# Numerical methods Roots finding 

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## Incremental search method



Figure: Incremental search method.

The choice of the increment size can influence the results.

## 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

## Bisection method

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

$$
\begin{equation*}
p_{1}=\frac{a+b}{2} \tag{1}
\end{equation*}
$$

If $f\left(p_{1}\right)=0, p=p_{0}$, and "That's all folks!"
If $f\left(p_{1}\right) \neq 0$ :

$$
\begin{aligned}
& \text { If } \operatorname{sign}\left(f\left(p_{1}\right)\right)=\operatorname{sign}(f(a)), a=p_{1} \\
& \text { If } \operatorname{sign}\left(f\left(p_{1}\right)\right)=\operatorname{sign}(f(b)), b=p_{1}
\end{aligned}
$$

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 $\left[x_{l}, x_{u}\right]$ and

$$
\begin{equation*}
f\left(x_{l}\right) f\left(x_{u}\right)<0 \tag{2}
\end{equation*}
$$

then there is at least one real root between $x_{l}$ and $x_{u}$

## Bisection method



Figure: Representation of bisection method.

## Stopping inequalities

## Typical stopping inequalities:

$$
\begin{gather*}
\left|p_{n}-p_{n-1}\right|<\varepsilon  \tag{3}\\
\frac{\left|p_{n}-p_{n-1}\right|}{\left|p_{n}\right|}<\varepsilon, \quad p_{n} \neq 0  \tag{4}\\
\left|f\left(p_{n}\right)\right|<\varepsilon \tag{5}
\end{gather*}
$$

## 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, $g^{\prime}(x)$ exists on $[a, b]$ and a positive constant $k>1$ exists with $\left|g^{\prime}(x)\right|<k$, then there is exactly one fixed point in $[a, b]$.


Figure: Fixed point for a function.

## Fixed-point method



Figure: Fixed point method representation.

## Fixed-point method - Algorithm

INPUT initial approximation $p_{0}$; tolerance $T O L$; 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 $p=g\left(p_{0}\right) . \quad\left(\right.$ Compute $\left.p_{i}.\right)$
Step 4 If $\left|p-p_{0}\right|<T O L$ then
OUTPUT $(p) ; \quad$ (The procedure was successful.) STOP.

Step 5 Set $i=i+1$.
Step 6 Set $p_{0}=p . \quad\left(\right.$ Update $\left.p_{0}.\right)$
Step 7 OUTPUT ('The method failed after $N_{0}$ iterations, $N_{0}=$ ', $N_{0}$ ); (The procedure was unsuccessful.) STOP.

Figure: Fixed point algorithm.

## Newton Raphson method

Taylor polynomial for $f(x)$ expanded about $p_{0}$ and evaluated at $x=p$

$$
\begin{equation*}
f(p)=f\left(p_{0}\right)+\left(p-p_{0}\right) f^{\prime}\left(p_{0}\right)+\frac{\left(p-p_{0}\right)^{2}}{2} f^{\prime \prime}(\xi) \tag{6}
\end{equation*}
$$

where $\xi \in\left[p_{0}, p\right]$.
Taking a first order approximation:

$$
\begin{gather*}
0 \approx f\left(p_{0}\right)+\left(p-p_{0}\right) f^{\prime}\left(p_{0}\right)  \tag{7}\\
p \approx p_{0}-\frac{f\left(p_{0}\right)}{f^{\prime}\left(p_{0}\right)} \tag{8}
\end{gather*}
$$

For an iterative process, we have:

$$
\begin{equation*}
p_{n}=p_{n-1}-\frac{f\left(p_{n-1}\right)}{f^{\prime}\left(p_{n-1}\right)}, \quad n \geq 1 \tag{9}
\end{equation*}
$$

## Newton Raphson



Figure: Representation of Newton Raphson method.

## Newton Raphson - Algorithm

INPUT initial approximation $p_{0}$; tolerance $T O L$; 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 $p=p_{0}-f\left(p_{0}\right) / f^{\prime}\left(p_{0}\right)$. (Compute $p_{i}$.)
Step 4 If $\left|p-p_{0}\right|<T O L$ then OUTPUT (p); (The procedure was successful.) STOP.
Step 5 Set $i=i+1$.
Step 6 Set $p_{0}=p . \quad\left(\right.$ Update $\left.p_{0}.\right)$
Step 7 OUTPUT ('The method failed after $N_{0}$ iterations, $N_{0}=$ ', $N_{0}$ ); (The procedure was unsuccessful.) STOP.

