CETI Engineering Maths Notes

Integration and ODEs

Laurence R. McGlashan, Cambridge, January 2011. **lrm29@cam.ac.uk**

Contents

1 Numerical Integration **1**
1.1 Series Expansion . . . 1
1.2 Trapezoidal Rule . . . 1
1.3 Simpson's Rule . . . 1

2 Solving ODEs **2**
2.1 Euler's Method and Modified Euler's Method . . . 2
2.2 Runge-Kutta Method . . . 2

3 Examples Paper 1 **3**

1 Numerical Integration

1.1 Series Expansion

The simplest method is to use a series expansion. Your answer's accuracy will correspond to the number of terms you include, and the smoothness of the function.

$$\sin x \equiv x - \frac{x^3}{3!} + \frac{x^5}{5!} - \ldots \tag{1}$$

$$\int_0^\pi \sin x \, \mathrm{d}x \equiv \int_0^\pi x \, \mathrm{d}x - \int_0^\pi \frac{x^3}{3!} \, \mathrm{d}x + \int_0^\pi \frac{x^5}{5!} \, \mathrm{d}x - \ldots \tag{2}$$

$$\equiv \left[\frac{x^2}{2}\right]_0^\pi - \left[\frac{x^4}{4!}\right]_0^\pi + \left[\frac{x^6}{6!}\right]_0^\pi - \ldots \tag{3}$$

Including 3 terms of the series expansion gives 2.21. The first 4 gives 1.98. The first five gives 2.002. The first 6 gives 1.9999.

1.2 Trapezoidal Rule

1. Divide the area under a curve into n strips of width δx.
2. Number and measure each ordinate: $y_1, y_2 \ldots y_{n+1}$.
3. $Area \approx \frac{\delta x}{2}\left(y_1 + y_{n+1} + 2\sum_{i=2}^{n} y_i\right)$

1.3 Simpson's Rule

1. Divide the area under a curve into n strips of width δx.
2. Number and measure each ordinate: $y_1, y_2 \ldots y_{n+1}$.
3. $Area \approx \frac{\delta x}{3}\left(y_1 + y_{n+1} + 4\sum_{i=2}^{n/2} y_{2i-2} + 2\sum_{i=2}^{n/2-1} y_{2i-1}\right)$

To derive Simpson's Rule, approximate $f(x) = Ax^2 + Bx + C$ in each section and integrate between $-a$ and a:

$$\begin{aligned}\int_{-a}^{a} f(x)\mathrm{d}x =& A\int_{-a}^{a} x^2\mathrm{d}x + B\int_{-a}^{a} x\mathrm{d}x + C\int_{-a}^{a}\mathrm{d}x \\ &= A\frac{2a^3}{3} + 2aC \\ &= \frac{a}{3}\left(2Aa^2 + 6C\right)\end{aligned}$$

We know that the quadratic goes through $(-a, y_0)$, $(0, y_1)$ and (a, y_2):

$$\begin{aligned}y_0 &= Aa^2 + Ba + C \\ y_1 &= C \\ y_2 &= Aa^2 - Ba + C\end{aligned}$$

So $2Aa^2 = y_0 - 2y_1 + y_2$ and $C = y_1$. Substituting into the equation above:

$$\begin{aligned}\int_{-a}^{a} f(x)\mathrm{d}x =& \frac{a}{3}\left(y_0 - 2y_1 + y_2 + 6y_1\right) \\ &= \frac{a}{3}\left(y_0 + 4y_1 + y_2\right)\end{aligned}$$

Now just sum this expression for each section to get Simpson's rule!

2 Solving ODEs

2.1 Euler's Method and Modified Euler's Method

Modified Euler's Method can be obtained from the Runge-Kutta algorithm.

input : x_0, y_0, h, N
for $n = 0, 1, ..., N-1$ **do**
  $x_{n+1} = x_n + h$
  $k_1 = h\ f(x_n, y_n)$
  $k_2 = h\ f(x_{n+1}, y_n + k_1)$
  $y_{n+1} = y_n + 0.5(k_1 + k_2)$
end
output: x_N, y_N

2.2 Runge-Kutta Method

We will make use of:

$$f'(x, y) = \frac{\partial f(x, y)}{\partial x} + \frac{\partial f(x, y)}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}x}$$

