Set 2: Representation, Conditioning and Error

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Finite Precision

- All discussions must make clear the assumptions made about the "numbers" used.
- Representation of numbers and related formulae can be symbolic and therefore exact, e.g., π , e^x , 1/3
- Arithmetic and manipulation is then symbolic and therefore exact.
- Computers store information using a finite number bits so even symbolic computation is limited by the size of memory.
- Numbers can also be represented in a manner that supports arithmetic operations rather than symbolic mathematics.
- Finite number of bits per number.
- Finite set of numbers so limited coverage and precision concerns.
- In this case arithmetic is not exact.

Finite Precision

Consequently,

- The problem stored in the computer is not necessarily the problem posed.
- The computed solution does not necessarily solve the problem posed or the problem stored in the computer.
- The computed solution may solve a problem that is not representable in the computer.

Numerical Analysis and Finite Precision

- Numerical error analysis addresses the effects of finite precision of representation and computation.
- Topics:
 - Representation
 - Arithmetic
 - Errors: forms and bounds
 - Conditioning of problem
 - Stability of an algorithm

Sources

In addition to the textbook the following are sources for this presentaion and useful references (see also their citations):

- What Every Computer Scientist Should Know About Floating-Point Arithmetic David Goldberg, ACM Computing Surveys, March, 1991. http://docs.sun.com/source/806-3568/ncg_goldberg.html
- *Matrix Algorithms, Volume 1: Basic Decompositions*, G. W. Stewart, SIAM, 1998.
- Accuracy and Stability of Numerical Algorithms, N. J. Higham, SIAM, Second Edition, 2002.
- *The Handbook of Mathematical Functions*, M. Abramowitz and I. Stegun, Tenth Printing, available on the web at several URLs

Integers – finite number exactly represented

Binary	unsigned	sign	excess	one's/two's
codeword		magnitude	three	complement
000	0	0	-3	0/0
001	1	1	-2	1/1
010	2	2	-1	2/2
011	3	3	0	3/3
100	4	-0	1	-3/-4
101	5	-1	2	-2/-3
110	6	-2	3	-1/-2
111	7	-3	4	-0/-1

Integers – finite number exactly represented

- one's complement flips bit of nonnegative integer
- two's complement adds 1 to the one's complement
- unsigned binary arithmetic implements signed integer arithmetic
- b bits has excess of $2^{b-1} 1$.
- finite range
- exact within range for integers
- ordering of codewords vs ordering of numbers represented
- choice depends on usage, e.g., arithmetic, exponent, communication

Real Number Representation

Real numbers can be written as decimal expansions:

$$\pi = 3.14159265358979\dots$$

$$\frac{1}{3} = 0.33333333...$$

$$98.6 = 986 \times 10^{-1} = 0.986 \times 10^{2} = \left(\frac{9}{10} + \frac{8}{100} + \frac{6}{1000}\right) \times 10^{2}$$

$$\forall x \in \mathbb{R} \ x = \pm 10^e \sum_{k=1}^{\infty} d_k \times 10^{-k}, \ 0 \le d_k \le 9, \ d_1 \ne 0, \ e \in \mathbb{Z}$$

Floating Point Representation

A floating point number system is characterized by four integers

 β the base or radix, t the precision, $L \le e \le U$ exponent bounds

Definition 2.1. A floating point number system $F \subset \mathbb{R}$ is a set of real numbers of the form

$$y = \pm m \times \beta^{e-t}$$

$$y = \pm \beta^e \sum_{k=1}^t d_k \times \beta^{-k} = \pm \beta^e (0.d_1 d_2 \dots d_t)$$

where $m \in \mathbb{Z}$, the $0 \le d_k < \beta$ are digits in $m, 0 \le m \le \beta^t - 1$.

