Roots of Equations

- Real roots of single variable function.
- Closed domain methods (bracketing).

Examples of nonlinear equations

- Equations of a single variable:

$$x^2 - 6x + 9 = 0$$
$$x^2 - \cos(x) = 0$$
$$\exp(x)\ln(x^2) - x\cos(x) = 0$$

- Equations of two variables:

$$y(x^3 - 1) = x^4$$
$$x^2 + y^2 = 1$$

Introduction

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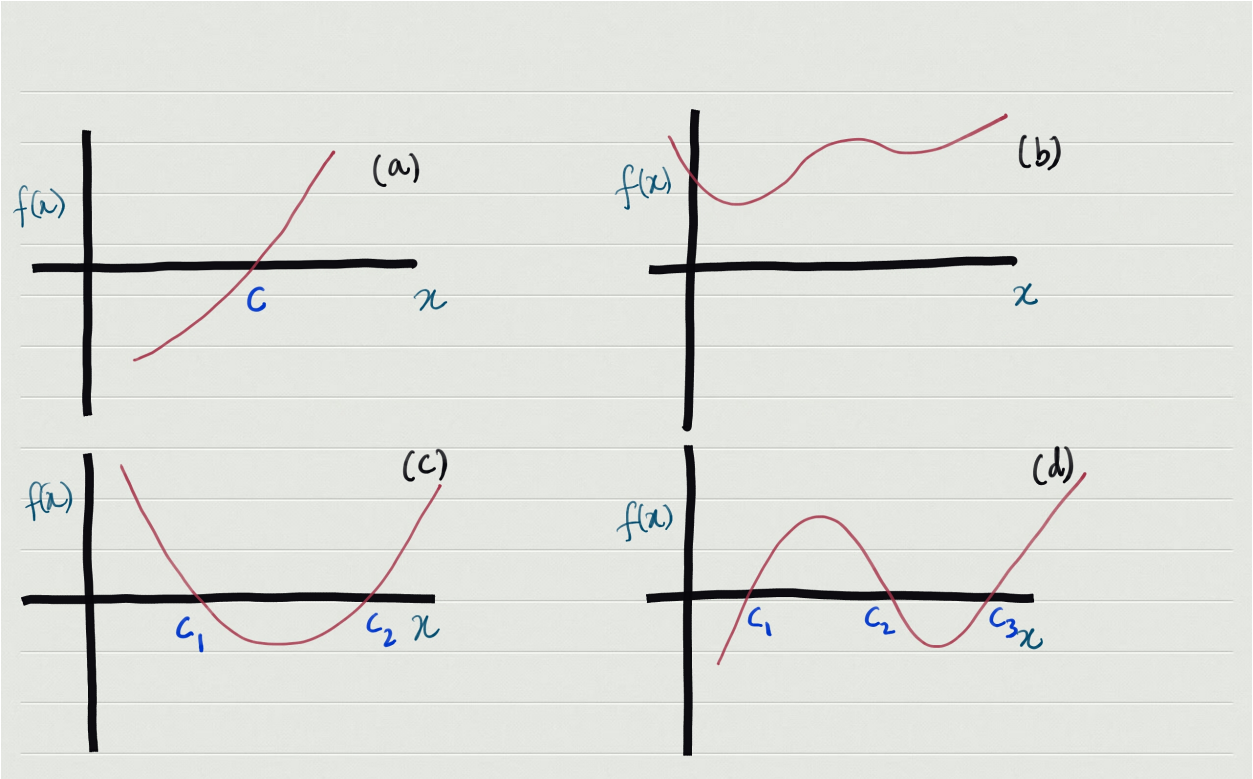
Behaviour of non-linear functions



(a) A single root.
(b) No real roots exist (complex roots might).
(c) Two simple roots.
(d) Three simple roots.

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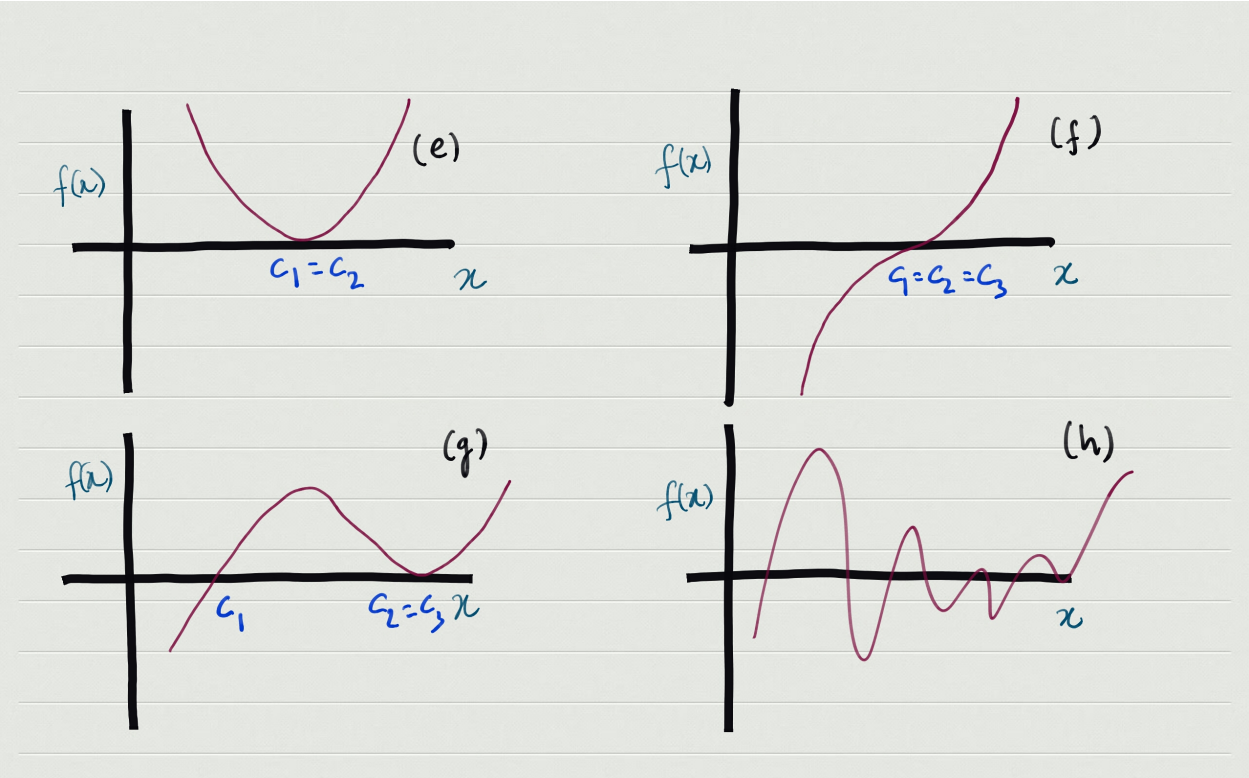

(e) Two multiple roots.

(f) Three multiple roots.

(g) One simple root and two multiple roots.

(h) Multiple roots.

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- So, it is crucial to have a good guess...

Bounding the solution

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- If possible, the root should be bracketed between two points at which the value of the non-linear function changes sign!

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- Previous solution in a sequence of solutions.

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- *There are numerous pitfalls in finding the roots of non linear equations*.
- An important question is when to stop the iteration –

$$\text{Absolute error:} |f_{i+1} - f_i|$$

$$\text{Relative error:} \left|\frac{f_{i+1} - f_i}{f_{i+1}}\right|$$

Types of Methods

There are two types of methods for finding roots of non linear equations:

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

Closed domain (bracketing) method

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  - False position method.
- In general, bracketing methods are quite robust – ie they are guaranteed to give a solution as the solution is bracketted in the interval.

Bisection Method

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- $f(x)$ a continuous function on $[a, b]$.
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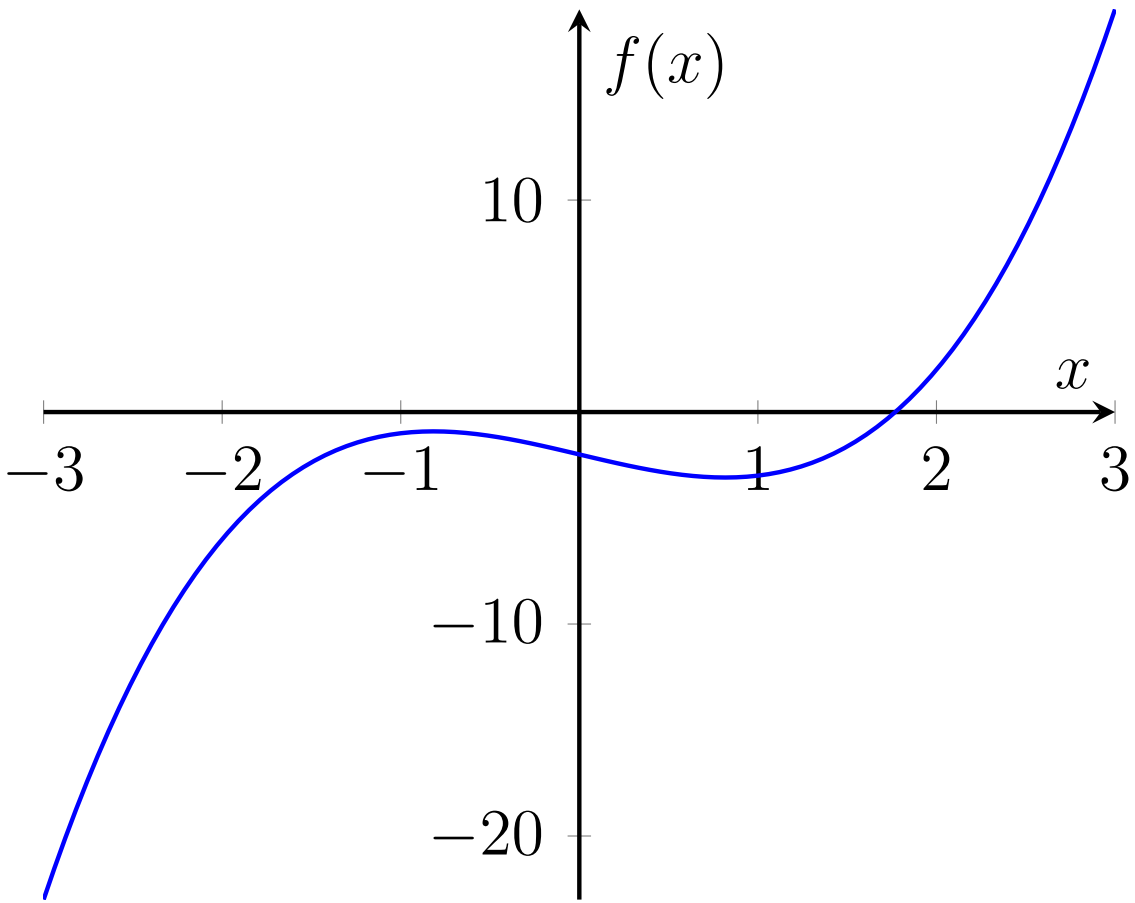
Consider an example: $f(x) = x^3 - 2x - 2$



Bisection Method: Algorithm

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$$\begin{aligned} &< 0 \text{ there is a root in } [a, c] \implies a = a, b = c \\ f(a)f(c) &> 0 \text{ there is a root in } [b, c] \implies a = c, b = b \\ &= 0 \text{ root is at } c \end{aligned}$$

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- Interval halving is an iterative procedure.
- Continue iterations till $|b - a| < \text{tol}$ or $|f(c)| < \text{tol}$ or both

