Roots of Nonlinear Equations

Examples of nonlinear equations

one-dimensional equations

$$x^2 - 6x + 9 = 0$$

$$x - \cos(x) = 0$$

$$\exp(x)\ln(x^2) - x\cos(x) = 0$$

two-dimensional equation

$$\begin{cases} y^2(1-x) = x^3 \\ x^2 + y^2 = 1 \end{cases}$$

Solving nonlinear equations = lots of fun in algebra classes?

Part 1.

Real Roots of a Single Variable Function

$$f(x) = 0$$

1.1 Introduction

Given - a continuous nonlinear function $f(x)$

find - the value $x = c$ such that $f(c) = 0.$

The nonlinear equation, $f(x) = 0$, may be

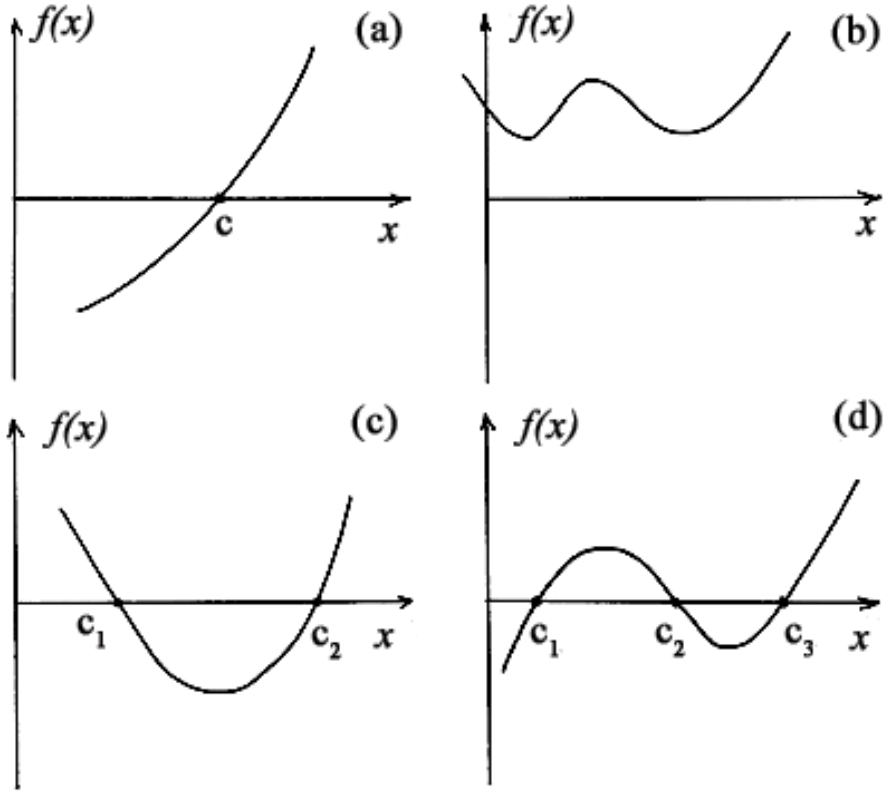
an algebraic equation

a transcendental equation

a solution of a differential equation

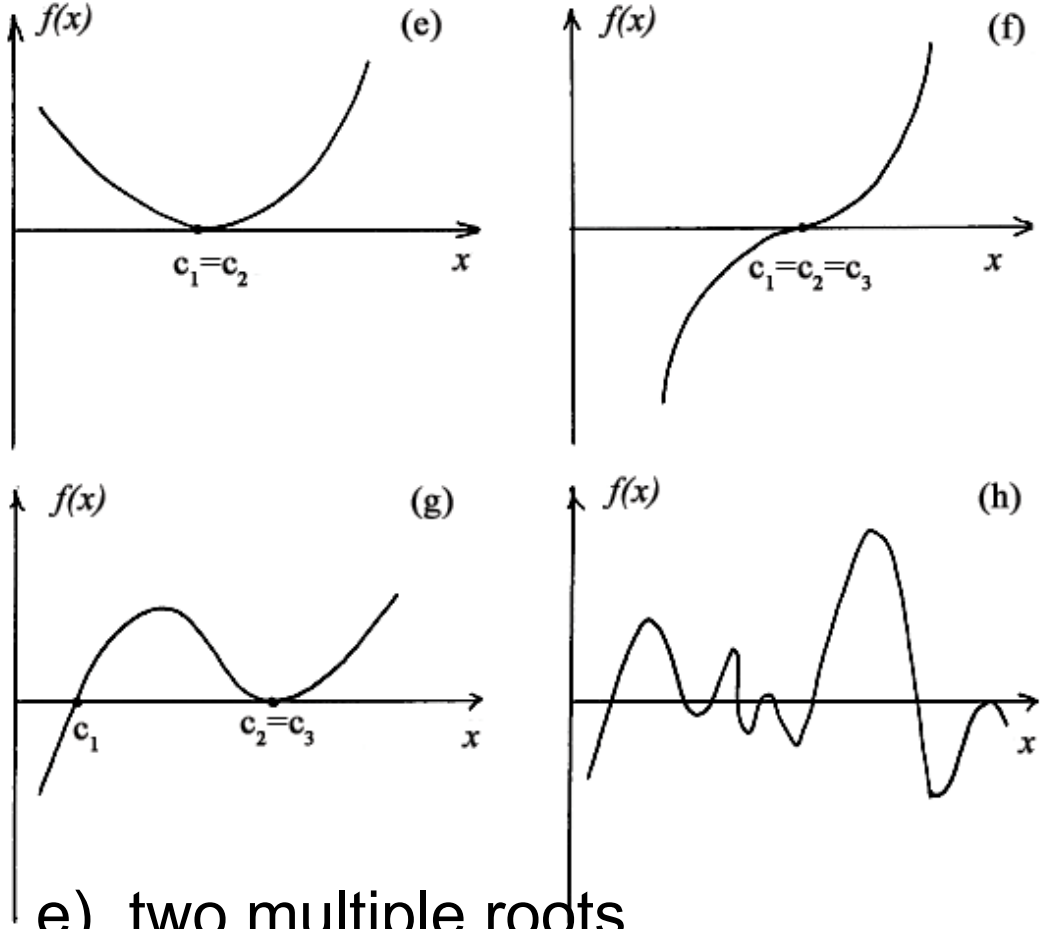
any nonlinear function of x.

