2.29 Numerical Fluid Mechanics
Fall 2011 – Lecture 2

REVIEW Lecture 1

1. Syllabus, Goals and Objectives
2. Introduction to CFD
3. From mathematical models to numerical simulations (1D Sphere in 1D flow)

   Continuum Model – Differential Equations

   => Difference Equations (often uses Taylor expansion and truncation)

   => Linear/Non-linear System of Equations

   => Numerical Solution (matrix inversion, eigenvalue problem, root finding, etc)
4. Error Types
   - Round-off error: due to representation by computers of numbers with a finite number of digits (significant digits)
   - Truncation error: due to approximation/truncation by numerical methods of "exact" mathematical operations/quantities
   - Other errors: model errors, data/parameter input errors, human errors.

REVIEW Lecture 1, Cont'd

- Approximation and round-off errors
  - Significant digits: Numbers that can be used with confidence
  - Absolute and relative errors $E_a = \hat{x}_a - \hat{x}\,, \quad \varepsilon_a = \frac{\hat{x}_a - \hat{x}}{\hat{x}_a}$
    - Iterative schemes and stop criterion: $|\varepsilon_a| = \left|\frac{\hat{x}_n - \hat{x}_{n-1}}{\hat{x}_n}\right| \leq \varepsilon_s$
  - For n digits: $\varepsilon_s = \frac{1}{2} 10^{-n}$

Numerical Fluid Mechanics – TODAY's Outline

- Approximation and round-off errors
  - Absolute and relative errors
  - Number representations
  - Arithmetic operations
  - Errors of arithmetic/numerical operations
  - Recursion algorithms (Heron, Horner's scheme, etc):
    - Order of computations matter

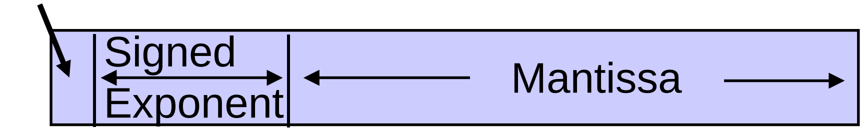
- Truncation Errors, Taylor Series and Error Analysis
  - Taylor series:
  - Use of Taylor Series to derive finite difference schemes (first-order Euler scheme and forward, backward and centered differences)
  - Error propagation – numerical stability
  - Error estimation
  - Error cancellation
  - Condition numbers

Reference: Chapra and Canale, Chaps 3.1-3.4 and 4.1-4.4

Number Representations

- Number Systems:
  - Base-10: $1{,}234_{10} = 1 \times 10^3 + 2 \times 10^2 + 3 \times 10^1 + 4 \times 10^0$
  - Computers (0/1): base-2 $1101_2 = 1 \times 2^3 + 1 \times 2^2 + 0 \times 2^1 + 1 \times 2^0 = 13_{10}$
- Integer Representation (signed magnitude method):
  - First bit is the sign (0,1), remaining bits used to store the number
  - For a 16-bits computer:
    - Example: -13_{10} = 1 0 0 0 0 0 0 0 0 0 0 0 1 1 0 1
    - Largest range of numbers: 2^{15}-1 largest number => -32,768 to 32,767 (from 0 to 111111111111111)
- Floating Number Representation

$$x = m\, b^e$$



m	Mantissa/Significand = fractional part
b	Base
e	Exponent

Floating Number Representation

Examples

Decimal $$0.00527 = 0.527_{10} \times 10^{-2_{10}}$$

Binary $$10.1_2 = 0.101_2 \times 2^{2_{10}} = 0.101_2 \times 2^{10_2}$$

Convention: Normalization of Mantissa m (so as to have no zeros on the left)

0.01234 => $0.1234\ 10^{-1}$

12.34 => $0.1234\ 10^{2}$

Decimal $$0.1 \leq m < 1.0$$

Binary $$0.1_2 = 0.5_{10} \leq m < 1.0$$

=> General $$b^{-1} \leq m < b^0$$

Example

(Chapra and Canale, pg 61)

Consider hypothetical Floating-Point machine in base-2

7-bits word =

- 1 for sign
- 3 for signed exp.
  (1 sign, 2 for exp.)
- 3 for mantissa

Largest and smallest positive number represented are ?

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Please see p.61 in:
Chapra, S., and R. Canale. *Numerical Methods for Engineers*. 6th ed. McGraw-Hill Higher Education, 2009, p. 61. ISBN: 9780073401065.

