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## Non-linear vs. linear equation.

Very many problems in physics require a solution of non-linear equation or function. And non-linear equations are much harder to solve. $\qquad$
Examples:
A system of linear equations vs. a system of non-linear equations, a $\qquad$ linear ordinary differential equation vs. a non-linear ODE, etc.
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Very often we try to transform a nonlinear problem to a linear one by using proper approximations.
$\qquad$ losing the essence of physics behind
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## Nonlinear vs. linear equation.

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In this lecture we consider as simple as possible form of nonlinear equations, namely a nonlinear function of one variable $f(x)=0$. $\qquad$ Statement of the problem:

Given the continuous nonlinear function $f(x)$, find the value(s) $x=c$ such that $f(c)=0$

The non-linear function $f(x)$ can be

- an algebraic equation
- a transcendental equation
- a solution of a differential equation
- ... any non-linear equation


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## Examples

## Simple equations of one variable

$$
\begin{aligned}
& x^{2}-6 x+9=0 \\
& x-\cos (x)=0 \\
& \exp (x) \ln \left(x^{2}\right)-x \cos (x)=0
\end{aligned}
$$

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Quantum mechanics: Solutions of the Schrodinger equation for a finite $\qquad$ square well $U(x)=-U_{0}$ for $|x|<a$, can be found from the following non-linear equations (for even and odd states

$$
\begin{aligned}
\sqrt{U_{0}-|E|} \tan \sqrt{2 m\left(U_{0}-|E|\right) a^{2} / \hbar^{2}} & =\sqrt{E}- \\
\sqrt{U_{0}-|E|} \cot \sqrt{2 m\left(U_{0}-|E|\right) a^{2} / \hbar^{2}} & =-\sqrt{E}-
\end{aligned}
$$

$\qquad$
$\qquad$ In textbooks these equations are solved only graphically.

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## Solutions of nonlinear functions


a) a single real root
b) no real roots exist (but complex roots may exist)
c) two simple roots
d) three simple roots

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Prelude for root finding

1. All non-linear equations can only be solved iteratively.
2. We must guess an approximate root to start an iterative procedure.
The better we guess, the more chances we have to find the right root in
shorter time.

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Bounding and refining
There are two distinct phases in finding the solution of at nonlinear
equation.

1. Bounding the solution
2. Refining the solution
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### 2.1 Bisectional method

The simplest but the most robust method!

1. let $f(x)$ be a continuous function on $[a, b]$
2. let $f(x)$ changes sign between $a$ and $b, f(a) f(b)<0$

## Example: function

$f(x)=x^{3}-2 x-2$

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## Bisectional method - algorithm

Divide $[a, b]$ into tow equal parts with $c=(a+b) / 2$ and if


$$
f(a) f(c) \begin{cases}<0 & \text { then there is a root in }[a, c], \text { set } a=a, b=c \\ >0 & \text { then there is a root in }[c, b], \text { set } a=c, b=b \\ =0 & \text { then } \mathrm{c} \text { is the root }\end{cases}
$$

Interval halving is an iterative procedure.
The iterations are continued until
$\left|b_{i}-a_{i}\right| \leq \varepsilon_{1}$ or $\left|f\left(c_{i}\right)\right| \leq \varepsilon_{2}$ or both

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## Bisectional method - summary

- The root is bracketed within the bounds of the interval, so the method is guaranteed to converge
- On each bisectional step we reduce by two the interval where the solution occurs. After n steps the original interval $[a, b]$ will be reduced to the $(b-a) / 2 n$ interval. The bisectional procedure is repeated till $(b-a) / 2 n$ is less than the given tolerance $\left(b_{n}-a_{n}\right)<\varepsilon$. thus, $n$ is given by

$$
n=\frac{1}{\ln 2} \ln \left(\frac{b_{0}-a_{0}}{b_{n}-a_{n}}\right)
$$

- The major disadvantage of the bisection method is that the solution converges slowly.
- The method does not use information about actual function behavior