Behavior 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

Behavior of Nonlinear Functions (cont.)



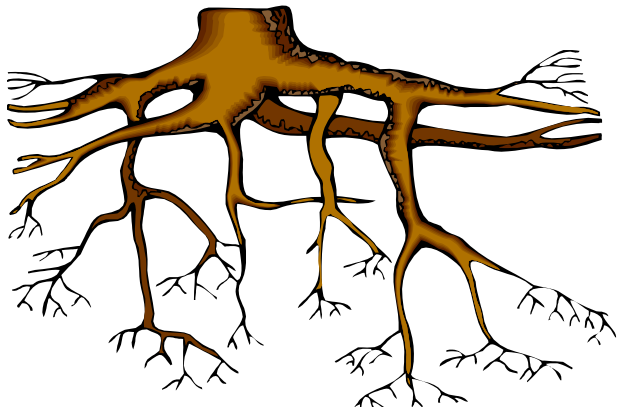
e) two multiple roots
f) three multiple roots
g) one simple root and two multiple roots
h) multiple roots

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.

$$f(x) = 0$$



Phase 1
Bounding the Solution

1. Graphing the function
2. Incremental search
3. Past experience with the problem or a similar one
4. Solution of a simplified approximate model
5. Previous solution in a sequence of solutions

Bounding the solution involves finding a rough estimate of the solution that can be used as the initial approximation, in an iterative procedure that refines the solution to a specified tolerance.

If possible, the root should be bracketed between two points at which the value of the nonlinear function has opposite signs.

"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)*

Phase 2

Iterative Refining the Solution

Two types of methods:

1. Closed domain (bracketing) methods
2. Open domain (non-bracketing) methods

Important question: How to stop an iteration?

Iterative refining the solution involves determining the solution to a specified tolerance by a systematic procedure.

There are numerous pitfalls in finding the roots of nonlinear equations.

abs. error $\left|g_{i+1} - g_i\right|$

rel. error $\left|\frac{g_{i+1} - g_i}{g_{i+1}}\right|$ never use $\left|1 - \frac{g_i}{g_{i+1}}\right|$

1.2 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:

1. Interval halving (bisection)
2. False position (regula falsi)

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

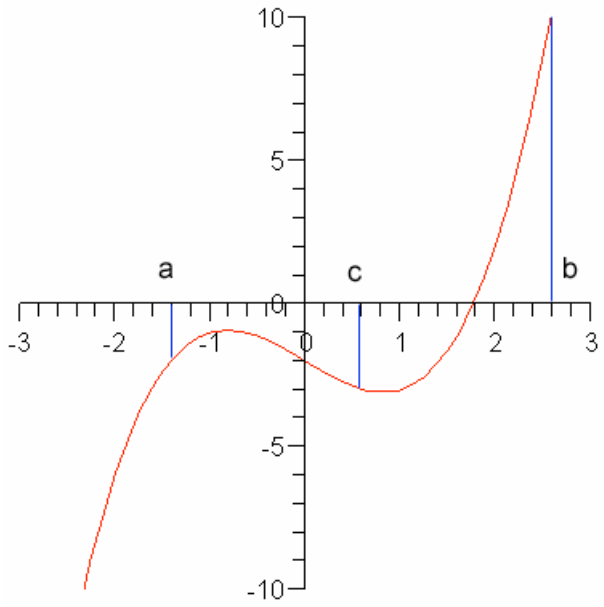
1.2.1 Bisectional method

the simplest but the most robust method!

- ✓ let f(x) be a continuous function on [a,b]
- ✓ let f(x) changes sign between a and b, f(a)f(b) < 0

Example: function

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



Bisectional method - algorithm

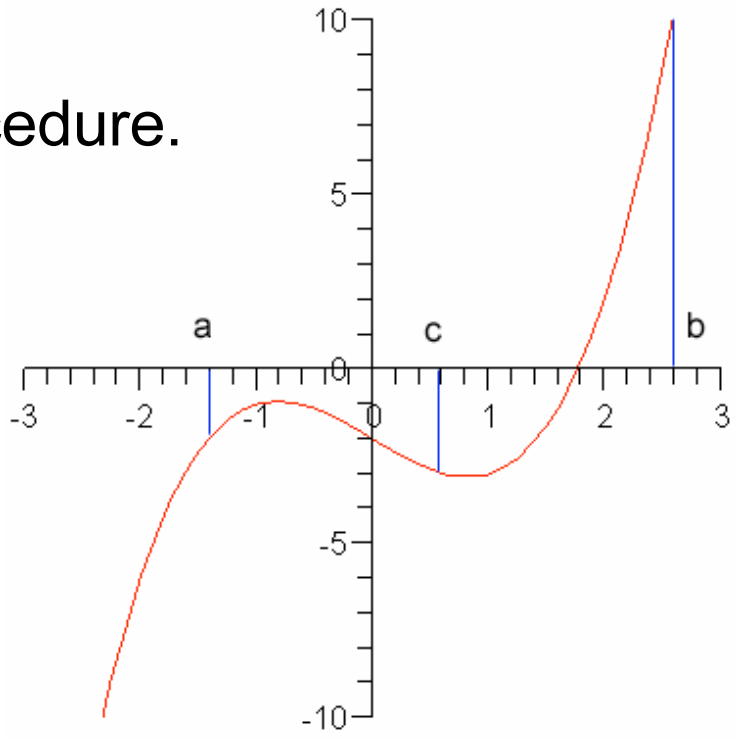
divide $[a,b]$ into two equal parts with $c = (a+b)/2$ then

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

Interval halving is an iterative procedure.

