3. Numerical Methods

The majority of equations of interest in actual practice do not admit any analytic solution. Even equations as simple as $x = e^{-x}$ and $I = \int e^{-x^2} dx$ have no exact solution. Such cases require numerical methods. Only a very brief survey is presented here.

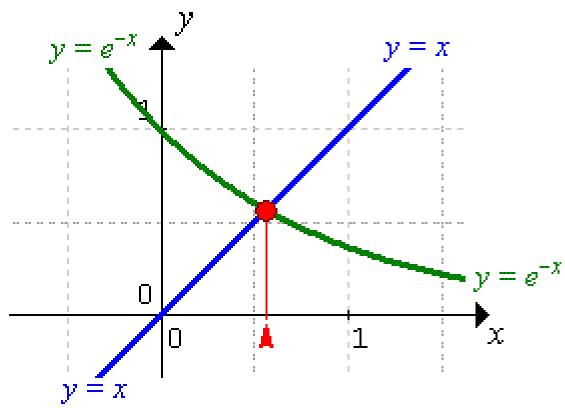
Sections in this Chapter:

3.01 Bisection

<u>Example 3.01.1</u>

Find the solution of $x = e^{-x}$, correct to 4 decimal places.

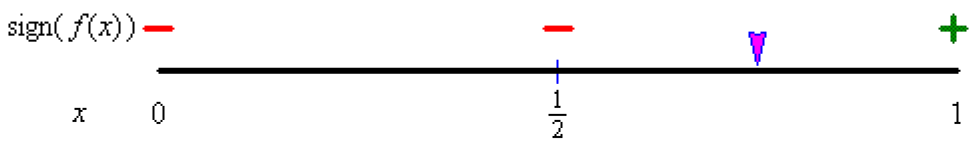
From a sketch of the two curves $y = x$ and $y = e^{-x}$, it is obvious that the only solution is somewhere in the interval (0, 1).



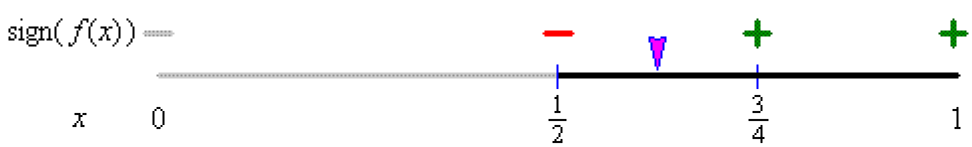
Let $f(x) = x - e^{-x}$.

Clearly $f(0) = -1 < 0$
and $f(1) = 1 - 1/e > 0$
$f(x)$ is continuous and changes sign only once inside (0, 1).

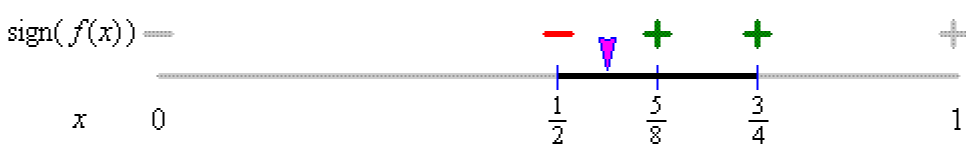
Halve the interval repeatedly and retain the half with a sign change:



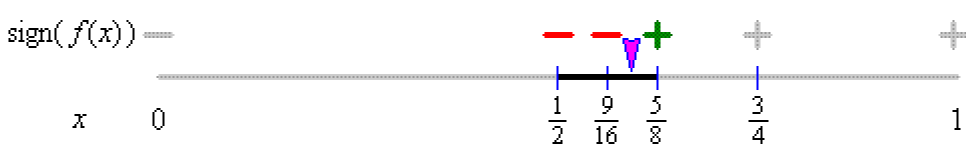
$f(0.50000) = -0.1065... < 0 \Rightarrow$ root is in (0.50000, 1.00000)



$f(0.75000) = +0.2776... > 0 \Rightarrow$ root is in (0.50000, 0.75000)



$f(0.62500) = +0.0897... > 0 \Rightarrow$ root is in (0.50000, 0.62500)

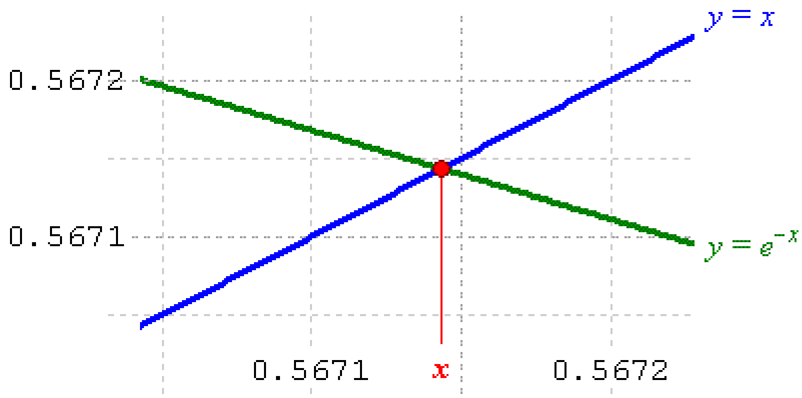


$f(0.56250) = -0.0072... < 0 \Rightarrow$ root is in (0.56250, 0.62500)