Floating Point Representation

Definition 2.2. A floating point number system $\mathcal{F} \subset \mathbb{R}$ is normalized if the mantissa, m, (or significand or fraction) satisfies $\beta^{t-1} \leq m < \beta^t$ when $y \neq 0$. This is the same as $d_1 \neq 0$. It is assumed that 0 has a special representation.

$$-9.9 = -0.99 \times 10^{1}$$
$$22 = +.1011 * 2^{5}$$
$$\frac{3}{8} = +.1200 \times 4^{0}$$

Example

The system with $\beta=2,\,t=3,\,L=-1,\,U=3$ has the following normalized positive numbers. Note the exponents are written as a base 10 integer for clarity.

$$.100 \times 2^{-1} = 0.25, \quad .101 \times 2^{-1} = 0.3125,$$

$$.110 \times 2^{-1} = 0.375, \quad .111 \times 2^{-1} = 0.4375$$

$$.100 \times 2^{0} = 0.5, \quad .101 \times 2^{0} = 0.625, \quad .110 \times 2^{0} = 0.75, \quad .111 \times 2^{0} = 0.875$$

$$.100 \times 2^{1} = 1.0, \quad .101 \times 2^{1} = 1.25, \quad .110 \times 2^{1} = 1.5, \quad .111 \times 2^{1} = 1.75$$

$$.100 \times 2^{2} = 2.0, \quad .101 \times 2^{2} = 2.5, \quad .110 \times 2^{2} = 3.0, \quad .111 \times 2^{2} = 3.5$$

$$.100 \times 2^{3} = 4.0, \quad .101 \times 2^{3} = 5.0, \quad .110 \times 2^{3} = 6.0, \quad .111 \times 2^{3} = 7.0$$

Floating Point Representation

- \mathcal{F} is a finite set with $1 + 2(U L + 1)(\beta 1)\beta^{t-1}$ elements
 - $(\beta 1)\beta^{t-1}$ normalized mantissas
 - (U-L+1) exponents
 - $-\pm \rightarrow 2$ values for each mantissa, exponent pair
 - 0 represented via special pattern
- 41 for $\beta = 2$, t = 3, L = -1, U = 3 example.
- $\beta^{L-1} \leq |y| \leq \beta^U (1 \beta^{-t})$ range of normalized FP's
- ullet absolute difference between normalized FP's is β^{e-t}
- machine epsilon is $\epsilon_M = \beta^{1-t}$. (distance from 1 to next $x \in \mathcal{F}$)
- magnitude of the relative distance varies periodically: 1/m(x).

Denormalized Numbers

Definition 2.3. Subnormal or denormalized elements are those with e = L, value $\pm m \times \beta^{L-t}$ and $d_1 = 0$. The smallest denormalized number is

$$\mu = \beta^{L-t} = \beta^{L-1}\beta^{1-t} = y_{min}\epsilon_M$$

- These are included in the system to facilitate what is known as gradual underflow.
- Since they keep explicitly the leading 0's they have less precision than normalized numbers in terms of number of signficant digits possible.
- e = L and $d_1 = 0$ can be viewed as one of two normalizations used, i.e., one for the interval of normalized FP's and one for the interval of denormalized FP's

Example

The system with $\beta=2,\,t=3,\,L=-1,\,U=3$ has the following denormalized numbers

$$.001 \times 2^{-1} = \frac{1}{16} = 0.0625$$
$$.010 \times 2^{-1} = \frac{1}{8} = 0.125$$
$$.011 \times 2^{-1} = \frac{3}{16} = 0.18755$$

- Every floating point number is a real number but not vice versa.
- We need a map $fl(x) : \mathbb{R} \to \mathcal{F}$.
- Care must be taken since the range of \mathcal{F} is limited.
- Many possible versions of the map fl(x) but not all are robust.

Suppose we have two consecutive positive normalized floating point numbers $f_1 < f_2$ and a real number $f_1 < x < f_2$.

$$x = (0.d_1 \dots d_{t-1} d_t d_{t+1} d_{t+2} \dots) \times \beta^e$$

$$f_1 = (0.d_1 \dots d_{t-1} d_t) \times \beta^e$$

$$f_2 = (0.d_1 \dots d_{t-1} \tilde{d}_t) \times \beta^e \text{ where } \tilde{d}_t = d_t + 1$$

$$fl(x) = f_1 \text{ called chopping}$$

$$\frac{x - fl(x)}{x} = \frac{(0.0 \dots 00d_{t+1} d_{t+2} \dots) \times \beta^e}{(0.d_1 \dots d_{t-1} d_t d_{t+1} d_{t+2} \dots) \times \beta^e} \leq \frac{\beta^{-t}}{\beta^{-1}} = \beta^{1-t} = \epsilon_M$$