The iterations are continued until

$|b_i - a_i| \le \varepsilon_1$, or $|f(c_i)| \le \varepsilon_2$, or both.



Bisectional method – summary

The root is bracketed within the bounds of the interval, so the method is guaranteed to converge

On the 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.

The major disadvantage of the bisection method is that the solution converges slowly.

The method does not use information about actual functions behavior.

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) >= eps)
    {
      x0 = (xr + xl)/2.0;
      if((f(xl) * f(x0)) <= 0.0 ) xr = x0;
      else xl = x0;
     }
     return x0;
}
```

Example for y = x - cos(x) on [0.0,4.0] for eps = 1.0e-6

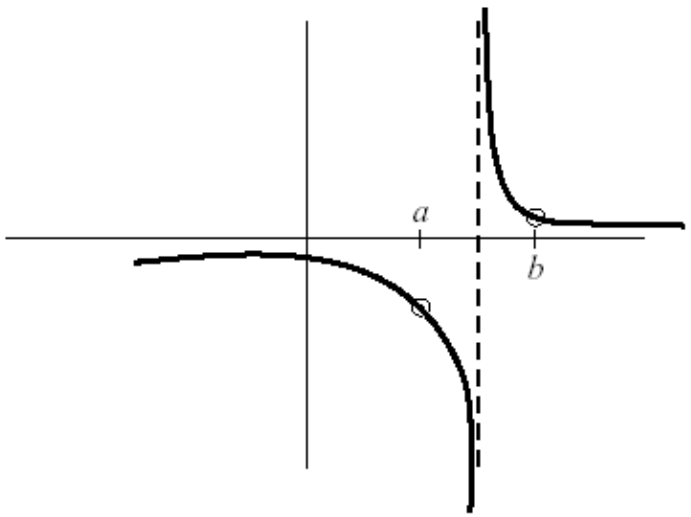
i	a	f(a)	b	f(b)	c	f(c)
1	0.00000	-1.00000	4.00000	4.65364	2.00000	2.41615
2	0.00000	-1.00000	2.00000	2.41615	1.00000	0.45970
3	0.00000	-1.00000	1.00000	0.45970	0.50000	-0.37758
4	0.50000	-0.37758	1.00000	0.45970	0.75000	0.01831
5	0.50000	-0.37758	0.75000	0.01831	0.62500	-0.18596
6	0.62500	-0.18596	0.75000	0.01831	0.68750	-0.08533
7	0.68750	-0.08533	0.75000	0.01831	0.71875	-0.03388
8	0.71875	-0.03388	0.75000	0.01831	0.73438	-0.00787
9	0.73438	-0.00787	0.75000	0.01831	0.74219	0.00520
10	0.73438	-0.00787	0.74219	0.00520	0.73828	-0.00135
11	0.73828	-0.00135	0.74219	0.00520	0.74023	0.00192
12	0.73828	-0.00135	0.74023	0.00192	0.73926	0.00029
13	0.73828	-0.00135	0.73926	0.00029	0.73877	-0.00053
14	0.73877	-0.00053	0.73926	0.00029	0.73901	-0.00012
15	0.73901	-0.00012	0.73926	0.00029	0.73914	0.00008
16	0.73901	-0.00012	0.73914	0.00008	0.73907	-0.00002
17	0.73907	-0.00002	0.73914	0.00008	0.73911	0.00003
18	0.73907	-0.00002	0.73911	0.00003	0.73909	0.00001
19	0.73907	-0.00002	0.73909	0.00001	0.73908	-0.00000
20	0.73908	-0.00000	0.73909	0.00001	0.73909	0.00000
21	0.73908	-0.00000	0.73909	0.00000	0.73908	-0.00000
22	0.73908	-0.00000	0.73909	0.00000	0.73909	0.00000

iterations	root
22	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 $x \rightarrow d$ would indicate that a discontinuity, not a root, is being found.



1.2.2 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 = α.

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).

False position method - algorithm

the slope of the linear function $g'(x)$ is given by

$g'(x) = \dfrac{f(b) - f(a)}{b - a}$ but at the same time $g'(x) = \dfrac{f(b) - f(c)}{b - c}$

solving the last equation for c with $f(c) = 0$ gives

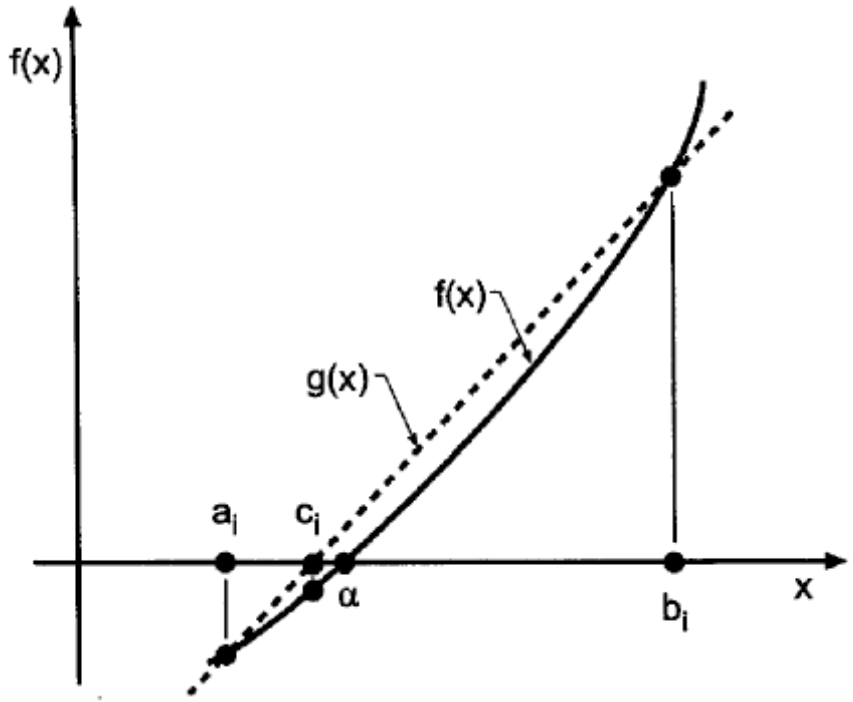
$c = b - \dfrac{f(b)}{g'(x)}$ and then

$c = b - f(b)\dfrac{b - a}{f(b) - f(a)}$

then like in bisectional method

if $f(a)f(c) < 0 \quad a = a, \quad b = c$

if $f(a)f(c) > 0 \quad a = c, \quad b = b$



Example: C++