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```
Example: C++
double bisect(double a, double b, double eps)
{ double xl,x0,xr;
    if( f(a)*f(b) > 0.0) return 999;
    xl=a;
    xr = b;
    while (fabs(xr - xl) >
        if((f(xl) * f(x0)) <= 0.0) xr = x0;
        else xl = x0;
        }
return x0;
}
```

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### 2.2 False position method

In the false position method, the nonlinear function $f(x)$ is assumed to be a linear function $g(x)$ in the interval $(a, b)$, and the root of the linear $\qquad$ function $g(x), x=c$, is taken as the next approximation of the root of the nonlinear function $f(x), x=c$.

The root of the linear function $g(x)$, that is, $x=c$, is not the root of the nonlinear function $f(x)$. It is a false position, which gives the method its name.
The method uses information about the function $f(x)$.

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### 2.2 False position method - algorithm

The slope of the linear function $g^{\prime}(x)$ is given by
$g^{\prime}(x)=\frac{f(b)-f(a)}{b-a}=\frac{f(b)-f(c)}{b-c}$
Setting $f(c)=0$ and solving for $c$ gives
$c=b-f(b) \frac{b-a}{f(b)-f(a)}$
then like for bisectional method
if $f(a) / f(c)<0 \quad a=a, b=c$
if $f(a) / f(c)>0 \quad a=c, b=b$


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## Example: C++

double false_p(double a, double b, double eps)
\{ double $x l, x 0, x r$;
if $(\mathrm{f}(\mathrm{a}) * \mathrm{f}(\mathrm{b})>0.0)$ return 999;
$x l=a$;
$x \mathrm{x}=\mathrm{b}$;
while (fabs(xr - xl) >= eps)
\{
$x 0=x r-f(x r) *(x r-x l) /(f(x r)-f(x l))$; if $\left.\left((f(x l))^{*} f(x 0)\right)<=0.0\right) \mathrm{xr}=\mathrm{x} 0$; else $x l=x 0$;
\}
\}
$\qquad$
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Example for $\mathrm{y}=\mathrm{x}-\cos (\mathrm{x})$ on $[0.0,4.0]$ for eps $=1.0 \mathrm{e}-6$ $\qquad$
$\qquad$
$\begin{array}{cccccc}1 & 0.00000 & f(a) & b & f(b) & c \\ -1.00000 & 4.00000 & 4.65364 & 0.70751 & f(c) \\ 0.0 .05248\end{array}$
$0.70751-0.05248 .00000 \quad 4.65364-0.70751-0.05248$ $\begin{array}{lllllll}0.70751 & -0.05248 & 4.00000 & 4.65364 & 0.74422 & 0.00861\end{array}$ $\begin{array}{llllll}0.70751 & -0.05248 & 0.74422 & 0.00861 & 0.73905 & -0.00006 \\ 0.73905 & -0.00006 & 0.74422 & 0.00861 & 0.73909 & -0.00000\end{array}$ $\begin{array}{llllll}0.73905 & -0.00006 & 0.74422 & 0.00861 & 0.73909 & -0.00000 \\ 0.73909 & -0.00000 & 0.74422 & 0.00861 & 0.73909 & -0.00000\end{array}$ $\begin{array}{llllll}0.73909 & -0.00000 & 0.74422 & 0.00861 & 0.73909 & -0.00000 \\ 0.73909 & -0.00000 & 0.74422 & 0.00861 & 0.73909 & -0.00000\end{array}$ $\qquad$ $\begin{array}{llllll}0.73909 & -0.00000 & 0.74422 & 0.00861 & 0.73909 & -0.00000\end{array}$ $\begin{array}{lllllll}8 & 0.73909 & -0.00000 & 0.74422 & 0.00861 & 0.73909 & 0.00000\end{array}$ $8_{8}^{0.73909}$
for bisectional method it takes 22 iterations
The false position method generally converges more rapidly than the bisection method, but it does not give a bound on the error of the solution.
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| Open domain methods |
| :--- |
| Open domain methods use information about the nonlinear function itself |
| to refine the estimates of the root. Thus, they are considerably more |
| efficient than bracketing ones. |
| However, such methods do not restrict the root to remain trapped in a |
| closed interval. Consequently, they are not as robust as bracketing |
| methods and can actually diverge. |
| Most popular open domain methods |
| 1. Newton's method |
| 2. The secant method |
| 3. Muller's method |

$\qquad$
Open domain methods use information about the nonlinear function itself to refine the estimates of the root. Thus, they are considerably more $\qquad$