To derive a 2nd order RK:

$$\begin{aligned}y_{i+1} &= y_i + h\left.\frac{\mathrm{d}y}{\mathrm{d}x}\right|_{x_i, y_i} + \frac{h^2}{2}\left.\frac{\mathrm{d}^2 y}{\mathrm{d}x^2}\right|_{x_i, y_i} + \mathcal{O}(h^3) \\ &= y_i + hf(x_i, y_i) + \frac{h^2}{2}f'(x_i, y_i) + \mathcal{O}(h^3) \\ &= y_i + hf(x_i, y_i) + \frac{h^2}{2}\left(\frac{\partial f}{\partial x}\right) + \frac{h^2}{2}\left(\frac{\partial f}{\partial y}f(x_i, y_i)\right)\end{aligned}$$

2nd order RK is $y_{i+1} = y_i + h(ak_1 + bk_2)$ where $k_1 = f(x_i, y_i)$ and $k_2 = f(x_i + \alpha h, y_i + \beta k_1 h)$. Take a Taylor series of k_2:

$$k_2 = f(x_i, y_i) + \alpha h \frac{\partial f}{\partial x} + \beta k_1 h \frac{\partial f}{\partial y} + \mathcal{O}(h^2)$$

Substituting into the above gives:

$$y_{i+1} = y_i + (a+b)hf(x_i, y_i) + b\alpha h^2 \frac{\partial f}{\partial x} + b\beta f(x_i, y_i) h^2 \frac{\partial f}{\partial y}$$

Now compare the coefficients of the second order Taylor series with the RK formula.

input : x_0, y_0, h, N
for $n = 0, 1, ..., N-1$ **do**
  $k_1 = h\ f(x_n, y_n)$
  $k_2 = h\ f(x_n + 0.5h, y_n + 0.5k_1)$
  $k_3 = h\ f(x_n + 0.5h, y_n + 0.5k_2)$
  $k_4 = h\ f(x_n + h, y_n + k_3)$
  $x_{n+1} = x_n + h$
  s $y_{n+1} = y_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$
end
output: x_N, y_N

3 Examples Paper 1

Question 1 Use the substitution $y = \dfrac{1}{\sqrt{z}}$.
This is necessary because $f(z)$ is undefined at $z = 0$. The new integrand is also smoother (rate of change of gradient is smaller).

$$I = \int_1^\infty \frac{2\ \mathrm{d}y}{y^2(1 + \exp(1/y))}$$

Exact answer is around 0.76.

Question 2 $f(x) = \sin x$. The exact solution $\displaystyle\int_0^\pi f(x)\ \mathrm{d}x = 2$.

(i) $h = \dfrac{\pi}{2}$

$$\begin{aligned}\int_0^\pi \sin x\ \mathrm{d}x &\approx \frac{h}{2}\left[f(0) + 2f(\pi/2) + f(\pi)\right] \\ &= \frac{\pi}{2} = 1.571\end{aligned}$$

(ii) $h = \dfrac{\pi}{4}$

$$\begin{aligned}\int_0^\pi \sin x\ \mathrm{d}x &\approx \frac{h}{2}\left[f(0) + 2\left(f(\pi/2) + f(\pi/2) + f(3\pi/4)\right) + f(\pi)\right] \\ &= \frac{\pi}{4}(1 + \sqrt{2}) = 1.896\end{aligned}$$

(iii) $h = \dfrac{\pi}{8}$

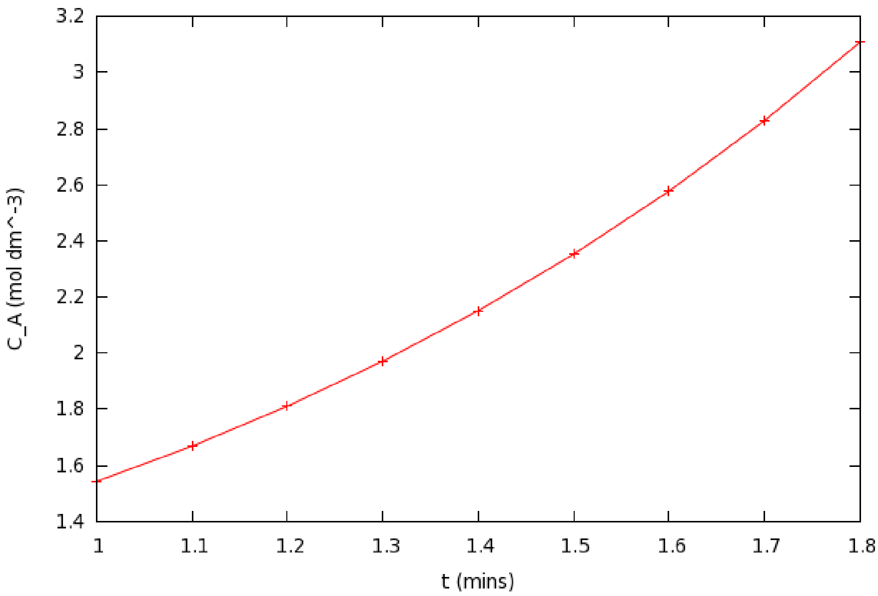
$$\begin{aligned}\int_0^\pi \sin x\ \mathrm{d}x &\approx \frac{h}{2}\left[f(0) + 2\left(f(\pi/8) + f(\pi/4) + f(3\pi/8) + f(\pi/2) + f(5\pi/8) + f(3\pi/4) + f(7\pi/8)\right) + f(\pi)\right] \\ &= 1.974\end{aligned}$$

