

Welcome to MA580-001
CSC.

Numerical analysis and Scientific Computing.

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An example. Data fitting and interpolation.

t	t_0	t_1	...	t_m	$m+1$ data
$y(t)$	y_0	y_1		y_m	

Find $y(t)$ at any time.

One approach: (polynomial fitting) other trig func.

$$y(t) = a_0 + a_1 t + \dots + a_n t^n$$

Want to find $\{a_i\}_{i=0}^n$

Hopefully

$$y(t_i) = y_i, \quad i=0, 1, \dots, m$$

other
trig func.
 $\frac{\sin at}{\cos nt}$
 $\sum a_n \cos + b_n \sin$
 $y(t) \approx a_0 e^{bt}$
Pade

$$t = t_0: \quad y_0 = a_0 + a_1 t_0 + a_2 t_0^2 + \dots + a_n t_0^n$$

$$t = t_1: \quad y_1 = a_0 + a_1 t_1 + a_2 t_1^2 + \dots + a_n t_1^n$$

$$Ax = b$$

$$t = t_i \quad y_i = \sum_{j=0}^n a_j t_i^j$$

$$i = 0, 1, \dots, m$$

Matrix-vector form

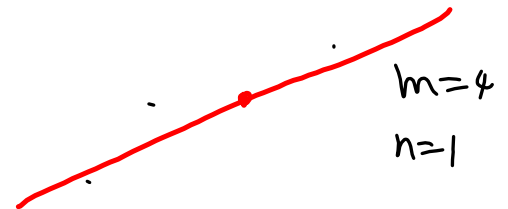
$$\underline{A} \underline{x} = \underline{b}$$

$$\begin{bmatrix} 1 & t_0 & t_0^2 & \dots & t_0^n \\ 1 & t_1 & t_1^2 & \dots & t_1^n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & t_m & t_m^2 & \dots & t_m^n \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_m \end{bmatrix}$$

(m+1) x (n+1)

$$n=0, \quad y(t) = a_0$$

$$n=1, \quad y(t) = a_0 + a_1 t$$



$n < m$, 'big data'; simple solution.

Q. Is there a classical solution to the problem? Can we find x^* such that

$Ax^* - b = 0$ In general, the answer is 'No'. There are too many constraints.

It's called an over-determined problem.

We will find the 'best' solution which is least squares solution.

$$n=0, \quad y(t) \approx a_0 = \left(\sum_{j=0}^m y_j \right) / (m+1)$$

The average?

$$n=m. \quad A \in \mathbb{R}^{(n+1) \times (n+1)}, \quad b \in \mathbb{R}^{n+1}. \quad Ax=b.$$

If $t_i \neq t_j$ if $i \neq j$, distinct sample points.

$$\det(A) \neq 0, \quad \det(A) = \prod_{i \neq j} (t_i - t_j) \neq 0$$

A^{-1} exist. There is a unique solution x^*
such that $Ax^* = b$

'Interpolation'



$n > m$ 'under-determined' $n = 3$

Not enough information to determine the $\{a_i\}$'s uniquely

$$\left. \begin{array}{l} m = 2 \\ n = 4 \\ 5 \text{ unknowns} \\ 3 \text{ equations} \end{array} \right\} \begin{cases} a_0 + a_1 t_0 + a_2 t_0^2 + a_3 t_0^3 + a_4 t_0^4 = y_0 \\ a_0 + a_1 t_1 + a_2 t_1^2 + a_3 t_1^3 + a_4 t_1^4 = y_1 \\ a_0 + a_1 t_2 + a_2 t_2^2 + a_3 t_2^3 + a_4 t_2^4 = y_2 \end{cases}$$

$$\begin{bmatrix} \text{---} \\ \text{---} \\ \text{---} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix} = \begin{bmatrix} y_0 \\ y_1 \\ y_2 \end{bmatrix}$$

SVD solution

There are infinite number

of x^* ,

x_{SVD}^* :

$$\min_{Ax^*=b} \|x^*\|_2, \text{ minimizes}$$

the two-norm of all possible solutions

Introduction: Continue.

What are our tasks in MATH580?

A math model: Data fitting & Interpolation

$$Ax = b, \quad A \in \mathbb{R}^{m \times n} \quad (m+1)(n+1)$$

- Wellposedness, existence/uniqueness / sensitivity Linear Algebra
- Numerical Analysis
 - Derive numerical methods using $\pm, \times, /$ and logic operation, include some packages
 - convergence/complexity
- Scientific computing
 - coding/debugging/validation
 - including round-off errors
 - Use packages

$m \geq n$

$$x = A \backslash b; \text{ is Matlab}$$

$$x = \text{pinv}(A) * b;$$

More expensive

$m < n$

$m = n$

$m > n$

$\mathbb{R}_C \Rightarrow$ Computer number systems: Floating point number system.

