

## Numerical Solution of Differential Equations

A **differential equation** (or "DE") contains **derivatives** or **differentials**. In a differential equation the unknown is a function, and the differential equation relates the function itself to its derivative(s). Our task is to **solve** the differential equation (i.e. find the unknown function).

### Why numerical solutions?

For many of the differential equations we need to solve in the real world, there is no "nice" algebraic solution. That is, we can't solve it using the techniques we have met before in calculus ([separation of variables](#), [integrable combinations](#), or [using an integrating factor](#)), or other similar means.

As a result, we need to resort to using numerical methods for solving such DEs. The concept is similar to the numerical approaches we saw in an earlier integration chapter ([Trapezoidal Rule](#) and [Simpson's Rule](#) ).

### Ordinary differential equations (Initial Value Problems)

In this section first order single ordinary differential equations will be considered.

#### The General Initial Value Problem

We are trying to solve problems that are presented in the following way:

$$\frac{dy}{dx} = f(x, y)$$

and  $y(a)$  (the initial value) is known. ( $y$  at  $x = a$  is known)

where  $f(x, y)$  is some function of the variables  $x$ , and  $y$  that are involved in the problem.

#### Examples of Initial Value Problems

1.  $\frac{dy}{dx} = 6 - 2\frac{y}{x}; y(3) = 1$
2.  $\frac{dy}{dx} = \frac{y \ln y}{x}; y(2) = e$
3.  $\frac{dy}{dx} = \frac{50x^2 - 10y}{3}; y(0) = 0$

Note that the right hand side is a function of  $x$  and  $y$ . Let's now see how to solve such problems using a numerical approach.

### Euler's Method

Euler's Method assumes our solution is written in the form of a Taylor's Series.

That is, we'll have a function of the form:

$$y(x + h) \approx y(x) + hy'(x) + \frac{h^2 y''(x)}{2!} + \frac{h^3 y'''(x)}{3!} + \dots$$

This gives us a reasonably good approximation if we take plenty of terms, and if the value of  $h$  is reasonably small.

For Euler's Method, we just take the first 2 terms only.

$$y(x + h) \approx y(x) + hy'(x)$$

The last term is just  $h$  times  $\frac{dy}{dx}$  expression, so we can write Euler's Method as follows:

$$y(x + h) \approx y(x) + h f(x, y)$$

### How do we use this formula?

We start with some known value for  $y$ , which we could call  $y_0$ . It has this value when  $x = x_0$ . (We make use of the initial value  $(x_0, y_0)$ )

The result of using this formula is the value for  $y$ , one  $h$  step to the right of the current value.

Let's call it  $y_1$ . So we have:

$$y_1 \approx y_0 + h f(x_0, y_0)$$

Where

$y_1$  is the next estimated solution value;

$y_0$  is the current value;

$h$  is the interval between steps; and

$f(x_0, y_0)$  is the value of the derivative at the starting point  $(x_0, y_0)$ .

Next value: To get the next value  $y_2$ , we would use the value we just found for  $y_1$  as follows:

$$y_2 \approx y_1 + h f(x_1, y_1)$$

Where

$$x_1 = x_0 + h$$

$f(x_1, y_1)$  is the value of the derivative at the current  $(x_1, y_1)$  point.

We continue this process for as many steps as required.

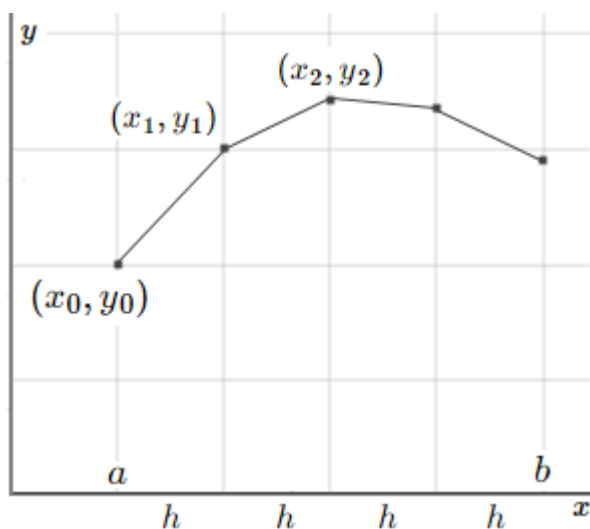
What's going on?

