Numerical methods Roots finding

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Numerical methods

August 21, 2018 1 / 33

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- 1 Incremental search method
  - Bisection method
    - Stopping inequalities
- 3 Fixed point method
- 4 Newton Raphson method
- 5 Error analysis for iterative methods
- 6 Newton Raphson (single variable)
- 🕖 Newton Raphson (multivariate)

## Incremental search method



Figure: Incremental search method.

The choice of the increment size can influence the results.

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## Bisection method

Bisection method is based on the Intermediate Value Theorem.

#### Intermediate Value Theorem

If f is continuous of a closed interval [a, b], and u is any number between f(a) and f(b) inclusive, there is at least one number  $c \in [a, b]$  so that f(c) = u.



Figure: Intermediate value theorem representation.

See: Intermediate Value Theorem - Khan Academy

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## Bisection method

To begin, let p be the middle point of the interval [a, b]:

$$p_1 = \frac{a+b}{2} \tag{1}$$

If  $f(p_1) = 0$ ,  $p = p_0$ , and "That's all folks!" If  $f(p_1) \neq 0$ : If  $sign(f(p_1)) = sign(f(a))$ ,  $a = p_1$ If  $sign(f(p_1)) = sign(f(b))$ ,  $b = p_1$ Then reapply the process to the new interval [a, b].

#### Bracketing methods

**Bracketing methods** are based on two initial guesses that "bracket" the root. If f(x) is a real and continuous in the interval  $[x_l, x_u]$  and

$$f(x_l)f(x_u) < 0 \tag{2}$$

then there is at least one real root between  $x_l$  and  $x_u$ 

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## Bisection method



Figure: Representation of bisection method.

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## Stopping inequalities

Typical stopping inequalities:

$$|p_n - p_{n-1}| < \varepsilon \tag{3}$$

$$\frac{|p_n - p_{n-1}|}{|p_n|} < \varepsilon, \quad p_n \neq 0$$

$$|f(p_n)| < \varepsilon$$
(4)

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- 31

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## Fixed-point method

The number p is a fixed point for a given function g if g(p) = p.

#### Theorem

If  $g \in C[a, b]$  and  $g(x) \in [a, b]$  for all  $x \in [a, b]$ , then g has at least one fixed point on [a, b].

If, in addition, g'(x) exists on [a,b] and a positive constant k > 1 exists with |g'(x)| < k, then there is exactly one fixed point in [a,b].



Figure: Fixed point for a function.

## Fixed-point method



Figure: Fixed point method representation.

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## Fixed-point method - Algorithm

- **INPUT** initial approximation  $p_0$ ; tolerance *TOL*; maximum number of iterations  $N_0$ .
- **OUTPUT** approximate solution *p* or message of failure.
- Step 1 Set i = 1.
- Step 2 While  $i \leq N_0$  do Steps 3–6.
  - Step 3 Set  $p = g(p_0)$ . (Compute  $p_i$ .)
  - Step 4 If  $|p p_0| < TOL$  then OUTPUT (p); (The procedure was successful.) STOP.
  - *Step 5* Set i = i + 1.
  - Step 6 Set  $p_0 = p$ . (Update  $p_0$ .)
- Step 7 OUTPUT ('The method failed after  $N_0$  iterations,  $N_0 = ', N_0$ ); (*The procedure was unsuccessful.*) STOP.

#### Figure: Fixed point algorithm.

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#### Newton Raphson method

Taylor polynomial for f(x) expanded about  $p_0$  and evaluated at x = p

$$f(p) = f(p_0) + (p - p_0)f'(p_0) + \frac{(p - p_0)^2}{2}f''(\xi)$$
(6)

where  $\xi \in [p_0, p]$ . Taking a first order approximation:

$$0 \approx f(p_0) + (p - p_0)f'(p_0) \tag{7}$$

$$p \approx p_0 - \frac{f(p_0)}{f'(p_0)}$$
 (8)

For an iterative process, we have:

$$p_n = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})}, \quad n \ge 1$$
 (9)

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## Newton Raphson



Figure: Representation of Newton Raphson method.