```
 double false_p(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) >= eps)
    {
      x0 = xr - f(xr)*(xr - xl)/(f(xr)-f(xl));
      if((f(xl) * f(x0)) <= 0.0 ) xr = x0;
      else xl = x0;
     }
     return x0;
}
```

Example for y = x - cos(x) on [0.0,4.0] for eps = 1.0e-6

i	a	f(a)	b	f(b)	c	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

iterations	root
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.

1.3 Open Domain Methods

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*.

However, they use information about the nonlinear function itself to refine the estimates of the root. Thus, they are considerably more efficient than bracketing ones.

Most popular open domain methods

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

1.3.1 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.

Key idea: A continuous function f(x) around the point x may be expanded in Taylor series

$$f(x) = f(x_0) + (x - x_0) f'(x_0) + (x - x_0)^2 \frac{f''(x_0)}{2!} + \ldots$$

Suppose that x is the solution for $f(x) = 0$.

If we keep two first terms in Taylor series,

$$f(x) = 0 = f(x_0) + (x - x_0) f'(x_0)$$

it follows that

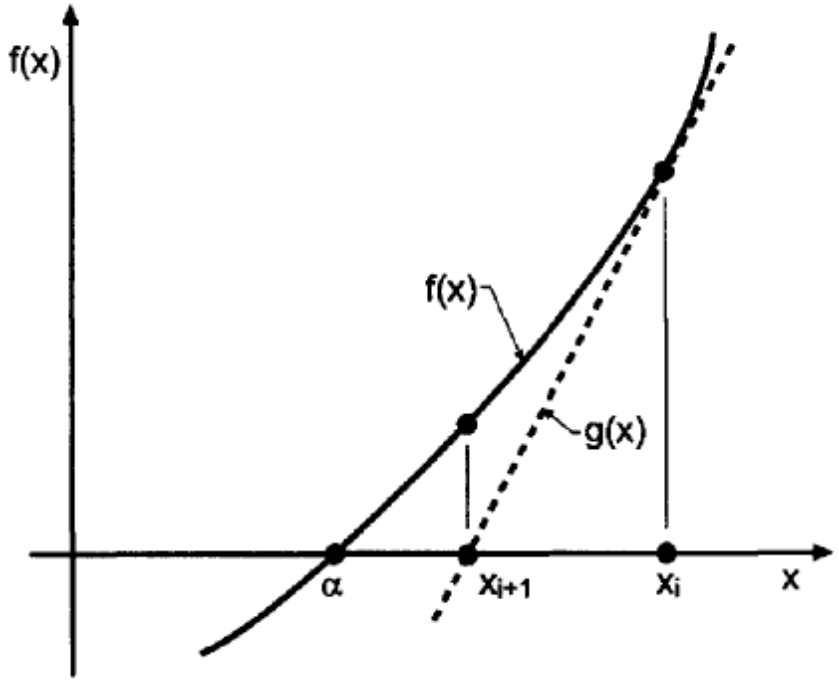
$$x = x_0 - \frac{f(x_0)}{f'(x_0)}$$

Newton's method - algorithm

We need $f(x)$ and $f'(x)$ to proceed

each next iteration is

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$



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;
    do {
        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;
}
```

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

```
iterations       root
      4        0.73909
```

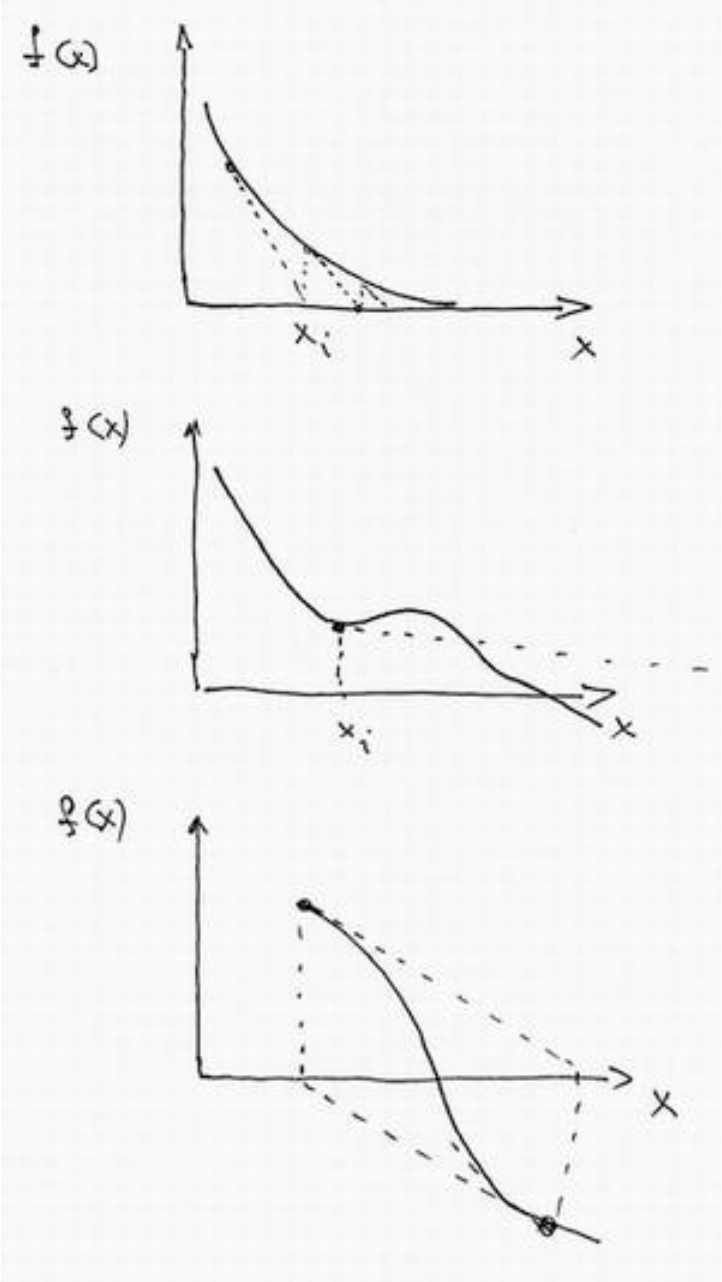
for bisectional method it takes 22 iterations

