UNIVERSITY OF MINNESOTA TWIN CITIES

C S C I 5304 Fall 2021

COMPUTATIONAL ASPECTS OF MATRIX THEORY

Class time	:	*MW 4:00 – 5:15 pm*
Room	:	*Keller 3-230 or Online*
Instructor	:	*Daniel Boley*

Lecture notes: http://www-users.cselabs.umn.edu/classes/Fall-2021/csci5304/

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FLOATING POINT ARITHMETIC - ERROR ANALYSIS

- **Brief review of floating point arithmetic**
- **Model of floating point arithmetic**
- **Notation, backward and forward errors**

Roundoff errors and floating-point arithmetic

➤ The basic problem: The set A of all possible representable numbers on a given machine is finite - but we would like to use this set to perform standard arithmetic operations (+,*,-,/) on an infinite set. The usual algebra rules are no longer satisfied since results of operations are rounded.

➤ Basic algebra breaks down in floating point arithmetic.

Example: In floating point arithmetic.

$$a + (b + c) \; != \; (a + b) + c$$

Matlab experiment: For 10,000 random numbers find number of instances when the above is true. Same thing for the multiplication..

Floating point representation:

Real numbers are represented in two parts: A mantissa (significand) and an exponent. If the representation is in the base β then:

$$x = \pm(.d_1 d_2 \cdots d_t)\beta^e$$

- $.d_1 d_2 \cdots d_t$ is a fraction in the base-β representation (Generally the form is normalized in that $d_1 \neq 0$), and e is an integer
- Often, more convenient to rewrite the above as:

$$x = \pm(m/\beta^t) \times \beta^e \equiv \pm m \times \beta^{e-t}$$

- Mantissa m is an integer with $0 \le m \le \beta^t - 1$.

Machine precision - machine epsilon

- Notation : $fl(x)$ = closest floating point representation of real number x ('rounding')
- When a number x is very small, there is a point when $1 + x == 1$ in a machine sense. The computer no longer makes a difference between 1 and $1 + x$.

Machine epsilon: The smallest number ϵ such that $1 + \epsilon$ is a float that is different from one, is called machine epsilon. Denoted by **macheps** or **eps**, it represents the distance from 1 to the next larger floating point number.

- With previous representation, **eps** is equal to $\beta^{-(t-1)}$.

Example: In IEEE standard double precision, $\beta = 2$, and $t = 53$ (includes 'hidden bit'). Therefore **eps** $= 2^{-52}$.

Unit Round-off A real number x can be approximated by a floating number $fl(x)$ with relative error no larger than $\underline{\mathbf{u}} = \frac{1}{2}\beta^{-(t-1)}$.

- $\underline{\mathbf{u}}$ is called Unit Round-off.
- In fact can easily show:

$$fl(x) = x(1 + \delta) \text{ with } |\delta| < \underline{\mathbf{u}}$$

✍₂ Matlab experiment: find the machine epsilon on your computer.

- Many discussions on what conditions/ rules should be satisfied by floating point arithmetic. The IEEE standard is a set of standards adopted by many CPU manufacturers.

Rule 1.

$$fl(x) = x(1+\epsilon), \quad \text{where} \quad |\epsilon| \le \mathbf{\underline{u}}$$

Rule 2. For all operations $\odot$ (one of $+, -, *, /$)

$$fl(x \odot y) = (x \odot y)(1+\epsilon_\odot), \quad \text{where} \quad |\epsilon_\odot| \le \mathbf{\underline{u}}$$

Rule 3. For $+, *$ operations

$$fl(a \odot b) = fl(b \odot a)$$

✍3 Matlab experiment: Verify experimentally Rule 3 with 10,000 randomly generated numbers a_i, b_i.

Example: Consider the sum of 3 numbers: $y = a + b + c$.