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### 3.1 Newton's method

Newton's method exploits the derivatives $f^{\prime}(x)$ of the function $f(x)$ to accelerate convergence for solving $f(x)=0$.
It always converges if the initial approximation is sufficiently close to the root, and it converges quadratically.

Its only disadvantage is that the derivative $f^{\prime}(x)$ of the nonlinear function $f(x)$ must be evaluated.

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## Newton's method - basics and algorithm

$$
f(x)=f\left(x_{0}\right)+\left(x-x_{0}\right) f^{\prime}\left(x_{0}\right)+\left(x-x_{0}\right)^{2} \frac{f^{\prime \prime}\left(x_{0}\right)}{2!}+\cdots
$$

Suppose that $x$ is the solution for $f(x)=0$.
If we keep two first terms in Taylor series $\qquad$
$f(x)=0=f\left(x_{0}\right)+\left(x-x_{0}\right) f^{\prime}\left(x_{0}\right)$
and then
$x=x_{0}-\frac{f\left(x_{0}\right)}{f^{\prime}\left(x_{0}\right)}$
We need $f(x)$ and $f^{\prime}(x)$ to proceed
Each next iteration is

$$
x_{k+1}=x_{k}-\frac{f\left(x_{k}\right)}{f^{\prime}\left(x_{k}\right)}
$$



## Example: C++

double newton(void(*f)(double, double\&, double\&), double $x$, double eps, int\& flag)
\{ double fx, fpx, xc
int $i$, iter $=1000$;
$\mathrm{i}=0$;
do $\left\{\begin{array}{l}i=1+1 ;\end{array}\right.$
$f(x, f x, f p x)$;
$\mathrm{xc}=\mathrm{x}-\mathrm{fx} / \mathrm{fpx}$;
$x=x c$;
if(i $>=$ iter $)$ break;
\} while (fabs(fx) >= eps)
flag $=i$;
f (i == iter) flag = 0;
return $x c$;

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Example for $\mathrm{y}=\mathrm{x}-\cos (\mathrm{x})$ on $[0.0,4.0]$ for $\mathrm{eps}=1.0 \mathrm{e}-6$ $\qquad$
Initial point is 1.0

| iterations | root |
| :---: | :---: |
| 4 | 0.73909 |

for bisectional method 22 iterations
for false position 8 iterations
Newton's method 4 iterations
Newton's method has excellent local convergence properties.
However, its global convergence properties can be very poor, due to the neglect of the higher-order terms in the Taylor series.

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## Comments to Newton's method

Newton's method is an excellent method for polishing roots obtained by other methods which yield results polluted by round-off errors $\qquad$

Newton's method has several disadvantages.

1. Some functions are difficult to differentiate analytically, and some functions cannot be differentiated analytically at all.
2. If the derivative is small the next iteration may end up very far from the root

Practical comment:
In any program we must check the size of the step for the next iteration. If it is improbably large - then reject it (or switch to some other method)

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### 3.2 Method of secants

The secant method is a variation of Newton's method when the evaluation of derivatives is difficult.
The nonlinear function $f(x)$ is approximated locally by the linear function $g(x)$, which is the secant to $f(x)$, and the root of $g(x)$ is taken as an improved approximation to the root of the nonlinear function $f(x)$.

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### 3.2 Method of secants - algorithm

$\qquad$
The derivative $f^{\prime}(x)$ at point $x_{k}$ can be approximated as

$$
f^{\prime}\left(x_{k}\right)=\frac{f\left(x_{k}\right)-f\left(x_{k-1}\right)}{x_{k}-x_{k-1}}
$$

From the Newton's method
$x_{k+1}=x_{k}-\frac{f\left(x_{k}\right)}{f^{\prime}\left(x_{k}\right)}=x_{k}-\frac{f\left(x_{k}\right)\left(x_{k}-x_{k-1}\right)}{f\left(x_{k}\right)-f\left(x_{k-1}\right)}$
One has to select two initial points to start


Note that the method of secant = the False position method
The only difference is about selecting two points to start the method $\qquad$ ${ }^{33}$ $\qquad$