for false position – 8 iterations

Newton's method has excellent *local* convergence properties. (4 iterations above for a good guess)

However, its global convergence properties can be very poor, due to the neglect of the higher-order terms in the Taylor series

possible problems



a very slow approach to the solution when f'(x) → 0 around the root

difficulty with local minima, sending the next iteration value x_{k+1} far away

lack of convergence for asymmetric functions
f(a+x)=-f(a-x)

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.
- ✓ 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)

1.3.2 Method of secants

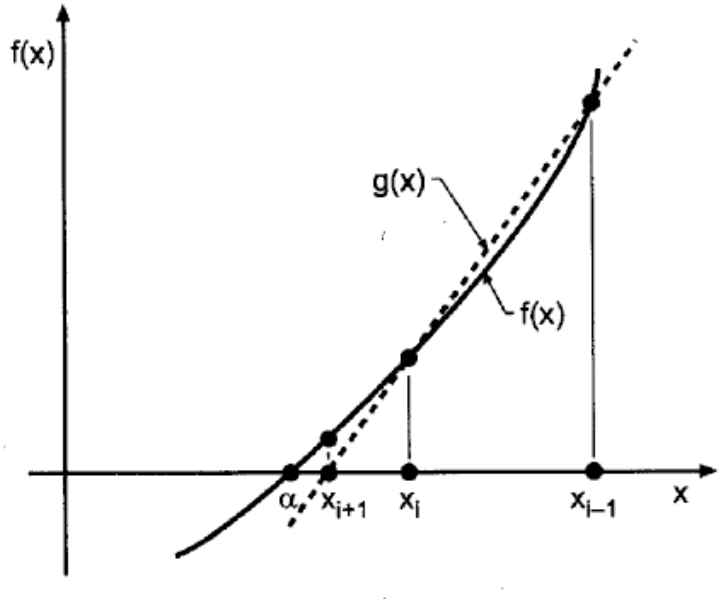
The secant method is a variation of Newton's method when the evaluation of derivatives is difficult.

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).

Method of secants - algorithm

The derivative f' of the continuum function f(x) at point x_k can be presented by