- Done as $fl(a+b+c) = fl(fl(a+b)+c)$

$$\begin{aligned} fl(a+b) &= (a+b)(1+\epsilon_1) \\ fl(a+b+c) &= [(a+b)(1+\epsilon_1)+c]\,(1+\epsilon_2) \\ &= a(1+\epsilon_1)(1+\epsilon_2) + b(1+\epsilon_1)(1+\epsilon_2) \\ &\qquad + c(1+\epsilon_2) \\ &= a(1+\theta_1) + b(1+\theta_2) + c(1+\theta_3) \end{aligned}$$

with $1+\theta_1 = 1+\theta_2 = (1+\epsilon_1)(1+\epsilon_2)$ and $1+\theta_3 = (1+\epsilon_2)$

For a longer sum we would have something like:

$$1+\theta_j = (1+\epsilon_1)(1+\epsilon_2)(\cdots)(1+\epsilon_{n-j})$$

- Remark on order of the sum. If $y_1 = fl(fl(a+b)+c)$:

$$\begin{aligned} y1 &= [(a+b+c)+(a+b)\epsilon_1)]\,(1+\epsilon_2) \\ &= (a+b+c)\left[1 + \frac{a+b}{a+b+c}\epsilon_1(1+\epsilon_2) + \epsilon_2\right] \end{aligned}$$

So disregarding the high order term $\epsilon_1\epsilon_2$

$$\begin{aligned} fl(fl(a+b)+c) &= (a+b+c)(1+\epsilon_3) \\ \epsilon_3 &\approx \frac{a+b}{a+b+c}\epsilon_1 + \epsilon_2 \end{aligned}$$

- If we redid the computation as $y_2 = fl(a + fl(b+c))$ we would find

$$\begin{aligned} fl(a+fl(b+c)) &= (a+b+c)(1+\epsilon_4) \\ \epsilon_4 &\approx \frac{b+c}{a+b+c}\epsilon_1 + \epsilon_2 \end{aligned}$$

- The error is amplified by the factor $(a+b)/y$ in the first case and $(b+c)/y$ in the second case.

- In order to sum n numbers accurately, it is better to start with small numbers first. [However, sorting before adding is not worth it.]

- But watch out if the numbers have mixed signs!

The absolute value notation

- For a given vector x, $|x|$ is the vector with components $|x_i|$, i.e., $|x|$ is the component-wise absolute value of x.
- Similarly for matrices:

$$|A| = \{|a_{ij}|\}_{i=1,\dots,m;\ j=1,\dots,n}$$

- An obvious result: The basic inequality

$$|fl(a_{ij}) - a_{ij}| \le \underline{\mathbf{u}}\ |a_{ij}|$$

translates into

$$|fl(A) - A| \le \underline{\mathbf{u}}\ |A|$$

- $A \le B$ means $a_{ij} \le b_{ij}$ for all $1 \le i \le m;\ 1 \le j \le n$

Backward and forward errors

- Assume the approximation $\hat{y}$ to $y = \text{alg}(x)$ is computed by some algorithm with arithmetic precision ϵ. Possible analysis: find an upper bound for the Forward error

$$|\Delta y| = |y - \hat{y}|$$

- This is not always easy.

Alternative question: find equivalent perturbation on initial data (x) that produces the result $\hat{y}$. In other words, find Δx so that:

$$\text{alg}(x + \Delta x) = \hat{y}$$

- The value of $|\Delta x|$ is called the backward error. An analysis to find an upper bound for $|\Delta x|$ is called Backward error analysis.

Example: $A = \begin{pmatrix} a & b \\ 0 & c \end{pmatrix} \quad B = \begin{pmatrix} d & e \\ 0 & f \end{pmatrix}$

Consider the product: $fl(A.B) =$

$$\left[\begin{array}{c|c} ad(1+\epsilon_1) & [ae(1+\epsilon_2) + bf(1+\epsilon_3)]\,(1+\epsilon_4) \\ \hline 0 & cf(1+\epsilon_5) \end{array}\right]$$

with $\epsilon_i \le \underline{\mathbf{u}}$, for $i = 1, \dots, 5$. Result can be written as:

$$\left[\begin{array}{c|c} a & b(1+\epsilon_3)(1+\epsilon_4) \\ \hline 0 & c(1+\epsilon_5) \end{array}\right] \left[\begin{array}{c|c} d(1+\epsilon_1) & e(1+\epsilon_2)(1+\epsilon_4) \\ \hline 0 & f \end{array}\right]$$