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Largest number is: $7 = 2^{(2+1)} (2^{-1}+ 2^{-2}+ 2^{-3})$

Sign nb	Sign exp	2^1	2^0	2^{-1}	2^{-2}	2^{-3}
0	0	1	1	1	1	1

Smallest positive number is: $0.5\ 2^{-3}$

Sign	Sign exp	2^1	2^0	2^{-1}	2^{-2}	2^{-3}
0	1	1	1	1	0	0

Consequence of Floating Point Reals

- Limited range of quantities can be represented
  - Min number (Underflow Error) and Max number (Overflow)
- Finite Number of quantities can be represented within the range (limited precision) => "**Quantizing errors**"
  - Quantizing errors treated either by round-off or chopping.
- Interval Δx between numbers increases as numbers grow in magnitude
  - For t = number of significant digits in mantissa and rounding,

$E = b^{1-t} =$ Machine Epsilon

Relative Error $$\frac{|\Delta x|}{|x|} \leq \frac{E}{2}$$

Absolute Error $$|\Delta x| \leq \frac{E}{2}|x|$$

```
%Determine machine epsilon in matlab
%
eps=1
while (eps+1>1)
  eps=eps/2;
end
eps*2
```

Arithmetic Operations

1. Addition and Subtraction

$$r_1 \pm r_2 = m_1 b^{e_1} \pm m_2 b^{e_2}$$

Shift mantissa of smallest number,

assuming $e_1 > e_2$

Result has exponent of largest number:

$$r_1 \pm r_2 = \left(m_1 \pm m_2 b^{e_2 - e_1} \right) b^{e_1} = m b^{e1}$$

Absolute Error

$$\bar{\epsilon} \leq \bar{\epsilon_1} + \bar{\epsilon_2}$$

Relative Error

$$\bar{\alpha} = \frac{|\bar{m} - m|}{|m|}$$

Unbounded for $m_1 \pm m_2 \rightarrow 0$

2. Multiplication and Division

$$r_1 \times r_2 = m_1 m_2 b^{e1+e2}$$

Multiplication:
Add exp, multiply mantissa, normalize and chop/round

$$m = m1m2 < 1$$

Division:
Subtract exp, divide mantissa, normalize and chop/round

$$0.1_2 \times 0.1_2 = 0.01_2$$

Relative Error

$$\bar{\alpha} \leq \bar{\alpha_1} + \bar{\alpha_2}$$

Bounded

Digital Arithmetics

Finite Mantissa Length

radd.m

Limited precision addition in MATLAB

```
function c = radd(a,b,n)
%
% function c = radd(a,b,n)
%
% Adds two real numbers a and b simulating an arithmetic unit with
% n significant digits, and rounding-off (not chopping-off) of numbers.
% If the inputs a and b provided do not have n digits, they are first
% rounded to n digits before being added.

%--- First determine signs
sa=sign(a);
sb=sign(b);

%--- Determine the largest number (exponent)
if (sa == 0)
    la=-200; %this makes sure that if sa==0, even if b is very small, it will have the largest exponent
else
la=ceil(log10(sa*a*(1+10^(-(n+1))))); %This determines the exponent on the base. Ceiling is used
                                      %since 0<log10(mantissa_base10)<=-1. The 10^etc. term just
                                      %properly increases the exponent estimated by 1 in the case
                                      %of a perfect log: i.e. log10(m b^e) is an integer,
                                      %mantissa is 0.1, hence log10(m)=-1, and
                                      %ceil(log10(m b^e(1+10^-(n+1))) ~< ceil(e +log10(m)+log10(1+10^-(n+1)))=e.
end
if (sb == 0)
    lb=-200;
else
    lb=ceil(log10(sb*b*(1+10^(-(n+1)))));
end
    lm=max(la,lb);
```