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Image: A matrix and a matrix

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#### Newton Raphson - Algorithm

- **INPUT** initial approximation  $p_0$ ; tolerance *TOL*; maximum number of iterations  $N_0$ .
- OUTPUT approximate solution p or message of failure.
- Step 1 Set i = 1.
- Step 2 While  $i \leq N_0$  do Steps 3–6.
  - **Step 3** Set  $p = p_0 f(p_0)/f'(p_0)$ . (Compute  $p_i$ .)
  - Step 4 If  $|p p_0| < TOL$  then OUTPUT (p); (The procedure was successful.) STOP.
  - *Step 5* Set i = i + 1.
  - Step 6 Set  $p_0 = p$ . (Update  $p_0$ .)
- Step 7 OUTPUT ('The method failed after  $N_0$  iterations,  $N_0 = ', N_0$ ); (*The procedure was unsuccessful.*) STOP.

#### Figure: Newton Raphson algorithm.

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#### Secant method

To circumvent the problem of derivative evaluation at each approximation in Newton's method, the Secant method gives an alternative. By definition:

$$f'(p_{n-1}) = \lim \frac{f(x) - f(p_{n-1})}{x - p_{n-1}}$$
(10)

Considering  $p_{n-2}$  is close to  $p_{n-1}$ , so:

$$f'(p_{n-1}) \approx \frac{f(p_{n-1}) - f(p_{n-2})}{p_{n-1} - p_{n-2}}$$
(11)

Using the Newton formula with this new derivative approximation, we obtain:

$$p_n = p_{n-1} - \frac{f(p_{n-1})(p_{n-1} - p_{n-2})}{f(p_{n-1}) - f(p_{n-2})}$$
(12)

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## Secant method



Figure: Secant method representation.

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Numerical methods

August 21, 2018 15 / 33

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## Secant method - Algorithm

- **INPUT** initial approximations  $p_0, p_1$ ; tolerance *TOL*; maximum number of iterations  $N_0$ .
- OUTPUT approximate solution p or message of failure.
- Step 1 Set i = 2;  $q_0 = f(p_0)$ ;  $q_1 = f(p_1)$ . Step 2 While  $i \le N_0$  do Steps 3–6. Step 3 Set  $p = p_1 - q_1(p_1 - p_0)/(q_1 - q_0)$ . (Compute  $p_{i\cdot}$ ) Step 4 If  $|p - p_1| < TOL$  then OUTPUT (p); (The procedure was successful.) STOP. Step 5 Set i = i + 1. Step 6 Set  $p_0 = p_1$ ; (Update  $p_0, q_0, p_1, q_1$ .)  $q_0 = q_1$ ;  $p_1 = p$ ;  $q_1 = f(p)$ .
- Step 7 OUTPUT ('The method failed after  $N_0$  iterations,  $N_0 = ', N_0$ ); (The procedure was unsuccessful.) STOP.

#### Figure: Secant method algorithm.

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Suppose  $\{p_n\}_{n=0}^{\infty}$  is a sequence that converges to p, with  $p_n \neq p$  for all n. If positive constants  $\lambda$  and  $\alpha$  exists with

$$\lim_{n \to \infty} \frac{|p_{n+1} - p_n|}{|p_n - p|^{\alpha}} = \lambda$$
(13)

then  $\{p_n\}_{n=0}^{\infty}$  converges to p of order  $\alpha$ , with asymptotic error constant  $\lambda$ .

## Newton Raphson (single variable)

Taylor polynomial for f(x) expanded about  $p_0$  and evaluated at x = p

$$f(p) = f(p_0) + (p - p_0)f'(p_0) + \frac{(p - p_0)^2}{2}f''(\xi)$$
(14)

where  $\xi \in [p_0, p]$ . Taking a first order approximation:

$$0 \approx f(p_0) + (p - p_0)f'(p_0)$$
(15)

$$p \approx p_0 - \frac{f(p_0)}{f'(p_0)}$$
 (16)

For an iterative process, we have:

$$p_n = p_{n-1} - \frac{f(p_{n-1})}{f'(p_{n-1})}, \quad n \ge 1$$
(17)

## Newton Raphson (single variable)



Figure: Representation of Newton Raphson method.

