Content

Problems in Mathematics & Experiments with Mathematica

4. The derivative and its applications

4.4 Approximation of zeros

The problem of zeros

Let the function f be continuous on the interval (a,b). Find the zeros of $f(x)$, that is the points $\overline{x} \in (a, b)$, for which $f(\overline{x})=0$.

- **Formal solution**

Use algebraic methods to find all the zeros of the equation

$$f(x)=0$$

- *Solution with Mathematica*

`Solve[eqn., x]`	Formal solution of equations
`NSolve[eqn., x]`	N[Solve[...]]

See the following chapters for details:
A short introduction to *Mathematica*
Exercises for the basic properties and graphs of elementary functions

Approximation of zeros: the secant method

- **The algorithm**

Let the function f be *continuous* (only!) on the interval (a,b). Let $f(x_0) < 0$ and $f(x_1) > 0$. By the mean value theorem for continuous functions, there is an $\overline{x}$ such that $f(\overline{x}) = 0$. Approximate the zero position $\overline{x}$ of f with the zero x_2 of the secant line

$$y = f(x_1) + \frac{f(x_0) - f(x_1)}{x_0 - x_1}(x - x_1)$$

that passes throught the points $(x_0, f(x_0))$ and $(x_1, f(x_1))$. Then, x_2 can be expressed by

$$x_2 = x_1 - f(x_1)\frac{x_1 - x_0}{f(x_1) - f(x_0)}.$$

Then, continue the process with $(x_1, x_2) \to x_3$, and so $(x_{n-1}, x_n) \to x_{n+1}$ till the desired accuracy is reached, where

$$x_{n+1} = x_n - f(x_n)\,\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})}$$

- **Convergence and error**

The method always converges if $f'(x)$ is nonzero and $f''(x)$ is continuous on an interval containing the zero $\bar{x}$. The error is

$$|\bar{x} - x_{n+1}| \approx C(|\bar{x} - x_n|)^p,$$

where

$$p = \frac{1+\sqrt{5}}{2} \text{ and } C = \sqrt[p]{\frac{|f''(\bar{x})|}{2|f'(\bar{x})|}}$$

- *Important remark*

The secant method can be applied even if the function *f(x)* is not differentiable. This is a "safe" method to approximate zeros of functions. The higher order derivatives are used only for the error estimation.

Exercises and problems for secant method

Mathematica initialization

```
SecantStep[f_, {x0_, x1_}] := x1 - (f[x1] (x1 - x0))/(f[x1] - f[x0])
SecantPlot[f_, {x0_, x1_}, n_, opt___] := Module[{data}, data =
        NestList[{#1[[2]], SecantStep[f, #1]} &, {x0, x1}, n];
   Return[
    Show[Table[{Graphics[{RGBColor[0, 0, 1], Line[{{data[[i, 1]],
           f[data[[i, 1]]]}, {data[[i, 2]], f[data[[i, 2]]]}}]}],
      Graphics[{RGBColor[1, 0, 0], Line[{{data[[i, 2]], 0},
          {data[[i, 2]], f[data[[i, 2]]]}}]}]},
     {i, 1, Length[data]}], opt]]];
```

Solved Problem 4.4.1

Perform the first n steps of the secant method to find a zero of the function *f(x)*. Use x_0 and x_1 as initial values. Verify your calculations with *Mathematica* using the above defined statements `SecantStep` and `SecantPlot`.

$$f(x\_) := \frac{1}{x^2+1} - \sin(x);\ x_0 = 0.;\ x_1 = 2.;\ n = 5;$$

- Solution

Problem 4.4.2

Perform the tasks in the previous problem for the following cases. Find other zeros by choosing different initial positions.

(1) $f(\text{x\_}) := \dfrac{x}{x^2+1} - \cos(x);\ x_0 = 0.;\ x_1 = 3.;\ n = 5;$

(2) $f(\text{x\_}) := \dfrac{1}{x+1} - \sin(x);\ x_0 = 2.;\ x_1 = 4.;\ n = 5;$

(3) $f(\text{x\_}) := e^{-x} - x^2;\ x_0 = 0.;\ x_1 = 2.;\ n = 5;$

The Newton method

• The algorithm

Let the function f be continuously differentiable on the interval (a,b) that contains a zero $\overline{x}$ of $f(x)$. To find $\overline{x}$, let $x_0 \in (a, b)$ be a first estimate of $\overline{x}$. Next, for a second estimate, take the zero x_1 of the tangent line

$$y - f(x_0) = f'(x_0)(x - x_0),$$

and x_1 is

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}.$$

Then, continue the process with $x_1 \to x_2$, and so $x_n \to x_{n+1}$ till the desired accuracy is reached, where