radd.m, continued

```
%--- Shift the two numbers magnitude to obtain two integers with n digits
f=10^(n);   %this is used in conjunction with the round function below
at=sa*round(f*sa*a/10^lm);  %sa*a/10^lm shifts the decimal point such that the number starts with 0.something
                            %the f*(*) then raises the number to a power 10^n, to get the desired accuracy
                            %of n digits above the decimal. After rounding to an integer, any figures that
                            %remain below are wiped out.
bt=sb*round(f*sb*b/10^lm);
% Check to see if another digit was added by the round. If yes, increase
% la (lb) and reset lm, at and bt.
ireset=0;
if ((at~=0) & (log10(at)>=n))
     la=la+1; ireset=1;
end
if ((bt~=0) & (log10(bt)>=n))
     lb=lb+1; ireset=1;
end
if (ireset)
     lm=max(la,lb);
     at=sa*round(f*sa*a/10^lm);
     bt=sb*round(f*sb*b/10^lm);
end
ct=at+bt;   %adds the two numbers
sc=sign(ct);

%The following accounts for the case when another digit is added when
%summing two numbers... ie. if the number of digits desired is only 3,
%then 999 +3 = 1002, but to keep only 3 digits, the 2 needs to be wiped out.
if (sc ~= 0)
    if (log10(sc*ct) >= n)
        ct=round(ct/10)*10;
%         'ct'
    end
end

%-----This basically reverses the operation on line 34,38
%  (it brings back the final number to its true magnitude)
c=ct*10^lm/f;
```

Matlab additions and quantizing effect

EXAMPLES

radd (100,4.9,1) = 100

radd (100,4.9,2) = 100

radd (100,4.9,3) = 105

```
>> radd (99.9,4.9,1)= 100
>> radd (99.9,4.9,2)= 100
>> radd (99.9,4.9,3) = 105
```

NOTE: Quantizing effect peculiarities

```
>> radd (0.095,-0.03,1) =0.06
>> radd (0.95,-0.3,1)= 1
```

Difference come from MATLAB round:

```
>> round(10^1*0.095/10^(-1))
    9
>> round(10^1*0.95/10^(0))
   10
```

Issues due to Digital Arithmetic

- Large number of additions/subtractions (recursion), e.g.
  - add 1 100,000 times vs.
  - add 0.00001 100,000 times.
- Adding large and small numbers
- Subtractive cancellation
  - Round-off errors induced when subtracting nearly equal numbers, e.g. roots of polynomials
- Smearing: occurs when terms in sum are larger than the sum
  - e.g. series of mixed/alternating signs
- Inner products: very common computation, but prone to round-off errors

Recursion: Heron's Device

Numerically evaluate square-root

$$\sqrt{s}\ , \quad s > 0$$

Initial guess x_0

$$x_0 \simeq \sqrt{s}$$

Test

$$x_0^2 < s \;\Rightarrow\; x_0 < \sqrt{s} \;\Rightarrow\; \frac{s}{x_0} > \sqrt{s}$$

$$x_0^2 > s \;\Rightarrow\; x_0 > \sqrt{s} \;\Rightarrow\; \frac{s}{x_0} < \sqrt{s}$$

Mean of guess and its reciprocal

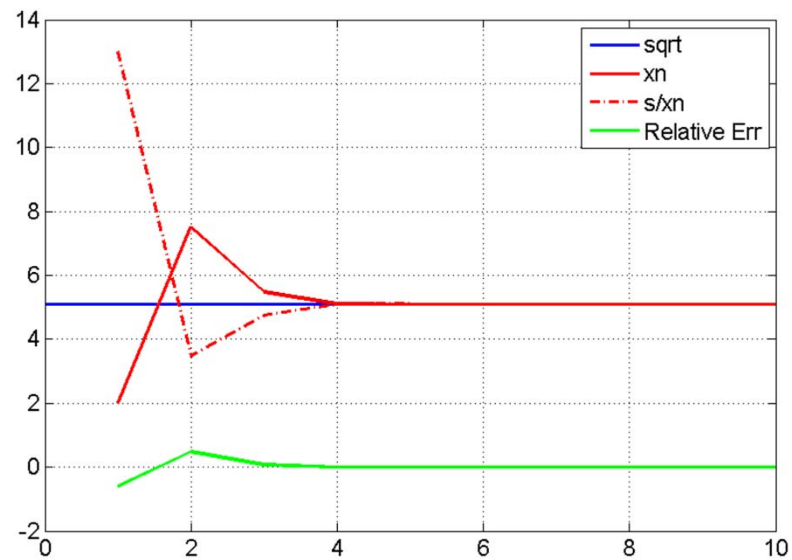
$$x_1 = \frac{1}{2}\left(x_0 + \frac{s}{x_0}\right)$$

