

Part 1: Prelude to the problem

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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. Examples:

A system of linear equations vs. a system of non-linear equations, a linear ordinary differential equation vs. a non-linear ODE, etc.

Very often we try to transform a nonlinear problem to a linear one by using proper approximations.

However, very many nonlinear problems cannot be linearized without losing the essence of physics behind.

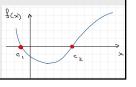
Nonlinear vs. linear equation.

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

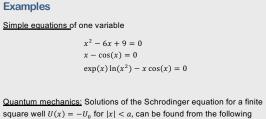
Given the continuous nonlinear function f(x), find the value(s) x = csuch that f(c) = 0

The non-linear function f(x) can be

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





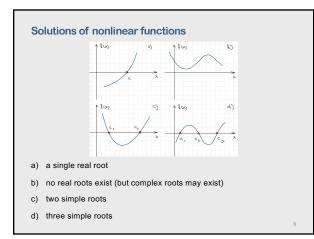


square well $U(x) = -U_0$ for |x| < a, can be found from the following non-linear equations (for even and odd states

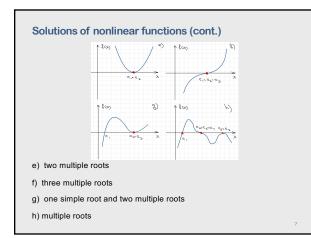
 $\sqrt{U_0 - |E|} \tan \sqrt{2m(U_0 - |E|) a^2/\hbar^2} = \sqrt{E}$

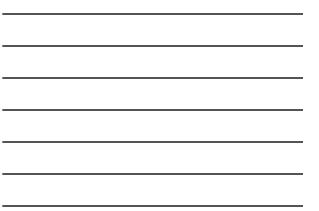
$$\sqrt{U_0 - |E|} \cot \sqrt{2m(U_0 - |E|) a^2/\hbar^2} = -\sqrt{E}$$

In textbooks these equations are solved only graphically.









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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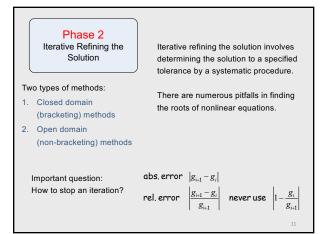
Bounding and refining

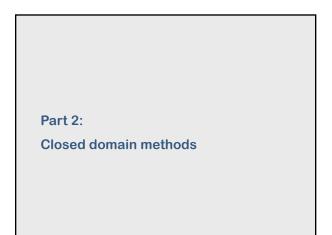
There are two distinct phases in finding the solution of at nonlinear equation.

- 1. Bounding the solution
- 2. Refining the solution

Phase 1 Bounding the Solution Bounding the solution involves finding a 1. Graphing the function rough estimate of the solution that can be 2. Incremental search used as the initial approximation, in an Past experience with the 3. iterative procedure that refines the problem or a similar one solution to a specified tolerance. Solution of a simplified 4 If possible, the root should be bracketed approximate model between two points at which the value of 5. Previous solution in a the nonlinear function has opposite signs. sequence of solutions "The hardest thing of all is to find a black cat in a dark room, especially if there is no cat." Confucius (551-479 AD)

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Closed Domain (Bracketing) Methods

Methods start with two values of x which bracket the root in the interval [a, b].

If f(a) and f(b) have opposite signs, and if the function is continuous, then at least one root must be in the interval.

Most common closed domain methods:

- Interval halving (bisection)
- False position (regula falsi)

Bracketing methods are robust (they are guaranteed to obtain a solution since the root is trapped in the closed interval).

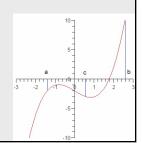
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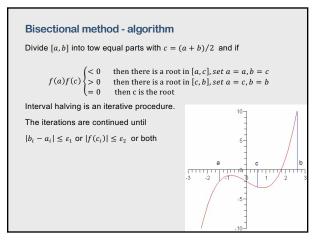
2.1 Bisectional method

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







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)/2n interval. The bisectional procedure is repeated till (b − a)/2n is less than the given tolerance (b_n−a_n) < ε. thus, n is given by

