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Hw3 analysis

Question 1

Considering a simple 1st order chemical reaction, substance A becomes B with rate constant k1, and B becomes C with rate constant k2. From mass conservation principles the governing equation for describing the time rate of change of the concentration for substance A, B and C can be expressed as

$$\frac{dA}{dt} = -k_1 A \qquad \frac{dB}{dt} = k_1 A - k_2 B \qquad \frac{dC}{dt} = k_2 B$$

Find the transient solution of the reaction system for the given initial conditions:

$$A(0) = A_0$$
 $B(0) = C(0) = 0$

<u>Answer</u>

Write equation in matrix nation

$$\frac{dx}{dt} = Ax = \begin{bmatrix} -k_1 & 0 & 0 \\ k_1 & -k_2 & 0 \\ 0 & k_2 & 0 \end{bmatrix} x$$

Which yields 3 eigenvalues

and 3 eigen vectors

$$X_1$$
 X_2 X_3 $AX = \lambda X$

For $\lambda_1=0$

$$\begin{bmatrix} -k_1 & 0 & 0 \\ k_1 & -k_2 & 0 \\ 0 & k_2 & 0 \end{bmatrix} X_1 = \lambda_1 X_1$$

$$\begin{bmatrix} -k_1 & 0 & 0 \\ k_1 & -k_2 & 0 \\ 0 & k_2 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}_1 = 0 \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}_1$$

This is equivalent to 3 equations

$$-k_1x_1 + 0x_2 + 0x_3 = 0x_1$$
$$k_1x_1 - k_2x_2 + 0x_3 = 0x_2$$
$$0x_1 + k_2x_2 + 0x_3 = 0x_3$$

Canceling terms

$$-k_1 x_1 = 0x_1$$

 $k_1 x_1 - k_2 x_2 = 0x_2$
 $k_2 x_2 = 0x_3$

$$X_1 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

I have the work done by hand but I did not type it up but it is done using the same technique

For $\lambda_2 = -k_2$

$$\begin{bmatrix} -k_1 & 0 & 0 \\ k_1 & -k_2 & 0 \\ 0 & k_2 & 0 \end{bmatrix} X_1 = \lambda_1 X_1$$

$$\begin{bmatrix} -k_1 & 0 & 0 \\ k_1 & -k_2 & 0 \\ 0 & k_2 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}_1 = -k_2 \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}_1$$

This is equivalent to 3 equations

$$-k_1x_1 + 0x_2 + 0x_3 = -k_2x_1$$

$$k_1x_1 - k_2x_2 + 0x_3 = -k_2x_2$$

$$0x_1 + k_2x_2 + 0x_3 = -k_2x_3$$

Canceling terms

$$-k_1 x_1 = -k_2 x_1$$

 $k_1 x_1 - k_2 x_2 = -k_2 x_2$

$$k_2 x_2 = -k_2 x_3$$

$$X_2 = \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix}$$

For $\lambda_3 = -k_1$

$$\begin{bmatrix} -k_1 & 0 & 0 \\ k_1 & -k_2 & 0 \\ 0 & k_2 & 0 \end{bmatrix} X_1 = \lambda_1 X_1$$

$$\begin{bmatrix} -k_1 & 0 & 0 \\ k_1 & -k_2 & 0 \\ 0 & k_2 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}_1 = -k_1 \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}_1$$

This is equivalent to 3 equations

$$-k_1x_1 + 0x_2 + 0x_3 = -k_1x_1$$
$$k_1x_1 - k_2x_2 + 0x_3 = -k_1x_2$$
$$0x_1 + k_2x_2 + 0x_3 = -k_1x_3$$

Canceling terms

$$-k_1x_1 = -k_1x_1 eq1$$

 $k_1x_1 - k_2x_2 = -k_1x_2 eq2$
 $k_2x_2 = -k_1x_3 eq3$

$$X_{3} = \begin{bmatrix} ? \\ -k_{1} \\ k_{2} \\ x_{3} \end{bmatrix} = \begin{bmatrix} \frac{k_{1}}{k_{2}} - 1 \\ -k_{1} \\ \frac{k_{2}}{k_{2}} \end{bmatrix}$$