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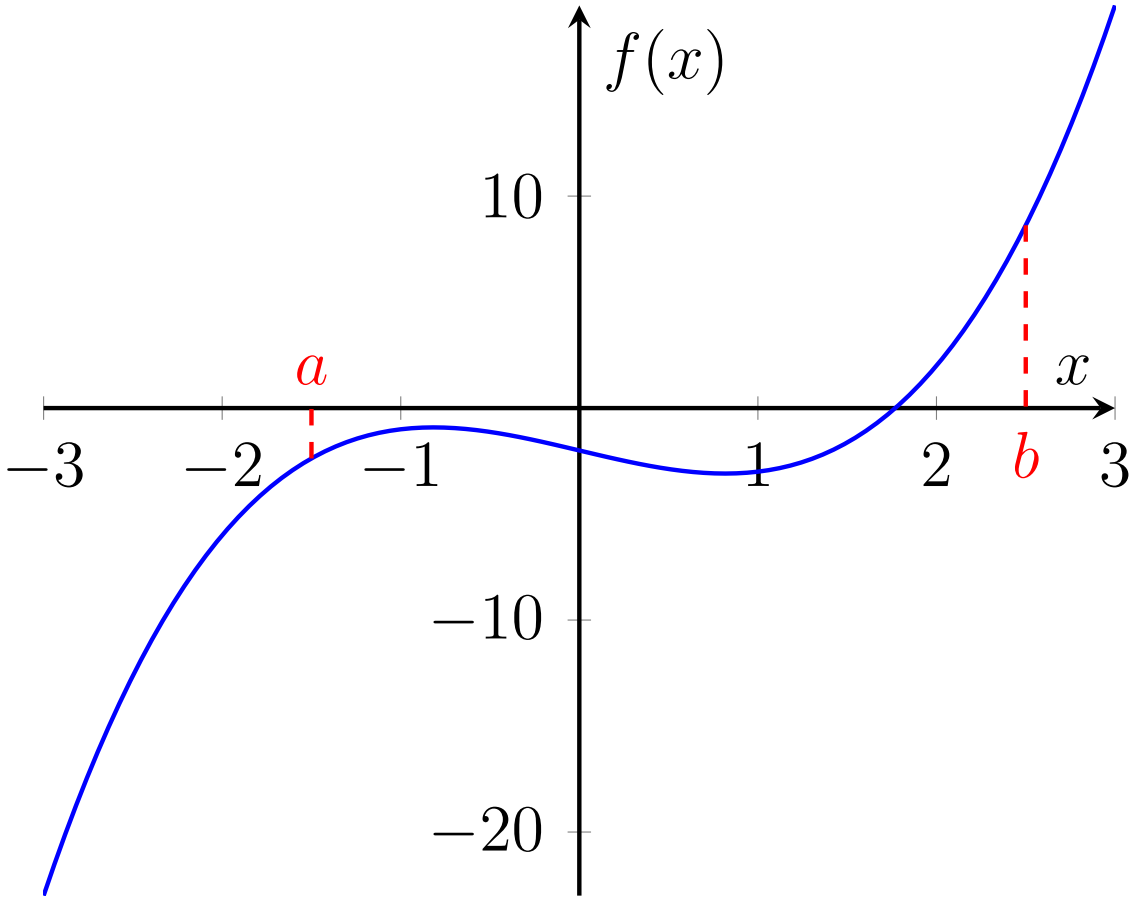

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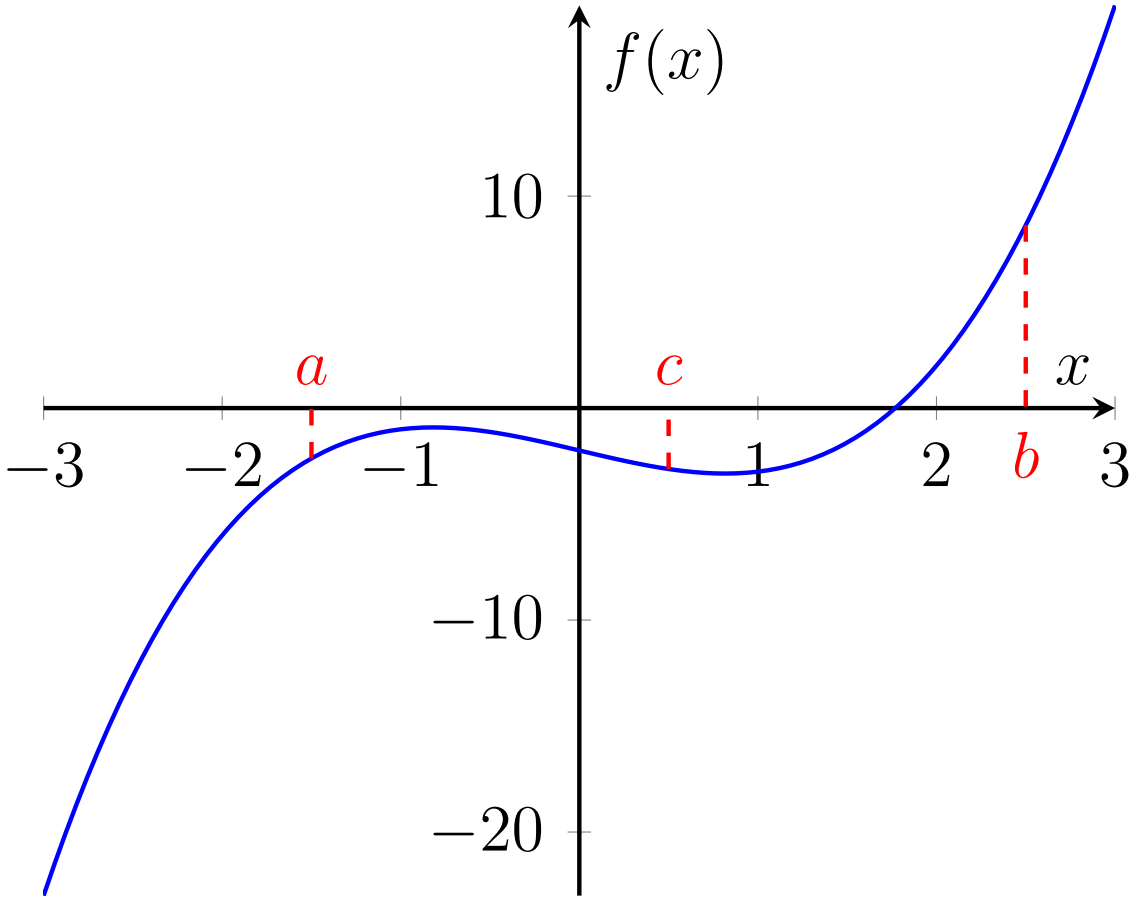

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- Notice that this method does not use any information about the function's behaviour!

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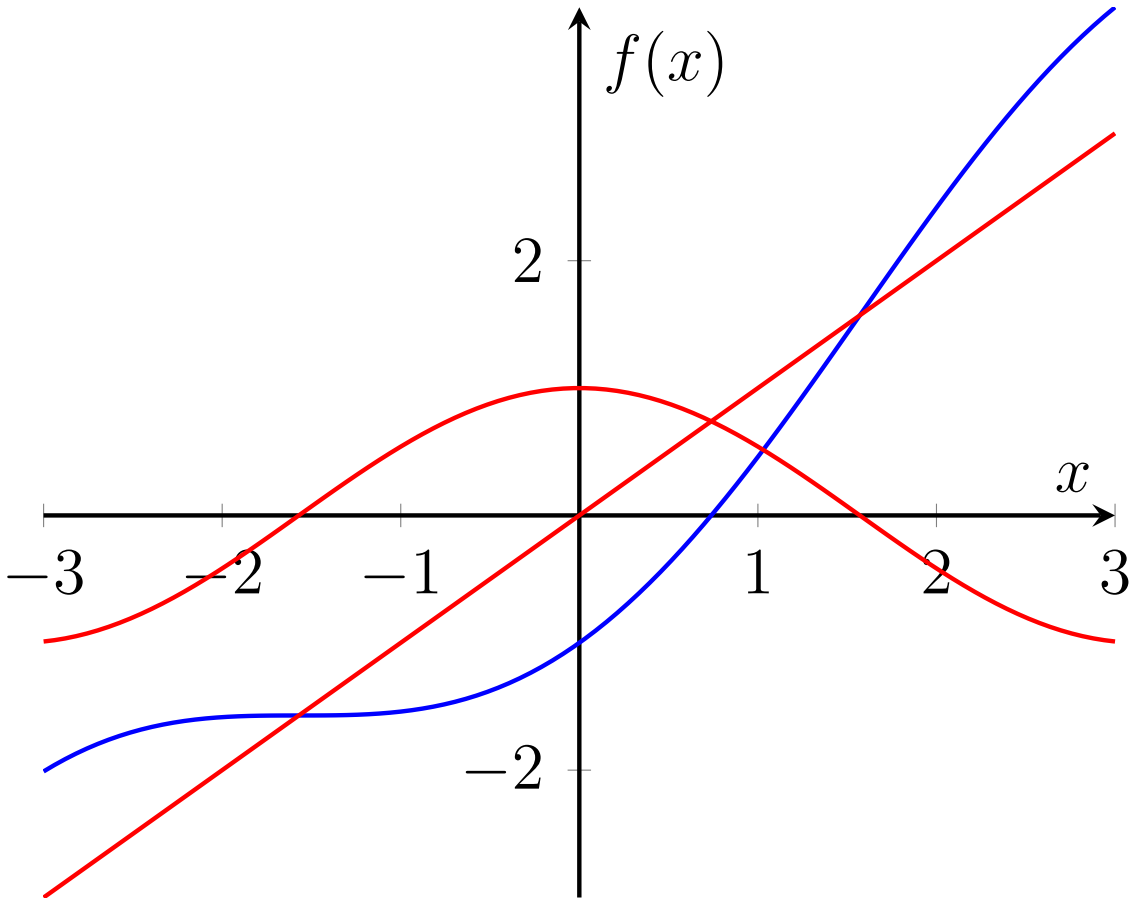

Bisection method: example

i	a	f(a)	b	f(b)	c	f(c)
1	0.000000	-1.000000	4.000000	4.653644	2.000000	2.416147
2	0.000000	-1.000000	2.000000	2.416147	1.000000	0.459698
3	0.000000	-1.000000	1.000000	0.459698	0.500000	-0.377583
4	0.500000	-0.377583	1.000000	0.459698	0.750000	0.018311
5	0.500000	-0.377583	0.750000	0.018311	0.625000	-0.185963
6	0.625000	-0.185963	0.750000	0.018311	0.687500	-0.085335
7	0.687500	-0.085335	0.750000	0.018311	0.718750	-0.033879
8	0.718750	-0.033879	0.750000	0.018311	0.734375	-0.007875
9	0.734375	-0.007875	0.750000	0.018311	0.742188	0.005196
10	0.734375	-0.007875	0.742188	0.005196	0.738281	-0.001345
11	0.738281	-0.001345	0.742188	0.005196	0.740234	0.001924
12	0.738281	-0.001345	0.740234	0.001924	0.739258	0.000289
13	0.738281	-0.001345	0.739258	0.000289	0.738770	-0.000528
14	0.738770	-0.000528	0.739258	0.000289	0.739014	-0.000120
15	0.739014	-0.000120	0.739258	0.000289	0.739136	0.000085
16	0.739014	-0.000120	0.739136	0.000085	0.739075	-0.000017
17	0.739075	-0.000017	0.739136	0.000085	0.739105	0.000034
18	0.739075	-0.000017	0.739105	0.000034	0.739090	0.000008
19	0.739075	-0.000017	0.739090	0.000008	0.739082	-0.000005
20	0.739082	-0.000005	0.739090	0.000008	0.739086	0.000002
21	0.739082	-0.000005	0.739086	0.000002	0.739084	-0.000001
22	0.739084	-0.000001	0.739086	0.000002	0.739085	0.000000

Root is: 0.739085197449

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- The root of the linear function, $g(x)$, $x = c$ is not the root of the non linear function $f(x)$. It is a *false position* and hence the name.
- Unlike bisection, this method uses some information about the function $f(x)$.