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$



from Newton's method follows

$$x_{i+1} = x_i - \frac{f(x_i)(x_i - x_{i-1})}{f(x_i) - f(x_{i-1})}$$

One has to select two initial points to start

By the way: the method of secant = the False position method

$$c = b - f(b)\frac{b - a}{f(b) - f(a)}$$

the only difference is about the two points to select

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)
    {
     i = i + 1;
     x3 = x2 - (f(x2)*(x2-x1))/(f(x2)-f(x1));
     x1 = x2;
     x2 = x3;
     if(i >= iter) break;
     }
    if (i == iter) flag = 0;
    return x3;
}
```

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 method it takes 22 iterations, but for Newton only 4 iterations.

The question of which method is more efficient, Newton's method or the secant method, was answered by Jeeves. He 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.

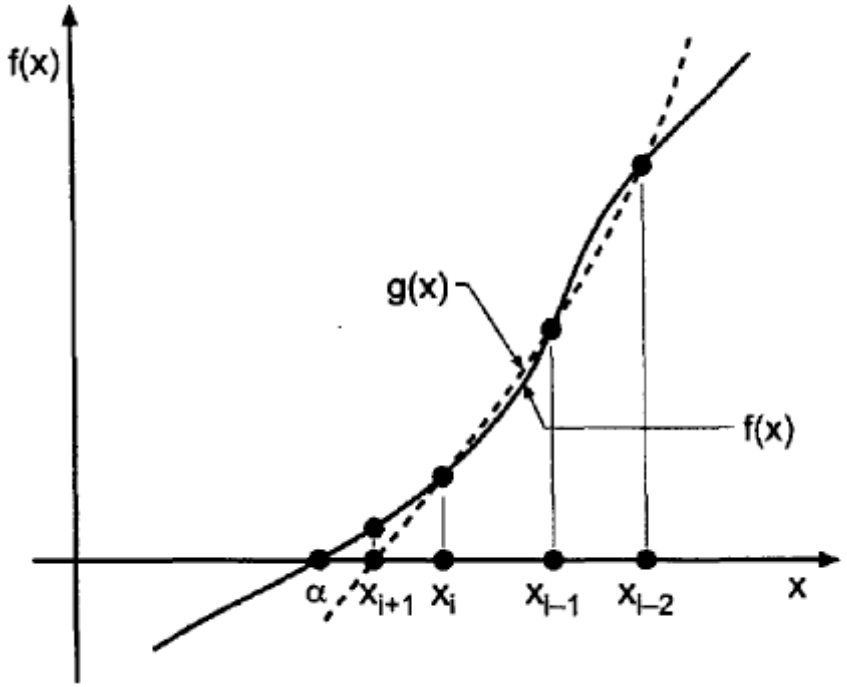
1.3.3 Muller's Method

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.

Muller's Method (cont.)

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.



1.3.4 Summary for the open 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.

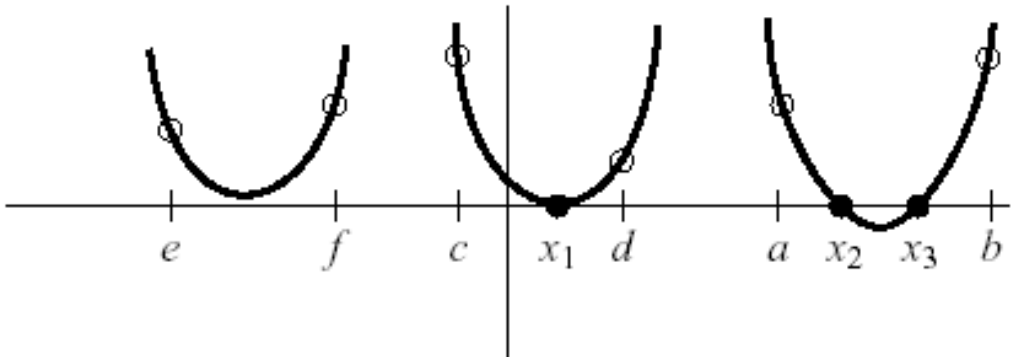
All three of the methods can find complex roots simply by using complex arithmetic.

Complications

there are no roots at all (see “the black cat” story)

there is one root but the function does not change the sign, as in the equation $x^2-2x+1=0$

there are two or more roots on an interval [a,b]

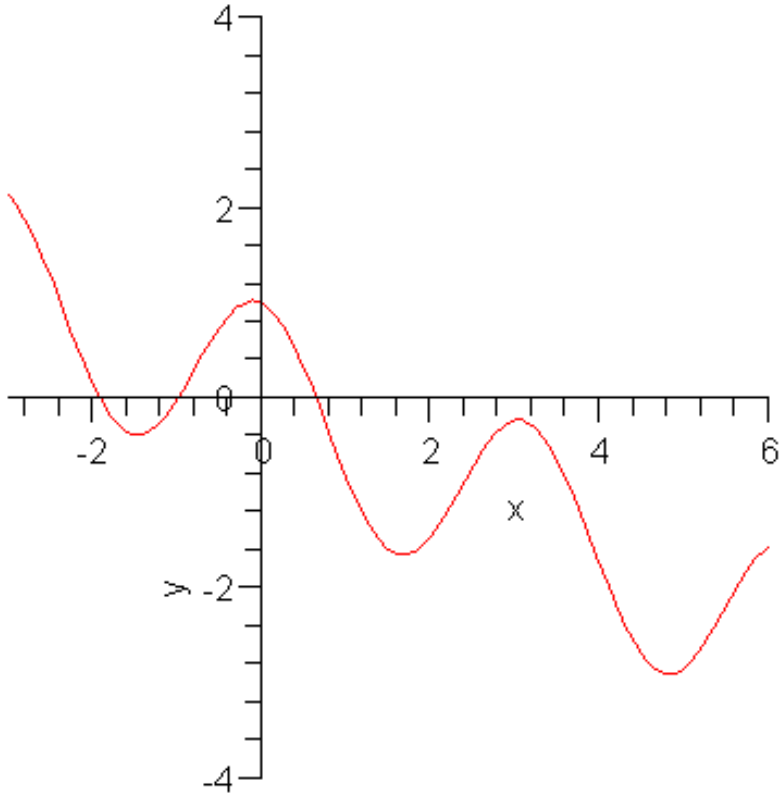


What will happen if we apply the bisectional method here?

How about Newton’s method?

More complications

there are many roots on an interval [a,b]

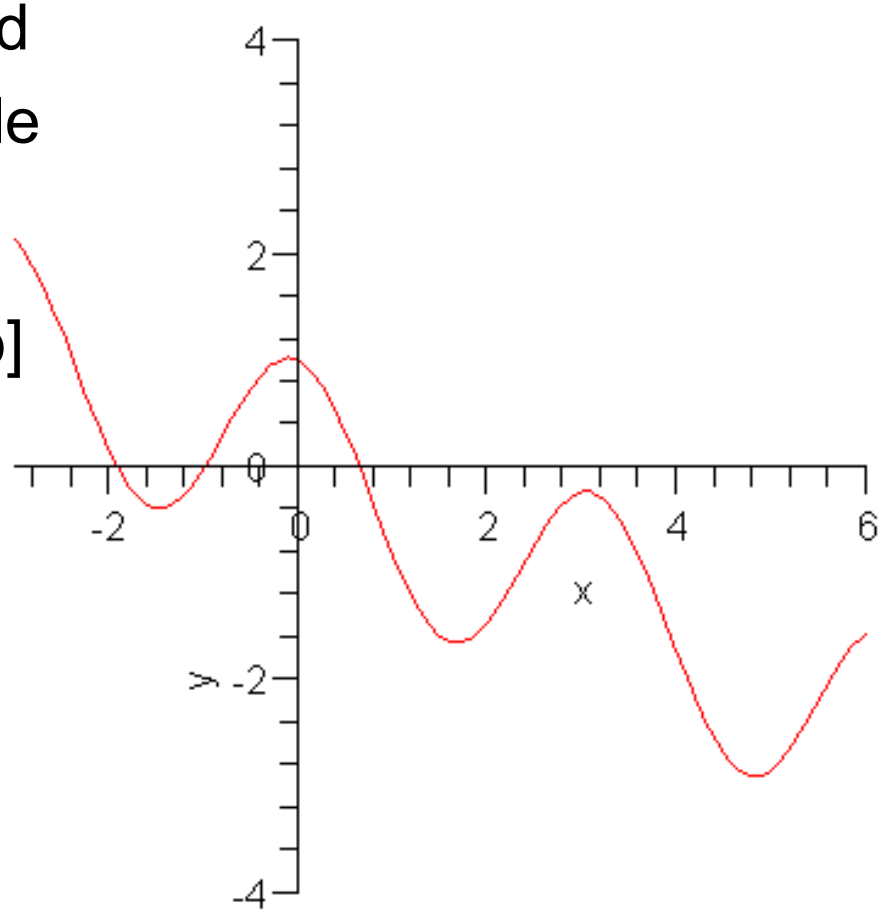


What root will you find with the bisectional method?

1.4 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 the each h.



Step size in brute force method

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 2.