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The method described for 1D functions can be generalized for a system of non-linear equations:

$$f_1(\mathbf{x}) = 0$$
$$f_2(\mathbf{x}) = 0$$
$$\dots$$
$$f_N(\mathbf{x}) = 0$$

where

$$\mathbf{x} = \begin{bmatrix} x_1 & x_2 & \cdots & x_N \end{bmatrix}^T \tag{18}$$

Defining a function vector:

$$\mathbf{f}(\mathbf{x}) = \begin{bmatrix} f_1(\mathbf{x}) & f_2(\mathbf{x}) & \cdots & f_N(\mathbf{x}) \end{bmatrix}$$
(19)

The system can be rewritten as:

$$f(\mathbf{x}) = 0 \tag{20}$$
Numerical methods August 21, 2018 20 / 33

Considering N = 2 (2D problem), the multidimensional equation can be geometrically interpreted as:



Figure: Visualization of the root finding problem in 2D.

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The Taylor expansion for each function  $f_i$  can be written as:

$$f_i(\mathbf{x} + \delta \mathbf{x}) = f_i(\mathbf{x}) + \sum_{j=1}^N \frac{\partial f_i(x_j)}{\partial x_j} + O(\delta \mathbf{x}^2) \approx f_i(\mathbf{x}) + \sum_{j=1}^N \frac{\partial f_i(x_j)}{\partial x_j} \delta \mathbf{x}$$
(21)

In the vector form, the above equation can be written as:

$$\mathbf{f}(\mathbf{x} + \delta \mathbf{x}) = \mathbf{f}(\mathbf{x}) + \mathbf{J}(\mathbf{x}) \,\delta \mathbf{x}$$
(22)

where  $\mathbf{J}(\mathbf{x})$  is the Jacobian matrix, which is defined as:

$$\mathbf{J}(\mathbf{x}) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_N}{\partial x_1} & \cdots & \frac{\partial f_N}{\partial x_N} \end{bmatrix}$$
(23)

Assuming  $f(x + \delta x) = 0$ , the roots are  $x + \delta x$ , where  $\delta x$  can be obtained from:

$$\mathbf{f}(\mathbf{x} + \delta \mathbf{x}) = \mathbf{f}(\mathbf{x}) + \mathbf{J}(\mathbf{x}) \,\delta \mathbf{x} \implies (24)$$

$$\delta \mathbf{x} = \mathbf{J}(\mathbf{x})^{-1}[\mathbf{f}(\mathbf{x} + \delta \mathbf{x}) - \mathbf{f}(\mathbf{x})] = -\mathbf{J}(\mathbf{x})^{-1}\mathbf{f}(\mathbf{x})$$
(25)

And, from an starting point x:

$$\mathbf{x} + \delta \mathbf{x} = \mathbf{x} - \mathbf{J}(\mathbf{x})^{-1} \mathbf{f}(\mathbf{x})$$
(26)

For nonlinear equations, the result above is only an approximation:

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \delta \mathbf{x}_k = \mathbf{x}_k - \mathbf{J}(\mathbf{x}_k)^{-1} \mathbf{f}(\mathbf{x}_k)$$
(27)

#### Example 1

Computes the roots of:

$$\begin{cases} x_1^2 - 2x_1 + x_2 + 7 = 0\\ 3x_1 - x_2 + 1 = 0 \end{cases}$$

Starting point:  $\mathbf{x} = \begin{bmatrix} 1.00 & 1.00 \end{bmatrix}^T$ 

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#### Example 2

Determine the points of intersection between the circle  $x^2 + y^2 = 3$  and the hyperbola xy = 1Starting point: x = 0.5; y = 1.5