False position method: Algorithm

The slope of linear function, $g'(x)$, is given by:

$$g'(x) = \frac{f(b) - f(a)}{b - a}$$

Assuming $f(c) = 0$, one can also write $g'(x)$ as:

$$g'(x) = \frac{f(b) - f(c)}{b - c} \implies c = b - \frac{f(b)}{g'(x)}$$

Combining with the first equation:

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

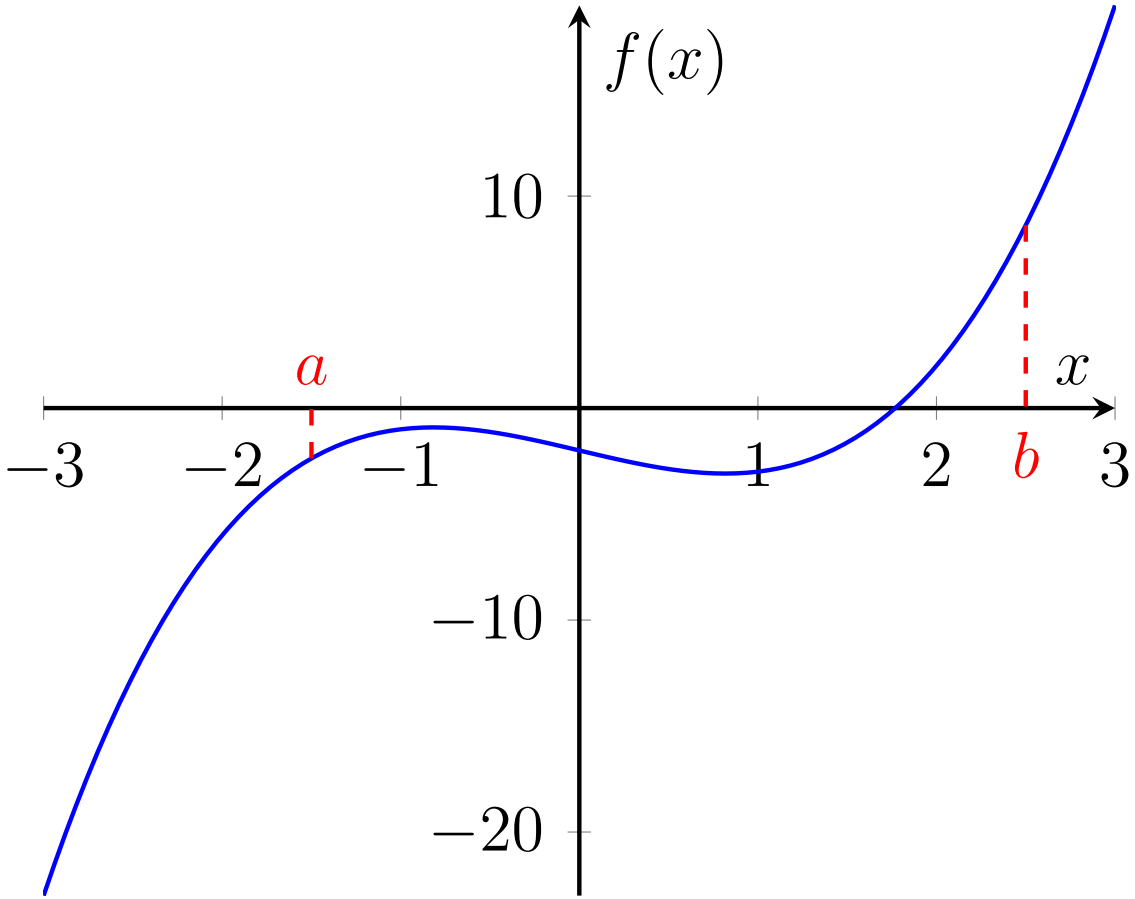
$$c = \frac{a * f(b) - b * f(a)}{f(b) - f(a)}$$

Then just like the bisection method:

$$\text{if } f(a) * f(c) < 0 \; a = a, b = c$$

$$\text{if } f(a) * f(c) > 0 \; a = c, b = b$$

False position method: Example



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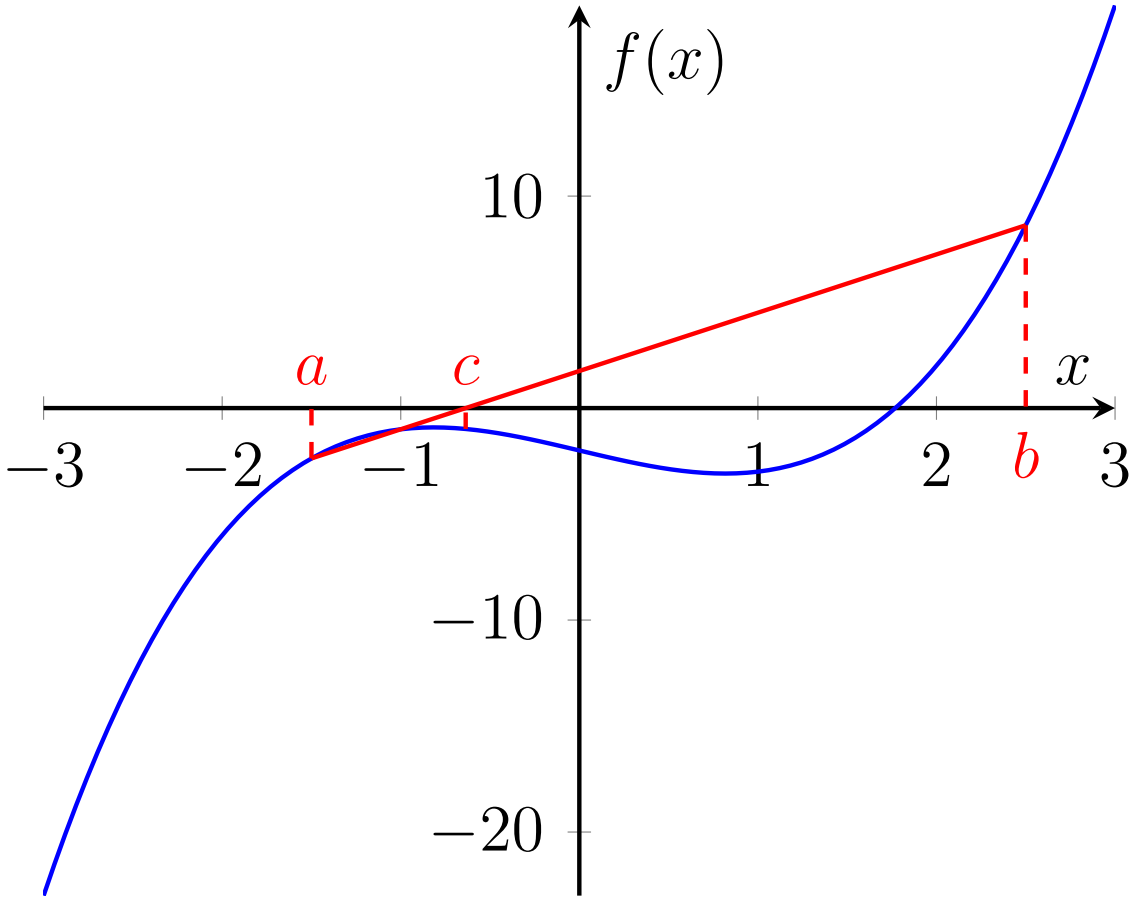

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2	0.707508	-0.052475	4.000000	4.653644	0.744221	0.008605
3	0.707508	-0.052475	0.744221	0.008605	0.739049	-0.000061
4	0.739049	-0.000061	0.744221	0.008605	0.739085	-0.000000

```
Root is: 0.739085092149
```

False position used 4 iterations compared to 22 in bisection!
Generally false position converges much faster than bisection.

Open domain methods

- Newton's iteration.
- Method of secants.
- Muller's method.
- Fixed point iteration.

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- As a result, these methods are not as *robust* as bracketing methods – these methods may not converge at all.
- They use information about the non linear function to refine the estimates of the root – can be considerably more efficient than bracketing methods.

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- It always converges *if the initial approximation is sufficiently close to the root*. Its rate of convergence is quadratic!
- However, it not only needs $f(x)$, it also needs the derivative $f'(x)$.

Newton's method: Key idea

A continuous function $f(x)$ can be expanded around a point x is terms of a Taylor's series:

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

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Using this we can write:

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

Newton's method: Algorithm

The iterations use $f(x)$ and $f'(x)$ to proceed in the following way:

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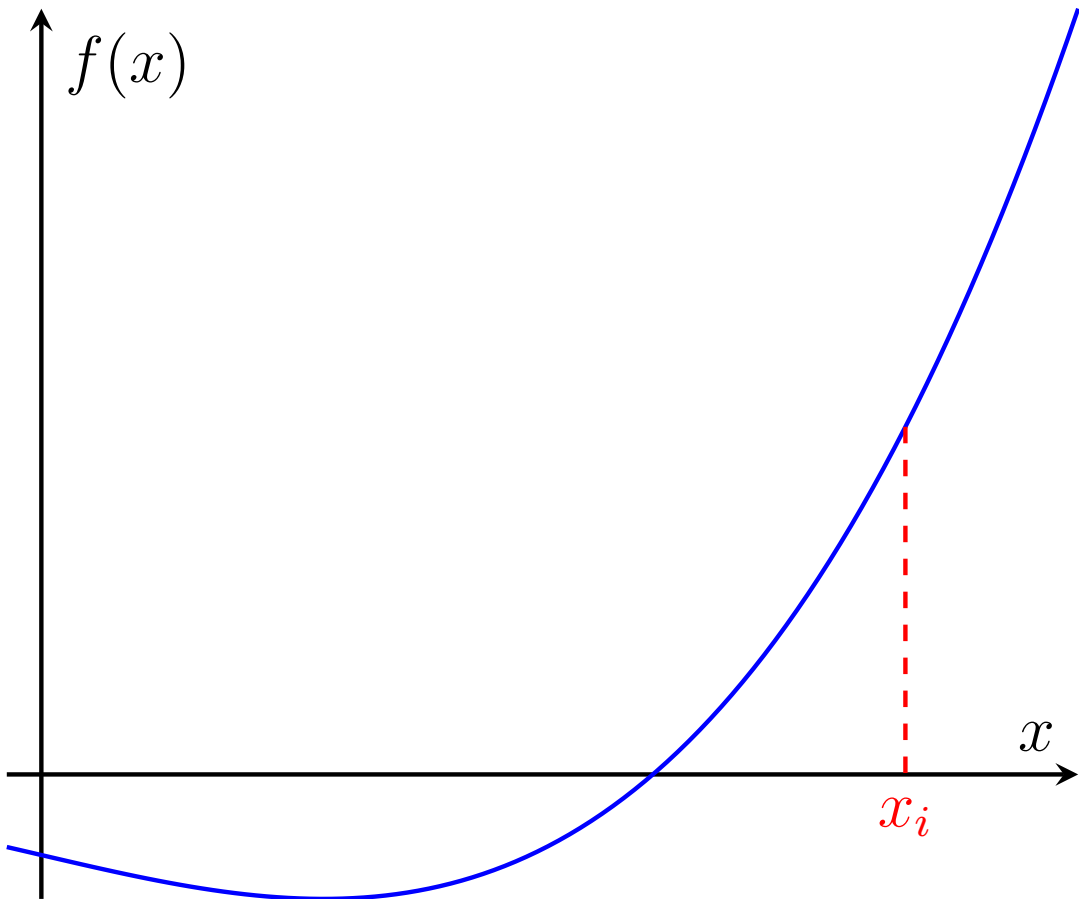