Floating point rounding:

$$fl(x) = \begin{cases} f_1 & \text{when } |x - f_1| < |x - f_2| \\ f_2 & \text{when } |x - f_2| < |x - f_1| \end{cases}$$

Ties can be broken in different ways. For example,

- round to even, i.e., d_t is even in fl(x), IEEE default
- round to odd, i.e., d_t is odd in fl(x)
- round towards 0 (round away from ∞ , chopping) applies to magnitude
- round towards ∞ (round away from 0) applies to magnitude

There are many others and a large literature analyzing their biases.

Lemma 2.1. For any x in the range of the floating point system $\mathcal{F}(\beta, t, L, U)$ we have

$$\frac{|fl(x) - x|}{|x|} \le \begin{cases} \beta^{1-t} = u & \text{for chopping} \\ \frac{1}{2}\beta^{1-t} = u & \text{for rounding} \end{cases}$$
$$fl(x) = x(1+\delta), \quad |\delta| < u$$

If x is outside the range of \mathcal{F} then fl(x) is said to overflow.

If $0 \le |x| \le y_{min} = \beta^{L-1}$ then then fl(x) is said to underflow. $(y_{min} \text{ is normalized } FP)$

u is called unit roundoff.

In practice, x will be a real number produced on the computer that has the form

$$x = (0.d_1 \dots d_{t-1} d_t d_{t+1} d_{t+2} \dots d_{t+g}) \times \beta^e$$

That is, it will have some extra digits called guard digits (and sometimes an extra sticky digit).

In this case rounding is based on the value of one or all of the digits $d_{t+1}d_{t+2} \dots d_{t+g}$, i.e., $x - f_1$ and $x - f_2$.

For example, rounding with a tie rounded up in magnitude is often described as

$$fl(x) = \begin{cases} f_1 & \text{if } d_{t+1} < \frac{\beta}{2} \\ f_2 & \text{if } d_{t+1} \ge \frac{\beta}{2} \end{cases}$$

Let
$$\beta = 10$$
 and $t = 5$

$$x = 142.52731$$

$$y = 142.52500$$

$$fl(x) = \begin{cases} 142.52 & \text{chopping} \\ 142.53 & \text{rounding to nearest - not a tie} \end{cases}$$

$$fl(y) = \begin{cases} 142.52 & \text{chopping} \\ 142.52 & \text{rounding to even} \end{cases}$$

IEEE Format

Single Precision:

- 32-bit FP number
- 1 bit, σ , for the sign of the mantissa
- 8-bit biased exponent, ϵ
- 23(+1)-bit normalized mantissa, μ .
- unit roundoff $u = 2^{-24} \approx 5.96 \times 10^{-8}$

The normalization is a leading hidden bit of 1 that with coefficient 2^0 that is not stored explicitly.

IEEE Format

Double Precision:

- 64-bit FP number
- 1 bit, σ , for the sign of the mantissa
- 11-bit biased exponent, ϵ
- 52(+1)-bit normalized mantissa, μ .
- unit roundoff $u = 2^{-53} \approx 1.11 \times 10^{-16}$

The normalization is a leading hidden bit of 1 that with coefficient 2^0 that is not stored explicitly.

Decoding

If σ , ϵ and μ are the decimal integer values of the bit patterns in the sign, exponent and mantissa fields respectively, then the number represented has the values:

Single precision: ($\epsilon=0$ and $\epsilon=255$ have special meanings.)

$$sp = (-1)^{\sigma} \quad 1. \ \mu \times 2^{\epsilon - 127}$$
$$1 \le \epsilon \le 254$$
$$10^{-38} \le sp \le 10^{38} \ roughly$$

$$\epsilon=255,\quad \mu\neq0\to NaN,\quad \text{e.g. }\sqrt{-1}$$

$$\epsilon=255,\quad \mu=0\to\pm\infty$$

$$\epsilon=0\to \text{denormalized number}$$

Decoding

Double precision: ($\epsilon = 0$ and $\epsilon = 2047$ have special meanings.)