The right hand side of the formula above means, "start at the known  $y$  value, then move one step  $h$  units to the right in the direction of the slope at that point, which is

$$\frac{dy}{dx} = f(x, y)$$

We will arrive at a good approximation to the curve's  $y$ -value at that new point."

We'll do this for each of the sub-points,  $h$  apart, from some starting value  $x = a$  to some finishing value,  $x=b$ , as shown in the graph below.



Let's see how it works with an example.

Example: Euler's Method

Solve the following differential equation:

$$\frac{dy}{dx} = \frac{y \ln y}{x}; \quad y(2) = e$$

### Step 1

We'll start at the point  $(x_0, y_0) = (2, e)$  and use step size of  $h=0.1$  and proceed for 10 steps. That is, we'll approximate the solution from  $t=2$  to  $t=3$  for our differential equation. We'll finish with a set of points that represent the solution, numerically.

We already know the first value, when  $x_0 = 2$ , which is  $y_0 = e$  (the initial value).

We now calculate the value of the derivative at this initial point. (This tells us the direction to move.)

$$\frac{dy}{dx} = f(2, e) = \frac{e \ln e}{2} = 1.3591409$$

This means the slope of the line from  $t=2$  to  $t=2.1$  is approximately 1.3591409.

### Step 2

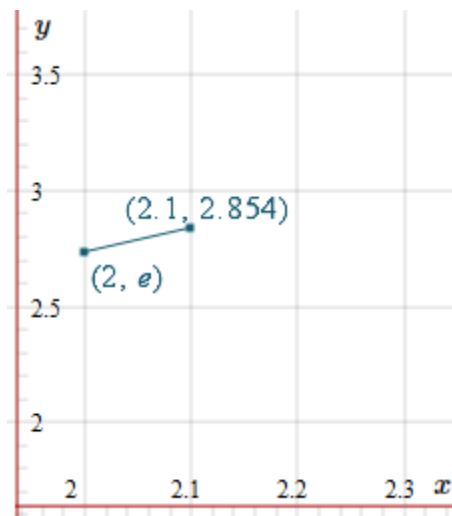
Now, for the second step,  $h = 0.1$ , the next point is  $x+h = 2+0.1 = 2.1$ , we substitute what we know into Euler's Method formula, and we have:

$$y(x+h) \approx y(x) + h f(x, y)$$

$$y(2.1) \approx y(2) + 0.1 \left( \frac{e}{2} \right) = 2.8541959$$

This means the approximate value of the solution when  $x=2.1$  is 2.8540959.

Let's see what we've done on a graph.



We'll need the new slope at this point, so we'll know where to head next.

$$\frac{dy}{dx} = f(2.1, 2.8541959) = \frac{2.8541959 \ln 2.8541959}{2.1} = 1.4254536$$

This means the slope of the approximation line from  $x=2.1$  to  $x=2.2$  is 1.4254536. So it's a little bit steeper than the first slope we found.

