

## Nonlinear Rootfinding (Introduction)

# Introduction

# Problem Statement

## Rootfinding Problem

Given a continuous scalar function of a scalar variable, find a real number  $r$  such that  $f(r) = 0$ .

- $r$  is a **root** of the function  $f$ .
- The formulation  $f(x) = 0$  is general enough; e.g., to solve  $g(x) = h(x)$ , set  $f = g - h$  and find a root of  $f$ .

# Iterative Methods

- Unlike the earlier linear problems, the root cannot be produced in a finite number of operations.
- Rather, a sequence of approximations that formally converge to the root is pursued.

**Iteration Strategy for Rootfinding.** To find the root of  $f$ :

- 1 Start with an initial iterate, say  $x_0$ .
- 2 Generate a sequence of iterates  $x_1, x_2, \dots$  using an *iteration algorithm* of the form

$$\underline{x_{k+1}} = \underline{g}(x_k), \quad k = 0, 1, \dots$$

- 3 Continue the iteration process until you find an  $x_i$  such that  $f(x_i) = 0$ . (In practice, continue until some member of the sequence seems to be “good enough”.)

# MATLAB's FZERO

**fzero** is MATLAB's general purpose rootfinding tool.

## Syntax:

```
x_zero = fzero( <function>, <initial iterate> )  
x_zero = fzero( <function>, <initial interval> )  
[x_zero, fx_zero] = ....
```

root  $r$

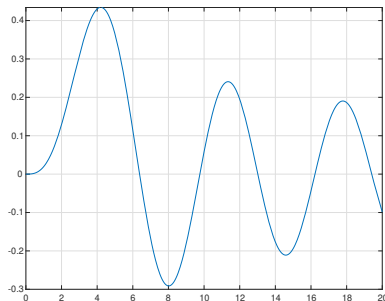
$f(r)$

# Example

The roots of  $J_m$ , a Bessel function of the first kind, is found by

- Plot the function.
- Find approximate locations of roots.

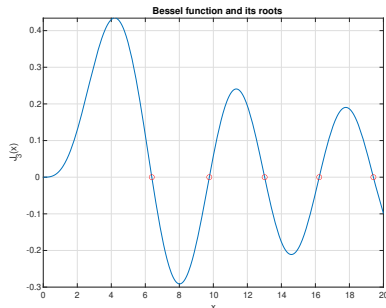
```
J3 = @(x) besselj(3,x);  
fplot(J3,[0 20])  
grid on  
guess = [6,10,13,16,19];
```



## Example (cont')

- Then use `fzero` to locate the roots:

```
omega = zeros(size(guess));  
for j = 1:length(guess)  
    omega(j) = fzero(J3,guess(j));  
end  
hold on  
plot(omega,J3(omega),'ro')
```



# Conditioning

- Sensitivity of the rootfinding problem can be measured in terms of the condition number:

$$(\text{absolute condition number}) = \frac{|\text{abs. error in output}|}{|\text{abs. error in input}|},$$

where, in the context of finding roots of  $f$ ,

- input:  $f$  (function)
- output:  $r$  (root)
- Denote the changes by:
  - error/change in input:  $\epsilon g$ , where  $\epsilon > 0$  is small  $(f \mapsto f + \epsilon g)$
  - error/change in output:  $\Delta r$   $(r \mapsto r + \Delta r)$



- The *perturbed equation*

$$f(r + \Delta r) + \epsilon g(r + \Delta r) = 0$$

is linearized to (Taylor expansion)

$$f(r) + f'(r)\Delta r + g(r)\epsilon + g'(r)\epsilon\Delta r \approx 0,$$

ignoring  $O((\Delta r)^2)$  terms<sup>1</sup>.

- Since  $f(r) = 0$ , we solve for  $\Delta r$  to get

$$\Delta r \approx -\epsilon \frac{g(r)}{f'(r) + \epsilon g'(r)} \approx -\epsilon \frac{g(r)}{f'(r)},$$

for small  $\epsilon$  compared with  $f'(r)$ .

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<sup>1</sup>That is, terms involving  $(\Delta r)^2$  and higher powers of  $\Delta r$

- Therefore, the absolute condition number of the rootfinding problem is

$$\kappa_{f \mapsto r} = \frac{1}{|f'(r)|},$$

which implies that the problem is highly sensitive whenever  $f'(r) \approx 0$ .

- In other words, if  $|f'|$  is small at the root, a computed *root estimate* may involve large errors.

# Residual and Backward Error

- Without knowing the exact root, we cannot compute the error.
- But the **residual** of a root estimate  $\tilde{r}$  can be computed:

$$(\text{residual}) = f(\tilde{r}).$$

- Small residual *might* be associated with a small error.
- The residual  $f(\tilde{r})$  is the *backward error* of the estimate.

# Multiple Roots

## Definition 1 (Multiplicity of Roots)

Assume that  $r$  is a root of the differentiable function  $f$ . Then if

$$0 = f(r) = f'(r) = \dots = f^{(m-1)}(r) \quad \text{but} \quad f^{(m)}(r) \neq 0,$$

we say that  $f$  has a root of **multiplicity**  $m$  at  $r$ .

- We say that  $f$  has a **multiple root** at  $r$  if the multiplicity is greater than 1.
- A root is called **simple** if its multiplicity is 1.
- If  $r$  is a multiple root, the condition number is infinite.
- Even if  $r$  is a simple root, we expect difficulty in numerical computation if  $f'(r) \approx 0$ .