## Figure: Newton Raphson algorithm.

## Secant method

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

$$
\begin{equation*}
f^{\prime}\left(p_{n-1}\right)=\lim \frac{f(x)-f\left(p_{n-1}\right)}{x-p_{n-1}} \tag{10}
\end{equation*}
$$

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

$$
\begin{equation*}
f^{\prime}\left(p_{n-1}\right) \approx \frac{f\left(p_{n-1}\right)-f\left(p_{n-2}\right)}{p_{n-1}-p_{n-2}} \tag{11}
\end{equation*}
$$

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

$$
\begin{equation*}
p_{n}=p_{n-1}-\frac{f\left(p_{n-1}\right)\left(p_{n-1}-p_{n-2}\right)}{f\left(p_{n-1}\right)-f\left(p_{n-2}\right)} \tag{12}
\end{equation*}
$$

## Secant method



Figure: Secant method representation.

## Secant method - Algorithm

INPUT initial approximations $p_{0}, p_{1}$; tolerance $T O L$; maximum number of iterations $N_{0}$. OUTPUT approximate solution $p$ or message of failure.

Step 1 Set $i=2$;

$$
\begin{aligned}
& q_{0}=f\left(p_{0}\right) \\
& q_{1}=f\left(p_{1}\right)
\end{aligned}
$$

Step 2 While $i \leq N_{0}$ do Steps 3-6.

```
Step 3 Set \(p=p_{1}-q_{1}\left(p_{1}-p_{0}\right) /\left(q_{1}-q_{0}\right) . \quad\left(\right.\) Compute \(\left.p_{i}.\right)\)
Step 4 If \(\left|p-p_{1}\right|<T O L\) then
        OUTPUT (p); (The procedure was successful.)
        STOP.
    Step 5 Set \(i=i+1\).
    Step 6 Set \(p_{0}=p_{1} ; \quad\left(\right.\) Update \(\left.p_{0}, q_{0}, p_{1}, q_{1}\right)\)
            \(q_{0}=q_{1} ;\)
            \(p_{1}=p\);
            \(q_{1}=f(p)\).
```

Step 7 OUTPUT ('The method failed after $N_{0}$ iterations, $N_{0}=$ ', $N_{0}$ ); (The procedure was unsuccessful.) STOP.

Figure: Secant method algorithm.

## Order of convergence

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

$$
\begin{equation*}
\lim _{n \rightarrow \infty} \frac{\left|p_{n+1}-p_{n}\right|}{\left|p_{n}-p\right|^{\alpha}}=\lambda \tag{13}
\end{equation*}
$$

then $\left\{p_{n}\right\}_{n=0}^{\infty}$ 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 $x=p$

$$
\begin{equation*}
f(p)=f\left(p_{0}\right)+\left(p-p_{0}\right) f^{\prime}\left(p_{0}\right)+\frac{\left(p-p_{0}\right)^{2}}{2} f^{\prime \prime}(\xi) \tag{14}
\end{equation*}
$$

where $\xi \in\left[p_{0}, p\right]$.
Taking a first order approximation:

$$
\begin{gather*}
0 \approx f\left(p_{0}\right)+\left(p-p_{0}\right) f^{\prime}\left(p_{0}\right)  \tag{15}\\
p \approx p_{0}-\frac{f\left(p_{0}\right)}{f^{\prime}\left(p_{0}\right)} \tag{16}
\end{gather*}
$$

For an iterative process, we have:

$$
\begin{equation*}
p_{n}=p_{n-1}-\frac{f\left(p_{n-1}\right)}{f^{\prime}\left(p_{n-1}\right)}, \quad n \geq 1 \tag{17}
\end{equation*}
$$

## Newton Raphson (single variable)



Figure: Representation of Newton Raphson method.