- So $fl(A.B) = (A + E_A)(B + E_B)$.
- Backward errors E_A, E_B satisfy:

$$|E_A| \le 2\underline{\mathbf{u}}\,|A| + O(\underline{\mathbf{u}}^{\,2})\ ; \qquad |E_B| \le 2\underline{\mathbf{u}}\,|B| + O(\underline{\mathbf{u}}^{\,2})$$

- When solving $Ax = b$ by Gaussian Elimination, we will see that a bound on $\|e_x\|$ such that this holds exactly:

$$A(x_{\text{computed}} + e_x) = b$$

is much harder to find than bounds on $\|E_A\|$, $\|e_b\|$ such that this holds exactly:

$$(A + E_A)x_{\text{computed}} = (b + e_b).$$

Note: In many instances backward errors are more meaningful than forward errors: if initial data is accurate only to 4 digits say, then my algorithm for computing x need not guarantee a backward error of less then 10^{-10} for example. A backward error of order 10^{-4} is acceptable.

Error Analysis: Inner product

➤ Inner products are in the innermost parts of many calculations. Their analysis is important.

Lemma: If $|\delta_i| \le \underline{\mathbf{u}}$ and $n\underline{\mathbf{u}} < 1$ then

$$\Pi_{i=1}^n (1+\delta_i) = 1 + \theta_n \quad \text{where} \quad |\theta_n| \le \frac{n\underline{\mathbf{u}}}{1-n\underline{\mathbf{u}}}$$

➤ Common notation $\gamma_n \equiv \frac{n\underline{\mathbf{u}}}{1-n\underline{\mathbf{u}}}$

✍D4 Prove the lemma [Hint: use induction]

➤ Can use the following simpler result:

Lemma: If $|\delta_i| \le \underline{\mathbf{u}}$ and $n\underline{\mathbf{u}} < .01$ then

$$\Pi_{i=1}^n (1+\delta_i) = 1 + \theta_n \quad \text{where} \quad |\theta_n| \le 1.01 n\underline{\mathbf{u}}$$

Example: Previous sum of numbers can be written

$$\begin{aligned} fl(a+b+c) &= fl(fl(a+b)+c) \\ &= [(a+b)(1+\epsilon_1)+c]\,(1+\epsilon_2) \\ &= a(1+\epsilon_1)(1+\epsilon_2) + b(1+\epsilon_1)(1+\epsilon_2) + \\ &\qquad\qquad c(1+\epsilon_2) \\ &= a(1+\theta_1) + b(1+\theta_2) + c(1+\theta_3) \\ &= \text{exact sum of slightly perturbed inputs,} \end{aligned}$$

where all θ_i's satisfy $|\theta_i| \le 1.01 n\underline{\mathbf{u}}$ (here $n = 2$).

➤ Backward error result (output is exact sum of perturbed input)

➤ Alternatively, can write 'forward' bound:
$|fl(a+b+c) - (a+b+c)| \le |a\theta_1| + |b\theta_2| + |c\theta_3|$.

(bound on | output - exact sum |)

Analysis of inner products (cont.)

Consider $\quad s_n = fl(x_1 * y_1 + x_2 * y_2 + \cdots + x_n * y_n)$

➤ In what follows η_i's come from $*$, ϵ_i's come from $+$

➤ They satisfy: $|\eta_i| \le \underline{\mathbf{u}}$ and $|\epsilon_i| \le \underline{\mathbf{u}}$.