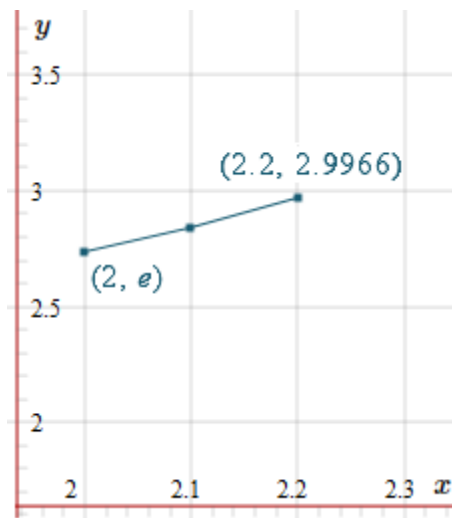
### Step 3

Now we are trying to find the solution value when  $x=2.2$ . We substitute our known values:

$$y(x+h) \approx y(x) + h f(x, y)$$

$$y(2.2) \approx 2.8541959 + 0.1(1.4254536) = 2.99664126$$

With this new value, our graph is now:



We'll need the new slope at this point, so we'll know where to head next.

$$\frac{dy}{dx} = f(2.2, 2.99664126) = \frac{2.99664126 \ln 2.99664126}{2.2} = 1.49490457$$

This means the slope of the approximation line from  $x = 2.3$  is 1.49490456. So it's a little steeper than the first 2 slopes we found.

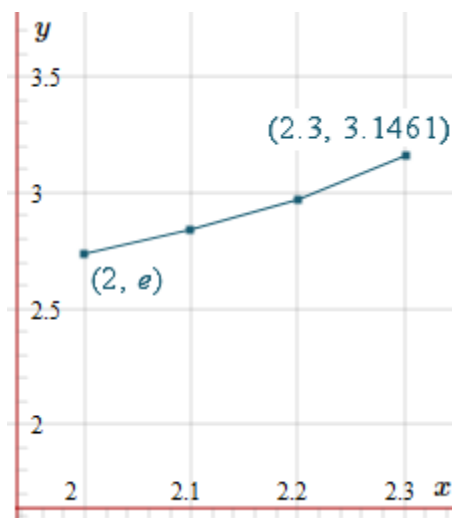
#### Step 4

Now we are trying to find the solution value when  $x=2.3$ . We substitute our known values:

$$y(x+h) \approx y(x) + h f(x, y)$$

$$y(2.3) \approx 2.99664126 + 0.1(1.49490457) = 3.1461317$$

With this new value, our graph is now:



### Subsequent Steps

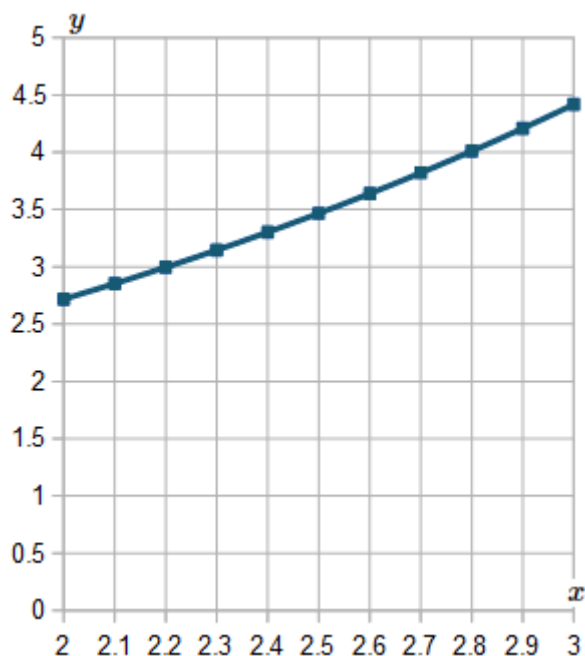
We present all the values up to  $x=3$  in the following table.

Of course, most of the time we'll use computers to find these approximations. I used a spreadsheet to obtain the following values. Don't use your calculator for these problems - it's very tedious and prone to error.