## Newton-Raphson method (multivariate)

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

$$
\begin{aligned}
f_{1}(\mathbf{x}) & =0 \\
f_{2}(\mathbf{x}) & =0 \\
& \ldots \\
f_{N}(\mathbf{x}) & =0
\end{aligned}
$$

where

$$
\mathbf{x}=\left[\begin{array}{lll}
x_{1} & x_{2} & \cdots x_{N} \tag{18}
\end{array}\right]^{T}
$$

Defining a function vector:

$$
\mathbf{f}(\mathbf{x})=\left[\begin{array}{llll}
f_{1}(\mathbf{x}) & f_{2}(\mathbf{x}) & \cdots & f_{N}(\mathbf{x}) \tag{19}
\end{array}\right]
$$

The system can be rewritten as:

$$
\begin{equation*}
\mathbf{f}(\mathbf{x})=\mathbf{0} \tag{20}
\end{equation*}
$$

## Newton-Raphson method (multivariate)

Considering $\mathrm{N}=2$ (2D problem), the multidimensional equation can be geometrically interpreted as:


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

## Newton-Raphson method (multivariate)

The Taylor expansion for each function $f_{i}$ can be written as:

$$
\begin{equation*}
f_{i}(\mathbf{x}+\delta \mathbf{x})=f_{i}(\mathbf{x})+\sum_{j=1}^{N} \frac{\partial f_{i}\left(x_{j}\right)}{\partial x_{j}}+O\left(\delta \mathbf{x}^{2}\right) \approx f_{i}(\mathbf{x})+\sum_{j=1}^{N} \frac{\partial f_{i}\left(x_{j}\right)}{\partial x_{j}} \delta \mathbf{x} \tag{21}
\end{equation*}
$$

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

$$
\begin{equation*}
\mathbf{f}(\mathbf{x}+\delta \mathbf{x})=\mathbf{f}(\mathbf{x})+\mathbf{J}(\mathbf{x}) \delta \mathbf{x} \tag{22}
\end{equation*}
$$

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

$$
\mathbf{J}(\mathbf{x})=\left[\begin{array}{ccc}
\frac{\partial f_{1}}{\partial x_{1}} & \cdots & \frac{\partial f_{1}}{\partial x_{N}}  \tag{23}\\
\vdots & \ddots & \vdots \\
\frac{\partial f_{N}}{\partial x_{1}} & \cdots & \frac{\partial f_{N}}{\partial x_{N}}
\end{array}\right]
$$

## Newton-Raphson method (multivariate)

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

$$
\begin{gather*}
\mathbf{f}(\mathbf{x}+\delta \mathbf{x})=\mathbf{f}(\mathbf{x})+\mathbf{J}(\mathbf{x}) \delta \mathbf{x} \Longrightarrow  \tag{24}\\
\delta \mathbf{x}=\mathbf{J}(\mathbf{x})^{-1}[\mathbf{f}(\mathbf{x}+\delta \mathbf{x})-\mathbf{f}(\mathbf{x})]=-\mathbf{J}(\mathbf{x})^{-1} \mathbf{f}(\mathbf{x}) \tag{25}
\end{gather*}
$$

And, from an starting point x :

$$
\begin{equation*}
\mathbf{x}+\delta \mathbf{x}=\mathbf{x}-\mathbf{J}(\mathbf{x})^{-1} \mathbf{f}(\mathbf{x}) \tag{26}
\end{equation*}
$$

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

$$
\begin{equation*}
\mathbf{x}_{k+1}=\mathbf{x}_{k}+\delta \mathbf{x}_{k}=\mathbf{x}_{k}-\mathbf{J}\left(\mathbf{x}_{k}\right)^{-1} \mathbf{f}\left(\mathbf{x}_{k}\right) \tag{27}
\end{equation*}
$$

## Newton-Raphson method (multivariate)

## Example 1

Computes the roots of:

$$
\left\{\begin{array}{c}
x_{1}^{2}-2 x_{1}+x_{2}+7=0  \tag{28}\\
3 x_{1}-x_{2}+1=0
\end{array}\right.
$$

Starting point: $\mathbf{x}=\left[\begin{array}{ll}1.00 & 1.00\end{array}\right]^{T}$