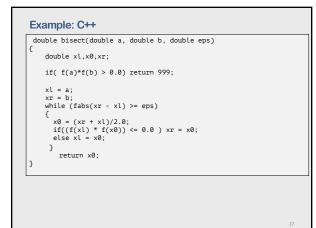
$$=\frac{1}{\ln 2}\ln\left(\frac{b_0-a_0}{b_n-a_n}\right)$$

n

- 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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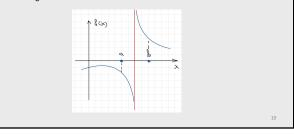
i	a	f(a)	b	f(b)	с	f(c)	
1	0.00000	-1.00000	4.00000	4.65364	2.00000	2.41615	
2	0.00000	-1.00000	2.00000	2.41615	1.00000	0.45970	
3	0.00000	-1.00000	1.00000	0.45970	0.50000	-0.37758	
4	0.50000	-0.37758	1.00000	0.45970	0.75000	0.01831	
5	0.50000	-0.37758	0.75000	0.01831	0.62500	-0.18596	
6	0.62500	-0.18596	0.75000	0.01831	0.68750	-0.08533	
7		-0.08533	0.75000	0.01831		-0.03388	1
8	0.71875	-0.03388	0.75000	0.01831	0.73438	-0.00787	
9		-0.00787	0.75000	0.01831	0.74219	0.00520	
10		-0.00787	0.74219	0.00520	0.73828		
11		-0.00135	0.74219	0.00520	0.74023	0.00192	*
12		-0.00135	0.74023	0.00192	0.73926	0.00029	
13		-0.00135	0.73926	0.00029		-0.00053	
14		-0.00053	0.73926	0.00029		-0.00012	
15		-0.00012	0.73926	0.00029	0.73914	0.00008	ч а к к к и к
16		-0.00012	0.73914	0.00008		-0.00002	
17		-0.00002	0.73914	0.00008	0.73911	0.00003	
18		-0.00002	0.73911	0.00003	0.73909	0.00001	
19		-0.00002	0.73909	0.00001	0.73908		
20		-0.00000	0.73909	0.00001	0.73909	0.00000	
21 22		-0.00000	0.73909	0.00000		-0.00000	
		-0.00000	0.73909	0.00000	0.73909	0.00000	
ite	rations 22	root 0.73909					



Bisectional method and singularity

If a nonlinear equation, such as f(x) = 1/(x - d) which has a singularity at x = d, is bracketed between a and b, interval halving will locate the discontinuity, x = d.

A check on |f(x)| as $x \to d$ would indicate that a discontinuity, not a root, is being found.



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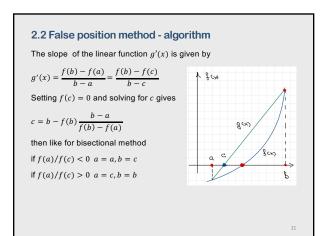
2.2 False position method

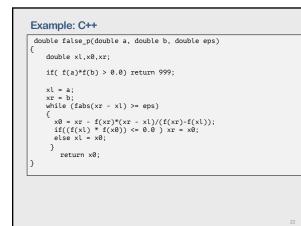
In the false position method, the nonlinear function f(x) is assumed to be a linear function g(x) in the interval (a, b), and the root of the linear function g(x), x = c, is taken as the next approximation of the root of the nonlinear function f(x), x = c.

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.

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The method uses information about the function f(x).





L	a	f(a)	b	f(b)	с	f(c)
1	0.00000	-1.00000	4.00000	4.65364	0.70751	-0.05248
2	0.70751	-0.05248	4.00000	4.65364	0.74422	0.00861
3	0.70751	-0.05248	0.74422	0.00861	0.73905	-0.00006
4	0.73905	-0.00006	0.74422	0.00861	0.73909	-0.00000
5	0.73909	-0.00000	0.74422	0.00861	0.73909	-0.00000
6	0.73909	-0.00000	0.74422	0.00861	0.73909	-0.00000
7	0.73909	-0.00000	0.74422	0.00861	0.73909	-0.00000
8	0.73909	-0.00000	0.74422	0.00861	0.73909	0.00000
ite	rations	root				
	8	0.73909				

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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Part 3:

Open domain methods

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.

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Most popular open domain methods

- 1. Newton's method
- 2. The secant method
- 3. Muller's method

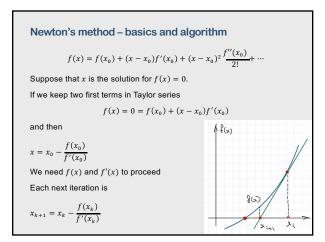
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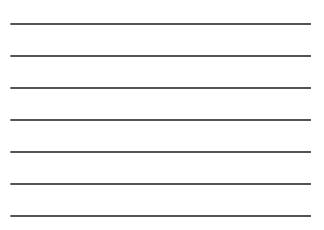
3.1 Newton's method

Newton's method exploits the derivatives f'(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.

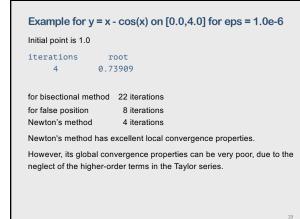
Its only disadvantage is that the derivative f'(x) of the nonlinear function f(x) must be evaluated.