$x$	$y$	$dx/dy$
2.0	$e = 2.7182818285$	$(e \ln e)/2 = 1.3591409142$
2.1	$e+0.1(e/2) = 2.8541959199$	$(2.8541959199 \ln 2.8541959199)/2 = 1.4254536226$
2.2	2.9967412821	1.4949999323
2.3	3.1462412754	1.5679341197
2.4	3.3030346873	1.6444180873
2.5	3.4674764961	1.7246216904
2.6	3.6399386651	1.8087230858
2.7	3.8208109737	1.8969091045
2.8	4.0105018841	1.9893756448
2.9	4.2094394486	2.08632809
3.0	4.4180722576	

(There's no final  $dy/dx$  value because we don't need it. We've found all the required  $y$  values.)

Here is the graph of our estimated solution values from  $x=2$  to  $x=3$ .



**Note:**

The problem with Euler's Method is that you have to use a small interval size to get a reasonably accurate result. That is, it's not very efficient.

**Runge-Kutta Methods**

The Runge-Kutta methods are a series of numerical methods for solving differential equations and systems of differential equations.

The error in the Euler's method is:

$$E = \frac{h^2 y''(x)}{2!} + \frac{h^3 y'''(x)}{3!} + \frac{h^4 y^{(4)}(x)}{4!} + \dots$$



If the term  $\frac{h^2 y''(x)}{2!}$  is included in the solution the method is second order RK method, if the term  $\frac{h^3 y'''(x)}{3!}$  the method is the third order RK method and if the term  $\frac{h^4 y''''(x)}{4!}$  the method is fourth order RK method.

### **Second order RK method**

The Runge-Kutta 2nd order method is a numerical technique used to solve an ordinary differential equation of the form

$$\frac{dy}{dx} = f(x, y); y(0) = y_0$$

Only first order ordinary differential equations can be solved by using the Runge-Kutta 2nd order method. In other sections, we will discuss how the Euler and Runge-Kutta methods are used to solve higher order ordinary differential equations or coupled (simultaneous) differential equations.

Note: Euler's method can be considered to be the Runge-Kutta 1st order method.

Runge and Kutta did write the 2nd order method as:

$$y(x + h) = y(x) + \frac{1}{2}(k_1 + k_2)$$

$$k_1 = h f(x, y)$$

$$k_2 = h f(x + h, y + k_1)$$

### **Runge-Kutta Method of Order 3**

As usual in this work, the more terms we take, the better the solution. In practice, the Order 2 solution is rarely used because it is not very accurate.

A better result is given by the Order 3 method:

$$y(x + h) = y(x) + \frac{1}{9}(2k_1 + 3k_2 + 4k_3)$$

$$k_1 = h f(x, y)$$

$$k_2 = h f\left(x + \frac{h}{2}, y + \frac{k_1}{2}\right)$$

$$k_3 = h f\left(x + \frac{3h}{4}, y + \frac{3k_2}{4}\right)$$

The most commonly used Runge-Kutta formula in use is the Order 4 formula (RK4), as it gives the best trade-off between computational requirements and accuracy.

### **Runge-Kutta Method of Order 4 Formula**

$$y(x + h) = y(x) + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

$$k_1 = h f(x, y)$$

$$k_2 = h f\left(x + \frac{h}{2}, y + \frac{k_1}{2}\right)$$

$$k_3 = h f\left(x + \frac{h}{2}, y + \frac{k_2}{2}\right)$$

$$k_4 = h f(x + h, y + k_3)$$

### **Example**

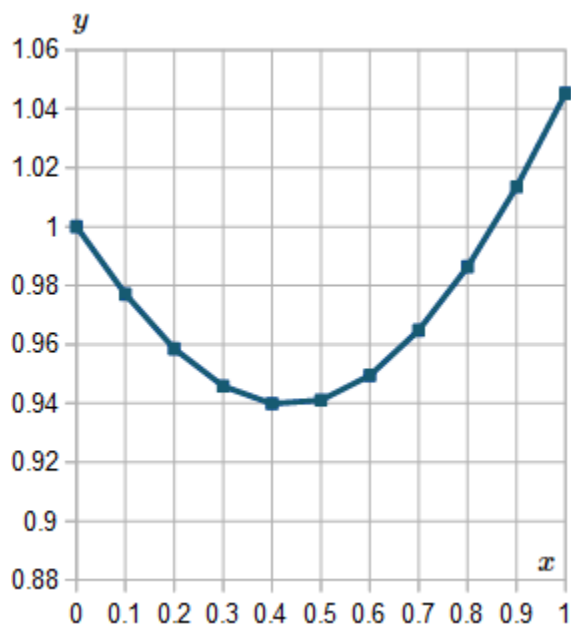
Use Runge-Kutta Method of Order 4 to solve the following, using a step size of  $h = 0.1$  for  $0 \leq x \leq 1$