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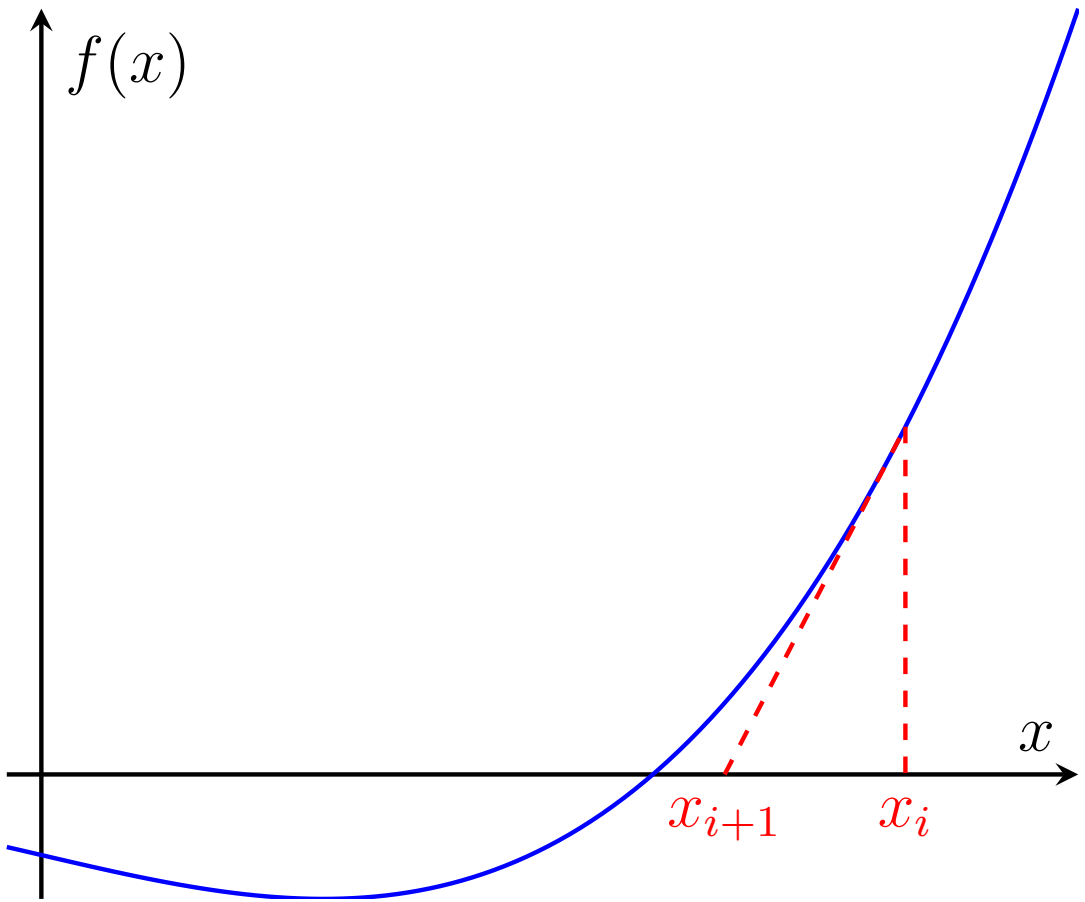

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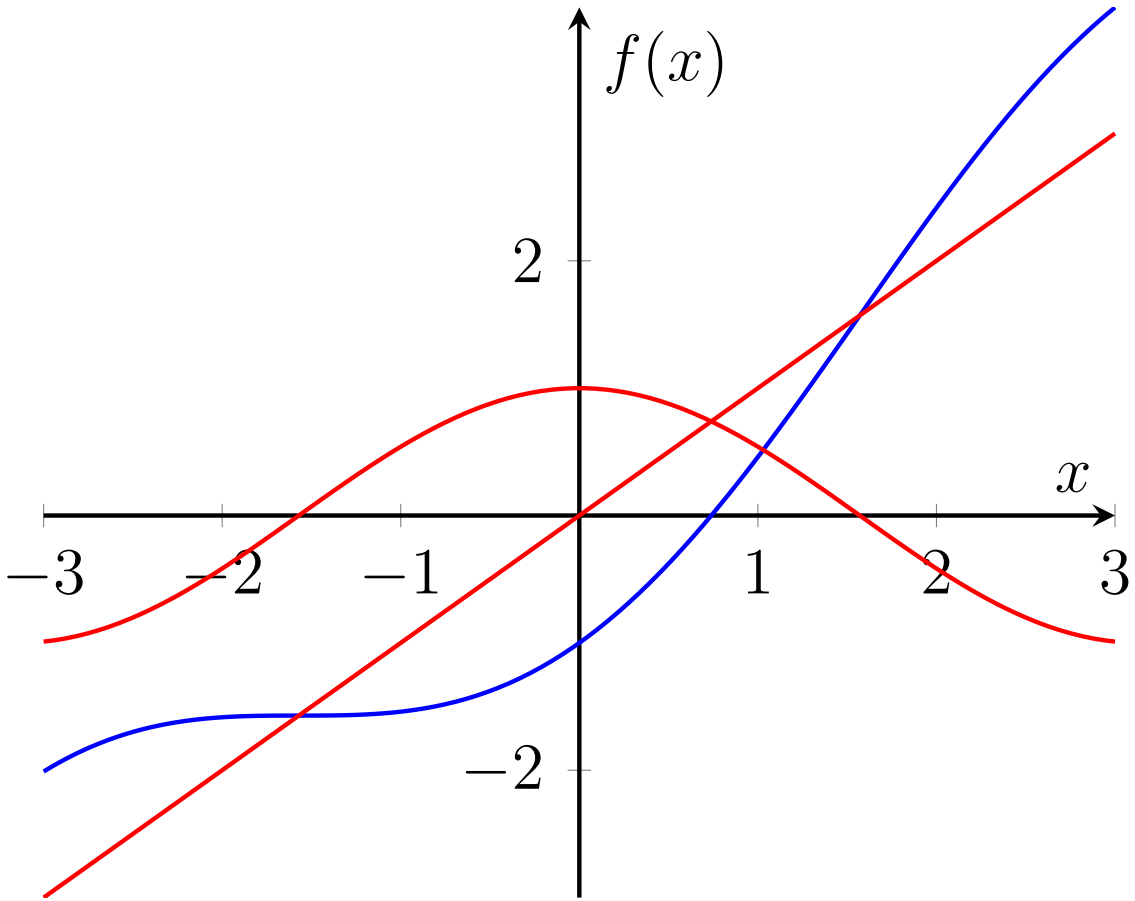


Initial guess $x = 1.0$.

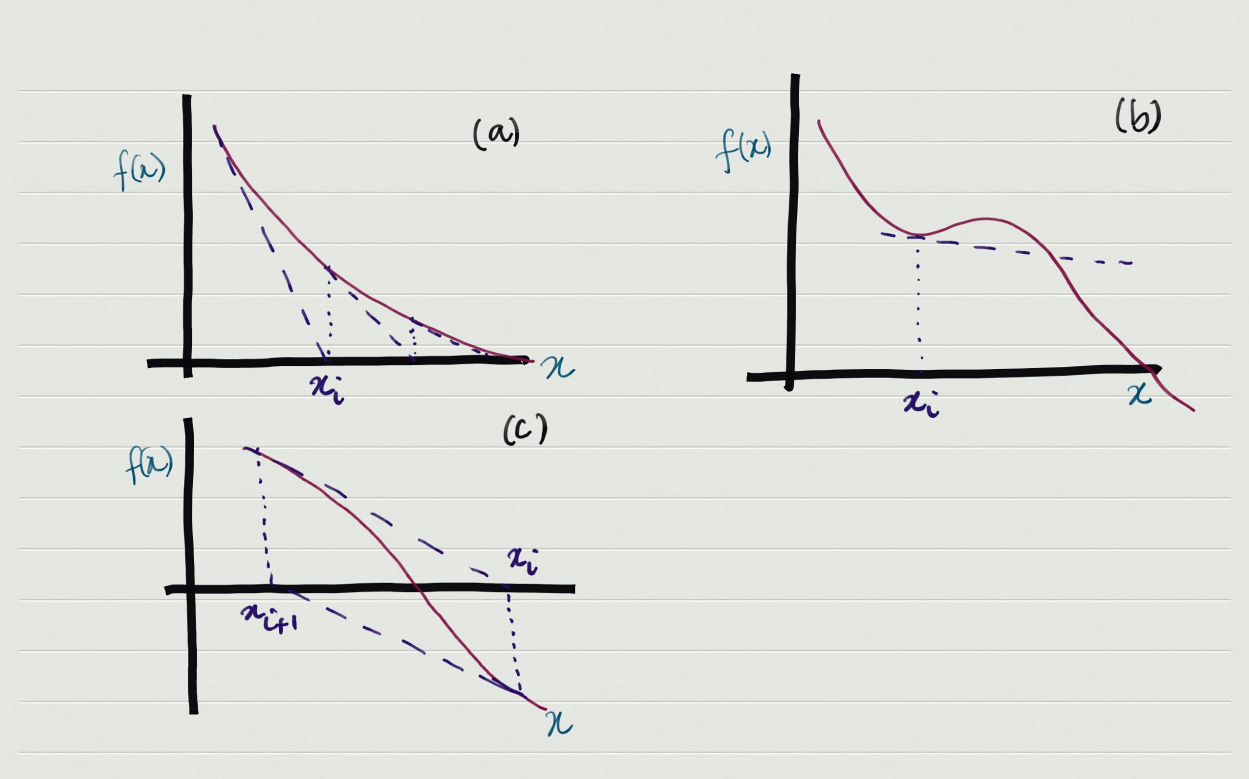
Newton's method: example

```
  i     x_i       f(x_i)     f'(x_i)   x_{i+1}   f(x_{i+1})
  1   1.000000  0.459698   1.841471   0.750364   0.018923
  2   0.750364  0.018923   1.681905   0.739113   0.000046
  3   0.739113  0.000046   1.673633   0.739085   0.000000

Root is: 0.739085133385
```

- False position used 4 iterations and bisection – 22 iterations!
- Newton's method has excellent local convergence properties.
- However, global convergence properties can be quite poor – due to neglect of higher order terms in the Taylor series expansion.

Possible problems



(a) Very slow approach to the root – $f'(x) \to 0$ near the root.

(b) Difficulty with local minima – may send the next iteration x_{i+1} very far from the root.

(c) Lack of convergence for asymmetric functions: $f(a+x) = -f(a-x)$

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- The method not only requires the function, but also its derivative. Besides being an additional computational expense, in some cases, it might not be possible to calculate the derivative easily...
- If the derivative becomes small – the method may end up not converging – as the next step might be far away from the root.

Method of secants

- The secant method is a variant of Newton's method – for the case when the evalulation of the derivative is difficult/impossible.

Method of secants

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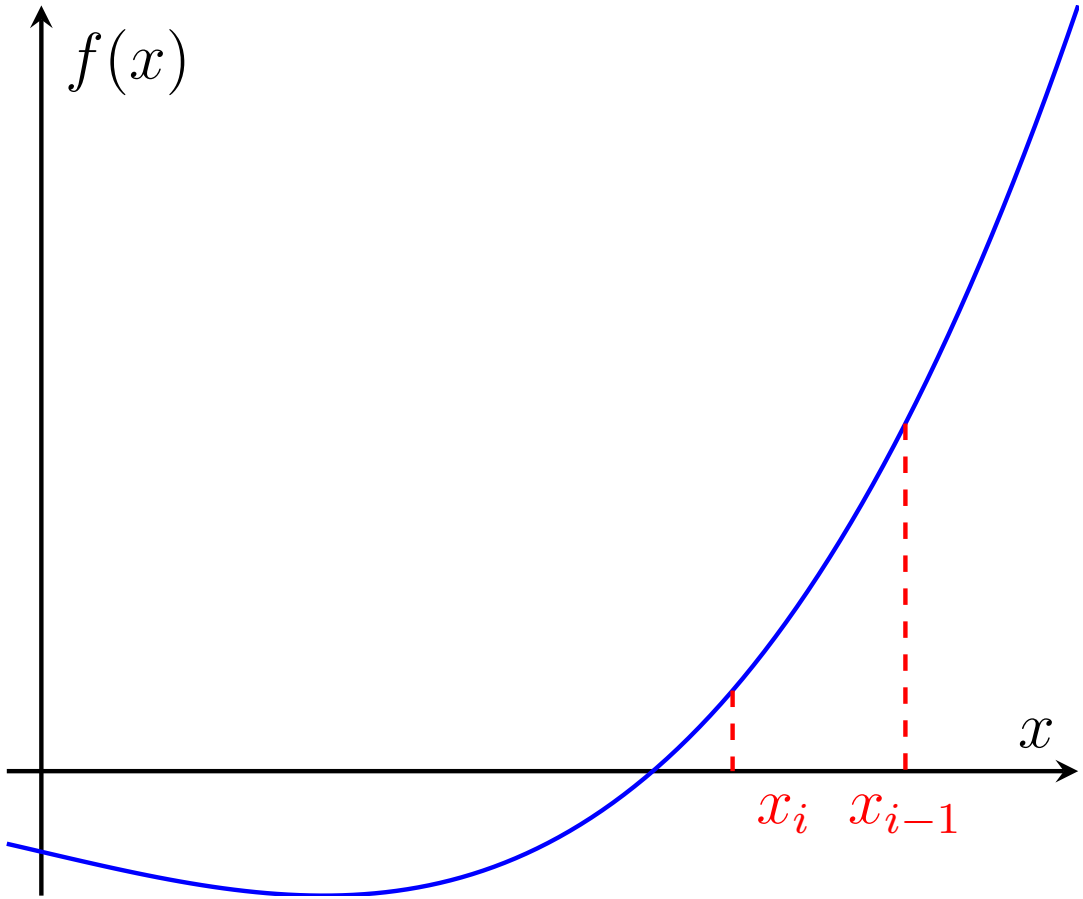
- Needs two initial points to start.
- Same as False position method – except for the points used!

