass formula combined