```
Example: C++
double secant (double(*f)(double), double x1,
double x2, double eps, int& flag)
{ double x3;
    int i, iter=1000;
    flag = 1;
    i = 0;
    while (fabs(x2 - x1) >= eps)
    {}\mp@subsup{}{i= = i + + 1;}{
        x3 = x2 - (f(x2)*(x2-x1))/(f(x2)-f(x1));
        x1 = x2;
        x1 = x2;
        if(i >= iter) break;
    if (i == iter) flag = 0;
    return x3;
}
```

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Example for $\mathrm{y}=\mathrm{x}-\cos (\mathrm{x})$ on $[0.0,4.0]$ for $\mathrm{eps}=1.0 \mathrm{e}-6$ $\qquad$
Initial point is 1.0

| iterations | root |
| :---: | :---: |
| 5 | 0.73909 |

for bisectional method 22 iterations
for false position 8 iterations
Newton's method 4 iterations
the secant method 5 iterations

Which method is more efficient?
Jeeves showed that if the effort required to evaluate $f(x)^{\prime}$ is less than 43 $\qquad$ percent of the effort required to evaluate $f(x)$, then Newton's method is
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$\qquad$ more efficient. Otherwise, the secant method is more efficient.
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### 3.2 Muller's and Brent's methods

Muller's method is based on locally approximating the nonlinear function $f(x)$ by a quadratic function $g(x)$, and the root of the quadratic function $\qquad$ $g(x)$ is taken as an improved approximation to the root of the nonlinear function $f(x)$.
Three initial approximations $x_{1}, x_{2}$, and $x_{3}$, (which are not required to
$\qquad$ bracket the root), are required to start the algorithm.

The only difference between Muller's method and the secant method is $\qquad$ that $g(x)$ is a quadratic function in Muller's method and a linear function in the secant method.
Brent's Method is a hybrid method-it uses parts of solving techniques from other methods.

Many numerical libraries, e.g. MatLab, implement a version of Brent's method.

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## Summary for the open domain methods

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- All three methods converge rapidly in the vicinity of a root.
- When the derivative $f^{\prime}(x)$ is difficult to determine or time consuming to evaluate, the secant method is more efficient.
- In extremely sensitive problems, all three methods may misbehave and require some bracketing technique.
- All three of the methods can find complex roots simply by using complex arithmetic
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## Complications

- there are no roots at all
- there is one root, but the function does not change the sign,

$$
f(x)=x^{2}-2 x+1
$$

- there are two or more roots on an interval $[a, b]$ $\qquad$

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$\qquad$
What will happen if we apply the bisectional method here?
How about Newton's method? $\qquad$
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Complications (cont.) $\qquad$
Many roots!


What root will you find with the bisectional method?
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Example 1:
$f(x)=x-\cos x$

\[

\]



$$
\begin{array}{ll}
\text { Brute force roots } \\
\text { number } & \\
\text { root } & \text { f(root) } \\
1 & 0.739085
\end{array}
$$


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Example 3:
$f(x)=4 x^{4}-6 x^{2}-11 / 4$

$$
\begin{array}{lrrr}
\text { Seant method } & 0.500012 & 18 & -4.000046 \\
\text { Matlab solution } & 1.366760 & & 0.00000
\end{array}
$$

$$
\begin{array}{ccc}
2 & 1.366760 \quad 0.000000 \\