Method of secants: Algorithm



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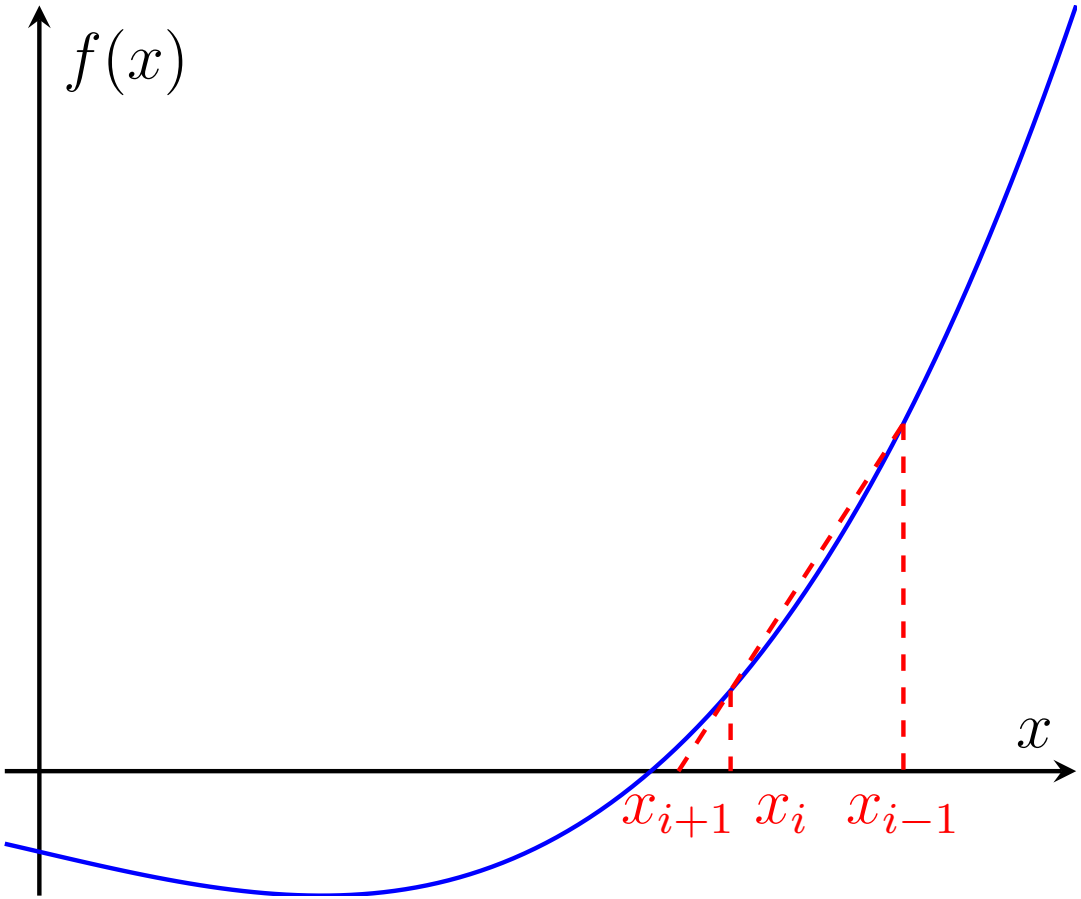

Method of secants: example

i	x_i	f(x_i)	x_{i-1}	f(x_{i-1})	x_{i+1}	f(x_{i+1})
1	1.000000	0.459698	1.500000	1.429263	0.762936	0.040126
2	0.762936	0.040126	1.000000	0.459698	0.740264	0.001974
3	0.740264	0.001974	0.762936	0.040126	0.739091	0.000010
4	0.739091	0.000010	0.740264	0.001974	0.739085	0.000000

Root is: 0.73908513481

- False position used 4 iterations and bisection – 22 iterations!
- Newton's method took 3 iterations.
- However, the question as to which method is more efficient depends not just on the number of iterations – as in the Newton's iteration, one also has to evaluate the derivative!

Muller's method

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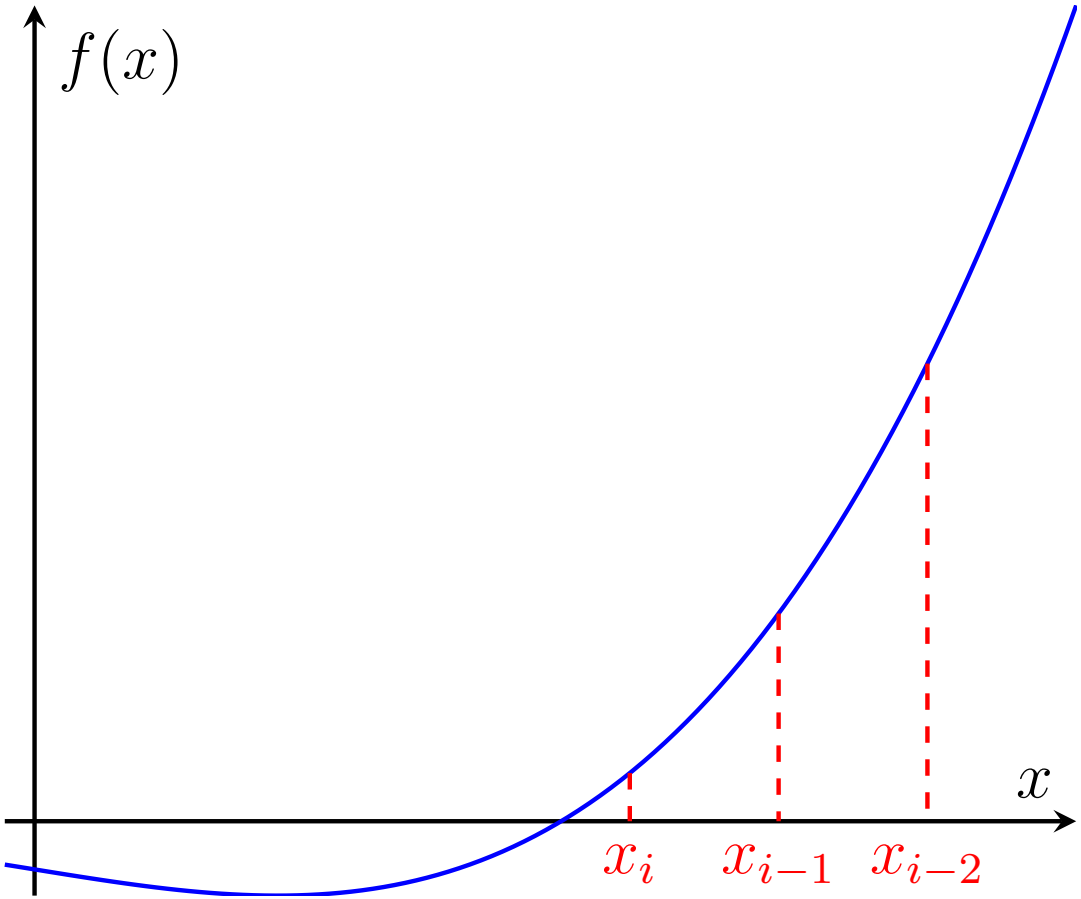
- The only difference between Muller's method and method of secants is that the $g(x)$ is quadratic function in Muller's method and linear function in secant method!
- Three initial approximations are required to start the algorithm (as opposed to two in secant method).

Muller's method: Algorithm



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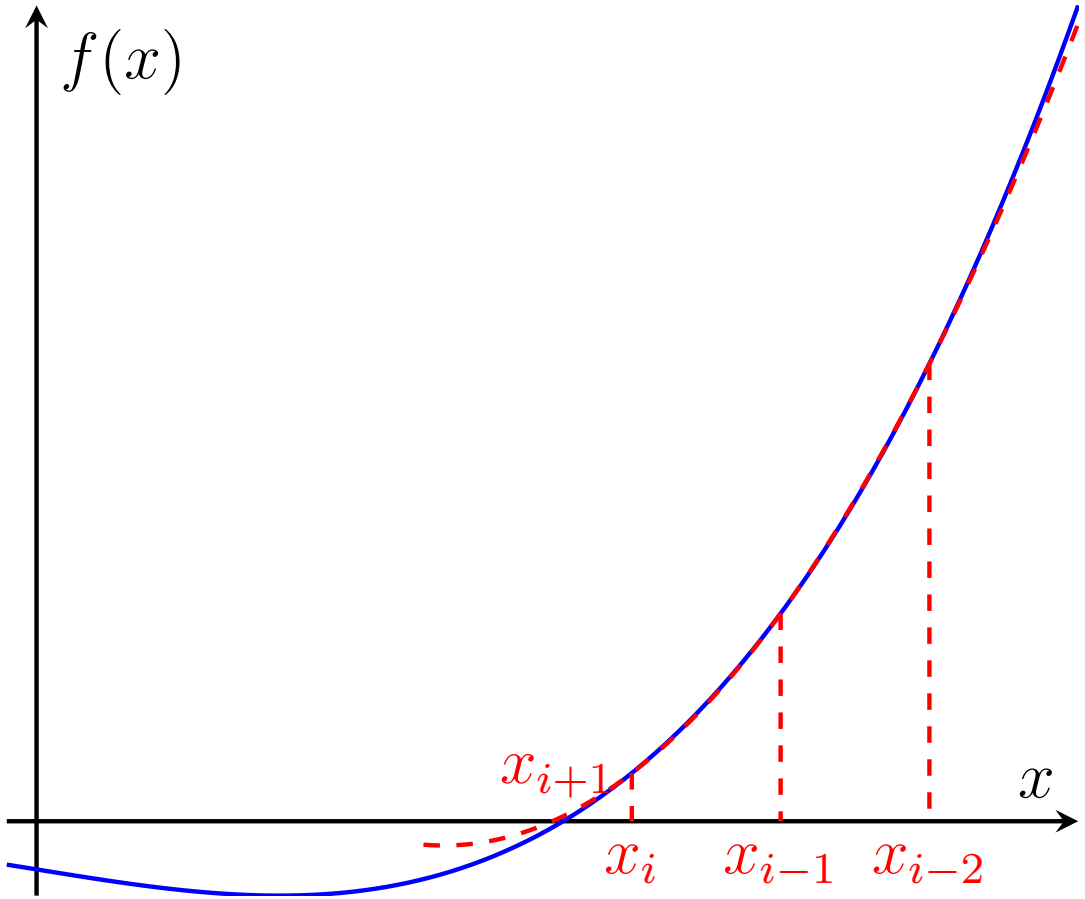