Recursion Algorithm

$$x_{n+1} = \frac{1}{2}\left(x_n + \frac{s}{x_n}\right)$$

MATLAB script
heron.m

```
a=26;   %Number for which the sqrt is to be computed
n=10;   %Number of iteration in recursion
g=2;    %Initial guess
% Number of Digits
dig=5;
     sq(1)=g;
     for i=2:n
      sq(i)= 0.5*radd(sq(i-1),a/sq(i-1),dig);
     end
     '      i       value    '
     [ [1:n]' sq']
     hold off
     plot([0 n],[sqrt(a) sqrt(a)],'b')
     hold on
     plot(sq,'r')
     plot(a./sq,'r-.')
     plot((sq-sqrt(a))/sqrt(a),'g')
     legend('sqrt','xn','s/xn','Relative Err')
     grid on
```



Recursion: Horner's scheme to evaluate polynomials by recursive additions

Goal: Evaluate polynomial

$$
\begin{aligned}
p(z) &= a_0 z^3 + a_1 z^2 + a_2 z + a_3 \\
&= ((a_0 z + a_1) z + a_2)\, z + a_3
\end{aligned}
$$

Horner's Scheme

$$
\begin{array}{ccccc}
 & a_0 & a_1 & a_2 & a_3 \\
+ & & zb_0 & zb_1 & zb_2 \\
\hline
(b_0 = a_0) & b_0 & b_1 & b_2 & b_3
\end{array}
$$

$$p(z) = b_3$$

General order n

$$p(z) = a_0 z^n + a_1 z^{n-1} + \cdots + a_{n-1} z + a_n$$

Recurrence relation

$$b_0 = a_0 \,, \quad b_i = a_i + z b_{i-1} \,, \quad i = 1, \ldots n$$

$$\boxed{p(z) = b_n}$$

horner.m

```
% Horner's scheme
% for evaluating polynomials
a=[ 1 2 3 4 5 6 7 8 9 10 ];
n=length(a) -1 ;
z=1;
b=a(1);
% Note index shift for a
for i=1:n
    b=a(i+1)+ z*b;
end
p=b
```

```
>> horner

p =

    55
```

For home suggestion: utilize radd.m for all additions above and compare the error of Horner's scheme to that of a brute force summation, for both z negative/positive

Recursion: Order of Operations Matter

Tends to: 0 1

$$y = f(x) = \sum_{n=1}^{\infty} [x^n + b\sin[\pi/2 - \pi/10n] - c\cos[pi/(10(n+1))]]$$

If $x = 0.5\,,\quad b = 0\,,\quad c = 0 \Rightarrow y = 1.0$

recur.m

```
N=20; sum=0; sumr=0;
b=1; c=1; x=0.5;
xn=1;
% Number of significant digits in computations
dig=2;
ndiv=10;
for i=1:N
  a1=sin(pi/2-pi/(ndiv*i));
  a2=-cos(pi/(ndiv*(i+1)));
% Full matlab precision
  xn=xn*x;
  addr=xn+b*a1;
  addr=addr+c*a2;
  ar(i)=addr;
  sumr=sumr+addr;
  z(i)=sumr;
% additions with dig significant digits
  add=radd(xn,b*a1,dig);
  add=radd(add,c*a2,dig);
% add=radd(b*a1,c*a2,dig);
% add=radd(add,xn,dig);
  a(i)=add;
  sum=radd(sum,add,dig);
  y(i)=sum;
end
sumr
```

Result of small, but significant term 'destroyed' by subsequent addition and subtraction of almost equal, large numbers.

Remedy:
Change order of additions

recur.m Contd.

```
'      i       delta      Sum    delta(approx) Sum(approx)'
res=[[1:1:N]' ar' z' a' y']

hold off
a=plot(y,'b'); set(a,'LineWidth',2);
hold on
a=plot(z,'r'); set(a,'LineWidth',2);
a=plot(abs(z-y)./z,'g'); set(a,'LineWidth',2);
legend([ num2str(dig) ' digits'],'Exact','Error');
```