From eq2, substitute into x_2 to get unknown value

$$k_1 x_1 - k_2 \frac{-k_1}{k_2} x_3 = -k_1 \frac{-k_1}{k_2} x_3$$
$$k_1 x_1 = \left[k_1 \frac{k_1}{k_2} - k_1 \right] x_3$$

$$x_1 = \left[\frac{k_1}{k_2} - 1\right] x_3$$

The general solution is

$$\begin{pmatrix} A \\ B \\ C \end{pmatrix} = c_1 X_1 \exp(\lambda_1 t) + c_2 X_2 \exp(\lambda_2 t) + c_3 X_3 \exp(\lambda_3 t)$$

$$\begin{pmatrix} A \\ B \\ C \end{pmatrix} = c_1 \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \exp(0 t) + c_2 \begin{bmatrix} 0 \\ -1 \\ 1 \end{bmatrix} \exp(-k_2 t) + c_3 \begin{bmatrix} \frac{k_1}{k_2} - 1 \\ -\frac{k_1}{k_2} \\ 1 \end{bmatrix} \exp(-k_1 t)$$

$$A = c_3 \left[\frac{k_1}{k_2} - 1 \right] \exp(-k_1 t)$$

$$B = -c_2 \exp(-k_2 t) - c_3 \left[\frac{k_1}{k_2} \right] \exp(-k_1 t)$$

$$C = c_1 + c_2 \exp(-k_2 t) + c_3 \exp(-k_1 t)$$

Using initial conditions

$$A(0) = A_0 B(0) = C(0) = 0$$

$$A_0 = c_3 \left[\frac{k_1}{k_2} - 1 \right] eq1$$

$$0 = -c_2 - c_3 \left[\frac{k_1}{k_2} \right] eq2$$

$$0 = c_1 + c_2 + c_3 eq3$$

From eq1 we get

$$c_3 = \frac{A_0}{\left[\frac{k_1}{k_2} - 1\right]}$$

From eq2 we get

$$c_2 = -c_3 \left[\frac{k_1}{k_2} \right] = -\frac{A_0}{\left[\frac{k_1}{k_2} - 1 \right]} \left[\frac{k_1}{k_2} \right] = \frac{A_0}{\left[1 - \frac{k_2}{k_1} \right]}$$

From eq3 we get

$$c_1 = -c_2 - c_3 = c_3 \left[\frac{k_1}{k_2} \right] - c_3 = c_3 \left[\frac{k_1}{k_2} - 1 \right] = \frac{A_0}{\left[\frac{k_1}{k_2} - 1 \right]} \left[\frac{k_1}{k_2} - 1 \right] = A_0$$

The following were helpful links for the problem:

"mathematics for physical chemistry" p256 books.google.com

http://books.google.com/books?id=QL0GXO4CeawC&lpg=PA256&ots=NL3J5xJFfY&dq=help%20what%20is%20the%20solution%20dA%2Fdt%20%3D%20-

k1%20A%20%20%20%20%20%20dB%2Fdt%20%3D%20k1A%20-

%20k2B%20dC%2Fdt%20%3D%20k2B&pg=PA256#v=onepage&q&f=false

also

http://www.boards.ie/vbulletin/showthread.php?p=70061453

Question 2:

Find the general solution of the 3rd order ODE:

$$y''' + y' = sec(x)$$

Solution:

First need the solutions of the homogeneous equation

$$y''' + y' = 0$$

That is a linear constant coefficient ODE with characteristic equation

$$r^3 + r = 0 = r(r^2 + 1)$$

It has a real root at 0

$$r_1 = 0$$

Hence

$$c_1 e^0 = c_1$$

Must be one term in the complementary function

When the

And two conjugate complex roots

$$r_{2,3} = 0 \mp i$$
 $r_2 = i$ $r_3 = -i$

Thus the complementary function must also contain

$$e^{0*t}(c_2\cos x + c_3\sin x) = c_2\cos x + c_3\sin x$$

Solution of the homogeneous equation is

$$y_h = c_1[1] + c_2[\cos x] + c_3[\sin x]$$

If y1 y2 and y3 are solution of the homogeneous equation

$$y_1 = 1$$
$$y_2 = \cos x$$
$$y_3 = \sin x$$

The wronskian is

$$W(y_1, y_2, y_3) \equiv \begin{vmatrix} y_1 & y_2 & y_3 \\ y_1' & y_2' & y_3' \\ y_1'' & y_2'' & y_3'' \end{vmatrix}$$

$$= (y_1)(y_2')(y_3'') + (y_2)(y_3')(y_1'') + (y_3)(y_1')(y_2'') - (y_1)(y_3')(y_2'')$$

$$- (y_2)(y_1')(y_3'') - (y_3)(y_2')(y_1'') \neq 0$$

Note: For this type of problem the particular solution is the whole solution, you don't need to and the homogeneous solution to the particular like the lower order ode

Variation of parameters methods assumes that general solution of the inhomogeneous equation takes the form:

$$y = v_1 * y_1 + v_2 * y_2 + v_3 y_3$$

The functions v1 v2 and v3 can be found by the integrals

$$v_i = \int \frac{W_i}{W} dx$$

W is the wronskian of the fundamental system. Wi is the same determinant as W, but column I is replaced by < 0, 0, f(x) > f(x) is the function on the RHS of the inhomgeneous equation