(iv)

n	$1/n^2$	ε
2	0.25	0.429
4	0.0625	0.104
8	0.015625	0.026

$$\therefore \varepsilon \propto \frac{1}{n^2}$$

Question 3 (Trapezium Rule) The data is plotted below:



The flowrate is constant at $V = 0.5$ dm^3 min^{-1}.
In general:

$$\int_{1.0}^{1.8} C_A \text{ d}t \approx \frac{h}{2}\left[f(1.0) + 2\left(\sum f(t)\right) + f(1.8)\right]$$

(i) $h = 0.1$

$$V\int_{1.0}^{1.8} C_A \text{ d}t \approx 0.8842$$

(ii) $h = 0.2$

$$V\int_{1.0}^{1.8} C_A \text{ d}t \approx 0.8864$$

(iii) $h = 0.4$

$$V\int_{1.0}^{1.8} C_A \text{ d}t \approx 0.8952$$

(iv) $C_A = \cosh t$.

$$V\int_{1.0}^{1.8} \cosh t \text{ d}t = V\left[\sinh t\right]_{1.0}^{1.8} = 0.8835$$

h	ε
0.1	0.0007
0.2	0.0029
0.4	0.0117

$$\therefore \varepsilon \propto h^2$$

Question 4 (Euler's Method)

$$\frac{\mathrm{d}y}{\mathrm{d}x} = \cos(xy) \qquad y(\pi/4) = 1$$

Euler's Method is based on a first order Taylor expansion:

$$\left.\frac{\mathrm{d}y}{\mathrm{d}x}\right|_{x_1,y_1} = \frac{y_2 - y_1}{x_2 - x_1} \qquad \therefore y_2 = y_1 + (x_2 - x_1)\left.\frac{\mathrm{d}y}{\mathrm{d}x}\right|_{x_1,y_1} + \mathcal{O}(h^2)$$

(i)

$$\begin{aligned}
y_1 &= 1.0 \\
y_2 &= 1.0 + 0.1\cos\left(\frac{\pi}{4}\right) = 1.071 \\
y_3 &= 1.07071 + 0.1\cos\left(1.07071\left(\frac{\pi}{4} + 0.1\right)\right) = 1.129
\end{aligned}$$

(ii)

$$\begin{aligned}
y_1 &= 1.0 \\
y_2 &= 1.0 + 0.05\cos\left(\frac{\pi}{4}\right) = 1.0354 \\
y_3 &= 1.0354 + 0.05\cos\left(1.0354\left(\frac{\pi}{4} + 0.05\right)\right) = 1.0678 \\
y_4 &= 1.0678 + 0.05\cos\left(1.0678\left(\frac{\pi}{4} + 0.1\right)\right) = 1.0971 \\
y_5 &= 1.0971 + 0.05\cos\left(1.0971\left(\frac{\pi}{4} + 0.15\right)\right) = 1.123
\end{aligned}$$