Example 3.01.1 (continued)

This method is slow and requires eighteen steps before the change in x is small enough to leave the fourth decimal place undisturbed with certainty:
$f(0.567142) = -0.0000... < 0 \quad \Rightarrow$ root is in (0.567142, 0.567146)

This method is equivalent to zooming in graphically by repeated factors of 2 until the desired accuracy is obtained. The result of a faster graphical zoom, sufficient to determine the solution to five decimal places, is displayed here:

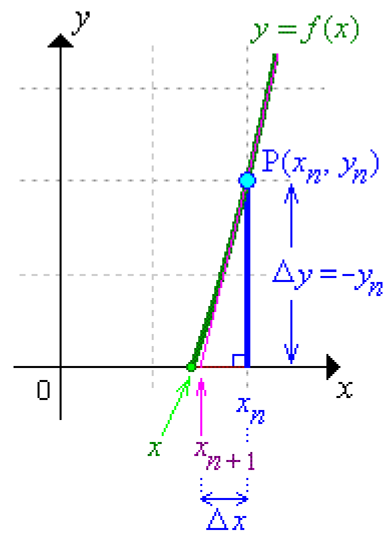


Correct to four decimal places, the solution to $x = e^{-x}$ is $\boldsymbol{x} = \mathbf{0.5671}$.

A calculator quickly confirms that $e^{-0.5671} \approx 0.5671$.

A spreadsheet to demonstrate the bisection method for this example is available from the course web site, at "`www.engr.mun.ca/~ggeorge/9420/demos/`".

3.02 Newton's Method



From the definition of the derivative, $\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{\Delta y}{\Delta x}$,

we obtain $\Delta y \approx \frac{dy}{dx} \Delta x$ or, equivalently,

$$\Delta x \approx \frac{\Delta y}{f'(x)}.$$

The tangent line to the curve $y = f(x)$ at the point $P(x_n, y_n)$ has slope $= f'(x_n)$.

Follow the tangent line down to its x axis intercept.
That intercept is the next approximation x_{n+1}.

$$\Delta y = y_{n+1} - y_n = 0 - y_n = -f(x_n) \text{ and}$$

$$\Delta x = x_{n+1} - x_n$$

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

If x_n is the n^{th} approximation to the equation $f(x) = 0$, then a better approximation may be

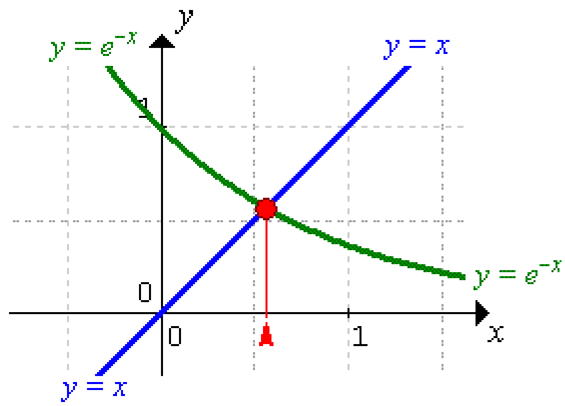
$$\boxed{x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}}$$

which is Newton's method.

Example 3.02.1

Find the solution of $x = e^{-x}$, correct to 4 decimal places.

From a sketch of the two curves $y = x$ and $y = e^{-x}$, it is obvious that the only solution is somewhere in the interval (0, 1). A reasonable first guess is $x_0 = \frac{1}{2}$.



$$f(x) = x - e^{-x} \quad \Rightarrow \quad f'(x) = 1 + e^{-x}$$

$$\Rightarrow \quad x_n - \frac{f(x_n)}{f'(x_n)} = x_n - \frac{x_n - e^{-x_n}}{1 + e^{-x_n}}.$$

Table of consecutive values:

x_n	$f(x_n) = x_n - e^{-x_n}$	$f'(x_n) = 1 + e^{-x_n}$	$\frac{f(x_n)}{f'(x_n)}$
0.500000	–0.106531	1.606531	–0.066311
0.566311	–0.001305	1.567616	–0.000832
0.567143	0.000000	1.567143	0.000000
0.567143			

Correct to four decimal places, the solution to $x = e^{-x}$ is $\boldsymbol{x = 0.5671}$.
In fact, we have the root correct to six decimal places, $x = 0.567143$.