Fixed point iteration

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$$x_1 = f(x_0)$$
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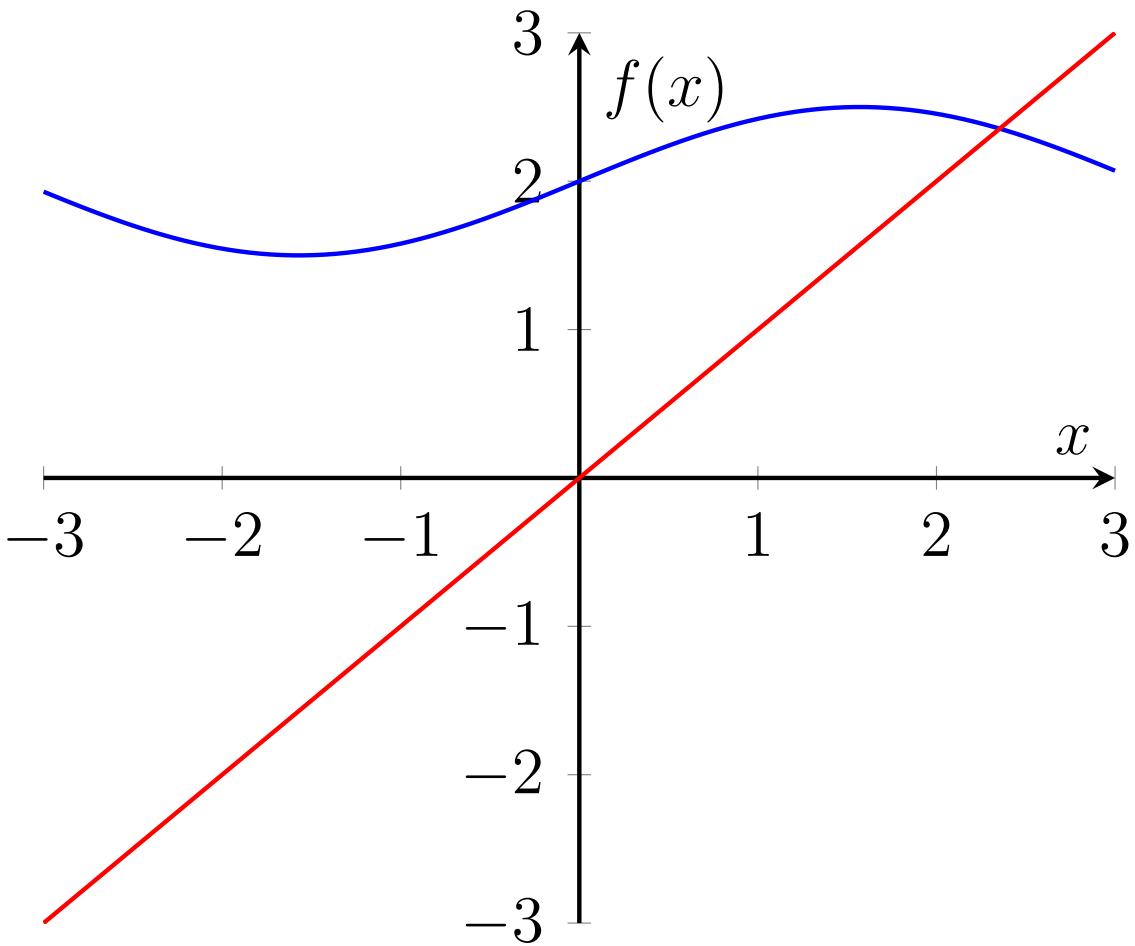
- If the sequence x_0, x_1 ... x_n belongs to an interval I, where $|f'(x)| < k < 1$ then the sequence has a limit L and L is the only root of $x = f(x)$ in the interval I.

Fixed point iteration: example

Consider an example: $f(x) = 2 + \frac{\sin(x)}{2}$

$$|f'(x)| = |\frac{\cos(x)}{2}| < 1.$$



Initial guess $x = 2.0$.

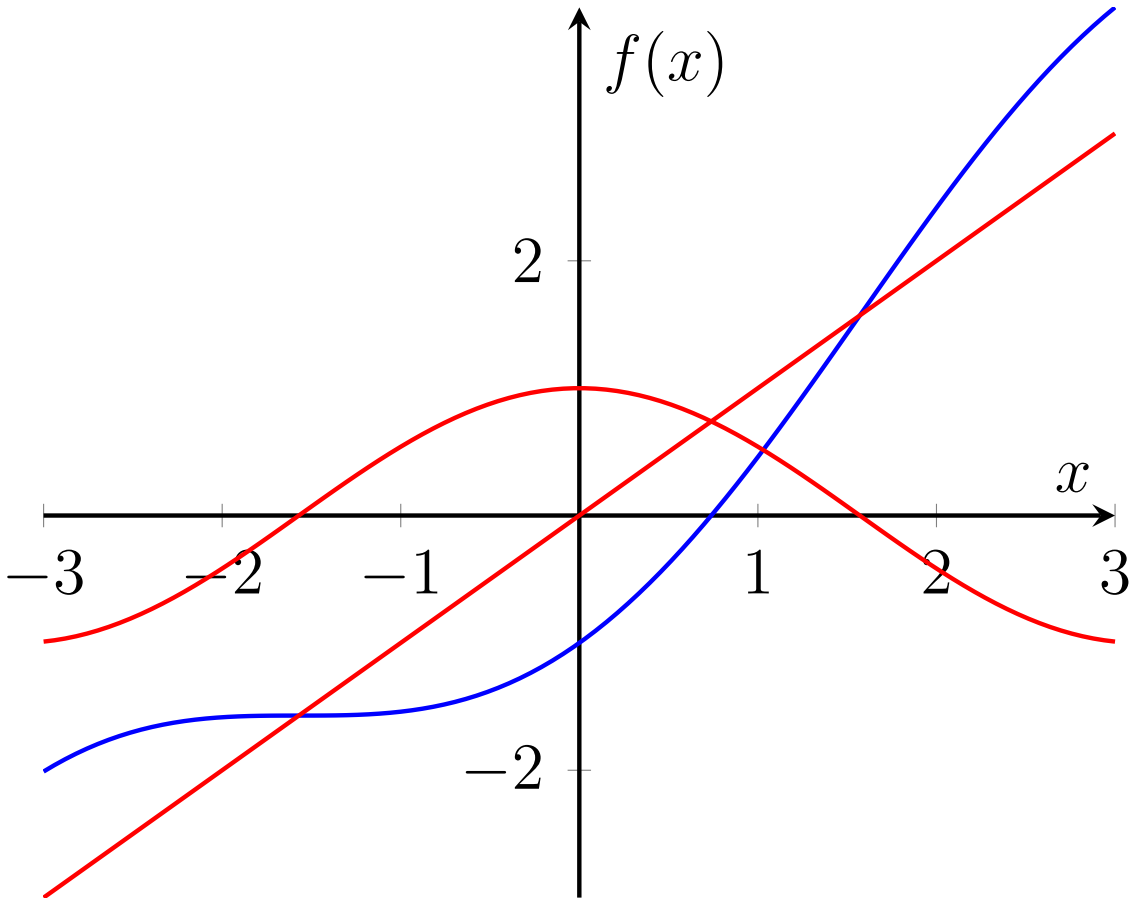
Fixed point iteration: example

```
 i     x_i       f(x_i)
 1   2.000000  2.454649
 2   2.454649  2.317089
 3   2.317089  2.367106
 4   2.367106  2.349675
 5   2.349675  2.355851
 6   2.355851  2.353675
 7   2.353675  2.354443
 8   2.354443  2.354172
 9   2.354172  2.354268
10   2.354268  2.354234
11   2.354234  2.354246
12   2.354246  2.354242
13   2.354242  2.354243

Root is: 2.35424314498
```

Fixed point iteration: Example

Consider an example: $f(x) = x - \cos(x)$



Initial guess $x = 1.0$.

Fixed point iteration: example

i	x_i	f(x_i)
1	1.000000	0.540302
2	0.540302	0.857553
3	0.857553	0.654290
4	0.654290	0.793480
5	0.793480	0.701369
6	0.701369	0.763960
7	0.763960	0.722102
8	0.722102	0.750418
9	0.750418	0.731404
10	0.731404	0.744237
11	0.744237	0.735605
12	0.735605	0.741425
13	0.741425	0.737507
14	0.737507	0.740147
15	0.740147	0.738369
16	0.738369	0.739567
17	0.739567	0.738760
18	0.738760	0.739304
19	0.739304	0.738938
20	0.738938	0.739184
21	0.739184	0.739018
22	0.739018	0.739130
23	0.739130	0.739055
24	0.739055	0.739106
25	0.739106	0.739071
26	0.739071	0.739094
27	0.739094	0.739079
28	0.739079	0.739089
29	0.739089	0.739082
30	0.739082	0.739087
31	0.739087	0.739084
32	0.739084	0.739086
33	0.739086	0.739085

Root is: 0.739084549575

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- We choose an r-value such that $1 + rg'(x_0) \approx 0$. Let $r_0 = \text{the chosen value}$.
- We apply iteration on $x = x + r_0 g(x)$ starting with $x = x_0$.

Fixed point iteration: example

We rewrite our function as $x = x - 0.54 * (x - \cos(x))$.

```
i     x_i        f(x_i)
1   1.000000   0.751763
2   0.751763   0.740273
3   0.740273   0.739199
4   0.739199   0.739096
5   0.739096   0.739086
6   0.739086   0.739085

Root is: 0.73908523492
```

- Huge difference in terms of the efficiency!!! From 33 iterations to 6 iterations.
- Careful choice/massaging of the equation can yield remarkable gains.

Open domain methods: General remarks

- All these methods converge rapidly in the vicinity of the root. When the derivative is difficult to compute or is time-consuming, the secant method is very efficient.

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- In sensitive cases, all these methods may misbehave! It may be required to use bracketing methods.
- Plotting of the functions can help in indetifying such cases.
- *All of these methods can find complex roots simply by using complex arithmetic!*

- Complications.
- Roots of polynomials.
- Non-linear systems of equations with multiple variables.
- Summary.

Complications

- There are no roots at all!

> The hardest thing of all is to find a black cat in a dark room, especially if there is no cat.
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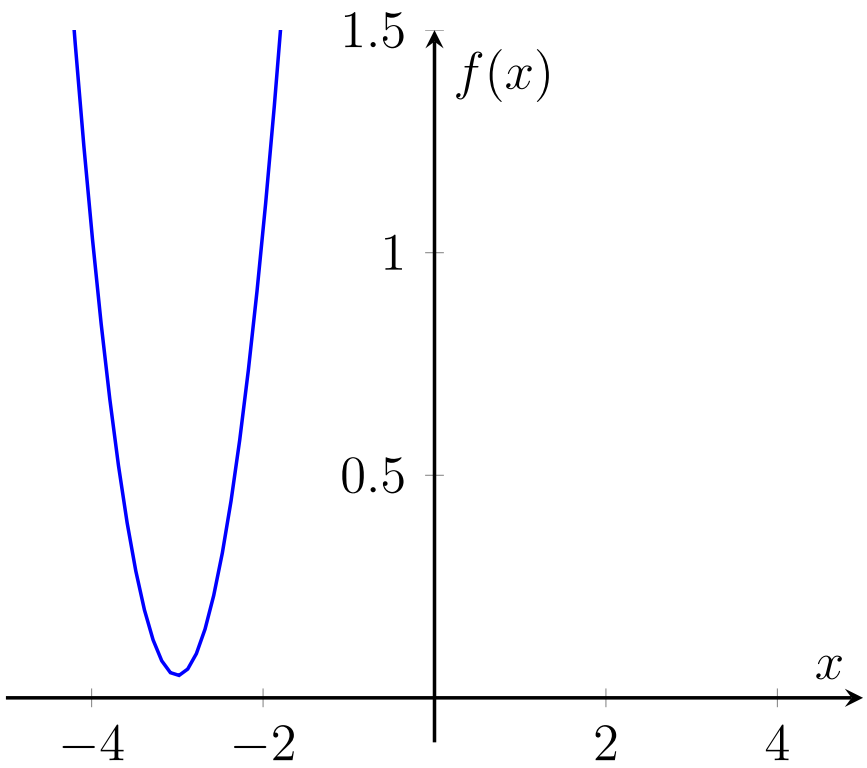