➤ The inner product s_n is computed as:

1. $s_1 = fl(x_1 y_1) = (x_1 y_1)(1+\eta_1)$

2. $s_2 = fl(s_1 + fl(x_2y_2)) = fl(s_1 + x_2y_2(1+\eta_2))$
$= (x_1y_1(1+\eta_1) + x_2y_2(1+\eta_2))\,(1+\epsilon_2)$
$= x_1y_1(1+\eta_1)(1+\epsilon_2) + x_2y_2(1+\eta_2)(1+\epsilon_2)$

3. $s_3 = fl(s_2 + fl(x_3y_3)) = fl(s_2 + x_3y_3(1+\eta_3))$
$= (s_2 + x_3y_3(1+\eta_3))(1+\epsilon_3)$

Expand: $s_3 = x_1y_1(1+\eta_1)(1+\epsilon_2)(1+\epsilon_3)$
$+x_2y_2(1+\eta_2)(1+\epsilon_2)(1+\epsilon_3)$
$+x_3y_3(1+\eta_3)(1+\epsilon_3)$

➤ Induction would show that [with convention that $\epsilon_1 \equiv 0$]

$$s_n = \sum_{i=1}^{n} x_iy_i(1+\eta_i) \prod_{j=i}^{n}(1+\epsilon_j)$$

Q: How many terms in the coefficient of x_iy_i do we have?

A:
- When $i > 1$: $1 + (n - i + 1) = n - i + 2$
- When $i = 1$: n (since $\epsilon_1 = 0$ does not count)

➤ Bottom line: always $\leq n$.

➤ For each of these products

$(1+\eta_i)\ \prod_{j=i}^{n}(1+\epsilon_j) = 1 + \theta_i,$ with $|\theta_i| \leq \gamma_n$ so:

$s_n = \sum_{i=1}^{n} x_iy_i(1+\theta_i)$ with $|\theta_i| \leq \gamma_n$ or:

$$\boxed{fl\left(\textstyle\sum_{i=1}^{n} x_iy_i\right) = \sum_{i=1}^{n} x_iy_i + \sum_{i=1}^{n} x_iy_i\theta_i \quad \text{with} \quad |\theta_i| \leq \gamma_n}$$

➤ This leads to the final result (forward form)

$$\left| fl\left(\sum_{i=1}^{n} x_iy_i\right) - \sum_{i=1}^{n} x_iy_i \right| \leq \gamma_n \sum_{i=1}^{n} |x_i||y_i|$$

➤ or (backward form)

$$fl\left(\sum_{i=1}^{n} x_iy_i\right) = \sum_{i=1}^{n} x_iy_i(1+\theta_i) \quad \text{with} \quad |\theta_i| \leq \gamma_n$$

Main result on inner products:

- Backward error expression:

$$fl(x^Ty) = [x .* (1 + d_x)]^T [y .* (1 + d_y)]$$

where $\|d_\Box\|_\infty \le 1.01 n \underline{\mathbf{u}}$, $\Box = x, y$.

- Can show equality valid even if one of the d_x, d_y absent.

- Forward error expression: $|fl(x^Ty) - x^Ty| \le \gamma_n \; |x|^T \; |y|$

with $0 \le \gamma_n \le 1.01 n \underline{\mathbf{u}}$.

- Elementwise absolute value $|x|$ and multiply $.*$ notation.

- Above assumes $n \underline{\mathbf{u}} \le .01$.
For $\underline{\mathbf{u}} = 2.0 \times 10^{-16}$, this holds for $n \le 4.5 \times 10^{13}$.

- Consequence for matrix products: ($A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{n \times p}$)

$$|fl(AB) - AB| \le \gamma_n \; |A||B|$$

- Another way to write the result (less precise) is

$$|fl(x^Ty) - x^Ty| \le \; n \; \underline{\mathbf{u}} \; |x|^T \; |y| + O(\underline{\mathbf{u}}^2)$$

✍D5 Assume you use single precision for which you have $\underline{\mathbf{u}} = 2. \times 10^{-6}$. What is the largest n for which $n\underline{\mathbf{u}} \le 0.01$ holds? Any conclusions for the use of single precision arithmetic?