recur.m

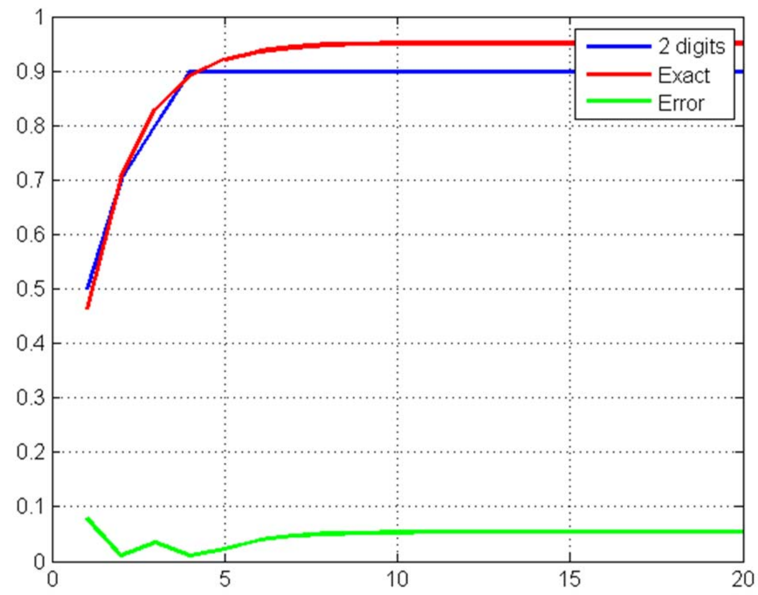
```
>> recur

b = 1; c = 1; x = 0.5;
dig=2

     i        delta       Sum     delta(approx) Sum(approx)

..\codes_2\recur.png
res =

    1.0000    0.4634    0.4634    0.5000    0.5000
    2.0000    0.2432    0.7065    0.2000    0.7000
    3.0000    0.1226    0.8291    0.1000    0.8000
    4.0000    0.0614    0.8905    0.1000    0.9000
    5.0000    0.0306    0.9212         0    0.9000
    6.0000    0.0153    0.9364         0    0.9000
    7.0000    0.0076    0.9440         0    0.9000
    8.0000    0.0037    0.9478         0    0.9000
    9.0000    0.0018    0.9496         0    0.9000
   10.0000    0.0009    0.9505         0    0.9000
   11.0000    0.0004    0.9509         0    0.9000
   12.0000    0.0002    0.9511         0    0.9000
   13.0000    0.0001    0.9512         0    0.9000
   14.0000    0.0000    0.9512         0    0.9000
   15.0000    0.0000    0.9512         0    0.9000
   16.0000   -0.0000    0.9512         0    0.9000
   17.0000   -0.0000    0.9512         0    0.9000
   18.0000   -0.0000    0.9512         0    0.9000
   19.0000   -0.0000    0.9512         0    0.9000
   20.0000   -0.0000    0.9512         0    0.9000
```



Error Propagation

Spherical Bessel Functions

ps: Bessel functions are only used as example, no need to know everything about them for this class.

Differential Equation

$$x^2\frac{d^2y}{dx^2} + 2x\frac{dy}{dx}(x^2 - n(n+1))y = 0$$

Solutions

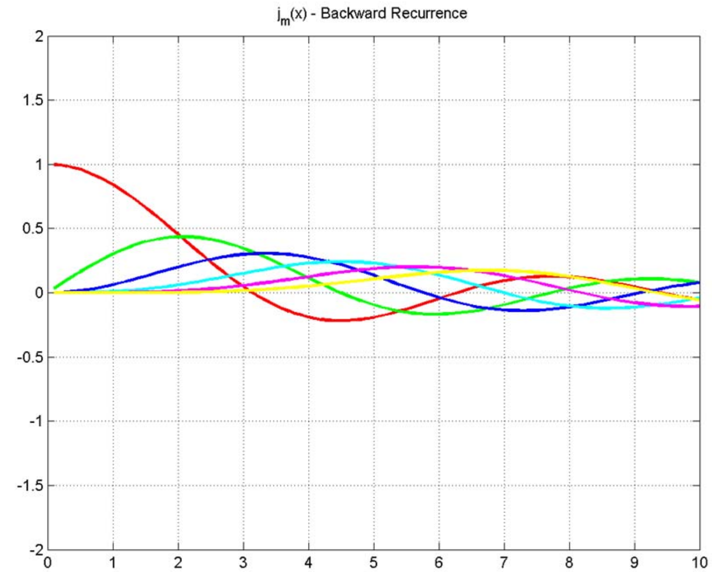
$$j_n(x) y_n(x)$$

n	$j_n(x)$	$y_n(x)$
0	$\frac{\sin x}{x}$	$-\frac{\cos x}{x}$
1	$\frac{\sin x}{x^2} - \frac{\cos x}{x}$	$-\frac{\cos x}{x^2} - \frac{\sin x}{x}$