$$dp = (-1)^{\sigma} \quad 1. \ \mu \times 2^{\epsilon - 1023}$$

$$1 \le \epsilon \le 2046$$

$$10^{-308} \le dp \le 10^{308} \ roughly$$

$$\epsilon=2047,\quad \mu\neq 0 \to NaN,\quad \text{e.g. } \sqrt{-1}$$

$$\epsilon=2047,\quad \mu=0 \to \pm\infty$$

$$\epsilon=0 \to \text{denormalized number}$$

Single Precision Example

32-bit word has fields:

$$\left[\begin{array}{c|c} \sigma & \epsilon & \mu \end{array}\right]$$

If x = -1.5 we have

$$x = -1.1 \times 2^{0}$$

$$\sigma = 1$$

$$\epsilon = 0 + 127 = 01111111$$

$$\mu = 1000000000000000000000000$$

Suppose we are to solve a problem specified by data d to yield a solution s. (d and s can be a collection of real scalars.)

The problem can be mathematically represented by

$$F(s,d) = 0 \text{ or } s = f(d)$$

Note this not an algorithm or a program. It is the mathematical specification of the mapping from the data d to the solution s.

Function evaluation:

$$d = \alpha \in \mathbb{R}, \quad s = f(d) \to y = e^{\alpha}$$

Root finding:

$$d = \begin{pmatrix} \alpha & \beta & \gamma \end{pmatrix}$$
 $s = \begin{pmatrix} x_+ & x_- \end{pmatrix}$ $\rightarrow F(d, s) = 0 = \alpha x^2 + \beta x + \gamma$

Solving linear systems:

$$d = (A \in \mathbb{R}^{n \times n}, b \in \mathbb{R}^n)$$
$$s = x \to F(s, d) = b - Ax \text{ or } s = x = f(d) = A^{-1}b$$

- s = f(d) desired.
- $fl(d) = d(1 + \delta)$ is stored.
- $\tilde{s} = f(fl(d))$ is exact solution to the perturbed problem.
- How much does the perturbation change the solution?

$$e_{abs} = \|\tilde{s} - s\|$$
 absolute error $e_{rel} = \frac{\|\tilde{s} - s\|}{\|s\|}$ relative error

- ullet these are **forward errors** resulting from uncertainty in the data d due to FP representation
- other sources of uncertainty in data also possible

Condition Number

- The condition number is a worst case bound on the effect of perturbations in a neighborhood around the original problem data.
- absolute and relative bounds

$$\kappa_{abs} = \sup \left\{ \frac{|f(d + \Delta d) - f(d)|}{|\Delta d|}, \ \Delta d \neq 0, \ d + \Delta d \in \mathcal{N}_d \right\}$$

$$\kappa_{rel} = \sup \left\{ \frac{|f(d+\Delta d) - f(d)|/|f(d)|}{|\Delta d|/|d|}, \quad \Delta d \neq 0, \quad d + \Delta d \in \mathcal{N}_d \right\}$$

Absolute Condition Number

Assume $s = f(d) : \mathbb{R} \to \mathbb{R}$ has a Taylor series approximation around points of interest. An estimate of the condition number based on an asymptotically small neighborhood/perturbation can be used.

$$f(d + \Delta d) = f(d) + \Delta df'(d) + O(\Delta d^{2})$$

$$f(d + \Delta d) - f(d) \approx \Delta df'(d)$$

$$|f(d + \Delta d) - f(d)| \le |f'(d)| |\Delta d|$$

$$e_{abs} = |\tilde{s} - s| \le \kappa_{abs} |\Delta d|$$

Relative Condition Number

Assume $s = f(d) : \mathbb{R} \to \mathbb{R}$ has a Taylor series approximation around points of interest.