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

• Convergence and error

The method converges if $f'(x)$ is nonzero and $f''(x)$ is continuous on an interval containing the zero $\overline{x}$. The error is

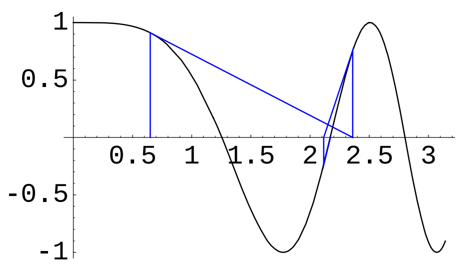
$$\left|\overline{x} - x_{n+1}\right| \approx C(|\overline{x} - x_n|)^2,$$

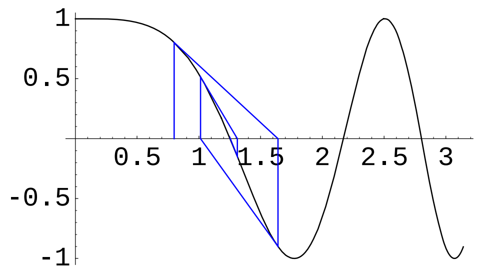
where

$$C = \frac{|f''(\overline{x})|}{\alpha|f'(\overline{x})|}$$

• *Important remark*

If the function f has several zeros, then the initial point has a main influence on the zero being approximated. Choose the initial point as good as possible to find the appropriate zero,. For illustration, see the following figures ($\cos(x^2)$, $x_0 = 0.65$, and $x_0 = 0.8$, respectively) and the problems below.





Exercises and problems for the Newton method

• Mathematica command for iteration

NestList[f, x_0, n]	*1, ..., n* iterations of function *f*

Mathematica initialization

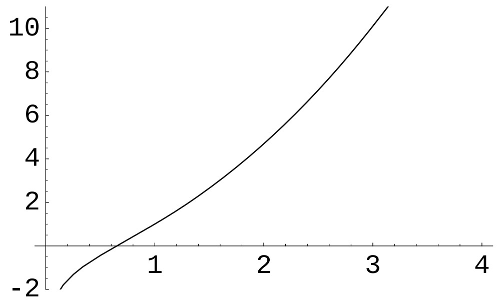
SOLVED PROBLEM 4.4.3

Perform the first *n* steps of the Newton method to find a zero of the function *f(x)*. Use x_0 as an initial value. Verify your calculations by computer.

$$f(x\_) := x^2 + \log(x);\ x_0 = 1.;\ n = 5;$$

○ SOLUTION

```
plt1 = Plot[f[x], {x, 0, 4}, PlotRange -> {-2, 11}];
```




```
x1 = NewtonStep[x0]
```

```
0.666667
```

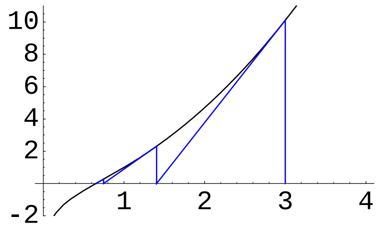
```
x2 = NewtonStep[x1]
```

```
0.652909
```

```
NestList[NewtonStep, x0, n]
```

```
{1., 0.666667, 0.652909, 0.652919, 0.652919, 0.652919}
```

```
Show[plt1, NewtonPlot[f, 3., 4, DisplayFunction -> Identity],
DisplayFunction -> $DisplayFunction];
```



PROBLEM 4.4.4

Do the tasks in the previous problem for the following cases. Find other zeros by choosing different initial positions.