## Newton-Raphson method (multivariate)

## Example 2

Determine the points of intersection between the circle $x^{2}+y^{2}=3$ and the hyperbola $x y=1$
Starting point: $x=0.5 ; y=1.5$
Solution: $\pm(0.618,1.618)$ and $\pm(1.618,0.618)$

## Newton-Raphson method (multivariate)

## Example 3

Computes the roots of:

$$
\left\{\begin{array}{c}
3 x_{1}-\cos \left(x_{2} x_{3}\right)-3 / 2=0  \tag{29}\\
4 x_{1}^{2}-625 x_{2}^{2}+2 x_{3}-1=0 \\
20 x_{3}+\exp \left(-x_{1} x_{2}\right)+9
\end{array}\right.
$$

Starting point: $\mathbf{x}=\left[\begin{array}{lll}1.00 & 1.00 & 1.00\end{array}\right]^{T}$
Solution: $x=\left[\begin{array}{lll}0.833282 & 0.035335 & -0.498549\end{array}\right]^{T}$

## Exercises

## 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

$$
\begin{aligned}
\beta_{i}^{4} & =\left(2 \pi f_{i}\right)^{2} \frac{m L^{3}}{E I} \\
f_{i} & =i \text { th natural frequency }(\mathrm{cps}) \\
m & =\text { mass of the beam } \\
L & =\text { length of the beam } \\
E & =\text { modulus of elasticity } \\
I & =\text { moment of inertia of the cross section }
\end{aligned}
$$

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 $7850 \mathrm{~kg} / \mathrm{m}^{3}$ and $E=200 \mathrm{GPa}$.

## Exercises

## Exercise 2



A steel cable of length $s$ is suspended as shown in the figure. The maximum tensile stress in the cable, which occurs at the supports, is

$$
\sigma_{\max }=\sigma_{0} \cosh \beta
$$

where

$$
\begin{aligned}
\beta & =\frac{\gamma L}{2 \sigma_{0}} \\
\sigma_{0} & =\text { tensile stress in the cable at } O \\
\gamma & =\text { weight of the cable per unit volume } \\
L & =\text { horizontal span of the cable }
\end{aligned}
$$

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 $\gamma=77 \times 10^{3} \mathrm{~N} / \mathrm{m}^{3}$ (steel), $L=1000 \mathrm{~m}$ and $s=1100 \mathrm{~m}$.

## Exercises

## Exercise 3



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

$$
\frac{Q^{2}}{2 g b^{2} h_{0}^{2}}+h_{0}=\frac{Q^{2}}{2 g b^{2} h^{2}}+h+H
$$

where

$$
\begin{aligned}
Q & =1.2 \mathrm{~m}^{3} / \mathrm{s}=\text { volume rate of flow } \\
g & =9.81 \mathrm{~m} / \mathrm{s}^{2}=\text { gravitational acceleration } \\
b & =1.8 \mathrm{~m}=\text { width of channel } \\
h_{0} & =0.6 \mathrm{~m}=\text { upstream water level } \\
H & =0.075 \mathrm{~m}=\text { height of bump } \\
h & =\text { water level above the bump }
\end{aligned}
$$

Determine $h$.

## Exercises

## Exercise 4



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

$$
\eta=\frac{\ln \left(T_{2} / T_{1}\right)-\left(1-T_{1} / T_{2}\right)}{\ln \left(T_{2} / T_{1}\right)+\left(1-T_{1} / T_{2}\right) /(\gamma-1)}
$$

where $T$ is the absolute temperature and $\gamma=5 / 3$. Find $T_{2} / T_{1}$ that results in $30 \%$ efficiency ( $\eta=0.3$ ).

## Exercises

## Exercise 5

$\square$ The equations

$$
\begin{aligned}
& \sin x+3 \cos x-2=0 \\
& \cos x-\sin y+0.2=0
\end{aligned}
$$

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

## Exercises

## Exercise 6



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

$$
\begin{aligned}
& x=(v \cos \theta) t \\
& y=-\frac{1}{2} g t^{2}+(\nu \sin \theta) t
\end{aligned}
$$

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

## Exercises

## Exercise 7

$\square$ 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 $b$.