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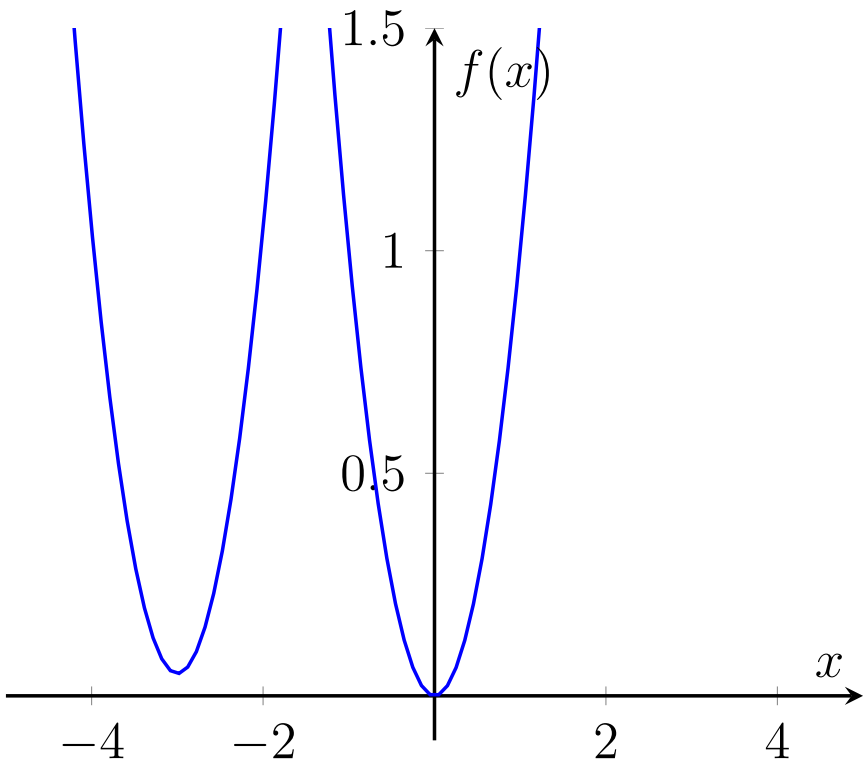

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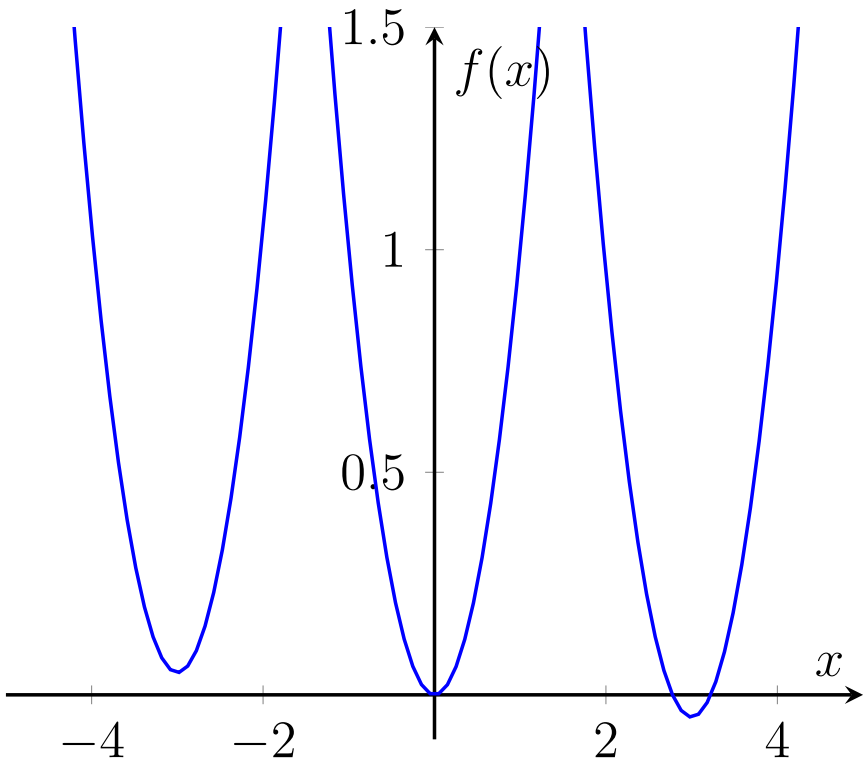
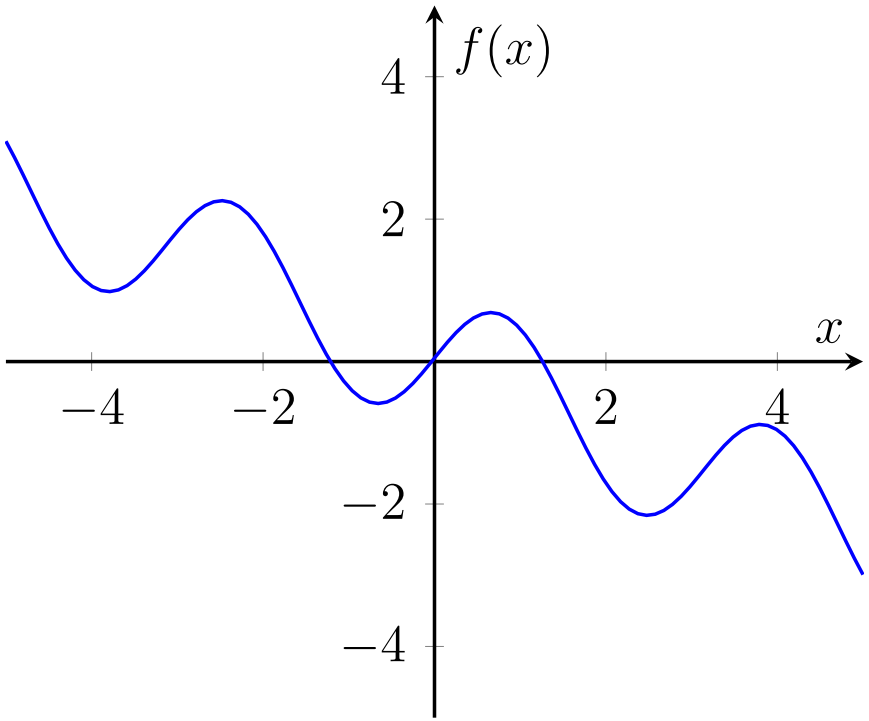
- There is one root but the function does not change sign.
- There are two or more roots in the interaval $[a, b]$.



More complications

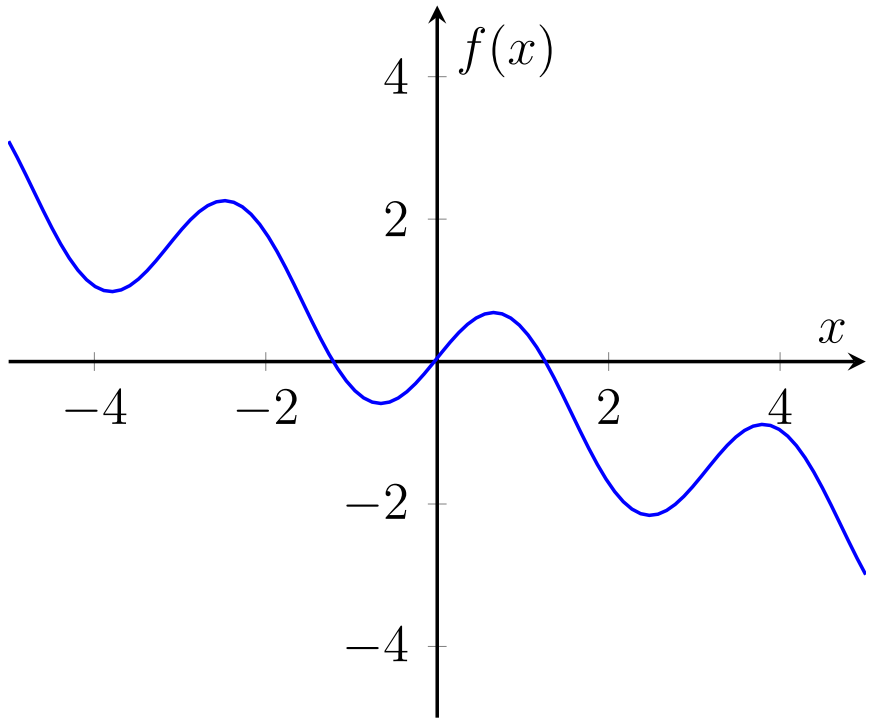
There are many roots.



What will happen if you use bracketing methods for this?

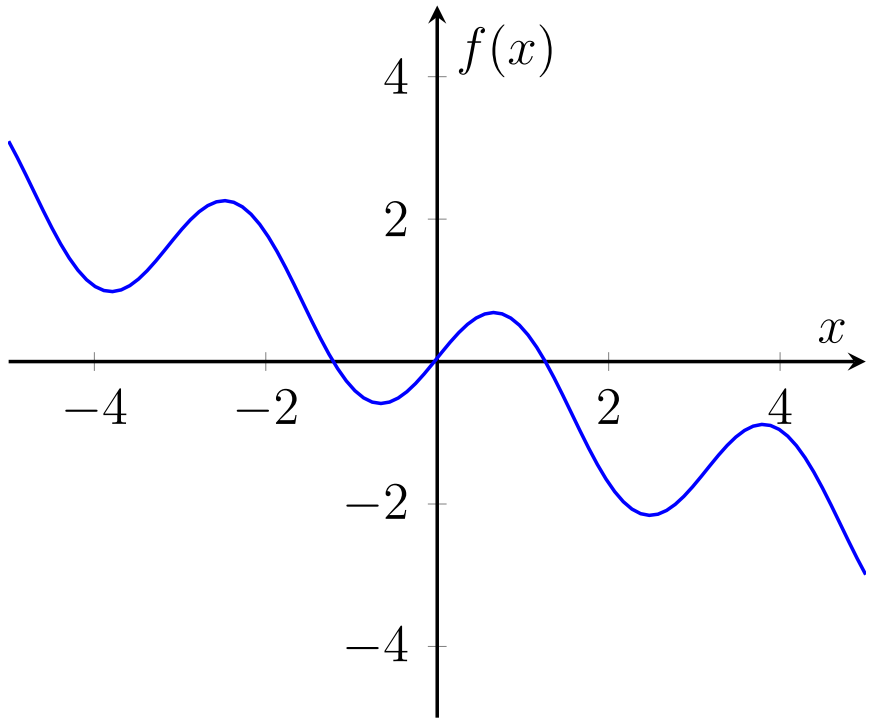
Multiple roots: Brute force method

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



Multiple roots: Brute force method

- The brute force method is a good method for dealing with multiple roots.
- One splits the original interval $[a, b]$ into smaller intervals with some step size (say h) and then applies the previously mentioned methods in each of the sub-intervals.



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- Choosing too small a step size will result in too many computations.
- A graphical analysis is very helpful in deciding the step size h.
- *It may be good to evaluate roots with h and then with $h/10$ to confirm that the number of roots remains unchanged.*

Some general comments on roots of polynomials

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- They can however be used to find repeated roots with odd multiplicity.
- Open domain methods are often more efficient than closed domain methods.

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- For complex roots – one just needs to use complex arithemetic – the algorithms remain the same.
- There are various modifications of the Newton's method which are often used to find roots. For eg. Bairstow's method.

Non linear system of equations: two variables

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$$f(x, y) = 0$$
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- Extension of bracketing methods is not obvious to systems of non linear equations.
- Open domain methods (especially Newton's method) are easily extended to solve such systems.
- One always needs a good guess!!!