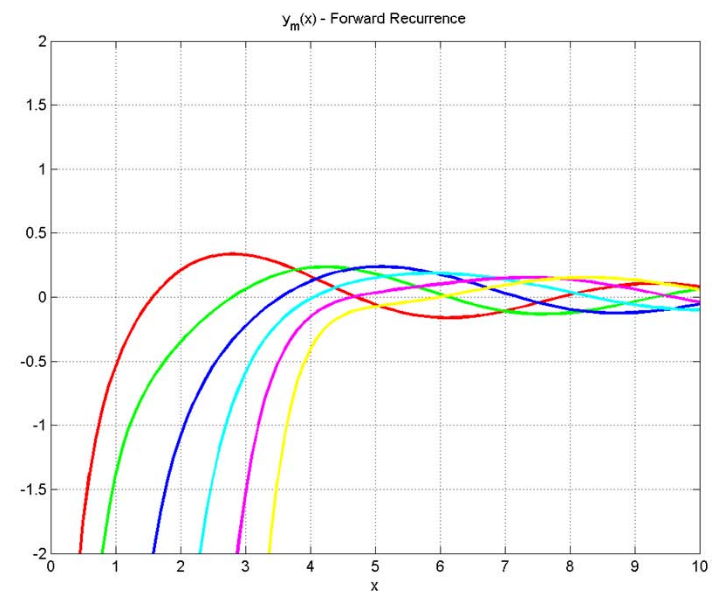
$$j_n(x) \to 0 \begin{cases} n \to \infty \\ x \to 0 \end{cases}$$

$$y_n(x) \to -\infty \begin{cases} n \to \infty \\ x \to 0 \end{cases}$$

$j_n(x)$



$y_n(x)$



Error Propagation

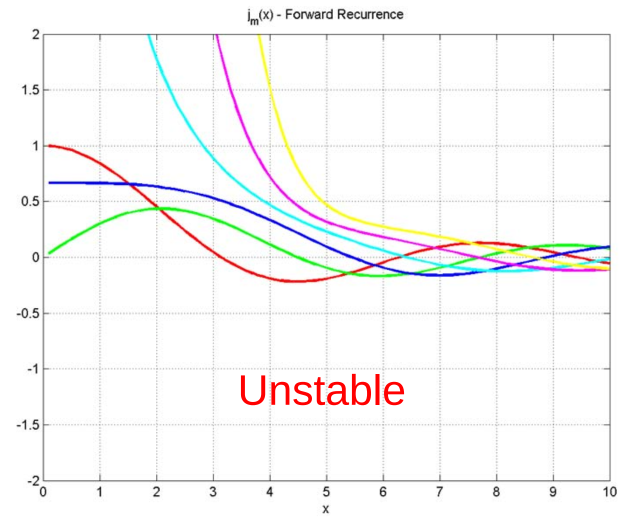
Spherical Bessel Functions

Forward Recurrence

$$j_{n+1}(x) = \frac{2n+1}{x} j_n(x) - j_{n-1}(x)$$

Forward Recurrence

$$\frac{2n+1}{x} j_n(x) \simeq j_{n-1}(x)$$



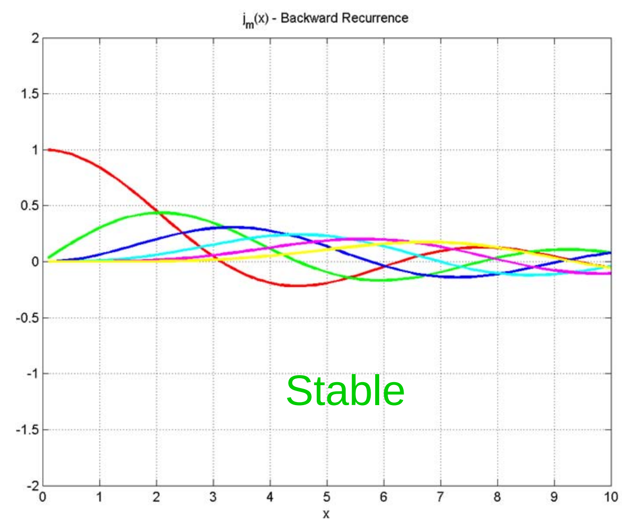
Backward Recurrence

$$j_{n-1}(x) = \frac{2n+1}{x} j_n(x) - j_{n+1}(x)$$

Miller's algorithm

$$j_N(x) = 1 \;,\; j_{N+1}(x) = 0 \;,\; j_0(x) = \frac{\sin x}{x}$$

with $N \sim x + 20$



Error Propagation Euler's Method

Differential Equation

$$\frac{dy}{dx} = f(x, y) \ , \ y_0 = p$$

Example

$$f(x, y) = x \ (y = x^2/2 + p)$$

Discretization

$$x_n = nh$$

Finite Difference (forward)