Roots of Polynomials

$$a_n x^n + a_{n-1} x^{n-1} + \ldots + a_1 x + a_0 = 0$$

Short notes on polynomials

The fundamental theorem of algebra states that a n^{th}-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).

Short notes on polynomials (cont.)

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.

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.

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.

The open methods for $P_n(x)$

There are various modifications of Newton's method for polynomials

Other methods for polynomials: Bairstow's method, Laguerre's method, Eigenvalue method, …

Part 3.

Nonlinear systems of equations

$$f(x, y) = 0$$

$$g(x, y) = 0$$

Short note on nonlinear systems

“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.

Newton method

Given: $f(x,y)=0$ and $g(x,y)=0$

find x^* and y^* such that $f(x^*,y^*) \sim 0$ and $g(x^*, y^*) = 0$.

two-variable Taylor series about (x,y),

$$f(x^*,y^*) \approx f(x,y) + f_x' \cdot (x^* - x) + f_y' \cdot (y^* - y) + \ldots$$

$$g(x^*,y^*) \approx g(x,y) + g_x' \cdot (x^* - x) + g_y' \cdot (y^* - y) + \ldots$$

keeping only first-order terms and considering that

$f(x^*,y^*) \approx 0$ and $g(x^*,y^*) \approx 0$ one have a system

of linear equations for x^* and y^* that gives

$$x^* = x + \frac{f_y' g(x,y) - f(x,y) g_y'}{f_x' g_y' - f_y' g_x'}$$

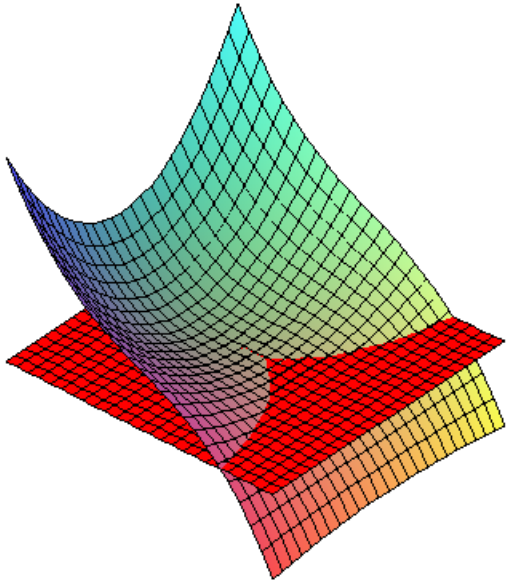
$$y^* = y + \frac{g_x' f(x,y) - g(x,y) f_x'}{f_x' g_y' - f_y' g_x'}$$

Example: C++

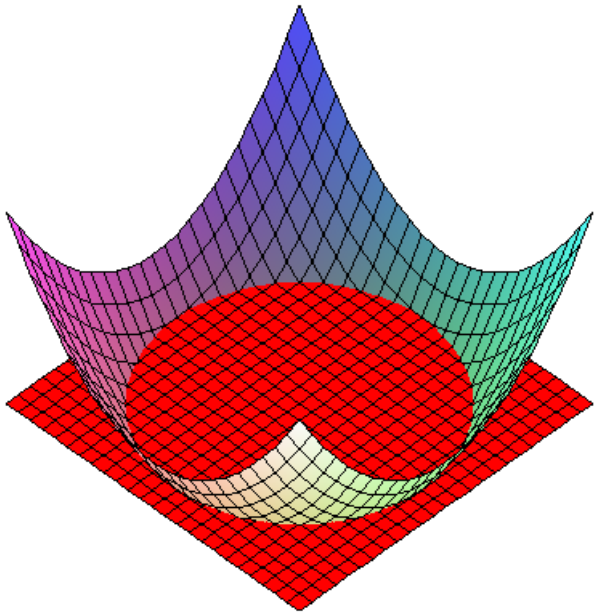
```
void newton2(double& x1, double& y1, double eps, int& i)
{
   double      f1, g1, fx, fy, gx, gy;
   double      del, x2, y2, dx, dy;
   int iter = 99;
   i = 0;
   do {
       i = i + 1;
       fg(x1, y1, f1, g1, fx, fy, gx, gy);
       del = fx*gy - fy*gx;
       dx=(fy*g1-f1*gy)/del;
       dy=(f1*gx-fx*g1)/del;
       x2=x1+dx;
       y2=y1+dy;
       x1=x2;
       y1=y2;