Extension of Newton's method to two variables

We are given two equations:

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

We have to find the solution (x^*, y^*) such that:

$$f(x^*, y^*) = 0$$
$$g(x^*, y^*) = 0$$

Taylor expanding about (x^*, y^*):

$$f(x, y) = f(x^*, y^*) + (x - x^*)f'_x + (y - y^*)f'_y + \dots$$
$$g(x, y) = g(x^*, y^*) + (x - x^*)g'_x + (y - y^*)g'_y + \dots$$

Extension of Newton's method to two variables

Keeping only first-order terms and given $f(x^*, y^*) = 0$ and $g(x^*, y^*) = 0$, one has a system of linear equations for x^* and y^* such that:

$$x^* = x + \frac{f'_y g(x,y) - g'_y f(x,y)}{f'_x g'_y - f'_y g'_x}$$

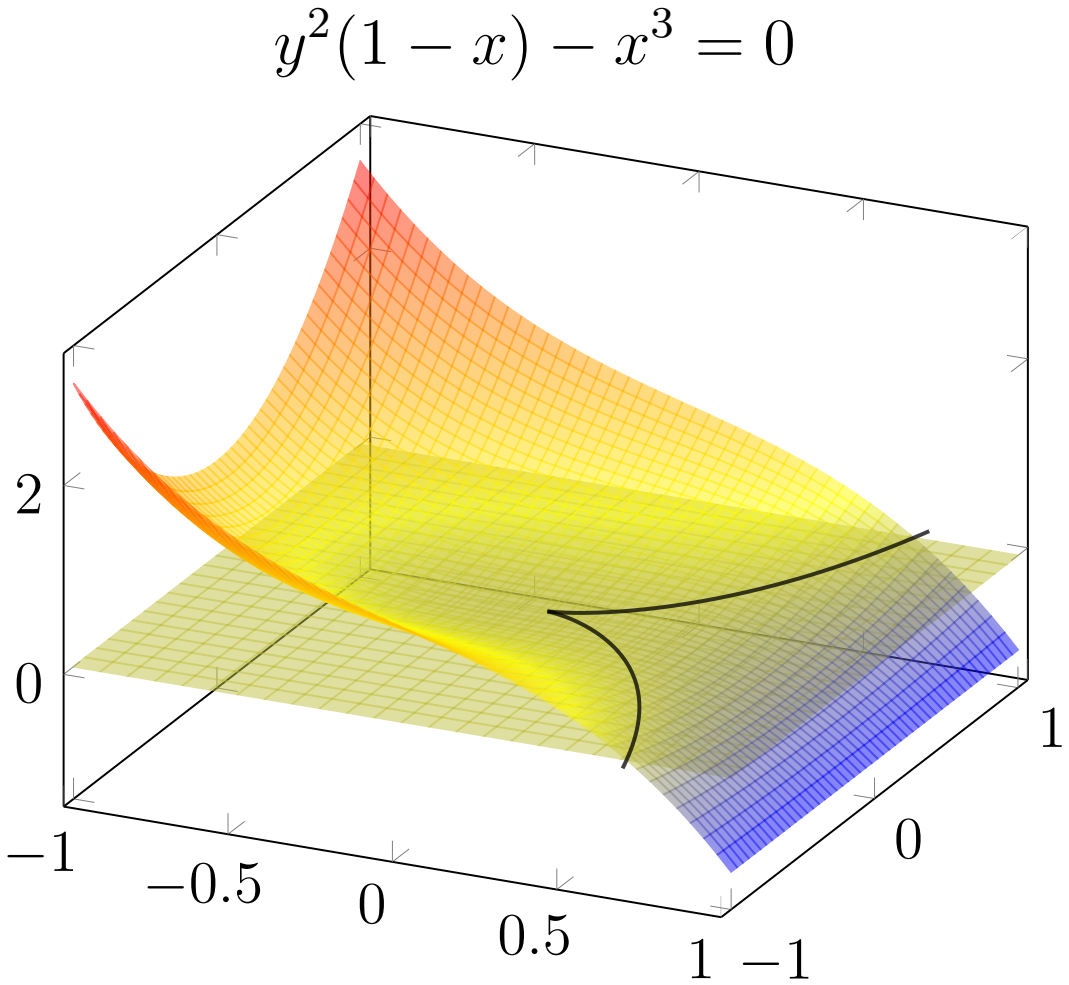
$$y^* = y + \frac{g'_x f(x,y) - f'_x g(x,y)}{f'_x g'_y - f'_y g'_x}$$

This method can be easily generalized to solving n non linear equations.

Non linear systems of equations: Example

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

Non linear systems of equations: Example



$h(x, y) = 0$ is also shown. The black line shows the intersection of the surface with $h(x, y) = 0$.

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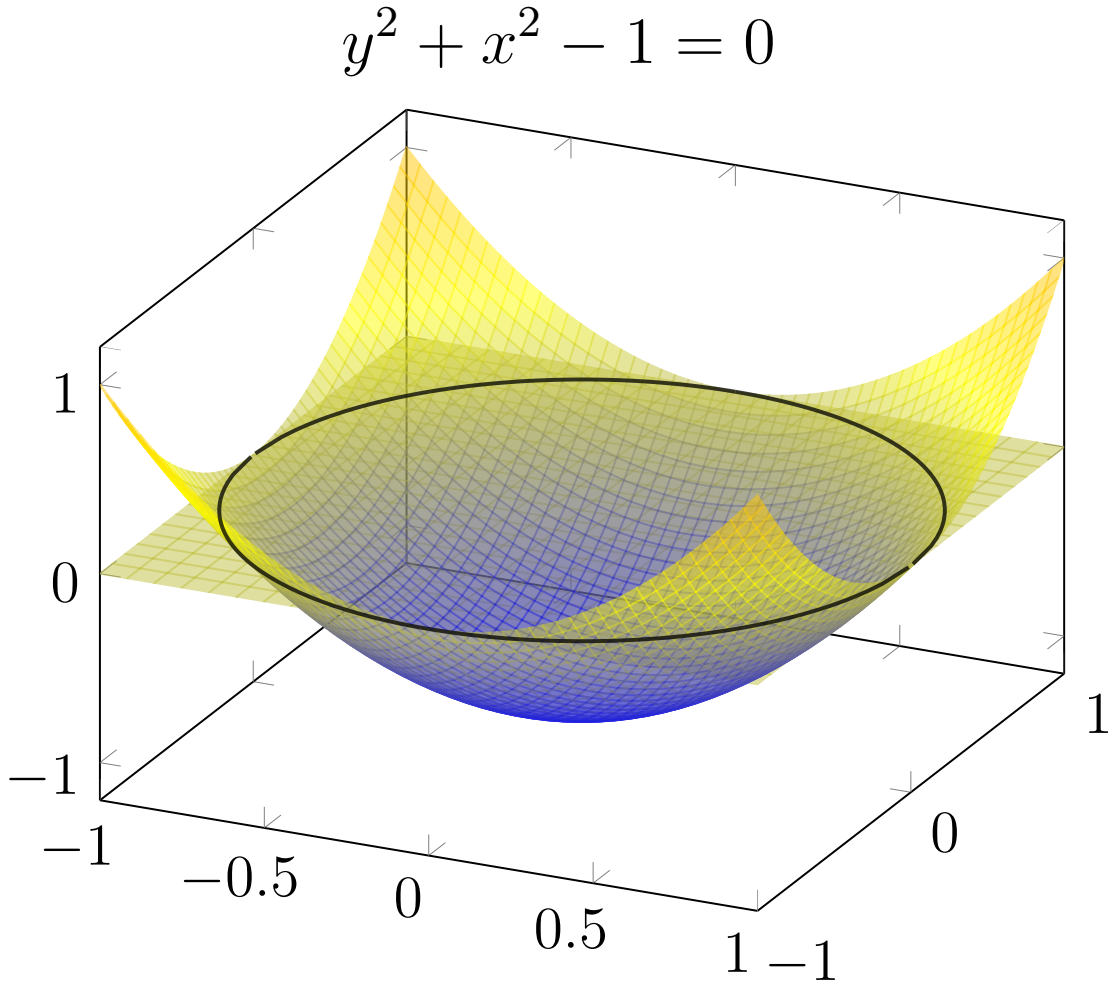

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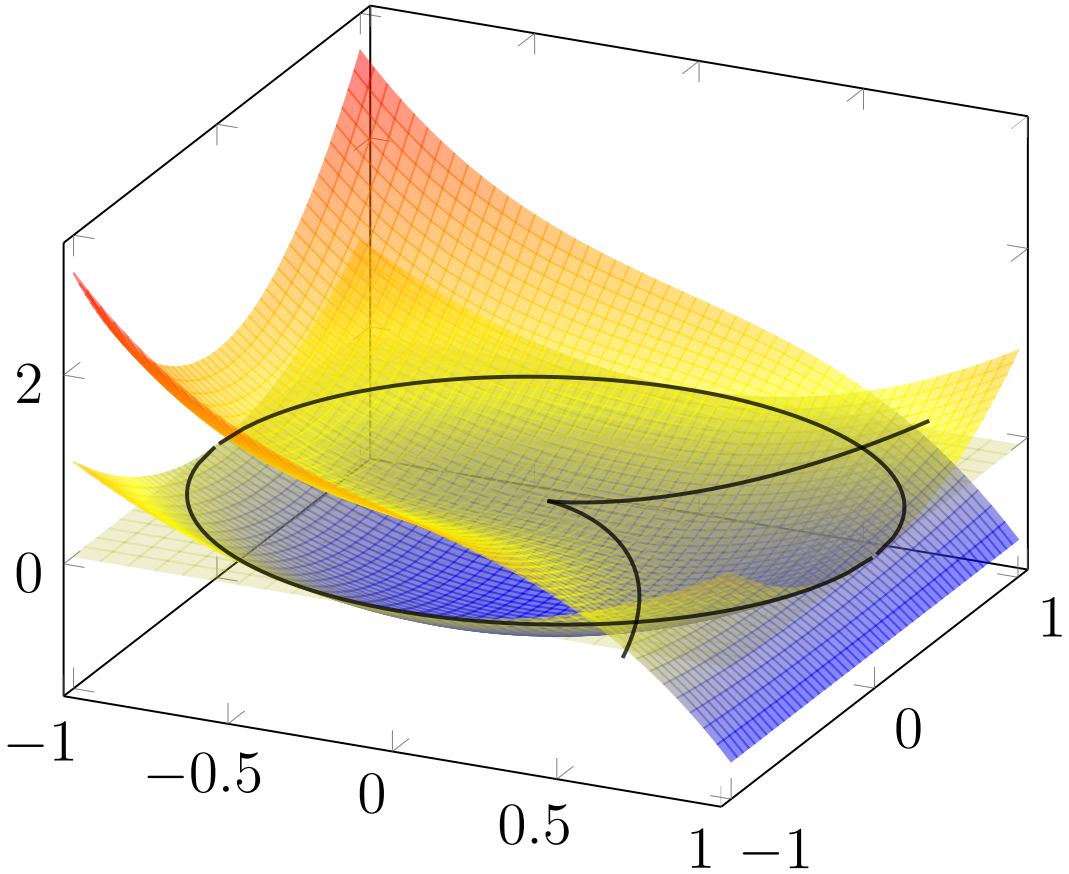

$h(x, y) = 0$ is also shown.

Newton's method: example

```
  i     x          y          f(x,y)     g(x,y)      dx          dy
  1  1.000000   1.000000 -1.000000   1.000000 -0.250000 -0.250000
  2  0.750000   0.750000 -0.281250   0.125000 -0.119048  0.035714
  3  0.630952   0.785714 -0.023352   0.015448 -0.012757  0.000414
  4  0.618195   0.786128 -0.000298   0.000163 -0.000161  0.000023
  5  0.618034   0.786151 -0.000000   0.000000
```

```
Root is: 0.618034012048126, 0.786151376237367
```

```
  i     x          y          f(x,y)     g(x,y)      dx          dy
  1  1.000000  -1.000000 -1.000000   1.000000 -0.250000  0.250000
  2  0.750000  -0.750000 -0.281250   0.125000 -0.119048 -0.035714
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```

Pitfalls of root finding

- Lack of good initial guess.

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- Choosing the right method is difficult – something that works in one equation can miserably fail in another.
- If possible, visualize the data – this helps a lot.