$$d + \Delta d = d(1 + \delta)$$

$$f(d + \Delta d) - f(d) \approx \Delta df'(d)$$

$$\frac{|f(d + \Delta d) - f(d)|}{|f(d)|} \leq \frac{|f'(d)|}{|f(d)|} |\Delta d|$$

$$\frac{|f(d + \Delta d) - f(d)|}{|f(d)|} \leq \frac{|df'(d)|}{|f(d)|} |\frac{\Delta d}{d}|$$

$$\frac{|f(d + \Delta d) - f(d)|}{|f(d)|} \leq \frac{|df'(d)|}{|f(d)|} |\delta|$$

$$e_{rel} = \frac{|\tilde{s} - s|}{|s|} \leq \kappa_{rel} |\delta|$$

Condition Numbers

- Definitions generalize to multidimensional data and solutions.
- κ_{abs} bounds the e_{abs} with an amplification of the magnitude of the absolute change in the data.
- κ_{rel} bounds the e_{rel} with an amplification of the magnitude of the relative change in the data
- The condition number is greater than 1, i.e.,

$$\kappa_{rel} = \max\left(1, \frac{|df'(d)|}{|f(d)|}\right), \quad \kappa_{abs} = \max\left(1, |f'(d)|\right)$$

• When |f'(d)| gets small, the asymptotic perturbation form may not be appropriate and the change over the neighborhood should be determined.

Condition Numbers

- Gives an idea of how much the uncertainty in the data specifying the problem can change the solution, i.e., how many digits may be lost.
- This does not involve the precision of the finite arithmetic only the precision of representation.
- No algorithm is involved. This is an analytical statement.
- Problems with large condition numbers are called ill-conditioned.
- Problems with condition number 1 are called perfectly conditioned.

A Simple Example

Consider the the condtioning of the sum of two numbers.

$$x=151.72899$$
 and $y=-151.71422$
$$x+y=0.01477$$

$$\tilde{x}=151.73 \text{ and } \tilde{y}=-151.71$$

$$\tilde{x}+\tilde{y}=0.02$$

- x and \tilde{x} agree to 4 digits; y and \tilde{y} agree to 4 digits
- relative error in the two sums 0.35 = (0.02 0.01477)/0.01477
- the respective sums do not agree to any digits
- Sum is ill-conditioned when magnitudes are close but signs are opposite.

Condition of Summation

$$s = \sum_{i=1}^{n} x_i \text{ and } \tilde{s} = \sum_{i=1}^{n} x_i (1 + \eta_i), \quad |\eta_i| \le \epsilon$$

$$\tilde{s} - s = \sum_{i=1}^{n} x_i \eta_i \to |\tilde{s} - s| \le \sum_{i=1}^{n} |x_i| \epsilon$$

$$|s| = |\sum_{i=1}^{n} x_i| \to \frac{|\tilde{s} - s|}{|s|} \le \kappa_{rel} \epsilon$$

$$\kappa_{rel} = \frac{|x_1| + \dots + |x_n|}{|x_1 + \dots + x_n|}$$

- $\kappa_{rel} = 1$ if all x_i have same sign.
- κ_{rel} large if the sum is small compared to the $|x_i|$, i.e., information is cancelled.

$$f(x) = e^{-x} \text{ and } f'(x) = -e^{-x}$$

$$\kappa_{rel} = \frac{|xe^{-x}|}{|e^{-x}|} = |x|$$

- Well-conditioned for x = O(1).
- If $x \approx 10^k$ we lose k digits in f(x) for every digit we alter in x.

$$x_0 = -5.5 \rightarrow e^{x_0} = 0.004086771...$$

 $x_1 = -(5.5 + 10^{-5}) = x_0(1 + \delta_1), \ \delta_1 = 1.8 \times 10^{-5}$

expect agreement to 4 or 5 digits since $|x_0||\delta_1| = 5.5 \times 1.8 \times 10^{-5}$

$$e^{x_1} = 0.004086731\dots$$

$$x_2 = -(5.5 + 10^{-4}) = x_0(1 + \delta_2), \ \delta_2 = 1.8 \times 10^{-4}$$

expect agreement to 3 to 4 digits since $|x_0||\delta_2| = 5.5 \times 1.8 \times 10^{-4}$

$$e^{x_2} = 0.004086363\dots$$

$$f(x) = \log x$$

$$f'(x) = \frac{1}{x}$$

$$\kappa_{rel} = \frac{|x|}{|x \log x|} = \left| \frac{1}{\log x} \right|$$

Ill-conditioned for $x \approx 1$.

