Computational Methods in Physics (PHY 365) FA23

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Lab 4

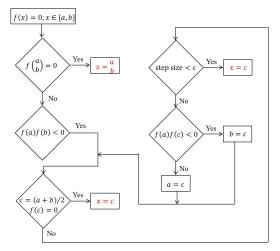


Figure: Flow chart for bisection method

Use the bisection algorithm to approximate the zero of the function $f(x) = 3x^2 - 5$, in the interval [1,2].

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■ Function

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■ Function

$$f = 3 * x 2 - 5;$$
 Error!!!

$$f = @ (x) 3 * x 2 - 5;$$

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■ Function

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 Error!!!
 $f = 0 (x) 3 * x ^2 - 5;$

- → @ creates a "function handle".
- \rightarrow A function handle is a data type that stores an association to a function.
- → Function handle can be used to construct anonymous functions or specify call back functions.

■ The interval

$$a = 1;$$

$$b = 2;$$

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■ Minimum interval length

$$\min_{\text{step}} = 10 - 4;$$

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```
\min_{\text{step}} = 10 - 4;
```

■ Checking for opposite signs at the endpoints

```
f_a = f(a);
f_b = f(b);
if f_a * f_b > 0
    error('Function has same sign at both endpoints.')
end
```

■ Calling the function

```
[ my_root , iterations ] = bisect_fun (f , a , b , min_step)
```

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```
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```

■ Displaying the result

```
formatspec = 'The calculated root is \%8.6f \n'; fprintf(formatspec, my root)
```

■ The function file (save with same name as the function)

```
function [my root, iterations] = bisect fun (f, a, b,
min step)
f = evalin ('base', 'f a');
iterations = 0;
step size = abs(a - b)/2;
x = (a + b)/2;
while step size > min step
  f x = f(x);
  if f x == 0
     iterations = iterations + 1;
     break
  end
```

```
% This code uses the bisection method to calculate roots of an equation
clear variables
close all
clc
format long
% The function
f = @(x) 3 * x .^2 - 5;
```

```
% The interval
a = 1;
b = 2;
% Minimum interval length
min step = 10 ^ - 4;
% Checking for opposite signs at the endpoints
fa = f(a);
fb = f(b);
if f a * f b > 0
   error('Function has same sign at both endpoints.')
end
```

```
% This is the function file for bisect code
function [my root, iterations] = bisect fun(f,a,b,min step)
f a = evalin('base', 'f a');
iterations = 0;
step size = abs(a - b) / 2;
x = (a + b) / 2;
```

```
while step_size > min_step

f_x = f(x);

if f_x == 0
    iterations = iterations + 1;

break
end

if f_a * f_x < 0
b = x;</pre>
```

```
else
        a = x;
    end
    x = (a + b) / 2;
    step size = abs(a - b) / 2;
    iterations = iterations + 1:
end
my root = x;
```

• Repeat the exercise for different functions, intervals and minimum step sizes.

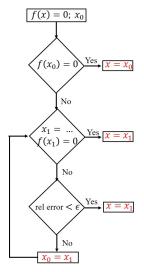


Figure: Flow chart for Newton-Raphson method

Use the Newton-Raphson method to approximate the zero of the function $f(x) = 3x^2 - 5$.

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■ Function

syms x

$$f = symfun (3 * x^2 - 5, x);$$

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■ Function

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■ Derivative of the function

$$f_{der} = diff(f, x);$$

Use the Newton-Raphson method to approximate the zero of the function $f(x) = 3x^2 - 5$.

■ Function

$$f = symfun (3 * x^2 - 5, x);$$

■ Derivative of the function

$$f_{der} = diff(f, x);$$

■ The initial guess

$$x_0 = 1;$$

■ Minimum error min_err = 10^-4;

- Minimum error min err = 10^-4;
- Calling the function

```
[x\_root, iterations] = new\_raph\_fun (f, f\_der, x\_0, min\_err);
```

- Minimum error min err = 10^-4;
- Calling the function

```
[x_root , iterations] = new_raph_fun (f , f_der , x_0 ,
min_err);
```

■ Displaying the result

```
fprintf ('\n')
disp ( ['Itertions = ', num2str(iterations) ] )
fprintf ('\n Root = \%3.7f \setminus n', x root)
```

■ The function file

```
function [x root, iterations] = new raph fun (f, f der,
x 0, min err)
x \text{ old} = x 0;
rel err = 1;
iterations = 0;
while rel err > min err
   f \times old = double (subs (f, x old));
   f der x old = double (subs (f der, x old));
   x \text{ new} = x \text{ old} - f x \text{ old} / f \text{ der } x \text{ old};
```

```
rel_err = abs (x_new - x_old);
x_old = x_new;
iterations = iterations + 1;
end
x_root = x_new;
```

```
% The function
syms x
f = symfun(3 * x ^ 2 - 5, x);
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
% Derivative of the function
f der = diff(f,x);
99999999999999999999999999999999999
% The initial guess
x 0 = 1.5;
% Minimum error
min err = 10 ^ -4;
```

```
% Calling the function
[x_root,iterations] = new_raph_fun(f,f_der,x_0,min_err);
% Displaying the result
fprintf('\n')
disp(['Itertions = ', num2str(iterations)])
fprintf('\n Root = %3.6f \n', x root)
```

```
function [x_root,iterations] = new_raph_fun(f,f_der,x_0,min_err)
 x \text{ old} = x 0;
 rel_err = 1;
 iterations = 0;
while rel_err > min_err
     f x old = double(subs(f, x old));
      f der x old = double(subs(f der,x old));
```

```
x_new = x_old - f_x_old / f_der_x_old;
rel_err = abs(x_new - x_old);
x_old = x_new;
iterations = iterations + 1;
-end
-x_root = x_new;
```

MATLAB fzero function

- fzero calculates root of nonlinear function.
- fzero cannot find a root of a function such as x^2 .
- x = fzero (fun, x0) tries to find a point x where fun (x) = 0.
- The solution is where fun (x) changes sign.

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- The solution is where fun (x) changes sign.
- Root from one point

fun = @ (x) exp (
$$-3 * x$$
) $-5 * x ^3 + 20$; % function $x0 = 3$; % initial point $x = fzero (fun ,x0)$;

MATLAB fzero function

■ Root within an interval

fun = @ (x) x
$$\hat{.}$$
 5 - 3 * x $\hat{.}$ 2 + 1;
x_int = [1,2]; % interval
x = fzero (fun, x_int)

MATLAB fsolve function

- x = fsolve (fun , x0) starts at x0 and tries to solve the equations fun (x) = 0, an array of zeros.
- \mathbf{x} = fsolve (fun, x0, options) solves the equations with the optimization options specified in options.
- [x , fval] = fsolve (___), for any syntax, returns the value of the objective function fun at the solution x.

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■ Example

fun = @ (x) exp (
$$-3 * x$$
) $-5 * x ^3 + 20$; % function $x0 = 3$; % initial point [x , fval] = fsolve (fun , x0);

References

- https://www.codesansar.com/numerical-methods/ bisection-method-using-matlab-output.html
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