$$\frac{dy}{dx} = \frac{5x^2 - y}{e^{x+y}}; y(0) = 1$$

Solving the problem using spread sheet will give the following data:

x	y	f(x,y)	k <sub>1</sub>	f(x+h/2,y+k <sub>1</sub> /2)	k <sub>2</sub>	f(x+h/2,y+k <sub>2</sub> /2)	k <sub>3</sub>	f(x+h,y+k <sub>3</sub> )	k <sub>4</sub>
0	1	-0.36788	-0.03679	-0.345422394	-0.03454	-0.345034753	-0.034503	-0.31544049	-0.03154
0.1	0.965596	-0.31544	-0.03154	-0.278770003	-0.02788	-0.278259299	-0.027826	-0.236479656	-0.02365
0.2	0.93783	-0.23648	-0.02365	-0.189271734	-0.01893	-0.188825458	-0.018883	-0.138593193	-0.01386
0.3	0.918975	-0.1386	-0.01386	-0.084793628	-0.00848	-0.084565823	-0.008457	-0.029804678	-0.00298
0.4	0.910523	-0.02981	-0.00298	0.026581644	0.002658	0.026506806	0.0026507	0.081973255	0.008197
0.5	0.913162	0.081977	0.008198	0.137235953	0.013724	0.136857301	0.0136857	0.189665443	0.018967
0.6	0.926826	0.189674	0.018967	0.240742061	0.024074	0.240128138	0.0240128	0.287672331	0.028767
0.7	0.950811	0.287686	0.028769	0.332382988	0.033238	0.331640987	0.0331641	0.372223842	0.037222
0.8	0.983943	0.372241	0.037224	0.409332877	0.040933	0.408574432	0.0408574	0.441391068	0.044139
0.9	1.024768	0.441411	0.044141	0.470511684	0.047051	0.469827563	0.0469828	0.494822386	0.049482
1	1.071716	0.494844	0.049484	0.516223978	0.051622	0.51567242	0.0515672	0.533332307	0.053333

The graph of the solution will be:



### Solving systems of ODE-IVPS

The following is a system of ODE-IVPs:

$$\frac{dy_1}{dt} = f_1(y_1, y_2, \dots, y_n, t); y_1(0) = y_{1_0}$$

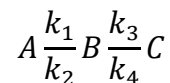
$$\frac{dy_2}{dt} = f_2(y_1, y_2, \dots, y_n, t); y_2(0) = y_{2_0}$$

$$\frac{dy_n}{dt} = f_n(y_1, y_2, \dots, y_n, t); y_n(0) = y_{n_0}$$

The only difference between solving a single ODE-IVP and solving a system of them is that all variables and functions become vectors. This is illustrated in the following example.

### Example: Solving a system of ODE-IVPS

Suppose the following chemical reactions take place in a continuous stirred tank reactor (CSTR):



Where the rate constants are as follows:

$$k_1 = 1 \text{ min}^{-1}, k_2 = 0 \text{ min}^{-1}, k_3 = 2 \text{ min}^{-1}, k_4 = 3 \text{ min}^{-1}$$

The initial charge to the reactor is all A, so the initial conditions are (in mol/L)

$$C_{A_0} = 1, C_{B_0} = 0, C_{C_0} = 0$$

An unsteady state mole balance on component leads to the following set of ODEs:

$$\frac{dC_A}{dt} = -k_1 C_A + k_2 C_B$$

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B - k_3 C_B + k_4 C_C$$

$$\frac{dC_C}{dt} = k_3 C_B - k_4 C_C$$

Solve the system of ODEs using the Euler's method for time only up to 0.13 min using  $h = 0.01$  min.