$x \in \mathbb{R} \longrightarrow fl(x) \quad \pi \neq fl(\pi)$

$fl(x) = \pm . d_1 d_2 \dots d_n \cdot \beta^s \longrightarrow$ exponential
 sign fraction base $0 \leq d_i \leq \beta - 1$

$\beta = 2$, binary

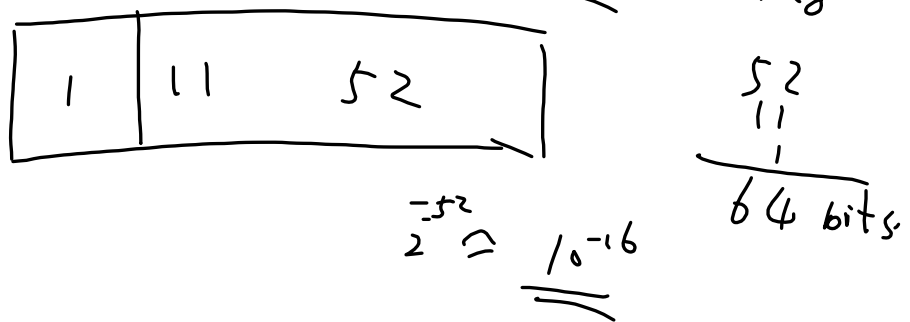
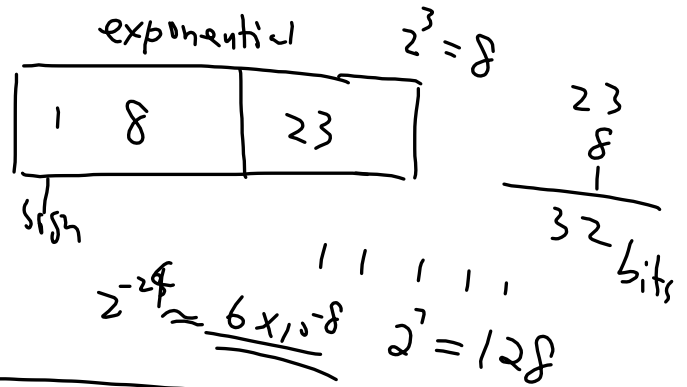
$\beta = 8$ octal

$\beta = 10$ decimal

$\beta = 16$ hexadecimal

64-bit

single precision $s_{min} \leq s \leq s_{max}$



Some examples of floating numbers

$- .1011 \cdot 2^5$ binary

$- .31416 \times 10^1$ ✓ $- .031416 \times 10^2$

Not unique! We should use the normalized

floating numbers. $x \neq 0, f(x) = \text{sign}(x) \cdot d_1 d_2 \dots$

$d_1 \neq 0$. In matlab $\tilde{x} = \text{sign}(x) \cdot d_1 d_2 \dots \dots d_n \cdot \beta^s$

$0.00001 \dots$ format short e $d_1 \neq 0$

long e

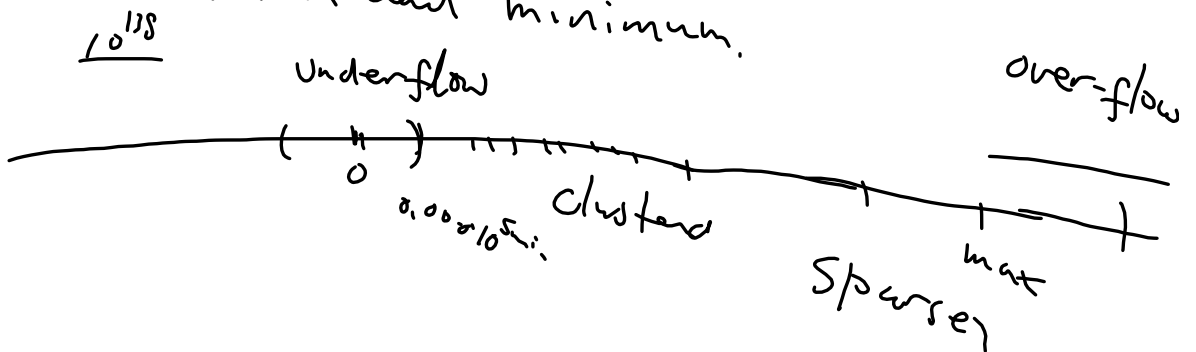
$0 = 0.00 \dots 0 \beta^0$

Properties of a computer number system.

- Finite numbers

Total = $2(\beta-1)\beta^{m-1}(S_{\max} - S_{\min} + 1) + 1$ ✓

- has maximum and minimum.



$\frac{f(x) \text{ or } f(y)}{0 \text{ + - } x \text{ } \frac{1}{\cdot}}$ may be out of computer system.

$$\frac{10^{13k}}{10^{13k}}$$

Usually underflow is not problem. simply put it as zero.

overflow means something is wrong. $\frac{y}{x}$
if x is not defined: double check!

$$\begin{array}{l} \text{Inf} \quad \text{NaN} \quad \lg(-5) \\ \frac{y}{x} \end{array} \quad \begin{array}{l} 10^{38} \\ \frac{10^{138}}{10^{138}} \end{array}$$

Most of time, a computer is adequate enough for many practical problem.

What's the best accuracy can we expect?

Single precision, 10^{-8}

double .. 10^{-16}

Round-off error analysis,

How do we measure errors.

$$x \rightarrow fl(x)$$

$$\pi \rightarrow fl(\pi)$$

Absolute error $x - fl(x)$ true - approximated

Ex: Error estimate for decimal = absolute error

$$x = 0.d_1 d_2 \dots d_n \overbrace{d_{n+1} \dots} \cdot 10^b$$

Round-off

$$fl(x) = \begin{cases} 0.d_1 d_2 \dots d_n \cdot 10^b & \text{if } d_{n+1} \geq 5 \\ 0.d_1 d_2 \dots (d_{n+1}) \cdot 10^b & \text{if } d_{n+1} < 5 \end{cases}$$

Truncating

rounding

$$x - fl(x) \text{ Varying with } x$$

$$|x - fl(x)|$$

Upper bound

$$\leq \begin{cases} 0.0 \dots 0 \overset{d_n}{5} 0 \dots 0 \cdot 10^b \dots 9999 \dots \\ 0.0 \dots 0 \overset{d_n}{5} 0 \dots 0 \cdot 10^b \end{cases}$$

$$\frac{1}{2} 10^{-n} \cdot 10^b$$

An upper bound