\text { but for } \times 0=1.0 \text { Secant method gives } 1.366760 \text { after } 11 \text { iterations }{ }^{43} \\
\hline
\end{array}
$$

$$
\begin{aligned}
& \text { Root(s) of } f(x) \\
& \begin{array}{l}
\text { Secant } x 0=0.5
\end{array} \\
& \text { Tolerance }=1.00 \mathrm{e}-08 \\
& \text { Bisectional: No root found } \\
& \text { False position: No root found } \\
& \begin{array}{ccc}
\text { number } & \text { root } & f \text { (root) } \\
1 & -1.366760 & 0.000000 \\
2 & 1.366760 & 0.000000
\end{array}
\end{aligned}
$$

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Part 4:
Roots of polynomials

$$
a_{n} x^{n}+a_{n-1} x^{n-1}+\cdots+a_{1} x+a_{0}=0
$$

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## Ideas

The fundamental theorem of algebra states that a nth-degree polynomial has exactly $n$ zeros, or roots.
The roots may be real or complex. If the coefficients are all real, complex roots always occur in conjugate pairs. The roots may be single (i.e., simple) or repeated (i.e., multiple).
Descartes' rule of signs, which applies to polynomials having real coefficients, states that the number of positive roots of $P_{n}(x)$ is equal to the number of sign changes in the nonzero coefficients of $P_{n}(x)$ or is smaller by an even integer.

The number of negative roots is found in a similar manner by considering $P_{n}(-x)$.
The bracketing methods for $\mathbf{P}_{\mathrm{n}}(\mathbf{x})$
The bracketing methods (bisection and false position), cannot be used to
find repeated roots with an even multiplicity, since the nonlinear function
$f(x)$ does not change sign at such roots.
Repeated roots with an odd multiplicity can be bracketed by monitoring
the sign of $f(x)$, but even in this case the open methods are more
efficient.
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## The open methods for $\mathrm{P}_{\mathrm{n}}(\mathrm{x})$

The open can be used to find the roots of polynomials: Newton's method, the secant method, and Muller's method.
These three methods also can be used for finding the complex roots of polynomials, provided that complex arithmetic is used, and reasonably good complex initial approximations are specified.
There are various modifications of Newton's method for polynomials
Other methods for polynomials: Bairstow's method, Laguerre's method, Eigenvalue method.

Matlab has a function roots to return roots of polynomials.

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## Systems of non-linear equations

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$$
\left\{\begin{array}{l}
f(x, y)=0 \\
g(x, y)=0
\end{array}\right.
$$

$\qquad$
"There are no good, general methods for solving systems of more than one nonlinear equation"
Numerical recipes in C by W. H Press et al.

- Bracketing methods are not readily extendable to systems of nonlinear equations.
- Newton's method, however, can be extended to solve systems of nonlinear equations. Quite often you need a good initial guess.
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```
Newton's method {}{\begin{array}{l}{f(x,y)=0}\\{g(x,y)=0}
Find \(x^{*}\) and \(y^{*}\) such that \(f\left(x^{*}, y^{*}\right) \approx 0, g\left(x^{*}, y^{*}\right) \approx 0\)
Using Taylor series about \((x, y)\)
\[
\begin{aligned}
& f\left(x^{*}, y^{*}\right)=f(x, y)+f_{x}^{\prime}(x, y)\left(x^{*}-x\right)+f_{y}^{\prime}(x, y)\left(y^{*}-y\right)+\cdots \\
& g\left(x^{*}, y^{*}\right)=g(x, y)+g_{x}^{\prime}(x, y)\left(x^{*}-x\right)+g_{y}^{\prime}(x, y)\left(y^{*}-y\right)+\cdots
\end{aligned}
\]
```