✍D6 What does the main result on inner products imply for the case when $y = x$? [Contrast the relative accuracy you get in this case vs. the general case when $y \ne x$]

✍D7 Show for any x, y, there exist $\Delta x, \Delta y$ such that

$$fl(x^Ty) = (x + \Delta x)^T y, \quad \text{with} \quad |\Delta x| \le \gamma_n |x|$$
$$fl(x^Ty) = x^T (y + \Delta y), \quad \text{with} \quad |\Delta y| \le \gamma_n |y|$$

✍D8 (Continuation) Let A an $m \times n$ matrix, x an n-vector, and $y = Ax$. Show that there exist a matrix ΔA such

$$fl(y) = (A + \Delta A) x, \quad \text{with} \quad |\Delta A| \le \gamma_n |A|$$

✍D9 (Continuation) From the above derive a result about a column of the product of two matrices A and B. Does a similar result hold for the product AB as a whole?

Error Analysis for linear systems: Triangular case

➤ Recall

ALGORITHM : 1. *Back-Substitution algorithm*

For $i = n : -1 : 1$ *do:*
 $t := b_i$
 For $j = i + 1 : n$ *do*
  $t := t - a_{ij} x_j$
 End
 $x_i = t / a_{ii}$
End

$$\left.\begin{array}{l} \text{For } j = i+1:n \text{ do} \\ \quad t := t - a_{ij}x_j \\ \text{End} \end{array}\right\} \begin{array}{l} t := t - (a_{i,i+1:n}, x_{i+1:n}) \\ \quad = t - \text{an inner product} \end{array}$$

➤ We must require that each $a_{ii} \neq 0$

➤ Round-off error (use previous results for $(\cdot, \cdot)$)?

The computed solution $\hat{x}$ of the triangular system $Ux = b$ computed by the back-substitution algorithm satisfies:

$$(U + E)\hat{x} = b$$

with

$$|E| \leq n\ \underline{\mathbf{u}}\ |U| + O(\underline{\mathbf{u}}^2)$$

➤ Backward error analysis. Computed x solves a slightly perturbed system.

➤ Backward error not large in general. It is said that triangular solve is "backward stable".

Error Analysis for Gaussian Elimination

If no zero pivots are encountered during Gaussian elimination (no pivoting) then the computed factors $\hat{L}$ and $\hat{U}$ satisfy

$$\hat{L}\hat{U} = A + H$$

with

$$|H| \leq 3(n-1)\ \times\ \underline{\mathbf{u}}\ \left(|A| + |\hat{L}|\ |\hat{U}|\right) + O(\underline{\mathbf{u}}^2)$$

Solution $\hat{x}$ computed via $\hat{L}\hat{y} = b$ and $\hat{U}\hat{x} = \hat{y}$ is s. t.

$$(A + E)\hat{x} = b \text{ with}$$

$$|E| \leq n\underline{\mathbf{u}}\ \left(3|A|\ + 5\ |\hat{L}|\ |\hat{U}|\right) + O(\underline{\mathbf{u}}^2)$$

➤ "Backward" error estimate.

➤ $|\hat{L}|$ and $|\hat{U}|$ are not known in advance – they can be large.

➤ What if partial pivoting is used?

➤ Permutations introduce no errors. Equivalent to standard LU factorization on matrix PA.

➤ $|\hat{L}|$ is small since $l_{ij} \leq 1$. Therefore, only U is "uncertain"

➤ In practice partial pivoting is "stable" – i.e., it is highly unlikely to have a very large U.

Supplemental notes: Floating Point Arithmetic

In most computing systems, real numbers are represented in two parts: A mantissa and an exponent. If the representation is in the base β then:

$$x = \pm(.d_1 d_2 \cdots d_m)_\beta \beta^e$$

- $.d_1 d_2 \cdots d_m$ is a fraction in the base-β representation
- e is an integer - can be negative, positive or zero.
- Generally the form is normalized in that $d_1 \neq 0$.

Example: In base 10 (for illustration)

1. 1000.12345 can be written as

$$0.100012345_{10} \times 10^4$$

2. 0.000812345 can be written as

$$0.812345_{10} \times 10^{-3}$$

- Problem with floating point arithmetic: we have to live with limited precision.

Example: Assume that we have only 5 digits of accuray in the mantissa and 2 digits for the exponent (excluding sign).