(1) $f(\text{x\_}) := e^{-x} - \sin(x);\ x_0 = 1.5;\ n = 5;$

(2) $f(\text{x\_}) := e^{-x} - \sin(x);\ x_0 = 2.5;\ n = 5;$

(3) $f(\text{x\_}) := x\, e^{x} \cos(x) - 1;\ x_0 = 0.;\ n = 5;$

(4) $f(\text{x\_}) := \cos(x^2);\ x_0 = 0.65;\ n = 5;$

(5) $f(\text{x\_}) := \cos(x^2);\ x_0 = 0.8;\ n = 5;$

Find zeros with Mathematica

FindRoot[eqn, {x, x_0}]	Newton method is applied
FindRoot[eqn, {x, {x_0, x_1}}]	Secant method is applied

The second form must be used if symbolic derivatives of the function cannot be found.

For technical details, see the chapter A short introduction to *Mathematica* .

- *Remark*

It is easy to read the coordinates of a point in a coordinate system. Select the Graphics object, push permanently the `Ctrl` button (or `Alt` in X-Windows systems). Then moving the mouse pointer, the coordinates of the actual point are printed in the left lower corner of the window.

SOLVED PROBLEM 4.4.5 Solve with *Mathematica*

Find the real zeros of the following function by using the `FindRoot` command.

(1) $f(\text{x\_}) := x^7 + 2\,x^6 + x^3 - 2\,x^3 - 1$

○ Solution

- *Try to use Solve*

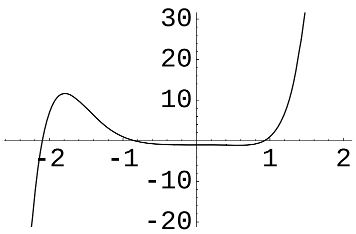
```
Solve[f[x] == 0, x]
```

$\{\{x\to \text{Root}[-1-\#1^3+2\,\#1^6+\#1^7\,\&,\ 1]\},$
$\{x\to \text{Root}[-1-\#1^3+2\,\#1^6+\#1^7\,\&,\ 2]\},$
$\{x\to \text{Root}[-1-\#1^3+2\,\#1^6+\#1^7\,\&,\ 3]\},$
$\{x\to \text{Root}[-1-\#1^3+2\,\#1^6+\#1^7\,\&,\ 4]\},$
$\{x\to \text{Root}[-1-\#1^3+2\,\#1^6+\#1^7\,\&,\ 5]\},$
$\{x\to \text{Root}[-1-\#1^3+2\,\#1^6+\#1^7\,\&,\ 6]\},$
$\{x\to \text{Root}[-1-\#1^3+2\,\#1^6+\#1^7\,\&,\ 7]\}\}$

No zeros could be found formally. We have to use a numerical method.

- *Use FindRoot*
- *Plot f(x)*

```
Plot[f[x], {x, -2.5, 2}];
```

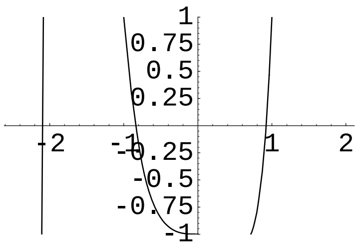


- *Initial estimates of the zeros*

It can be seen from the graph, and it can be proved that there are no more zeros less than $x_1 \approx$-2, and greater than $x_3 \approx 1$. In addition, there is another zero $x_2 \approx -1$. Detailed investigation can also prove that there are no more zeros in the interval (x_1, x_3).

Zoom in the zeros to find good initial values:

```
Plot[f[x], {x, -2.5, 2}, PlotRange -> {-1, 1}];
```



- *Find x_1*

```
FindRoot[f[x] == 0, {x, -2.}]
```

$\{x\to -2.09672\}$

- *Find x_2*

```
FindRoot[f[x] == 0, {x, -1.}]
```

```
{x → -0.839955}
```

- *Find x_3*

```
FindRoot[f[x] == 0, {x, 1.}]
```

```
{x → 0.920843}
```

- *A better program to find all the zeros in one step*

Collect the initial points into a list:

```
xinit = {-2, -1., 1.};
```

Find the zeros:

```
Map[FindRoot[f[x] == 0, {x, #}] &, xinit]
```

```
{{x → -2.09672}, {x → -0.839955}, {x → 0.920843}}
```

PROBLEM 4.4.6

Find the real zeros of the following functions by using the `FindRoot` command.

(1) $f(x\_) := 2x^6 + 3x^3 - x^2 - 1$

(2) $f(x\_) := x^{11} + 3x^{10} - x^5 - 2x^3 - 1$

PROBLEM 4.4.7

Use `FindRoot` to solve the problems stated above for the secant and Newton method.