Conditioning w/r to a Parameter

Given $p(x) = x^2 - 4x + \gamma$ consider roots.

$$x^{2} - 4x + \gamma = 0 \to x_{\pm} = 2 \pm \sqrt{4 - \gamma}$$

$$\gamma_{0} = 4 \to x_{\pm} = 2$$

$$\gamma = \gamma_{0} - 10^{-7} \to \tilde{x}_{\pm} = 2 \pm 10^{-3.5}$$

$$\Delta \gamma_{rel} = \frac{|\gamma - \gamma_{0}|}{|\gamma_{0}|} = \frac{10^{-7}}{4} = 2.5 \times 10^{-8}$$

$$\Delta x_{rel} = \frac{|\tilde{x} - x|}{|x|} = \frac{10^{-3.5}}{2} \approx 1.6 \times 10^{-4}$$

$$\frac{\Delta x_{rel}}{\Delta \gamma_{rel}} = \frac{1.6 \times 10^{-4}}{2.5 \times 10^{-8}} = 6400$$

Parameter agreed to 7 digits root agreed to 3 digits loss of 4 digits characterized by lower bound on condition number of 6400

Conditioning w/r to a Parameter

Choice of parameterization matters. Given

$$p(x) = x^2 - 4x + \gamma_0 = x^2 - 4x + 4 = (x - 2)^2$$

Suppose we view this as an instance of

$$\alpha(x-\rho_1)(x-\rho_2)$$

and discuss change in roots subject to parameters α , ρ_1 , and ρ_2 .

In this contrived parameterization the roots are perfectly conditioned.

See the text p. 35 and p. 39 for a more sophisticated version of this reparameterization with repeated roots.

Conditioning of Linear System Solving

Consider Ax = b

$$\begin{pmatrix} 0.300 & 0.401 \\ 0.374 & 0.500 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} -0.101 \\ -0.126 \end{pmatrix}$$
$$\begin{pmatrix} 0.300 & 0.401 \\ 0.374 & 0.500 \end{pmatrix} \begin{pmatrix} -0.337 \\ 0 \end{pmatrix} = \begin{pmatrix} -0.1011 \\ -0.126038 \end{pmatrix}$$
$$\Delta A = 0, \Delta b = \begin{pmatrix} -1 \times 10^{-4} \\ -3.8 \times 10^{-5} \end{pmatrix}$$

original solution and solution to perturbed equation disagree in all digits!

Conditioning of Linear System Solving

Consider Ax = b

$$\begin{pmatrix} 0.3001 & 0.4012 \\ 0.374002 & 0.50004 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} -0.1011 \\ -0.126038 \end{pmatrix}$$

$$\Delta A = \begin{pmatrix} 1 \times 10^{-4} & 2 \times 10^{-4} \\ 2 \times 10^{-6} & 4 \times 10^{-5} \end{pmatrix} \Delta b = \begin{pmatrix} -1 \times 10^{-4} \\ -3.8 \times 10^{-5} \end{pmatrix}$$

original solution and solution to perturbed equation are the same!

Conditioning of Linear System Solving

- The problem is ill-conditioned.
- We will define a condition number later using matrix norms.
- For this matrix, $||A||_{\infty} = 0.874$, $||A^{-1}||_{\infty} = 3.8 \times 10^4$ and $\kappa \approx 10^4$.
- Ill-conditioning does not imply that all perturbations to the data result in large changes to the solution.
- The condition number is a worst case bound on the effect of perturbations in a neighborhood around the original problem data.

Backward Error

Conditioning relates perturbations in input data, d, to FORWARD
 ERROR

$$e_{rel} = \frac{\|f(d + \Delta d) - f(d)\|}{\|f(d)\|}$$

- conditioning addresses uncertainty analytically
- BACKWARD ERROR reverses the question.
- Given s = f(d) and $\tilde{s} \neq f(d)$, find Δd such that

$$\tilde{s} = f(d + \Delta d)$$

• That is, show that \tilde{s} is the solution to another problem.

Backward Error

- technique often shows existence of such a problem within some neighborhood of d.
- nearby problem may not exist in same "class" of problems
- turns stability analysis into a perturbation analysis