$.d_1$	d_2	d_3	d_4	d_5	e_1	e_2

Try to add 1000.2 = .10002e+03 and 1.07 = .10700e+01:

1000.2 =

.1	0	0	0	2	0	4

;

1.07 =

.1	0	7	0	0	0	1

First task: align decimal points. The one with smallest exponent will be (internally) rewritten so its exponent matches the largest one:

$$1.07 = 0.000107 \times 10^4$$

Second task: add mantissas:

$$\begin{array}{rl} & 0.\ 1\ 0\ 0\ 0\ 2 \\ + & 0.\ 0\ 0\ 0\ 1\ 0\ 7 \\ \hline = & 0.\ 1\ 0\ 0\ 1\ 2\ 7 \end{array}$$

Third task:
round result. Result has 6 digits - can use only 5 so we can

- Chop result: $\boxed{.1\,|\,0\,|\,0\,|\,1\,|\,2}$;
- Round result: $\boxed{.1\,|\,0\,|\,0\,|\,1\,|\,3}$;

Fourth task:
Normalize result if needed (not needed here)

result with rounding: $\boxed{.1\,|\,0\,|\,0\,|\,1\,|\,3\,|\,0\,|\,4}$;

✍10 Redo the same thing with 7000.2 + 4000.3 or 6999.2 + 4000.3.

The IEEE standard

32 bit (Single precision) :

$\pm$	8 bits	$\leftarrow$ 23 bits $\rightarrow$
sign	exponent	mantissa

➤ Number is scaled so it is in the form $1.d_1 d_2 ... d_{23} \times 2^e$ - but leading one is not represented.

➤ e is between -126 and 127.

➤ [Here is why: Internally, exponent e is represented in "biased" form: what is stored is actually $c = e + 127$ – so the value c of exponent field is between 1 and 254. The values $c = 0$ and $c = 255$ are for special cases (0 and ∞)]

64 bit (Double precision) :

$\pm$	11 bits	$\leftarrow$ 52 bits $\rightarrow$
sign	exponent	mantissa

➤ Bias of 1023 so if e is the actual exponent the content of the exponent field is $c = e + 1023$

➤ Largest exponent: 1023; Smallest = -1022.

➤ $c = 0$ and $c = 2047$ (all ones) are again for 0 and ∞

➤ Including the hidden bit, mantissa has total of 53 bits (52 bits represented, one hidden).

➤ In single precision, mantissa has total of 24 bits (23 bits represented, one hidden).

✍11 Take the number 1.0 and see what will happen if you add $1/2, 1/4, ..., 2^{-i}$. Do not forget the hidden bit!

Hidden bit (Not represented)

Expon. $\downarrow$ $\leftarrow$ 52 bits $\rightarrow$

e	1	1	0	0	0	0	0	0	0	0	0	0
e	1	0	1	0	0	0	0	0	0	0	0	0
e	1	0	0	1	0	0	0	0	0	0	0	0

....

e	1	0	0	0	0	0	0	0	0	0	0	1
e	1	0	0	0	0	0	0	0	0	0	0	0

(Note: The 'e' part has 12 bits and includes the sign)

➤ Conclusion

$fl(1 + 2^{-52}) \neq 1$ but: $fl(1 + 2^{-53}) == 1$!!

Special Values

➤ Exponent field = 00000000000 (smallest possible value)
No hidden bit. All bits == 0 means exactly zero.

➤ Allow for unnormalized numbers,
leading to gradual underflow.

➤ Exponent field = 11111111111 (largest possible value)
Number represented is "Inf" "-Inf" or "NaN".

Recent trend: GPUs

- Graphics Processor Units: Very fast boards attached to CPUs for heavy-duty computing
- e.g., NVIDIA V100 can deliver 112 Teraflops (1 Teraflops = 10^{12} operations per second) for certain types of computations.
- Single precision much faster than double ...
- ... and there is also "half-precision" which is ≈ 16 times faster than standard 64bit arithmetic
- Used primarily for Deep-learning