The error for Euler's method may be approximated by $\varepsilon_i(x) = \frac{h^2}{2}\frac{\mathrm{d}^2y}{\mathrm{d}x^2}$, so the global error is:

$$\begin{aligned}
\varepsilon_g(x) &= \sum \frac{h^2}{2}\frac{\mathrm{d}^2y}{\mathrm{d}x^2} \\
&= n\frac{h^2}{2}\overline{\frac{\mathrm{d}^2y}{\mathrm{d}x^2}} \\
&= \frac{h}{2}(x_1 - x_0)\overline{\frac{\mathrm{d}^2y}{\mathrm{d}x^2}}
\end{aligned}$$

i.e. the error is proportional to the step size ($\varepsilon \propto h$). Using this:

$$\begin{aligned}
y_{exact} &= 1.129 + k\ 0.1 \\
y_{exact} &= 1.123 + k\ 0.05
\end{aligned}$$

Solving the above simultaneous equations gives $y_{exact} = 1.117$.
Discrepancy between exact and extrapolated solutions is due to the error only incorporating the second order term of the Taylor expansion and not including higher order terms.

Question 5 (Runge-Kutta)
Modified Euler is a special case of a 2nd order RK. Simpson's Rule can be recovered from 4th order RK for one variable.

$$\frac{\mathrm{d}y}{\mathrm{d}x} = f(x, y) = \frac{1}{x + y}\ , \qquad y(0) = 2$$

Step 1 ($h = 0.2$):

$$
\begin{aligned}
k_1 &= hf(x_0, y_0) = 0.1\\
k_2 &= hf(x_0 + 0.5h, y_0 + 0.5k_1) = 0.093\\
k_3 &= hf(x_0 + 0.5h, y_0 + 0.5k_2) = 0.0932\\
k_4 &= hf(x_0 + h, y_0 + k_3) = 0.0872\\
y_1 &= y_0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) = 2.0933
\end{aligned}
$$

Step 2:

$$
\begin{aligned}
k_1 &= hf(x_1, y_1) = 0.0872\\
k_2 &= hf(x_1 + 0.5h, y_1 + 0.5k_1) = 0.0821\\
k_3 &= hf(x_1 + 0.5h, y_1 + 0.5k_2) = 0.0822\\
k_4 &= hf(x_1 + h, y_1 + k_3) = 0.0777\\
y_2 &= y_1 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) = 2.1755
\end{aligned}
$$

Question 6 (Modified Euler)

$$
\frac{\mathrm{d}x}{\mathrm{d}t} = xy + t \qquad \frac{\mathrm{d}y}{\mathrm{d}t} = x - t \qquad\qquad x(0) = 0\ , \quad y(0) = 1
$$

Using Euler's Method:

$$
\begin{aligned}
x(h) &= x(0) + h\ \ [x(0)y(0) + 0] = 0.0\\
y(h) &= y(0) + h\ \ [x(0) - 0] = 1\\
x(2h) &= x(h) + h\ \ [x(h)y(h) + h] = 0.04\\
y(2h) &= y(h) + h\ \ [x(h) - h] = 0.96\\
x(3h) &= x(2h) + h\ \ [x(2h)y(2h) + 2h] = 0.1277\\
y(3h) &= y(2h) + h\ \ [x(2h) - 2h] = 0.888
\end{aligned}
$$

Using Modified Euler's Method:

$$
\begin{aligned}
x^*(h) &= x(0) + h\ \ [x(0)y(0) + 0] = 0.0\\
y^*(h) &= y(0) + h\ \ [x(0) - 0] = 1\\
x(h) &= x(0) + \frac{h}{2}\,[x(0)y(0) + 0 + x^*(h)y^*(h) + 0.2] = 0.02\\
y(h) &= y(0) + \frac{h}{2}\,[x(0) - 0 + x^*(h) - 0.2] = 0.98
\end{aligned}
$$

$$
\begin{aligned}
x^*(2h) &= x(h) + h\ \ [x(h)y(h) + h] = 0.06392\\
y^*(2h) &= y(h) + h\ \ [x(h) - h] = 0.944\\
x(2h) &= x(h) + \frac{h}{2}\,[x(h)y(h) + h + x^*(2h)y^*(2h) + 2h] = 0.08799\\
y(2h) &= y(h) + \frac{h}{2}\,[x(h) - h + x^*(2h) - 2h] = 0.92839
\end{aligned}
$$

$$
\begin{aligned}
x^*(3h) &= x(2h) + h\ \ [x(2h)y(2h) + 2h] = 0.1843\\
y^*(3h) &= y(2h) + h\ \ [x(2h) - 2h] = 0.866\\
x(3h) &= x(2h) + h\ \ [x(2h)y(2h) + 2h + x^*(2h)y^*(2h) + 3h] = 0.212\\
y(3h) &= y(2h) + h\ \ [x(2h) - 2h + x^*(2h) - 3h] = 0.856
\end{aligned}
$$

If we instead use $x^*(h)$ when we calculate $y(h)$ then we'll converge faster to the values $x(0.6) = 0.212$ and $y(0.6) = 0.8628$.