Solution:  $\pm (0.618, 1.618)$  and  $\pm (1.618, 0.618)$ 

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#### Example 3

Computes the roots of:

$$\begin{cases} 3x_1 - \cos(x_2x_3) - 3/2 = 0\\ 4x_1^2 - 625x_2^2 + 2x_3 - 1 = 0\\ 20x_3 + \exp(-x_1x_2) + 9 \end{cases}$$

Starting point:  $\mathbf{x} = [1.00 \ 1.00 \ 1.00]^T$ 

Solution:  $x = [0.833282 \quad 0.035335 \quad -0.498549]^T$ 

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#### Exercise 1

The natural frequencies of a uniform cantilever beam are related to the roots  $\beta_i$  of the frequency equation  $f(\beta) = \cosh \beta \cos \beta + 1 = 0$ , where

$$\beta_i^4 = (2\pi f_i)^2 \frac{mL^3}{EI}$$

 $f_i = i$ th natural frequency (cps)

m = mass of the beam

$$L =$$
length of the beam

E =modulus of elasticity

I =moment of inertia of the cross section

Determine the lowest two frequencies of a steel beam 0.9 m. long, with a rectangular cross section 25 mm wide and 2.5 mm in. high. The mass density of steel is 7850 kg/m<sup>3</sup> and E = 200 GPa.

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#### Exercises Exercise 2

# $\frac{\frac{L}{2}}{\text{Length} = s} = \frac{L}{0}$



$$\sigma_{\rm max} = \sigma_0 \cosh \beta$$

where

 $\beta = \frac{\gamma L}{2\sigma_0}$   $\sigma_0 = \text{tensile stress in the cable at } O$   $\gamma = \text{weight of the cable per unit volume}$ L = horizontal span of the cable

The length to span ratio of the cable is related to  $\beta$  by

$$\frac{s}{L} = \frac{1}{\beta} \sinh \beta$$

Find  $\sigma_{\text{max}}$  if  $\gamma = 77 \times 10^3 \text{ N/m}^3$  (steel), L = 1000 m and s = 1100 m.

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#### Exercise 3



Bernoulli's equation for fluid flow in an open channel with a small bump is

$$\frac{Q^2}{2gb^2h_0^2} + h_0 = \frac{Q^2}{2gb^2h^2} + h + H$$

where

 $Q = 1.2 \text{ m}^3/\text{s} = \text{volume rate of flow}$   $g = 9.81 \text{ m/s}^2 = \text{gravitational acceleration}$  b = 1.8 m = width of channel  $h_0 = 0.6 \text{ m} = \text{upstream water level}$  H = 0.075 m = height of bumph = water level above the bump

Determine h.

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#### Exercise 4



The figure shows the thermodynamic cycle of an engine. The efficiency of this engine for monoatomic gas is

$$\eta = \frac{\ln(T_2/T_1) - (1 - T_1/T_2)}{\ln(T_2/T_1) + (1 - T_1/T_2)/(\gamma - 1)}$$

where *T* is the absolute temperature and  $\gamma = 5/3$ . Find  $T_2/T_1$  that results in 30% efficiency ( $\eta = 0.3$ ).

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#### Exercise 5

■ The equations

 $\sin x + 3\cos x - 2 = 0$  $\cos x - \sin y + 0.2 = 0$ 

have a solution in the vicinity of the point (1, 1). Use the Newton–Raphson method to refine the solution.

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#### Exercise 6



A projectile is launched at *O* with the velocity *v* at the angle  $\theta$  to the horizontal. The parametric equations of the trajectory are

$$x = (v\cos\theta)t$$
$$y = -\frac{1}{2}gt^{2} + (v\sin\theta)t$$

where *t* is the time measured from the instant of launch, and  $g = 9.81 \text{ m/s}^2$  represents the gravitational acceleration. If the projectile is to hit the target at the 45° angle shown in the figure, determine v,  $\theta$  and the time of flight.

#### Exercise 7

■ The equation of a circle is

$$(x-a)^2 + (y-b)^2 = R^2$$

where R is the radius and (a, b) are the coordinates of the center. If the coordinates of three points on the circle are

x	8.21	0.34	5.96
y	0.00	6.62	-1.12

determine R, a and b.

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