       if(i >= iter) break;
   } while (fabs(dx) >= eps && fabs(dy) >=eps);
   i = i+1;
}
```

Example: $\begin{cases} y^2(1-x) = x^3 \\ x^2 + y^2 = 1 \end{cases}$

$f(x,y) = y^2(1-x) - x^3$
$h(x,y) = 0$



$g(x,y) = x^2 + y^2 - 1$
$h(x,y) = 0$



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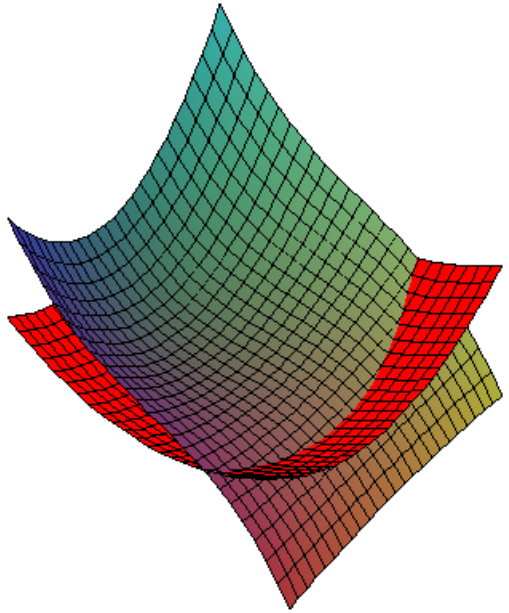


Example:

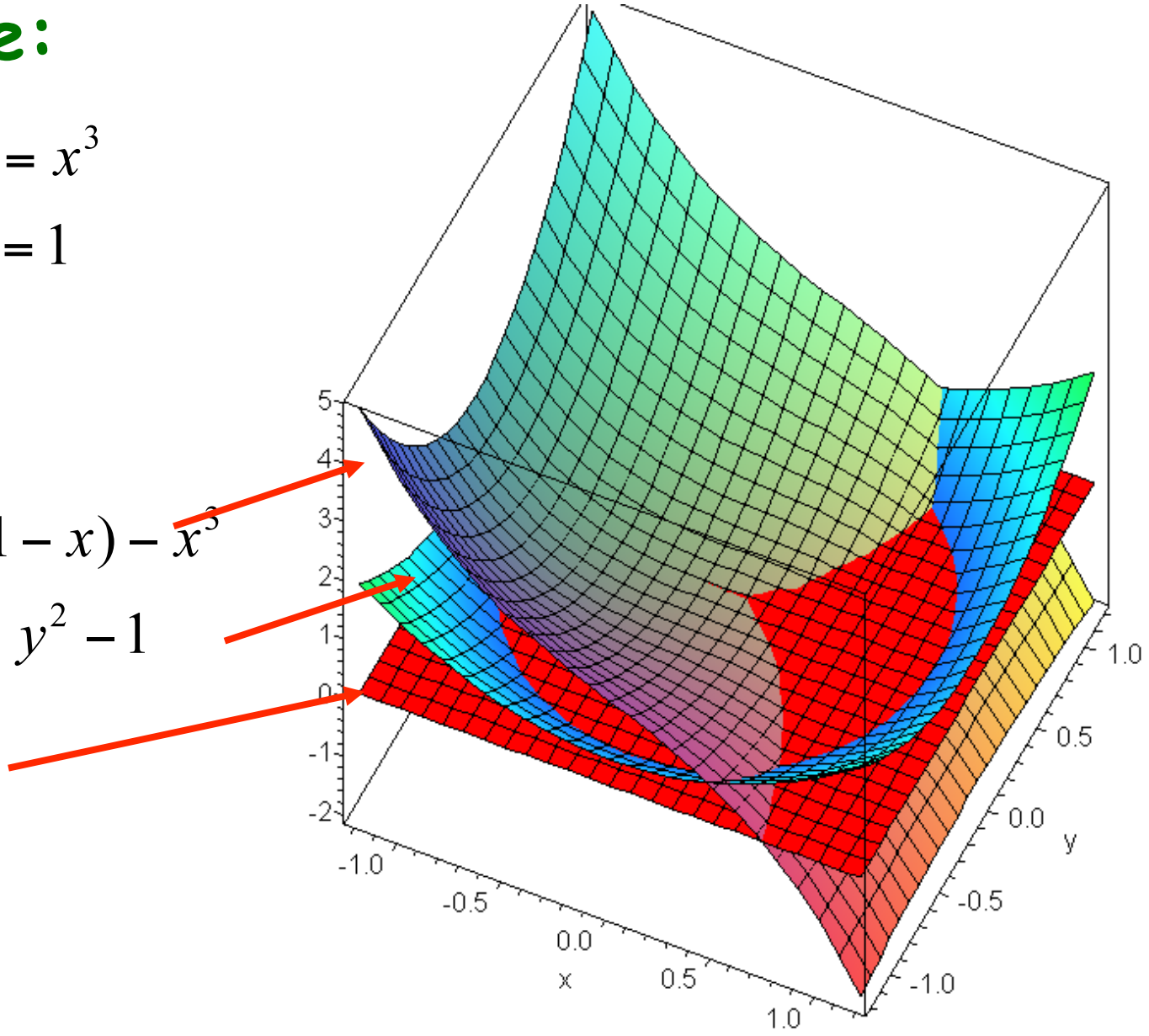
$$\begin{cases} y^2(1-x) = x^3 \\ x^2 + y^2 = 1 \end{cases}$$

plots:

$f(x,y) = y^2(1-x) - x^3$

$g(x,y) = x^2 + y^2 - 1$

$h(x,y) = 0$



$$\begin{cases} y^2(1-x) = x^3 \\ x^2 + y^2 = 1 \end{cases}$$

Example with various initial points

Newtons method for two coupled nonlinear equations

i	x	y	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		

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5	0.61803	-0.78615	-0.00000	0.00000	-0.00000	-0.00000
6	0.61803	-0.78615	-0.00000	0.00000		

Part 4.

Summary

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
- ✓ 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.

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

more comments

1. Good initial approximations are extremely important.
2. For smoothly varying functions, most algorithms will always converge if the initial approximation is close enough.
3. Many, if not most, problems in engineering and science are well behaved and straightforward.
4. 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.
5. If a nonlinear equation has complex roots, that must be anticipated when choosing a method.
6. Analyst's time versus computer time must be considered when selecting a method.

Root-finding algorithms should contain the following features:

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

Some thoughts

- ✓ Choosing right computational method for finding roots is a difficult skill for beginners.
- ✓ A method that was efficient for one equation may fail miserably for another
- ✓ Any method should be used intellingently!