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keeping only first-order terms and setting $f\left(x^{*}, y^{*}\right) \approx 0, g\left(x^{*}, y^{*}\right) \approx 0$
one has a system of linear equations for $x^{*}$ and $y^{*}$. Solving it gives

$$
\begin{aligned}
& x^{*}=x+\frac{f_{y}^{\prime}(x, y) g(x, y)-f(x, y) g_{y}^{\prime}(x, y)}{f_{x}^{\prime}(x, y) g_{y}^{\prime}(x, y)-f_{y}^{\prime}(x, y) g_{x}^{\prime}(x, y)} \\
& y^{*}=y+\frac{f(x, y) g_{x}^{\prime}(x, y)-f_{x}^{\prime}(x, y) g(x, y)}{f_{x}^{\prime}(x, y) g_{y}^{\prime}(x, y)-f_{y}^{\prime}(x, y) g_{x}^{\prime}(x, y)}
\end{aligned}
$$

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## Example: C++

void newton2(double\& x1, double\& y1, double eps, int\& i)
double f1, g1, fx, fy, gx, gy;
double del, $x 2, y 2, d x, d y$;
int iter $=99$;
$\mathrm{i}=0$;
do $\left\{\begin{array}{l}i=1+1 ; ~\end{array}\right.$ fg(x1, y1, f1, g1, fx, fy, gx, gy);
del $=f x^{*} g y-f y^{*} g x$;
$d x=(f y * g 1-f 1 * g y) / d e l ; ~$
$d y=(f 1 * g x-f x * g 1) / d e l ; ~$
$d y=\left(f 1 * g x-f x^{*} g 1\right) / d e l ; ~$
$x 2=x 1+d x ;$
$\mathrm{x} 2=\mathrm{x} 1+\mathrm{dx}$;
$y 2=y 1+d y$;
$\mathrm{x} 1=\mathrm{x} 2$;
$\mathrm{y} 1=\mathrm{y} 2$
$\mathrm{y} 1=\mathrm{y} 2$;
if(i $>=$ iter $)$ break;
\} while (fabs(dx) >=eps \&\& fabs(dy) >=eps);
$i=i+1 ;$
\}
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Example with various initial points


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## Root-finding algorithms should contain:

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1. An upper limit on the number of iterations.
2. If the method uses the derivative $f^{\prime}(x)$, it should be monitored to $\qquad$ ensure that it does not approach zero.
3. A convergence test for the magnitude of the solution, $\left|x_{i+1}-x_{i}\right| \leq \varepsilon$, $\qquad$ or/and the magnitude of the nonlinear function, $\left|f\left(x_{i+1}\right)\right| \leq \varepsilon$, must be included.
4. When convergence is indicated, the final root estimate should be inserted into the nonlinear function $f(x)$ to guarantee that $f(x)=0$ within the desired tolerance. $\qquad$
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## Summary 1:

1. Bisection and false position methods converge very slowly but are certain to converge because the root lies in a closed domain. $\qquad$
2. Newton's method and the secant method are both effective methods for solving nonlinear equations. Both methods generally require $\qquad$ reasonable initial approximations.
3. Polynomials can be solved by any of the methods for solving nonlinear equations.
However, the special features of polynomials should be taken into account.
$\qquad$
$\qquad$
$\qquad$ 60 $\qquad$

## Summary 2:

3. Multiple roots can be evaluated using Newton's basic method or its variations, or brute force method
4. Complex roots can be evaluated by Newton's method or the secant method by using complex arithmetic.
5. Solving systems of nonlinear equations is a difficult task. For systems of nonlinear equations which have analytical partial derivatives, Newton's method can be used.
Otherwise, multidimensional minimization techniques may be preferred.
No single approach has proven to be the most effective.
Solving systems of nonlinear equations remains a difficult problem.

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## Summary 3:

6. Good initial approximations are extremely important.
7. For smoothly varying functions, most algorithms will always converge if the initial approximation is close enough.
8. Many, if not most, problems in engineering and science are well behaved and straightforward.
9. When a problem is to be solved only once or a few times, the efficiency of the method is not of major concern. However, when a problem is to be solved many times, efficiency of the method is of major concern. $\qquad$
10. If a nonlinear equation has complex roots, that must be anticipated when choosing a method.
11. Analyst's time versus computer time must be considered when selecting a method.

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## Pitfalls of Root Finding Methods

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1. Lack of a good initial approximation
2. Convergence to the wrong root $\qquad$
3. Closely spaced roots
4. Multiple roots $\qquad$
5. Inflection points
6. Complex roots $\qquad$
7. III-conditioning of the nonlinear equation
8. Slow convergence $\qquad$
$\qquad$

## Other Methods of Root Finding

Brent's method uses a superlinear method (i.e., inverse quadratic interpolation) and monitors its behavior to ensure that it is behaving properly.
For finding the roots of polynomials: Graeff's root squaring method, the Lehmer-Schur method, and the QD (quotient-difference) method. Two of the more important additional methods for polynomials are Laguerre's method and the Jenkins-Traub method
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## Packages for non-linear equations

Numerous libraries and software packages are available for solving nonlinear equations. Many workstations and mainframe computers have such libraries attached to their operating systems

Many commercial software packages contain nonlinear equation solvers
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(e.g. Matlab, Mathematica, Maple, Mathcad)

More sophisticated packages can be found in IMSL, NAG
The book Numerical Recipes (Press et al., many editions) contains numerous subroutines for solving nonlinear equations.

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## Final thoughts

1. Choosing right computational method for finding roots is a difficult skill for beginners. $\qquad$
2. A method that was efficient for one equation may fail miserably for another
3. Any method should be used intelligently!
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