Question 7 (Euler's Method)

$$4\frac{\mathrm{d}^2 z}{\mathrm{d}t^2} + 5\frac{\mathrm{d}z}{\mathrm{d}t} + z = 4\exp\left(-t^2\right) \qquad \left.\frac{\mathrm{d}z}{\mathrm{d}t}\right|_{t=0} = 1\ , \quad z(0) = 0$$

Make the substitutions: $y_1 = z\ , \quad y_2 = \frac{\mathrm{d}z}{\mathrm{d}t}$.

$$4\frac{\mathrm{d}y_2}{\mathrm{d}t} + 5y_2 + y_1 = 4\exp\left(-t^2\right) \qquad y_2(0) = 1\ , \quad y_1(0) = 0$$

Step 1:

$$\begin{aligned}
y_1(h) &= y_1(0) + hy_2(0) = h = 0.1 \\
y_2(h) &= y_2(0) + h\frac{\mathrm{d}y_2}{\mathrm{d}t} \\
&= 1 + h\left(\exp(-h^2) - \frac{y_1(0)}{4} - \frac{5y_2(0)}{4}\right) = 0.974
\end{aligned}$$

Step 2:

$$\begin{aligned}
y_1(2h) &= y_1(h) + h\ y_2(h) \\
&= 0.1 + 0.1 \times 0.974 = 0.1974
\end{aligned}$$

Question 8 (Stiffness) To get an analytical solution, you should recognise that this can be solved using integrating factors:

$$\frac{\mathrm{d}y}{\mathrm{d}x} + P(x)y = Q(x)$$

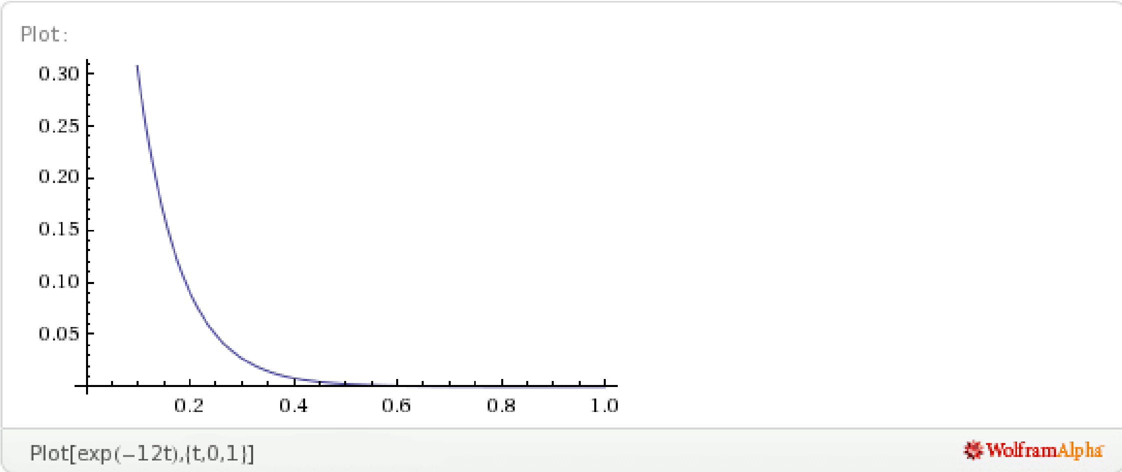
Multiply by an Integrating Factor $I(x)$:

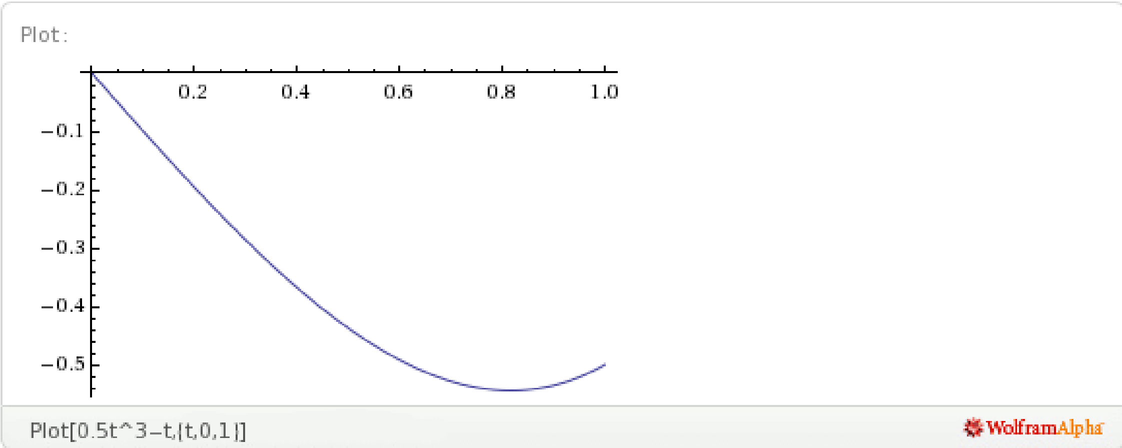
$$\begin{aligned}
I(x)\frac{\mathrm{d}y}{\mathrm{d}x} + I(x)P(x)y &= I(x)Q(x) \\
\frac{\mathrm{d}\left[I(x)y\right]}{\mathrm{d}x} &= I(x)Q(x)
\end{aligned}$$

Clearly for this to be true then $\frac{\mathrm{d}I(x)}{\mathrm{d}x} = I(x)P(x)$. So $I(x) = \exp\left(\int P(x)\mathrm{d}x\right)$. Going back to the given problem:

$$\begin{aligned}
\frac{\mathrm{d}P}{\mathrm{d}t} + 12P &= 6t^3 + \frac{3}{2}t^2 - 12t - 1 \quad , \qquad P(0) = a \\
\Rightarrow \frac{\mathrm{d}\left[P\exp(12t)\right]}{\mathrm{d}t} &= \exp(12t)\left(6t^3 + \frac{3}{2}t^2 - 12t - 1\right) \\
\Rightarrow \int_{t=0,P=a}^{t=t,P=P} \mathrm{d}[P\exp(12t)] &= \int_0^t \exp(12t)\left(6t^3 + \frac{3}{2}t^2 - 12t - 1\right)\mathrm{d}t \\
\Rightarrow P\exp(12t) - a &= \exp(12t)\left(\frac{t^3}{2} - t\right) \\
\Rightarrow P &= \frac{t^3}{2} - t + a\exp(-12t)
\end{aligned}$$

You can see that this is going to be stiff (stiffness is usually associated with high values of the derivative of the variable you are solving for):





Question 9 (Discontinuities)

$$\frac{dC_1}{dt} = \frac{C_0 - C_1}{1000} - 0.002C_1 \quad , \qquad C_0(0) = 3, \quad C_1(0) = 2, \quad C_2(0) = 1$$
$$\frac{dC_2}{dt} = \frac{C_1 - C_2}{500} - 0.002C_2$$

(a) $h = 250$

$$C_1(250) = C_1(0) + 250\left(\frac{C_0(0) - C_1(0)}{1000} - 0.002\ C_1(0)\right) = 1.25$$
$$C_2(250) = C_2(0) + 250\left(\frac{C_1(0) - C_2(0)}{500} - 0.002\ C_2(0)\right) = 1.0$$
$$C_1(500) = C_1(250) + 250\left(\frac{C_0(250) - C_1(250)}{1000} - 0.002\ C_1(250)\right) = 1.0625$$
$$C_2(500) = C_2(250) + 250\left(\frac{C_1(250) - C_2(250)}{500} - 0.002\ C_2(250)\right) = 0.625$$

(b) Go from $t = 500$ to $t = 600$, $h = 100$

$$C_1(600) = C_1(500) + 100\left(\frac{C_0(500) - C_1(500)}{1000} - 0.002\ C_1(500)\right) = 1.04375$$
$$C_2(600) = C_2(500) + 100\left(\frac{C_1(500) - C_2(500)}{500} - 0.002\ C_2(500)\right) = 0.5875$$

Go from $t = 600$ to $t = 750$, $h = 150$ and $C_0(600) = 6$:

$$C_1(750) = C_1(600) + 150\left(\frac{C_0(600) - C_1(600)}{1000} - 0.002\ C_1(600)\right) = 1.4741$$
$$C_2(750) = C_2(600) + 150\left(\frac{C_1(600) - C_2(600)}{500} - 0.002\ C_2(600)\right) = 0.5481$$