A spreadsheet to demonstrate Newton's method for this example is available from the course web site, at "`www.engr.mun.ca/~ggeorge/9420/demos/`".

This method converges much more rapidly than bisection, but requires more computational effort.

Note that Newton's method can fail if $f'(x) = 0$ in the neighbourhood of the root. A shallow tangent line could result in a sequence of approximations that fails to converge to the correct value.

3.03 Euler's Method for First Order ODEs

One of the simplest methods for obtaining the numerical values of solutions of initial value problems of the form

$$y' = f(x, y), \qquad y(x_0) = y_0$$

is Euler's method.

From the definition of the derivative, $\dfrac{dy}{dx} = \lim\limits_{\Delta x \to 0} \dfrac{\Delta y}{\Delta x}$, we obtain $\Delta y \approx \dfrac{dy}{dx} \Delta x$.
If we seek values of the solution $y(x)$ at successive evenly spaced values of x, then we have $\Delta y = y_{n+1} - y_n \quad \Rightarrow \quad y_{n+1} = y_n + \Delta y \approx y_n + f(x_n, y_n) \Delta x$.
With (by convention) $h = \Delta x$, we have the iterative scheme

$$\boxed{y_{n+1} = y_n + h\, f(x_n, y_n)}$$

However, errors propagate rapidly unless the step size h is very small, which requires a proportionate increase in the number of computations. Several modifications to Euler's method have been proposed, that replace the derivative $y' = f(x_n, y_n)$ by a weighted average of values of f at points around (x_n, y_n).

One of the most popular modifications is the fourth order Runge-Kutta method (RK4).

3.04 Fourth Order Runge-Kutta Procedure (RK4)

Values (x_n, y_n) [with $x_n = x_0 + nh$] of the solution $y(x)$ to the initial value problem

$$y' = f(x, y), \qquad y(x_0) = y_0$$

are given by the iterative scheme

$$\begin{aligned}
k_1 &= f(x_n, y_n) \\
k_2 &= f\left(x_n + \tfrac{1}{2}h,\ y_n + \tfrac{1}{2}h k_1\right) \\
k_3 &= f\left(x_n + \tfrac{1}{2}h,\ y_n + \tfrac{1}{2}h k_2\right) \\
k_4 &= f\left(x_n + h,\ y_n + h k_3\right) \\
y_{n+1} &= y_n + \frac{h}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)
\end{aligned}$$

Example 3.04.1

Use the RK4 procedure with step size $h = 0.1$ to obtain an approximation to $y(1.5)$ for the solution of the initial value problem $y' = 2xy$, $y(1) = 1$.

$x_0 = 1$, $h = 0.1$ and we want $y(1.5)$. $1.5 = 1 + 5\times0.1$, so we need to find y_5.
$(x_0, y_0) = (1, 1)$ and $f(x, y) = 2xy$.

For $n = 0$:

$$k_1 = f(x_0, y_0) = 2x_0y_0 = 2\times1\times1 = 2$$

$$k_2 = 2\left(1+\tfrac{1}{2}(0.1)\right)\left(1+\tfrac{1}{2}(0.1)2\right) = 2.31$$

$$k_3 = 2\left(1+\tfrac{1}{2}(0.1)\right)\left(1+\tfrac{1}{2}(0.1)2.31\right) = 2.34255$$

$$k_4 = 2(1+0.1)\left(1+(0.1)2.34255\right) = 2.715361$$

$$y_1 = y_0 + \frac{h}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right) = 1 + \frac{0.1}{6}\left(2 + 2(2.31) + 2(2.34255) + 2.715361\right)$$

Therefore $y(1.1) \approx y_1 = 1.23367435$

We can proceed with a similar chain of calculations to find y_2, y_3, y_4 and finally y_5.

<u>Example 3.04.1</u> (continued)

n	x_n	y_n	k_1	k_2	k_3	k_4
0	1.000000	1.000000	2.000000	2.310000	2.342550	2.715361
1	1.100000	1.233674	2.714084	3.149571	3.199652	3.728735
2	1.200000	1.552695	3.726469	4.347547	4.425182	5.187555
3	1.300000	1.993687	5.183586	6.082738	6.204124	7.319478
4	1.400000	2.611633	7.312573	8.634059	8.825675	10.482602
5	**1.500000**	**3.490211**				

Therefore $y(1.5) \approx \mathbf{3.4902}$.

This initial value problem happens to have an exact solution, $y = e^{x^2-1}$.
We can therefore test the accuracy of the RK4 procedure in this case.

The exact value of $y(1.5)$ is 3.4903..., an absolute error of less than 0.0002 and a relative error of less than 0.01%. Euler's method, in contrast, has an error exceeding 16%!

END OF CHAPTER 3