**Solution:**

The following spreadsheet displays a solution to this system using the Euler's method for time only up to 0.13 min:

Time	C <sub>A</sub>	dC <sub>A</sub> /dt	C <sub>B</sub>	dC <sub>B</sub> /dt	C <sub>C</sub>	dC <sub>C</sub> /dt
0	1	-1	0	1	0	0
0.01	0.99	-0.99	0.01	0.97	0	0.02
0.02	0.9801	-0.9801	0.0197	0.9413	0.0002	0.0388
0.03	0.970299	-0.9703	0.029113	0.913837	0.000588	0.056462
0.04	0.960596	-0.9606	0.038251	0.887551	0.001153	0.073045
0.05	0.95099	-0.95099	0.047127	0.862385	0.001883	0.088605
0.06	0.94148	-0.94148	0.055751	0.838286	0.002769	0.103194
0.07	0.932065	-0.93207	0.064134	0.815201	0.003801	0.116864
0.08	0.922745	-0.92274	0.072286	0.793083	0.00497	0.129662
0.09	0.913517	-0.91352	0.080216	0.771883	0.006266	0.141634
0.1	0.904382	-0.90438	0.087935	0.75156	0.007683	0.152823
0.11	0.895338	-0.89534	0.095451	0.732069	0.009211	0.163269
0.12	0.886385	-0.88638	0.102772	0.713372	0.010844	0.173012
0.13	0.877521	-0.87752	0.109905	0.695432	0.012574	0.182089

**Note:**

We used this formula with A, B and C in each row.

$$y(x + h) \approx y(x) + hy'(x)$$

**Homework:** Solve the above example using the second order RK method.

### Example: Penicillin Fermentation

A model for a batch reactor in which penicillin is produced by fermentation has been derived as follows for cell production and penicillin synthesis, respectively:

$$\frac{dy}{dt} = 13.1 y - 13.94 y^2; y(0) = 0.03$$

$$\frac{dx}{dt} = 1.71 y; x(0) = 0.0$$

where:

y = dimensionless concentration of cell mass

x = dimensionless concentration of penicillin

t = dimensionless time,  $0 \leq t \leq 1$

- Solve this ODE-IVP using the Euler method and Excel.
- Solve this ODE-IVP using the second-order RK method and Excel.

Use  $h = 0.1$ .

Solution:

- Euler's method

t	y	x	dy/dt	dx/dt
0	0.03	0	0.380454	0.0513
0.1	0.068045	0.00513	0.82685	0.116358
0.2	0.15073	0.016766	1.657856	0.257749
0.3	0.316516	0.042541	2.749817	0.541242
0.4	0.591498	0.096665	2.871438	1.011461
0.5	0.878642	0.197811	0.748371	1.502477
0.6	0.953479	0.348059	-0.18258	1.630449
0.7	0.93522	0.511104	0.058947	1.599227
0.8	0.941115	0.671026	-0.01801	1.609307
0.9	0.939313	0.831957	0.005608	1.606226
1	0.939874	0.99258	-0.00174	1.607185