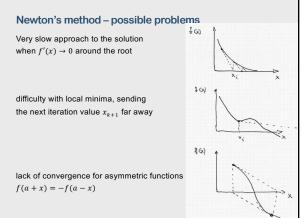


Example: C++ double newton(void(*f)(double, double&, double&),double x, double eps, int& flag) { double fx, fpx, xc; int i, iter=1000; i = 0; double fx i = do { i = i + 1; fx,fpx i = i + 1; f(x,fx,fpx); xc = x - fx/fpx; x = xc; if(i = iter) break; } while (fabs(fx) >= eps); flag = i; if (i == iter) flag = 0; return xc; }

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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

Newton's method has several disadvantages.

- 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)

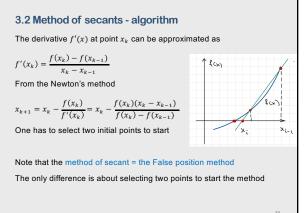
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3.2 Method of secants

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

iterations	root
5	0.73909
for bisectional me	thod 22 iterations
for false position	8 iterations
Newton's method	4 iterations
the secant method	d 5 iterations

Which method is more efficient?

Jeeves showed that if the effort required to evaluate f(x)' is less than 43 percent of the effort required to evaluate f(x), then Newton's method is 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 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 bracket the root), are required to start the algorithm.

The only difference between Muller's method and the secant method is 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.

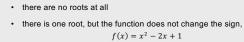


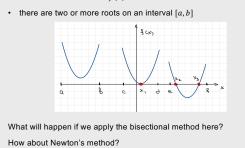
Summary for the open domain methods

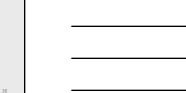
- · All three methods converge rapidly in the vicinity of a root.
- When the derivative f'(x) is difficult to determine or time consuming to evaluate, the secant method is more efficient.
- In extremely sensitive problems, all three methods may misbehave and require some bracketing technique.
- All three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

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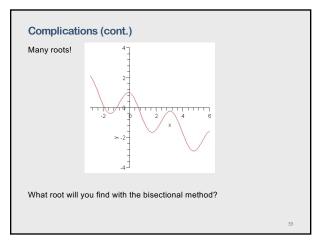
Complications







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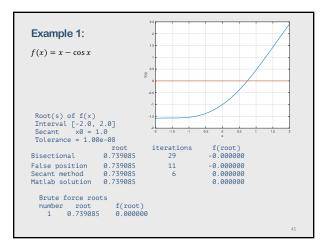
Multiple roots: "brute force" method

The brute force method is a good approach for dealing with multiple roots.

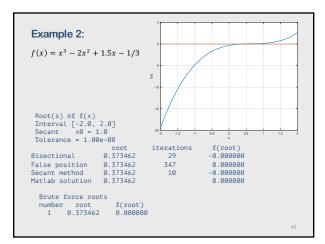
You split the original interval [a,b] into smaller intervals with some step h applying some of the methods for single roots to each subinterval.

Choosing a step size

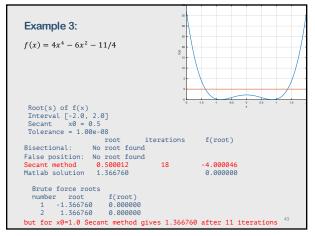
- · If the step size is too large, we may miss multiple zeros.
- Choosing too small steps may result in time consuming calculations.
- A graphical analysis of the equation may help to decide for the most reasonable step for h.
- A good idea evaluate roots for steps h and h/10 whether the number of roots stay the same.



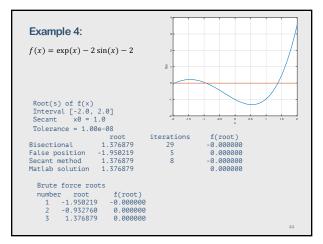


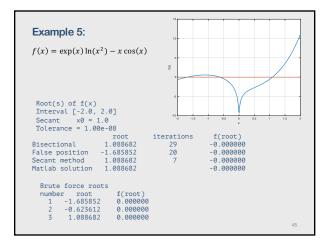


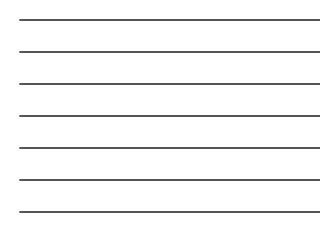


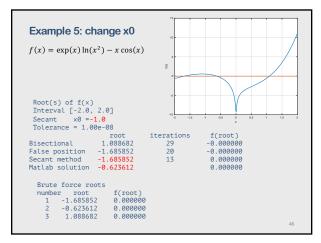














Part 4: Roots of polynomials $a_n x^n + a_{n-1} x^{n-1} + \dots + a_1 x + a_0 = 0$

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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 $P_n(x)$

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 P_n(x)

The open can be used to find the roots of polynomials: Newton's method, the secant method, and Muller's method.