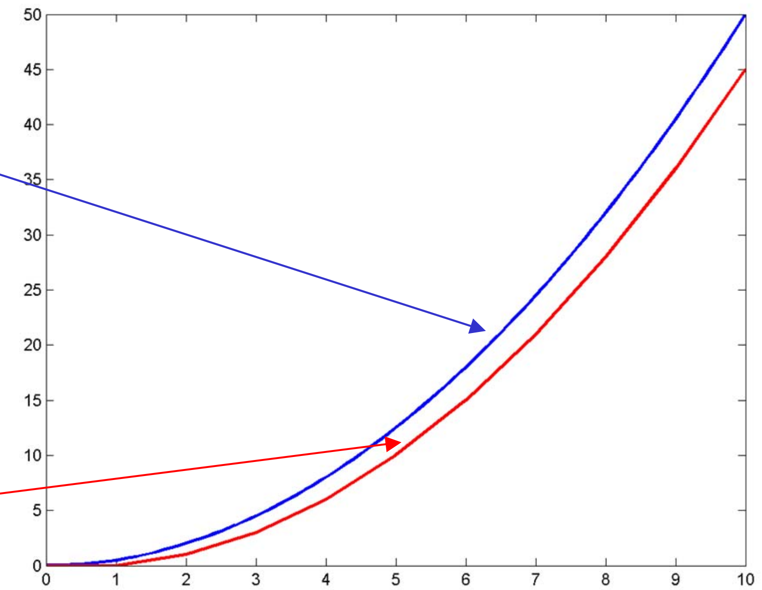
$$\frac{dy}{dx}|_{x=x_n} \simeq \frac{y_{n+1} - y_n}{h}$$

Recurrence

$$y_{n+1} = y_n + hf(nh, y)$$

Central Finite Difference

$$\frac{dy}{dx}|_{x=x_n} \simeq \frac{y_{n+1} - y_{n-1}}{2h}$$



euler.m

Error Analysis
Numerical Instability Example

Evaluate Integral

$$y_n = \int_0^1 \frac{x^n}{x+5} dx \;, n = 0, 2 \ldots \infty$$

Recurrence Relation: $y_n = \frac{1}{n} - 5y_{n-1}$

Proof :

$$y_n + 5y_{n-1} = \int_0^1 \frac{x^n + 5x^{n-1}}{x+5} dx = \int_0^1 \frac{x^{n-1}(x+5)}{x+5} dx = \int_0^1 x^{n-1} dx = \frac{1}{n}$$

3-digit Recurrence:

$$\begin{aligned}
y_0 &= \int_0^1 \frac{dx}{x+5} = [\log_e(x+5)]_0^1 = \log_e 6 - \log_e 5 = 0.182 \\
y1 &= 1 - 5y_0 = 1 - 0.910 \simeq 0.0090 \\
y2 &= 0.5 - 5y_1 \simeq 0.050 \\
y3 &= 0.333 - 5y_2 \simeq 0.083 \\
y4 &= 0.25 - 5y_3 \simeq -0.165
\end{aligned}$$

> y2 !! (y3)

< 0 !! (y4)

Backward Recurrence

$$y_{n-1} = \frac{1}{5n} - \frac{y_n}{5}$$

$$\begin{aligned}
y_{10} &\simeq y_9 \Rightarrow y_9 + 5y_9 = 0.1 \Rightarrow y_9 = 0.017 \\
y_8 &= 1/45 - y_9/5 = 0.019 \\
y_7 &= 1/40 - y_8/5 = 0.021 \\
y_6 &= 0.025 \\
&\cdot \\
&\cdot \\
&\cdot \\
y_1 &= 0.088 \\
y_0 &= 0.182
\end{aligned}$$

Correct

Exercise: Make MATLAB script

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