b) Second order RK method

t	y	x	dy/dt	dx/dt	y		x	
					k1	k2	k1	k2
0	0.03	0	0.380454	0.0513	0.038045	0.084046	0.00513	0.006007
0.1	0.091046	0.005569	1.077145	0.155688	0.107715	0.20928	0.015569	0.018231
0.2	0.249543	0.022469	2.400946	0.426719	0.240095	0.317014	0.042672	0.049969
0.3	0.528097	0.068789	3.030394	0.903046	0.303039	0.142453	0.090305	0.105747
0.4	0.750843	0.166814	1.977153	1.283942	0.197715	0.007313	0.128394	0.15035
0.5	0.853357	0.306186	1.027612	1.459241	0.102761	-0.00271	0.145924	0.170877
0.6	0.903385	0.464587	0.457842	1.544789	0.045784	0.006509	0.154479	0.180895
0.7	0.929532	0.632274	0.132295	1.5895	0.013229	0.014887	0.15895	0.18613
0.8	0.94359	0.804814	-0.05062	1.613539	-0.00506	0.020358	0.161354	0.188945
0.9	0.951238	0.979964	-0.15245	1.626617	-0.01524	0.02361	0.162662	0.190477
1	0.955421	1.156533	-0.20883	1.63377	-0.02088	0.025469	0.163377	0.191314

**HIGHER-ORDER ODES**

Consider a general second-order ODE-IVP of the form:

$$\frac{d^2y}{dt^2} = f(y, y', t); y(0) = y_0, \quad y'(0) = y'_0$$

Since all of the methods discussed apply only to first-order equations, one way to solve those of the form of the above equation is to convert them into two simultaneous first-order equations. This is easily accomplished by defining a new variable z as follows:

$$\frac{dy}{dt} = z; y(0) = y_0$$

The above equation is a first-order ODE-IVP involving both y and z. If this equation is differentiated with respect to t and substituted into the equation  $[\frac{d^2y}{dt^2} = f(y, y', t)]$ , there results:

$$\frac{dz}{dt} = f(y, z, t); z(0) = y'(0)$$

The two equations:

$$\frac{dy}{dt} = z; y(0) = y_0$$

$$\frac{dz}{dt} = f(y, z, t); z(0) = y'(0)$$

constitute a system of coupled ODE-IVPs. This system can be solved numerically by any of the methods previously discussed.

**Example:**

Solve the following differential equation using Euler's method

$$\frac{d^2y}{dt^2} + \frac{dy}{dt} + y = 1; y(0) = y'(0) = 0$$

Use  $h = 0.1$  for  $t$  up to 2.

**Solution:**

In order to solve this model equation numerically with, for example, the Euler method, it must be converted into two first-order equations as follows:

Define a new variable  $z$  such that:

$$\frac{dy}{dt} = z; y(0) = y_0$$

Differentiating this expression with respect to  $t$

$$\frac{d^2y}{dt^2} = \frac{dz}{dt}$$

and substituting into the original model equation, there results

$$\frac{dz}{dt} + z + y = 1$$

$$\frac{dz}{dt} = 1 - z - y = 1; z(0) = y'(0)$$

The two equations:

$$\frac{dy}{dt} = z; y(0) = y_0 = 0$$

$$\frac{dz}{dt} = 1 - z - y = 1; z(0) = y'(0)$$



are two first-order ODE-IVPs that can be solved by any of the methods previously described.

The solution by Euler's method will be as shown in the following table (using Excel spread sheet).

t	y	z=dy/dt	dz/dt
0	0	0	1
0.1	0	0.1	0.9
0.2	0.01	0.19	0.8
0.3	0.029	0.27	0.701
0.4	0.056	0.3401	0.6039
0.5	0.09001	0.40049	0.5095
0.6	0.130059	0.45144	0.418501
0.7	0.175203	0.49329	0.331507
0.8	0.224532	0.526441	0.249027
0.9	0.277176	0.551344	0.17148
1	0.33231	0.568492	0.099198
1.1	0.38916	0.578411	0.032429
1.2	0.447001	0.581654	-0.02865
1.3	0.505166	0.578789	-0.08395
1.4	0.563045	0.570393	-0.13344
1.5	0.620084	0.557049	-0.17713
1.6	0.675789	0.539336	-0.21513
1.7	0.729723	0.517824	-0.24755
1.8	0.781505	0.493069	-0.27457
1.9	0.830812	0.465611	-0.29642
2	0.877373	0.435969	-0.31334