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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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Part 5:

Nonlinear systems of equations

Systems of non-linear equations

 $\begin{cases} f(x, y) = 0\\ g(x, y) = 0 \end{cases}$

"There are no good, general methods for solving systems of more than one nonlinear equation"

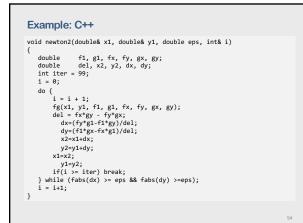
Numerical recipes in C by W. H Press et al.

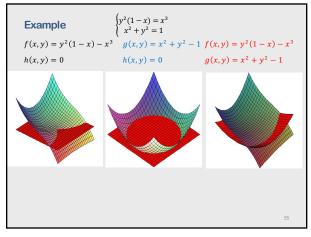
- Bracketing methods are not readily extendable to systems of nonlinear equations.
- Newton's method, however, can be extended to solve systems of nonlinear equations. Quite often you need a good initial guess.

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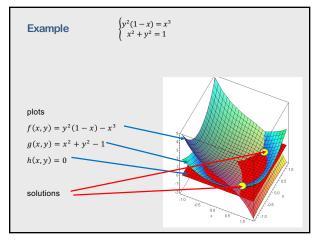
Newton's method $\begin{cases} f(x,y) = 0\\ g(x,y) = 0 \end{cases}$ Find x^* and y^* such that $f(x^*, y^*) \approx 0$, $g(x^*, y^*) \approx 0$ Using Taylor series about (x, y) $f(x^*, y^*) = f(x, y) + f'_x(x, y)(x^* - x) + f'_y(x, y)(y^* - y) + \cdots$ $g(x^*, y^*) = g(x, y) + g'_x(x, y)(x^* - x) + g'_y(x, y)(y^* - y) + \cdots$ keeping only first-order terms and setting $f(x^*, y^*) \approx 0$, $g(x^*, y^*) \approx 0$ one has a system of linear equations for x^* and y^* . Solving it gives $x^* = x + \frac{f'_y(x, y)g(x, y) - f(x, y)g'_y(x, y)}{f'_x(x, y)g'_y(x, y) - f'_y(x, y)g'_x(x, y)}$ $y^* = y + \frac{f(x, y)g'_x(x, y) - f'_x(x, y)g(x, y)}{f'_x(x, y)g'_y(x, y) - f'_y(x, y)g'_x(x, y)}$

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Newt	ons method	for two c	oupled non	linear equ	ations	
i	x	У	f	g	dx	dy
1	1.00000	1.00000	-1.00000	1.00000	-0.25000	-0.25000
2	0.75000	0.75000	-0.28125	0.12500	-0.11905	0.03571
3	0.63095	0.78571	-0.02335	0.01545	-0.01276	0.00041
4	0.61819	0.78613	-0.00030	0.00016	-0.00016	0.00002
5	0.61803	0.78615	-0.00000	0.00000	-0.00000	0.00000
6	0.61803	0.78615	-0.00000	0.00000		
	ons method		oupled non	1		
i 1	× 1.00000	y -1.00000	f -1.00000	9 1.00000	dx -0.25000	dy 0.25000
_			-		-0.25000	
1	1.00000	-1.00000	-1.00000	1.00000	-0.25000 -0.11905	0.25000
1 2	1.00000 0.75000	-1.00000 -0.75000	-1.00000 -0.28125	1.00000 0.12500	-0.25000 -0.11905 -0.01276	0.25000 -0.03571 -0.00041
1 2 3	1.00000 0.75000 0.63095	-1.00000 -0.75000 -0.78571	-1.00000 -0.28125 -0.02335	1.00000 0.12500 0.01545	-0.25000 -0.11905 -0.01276	0.25000 -0.03571 -0.00041



Part 6:

Summary

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Root-finding algorithms should contain:

- 1. An upper limit on the number of iterations.
- If the method uses the derivative f'(x), it should be monitored to ensure that it does not approach zero.
- A convergence test for the magnitude of the solution, |x_{i+1} x_i| ≤ ε, or/and the magnitude of the nonlinear function, |f(x_{i+1})| ≤ ε, 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.

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Summary 1:

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

Summary 2:

- 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.
- 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.
- 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.
- 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. $$_{\odot}$$

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Pitfalls of Root Finding Methods

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

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 (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.
- 2. A method that was efficient for one equation may fail miserably for another
- 3. Any method should be used intelligently!