For the given equation

$$W(y_1, y_2, y_3) \equiv \begin{vmatrix} y_1 & y_2 & y_3 \\ y_1' & y_2' & y_3' \\ y_1'' & y_2'' & y_3'' \end{vmatrix} = \begin{vmatrix} 1 & \sin x & \cos x \\ 0 & \cos x & -\sin x \\ 0 & -\sin x & -\cos x \end{vmatrix}$$

$$= (y_1)(y_2')(y_3'') + (y_2)(y_3')(y_1'') + (y_3)(y_1')(y_2'') - (y_1)(y_3')(y_2'') - (y_2)(y_1')(y_3'') - (y_3)(y_2')(y_1'') =$$

$$= (1)(\cos x)(-\cos x) - (1)(-\sin x)(-\sin x) = -1$$

For W1

$$W_{1} = \begin{vmatrix} 0 & y_{2} & y_{3} \\ 0 & y_{2}' & y_{3}' \\ f(x) & y_{2}'' & y_{3}'' \end{vmatrix} = \begin{vmatrix} 0 & \sin x & \cos x \\ 0 & \cos x & -\sin x \\ \sec x & -\sin x & -\cos x \end{vmatrix}$$

$$= (0)(y_{2}')(y_{3}'') + (y_{2})(y_{3}')(f(x)) + (y_{3})(0)(y_{2}'') - (0)(y_{3}')(y_{2}'') - (y_{2})(0)(y_{3}'')$$

$$- (y_{3})(y_{2}')(f(x)) =$$

$$= (y_{2})(y_{3}')(f(x)) - (y_{3})(y_{2}')(f(x)) = (\sin x)(-\sin x)(\sec x) - (\cos x)(\cos x)(\sec x) =$$

Note: $\sec x = 1/(\cos x)$ and $\tan x = (\sin x)/(\cos x)$

$$= -(\sin x)(\tan x) - (\cos x) =$$

For W2

$$W_{2} = \begin{vmatrix} y_{1} & 0 & y_{3} \\ y_{1}' & 0 & y_{3}' \\ y_{1}" & f(x) & y_{3}" \end{vmatrix} = \begin{vmatrix} 1 & 0 & \cos x \\ 0 & 0 & -\sin x \\ 0 & \sec x & -\cos x \end{vmatrix}$$

$$= (y_{1})(0)(y_{3}") + (0)(y_{3}')(y_{1}") + (y_{3})(0)(f(x)) - (y_{1})(y_{3}')(f(x)) - (0)(y_{1}')(y_{3}") - (y_{3})(0)(0) =$$

$$= (y_{1})(y_{3}')(f(x)) =$$

$$= (1)(-\sin x)(\sec x) = -\tan x$$

For W3

$$W_{3} = \begin{vmatrix} y_{1} & y_{2} & 0 \\ y_{1}' & y_{2}' & 0 \\ y_{1}" & y_{2}" & f(x) \end{vmatrix} = \begin{vmatrix} 1 & \sin x & 0 \\ 0 & \cos x & 0 \\ 0 & -\sin x & \sec x \end{vmatrix}$$
$$= (1)(y_{2}')(f(x)) + (y_{2})(0)(0) + (0)(0)(y_{2}") - (1)(0)(y_{2}") - (y_{2})(0)(f(x)) - (0)(y_{2}')(0) =$$
$$= (y_{2}')(f(x)) = (\cos x)(\sec x) = 1$$

For v1

$$v_1 = \int \frac{W_1}{W} dx = \int [(\sin x)(\tan x) + (\cos x)] dx =$$

$$v_1 = \int \frac{W_1}{W} dx = \int [(\sin x)(\tan x)] dx + \int [\cos x] dx =$$

$$\int [(\sin x)(\tan x)] dx = \int [(\sin x)^2/(\cos x)] dx = \int \left[\frac{(1-\cos^2 x)}{(\cos x)}\right] dx = \int [\sec x - \cos x] dx$$

$$v_1 = \int \frac{W_1}{W} dx = \ln|\sec(x) + \tan(x)| - \sin(x) + C_{1a} + \sin x + C_{1b} =$$

$$v_1 = \int \frac{W_1}{W} dx = \ln|\sec(x) + \tan(x)| + C_1$$

For v2

$$v_2 = \int \frac{W_2}{W} dx = \int \tan x dx = \int \left[\frac{\sin x}{\cos x} \right] dx$$

Set

$$u = \cos x$$

Then we find

$$du = -\sin x \ dx$$

Substitute $du = -\sin x$, $u = \cos x$

$$\int \left[\frac{\sin x}{\cos x} \right] dx = -\int \left[\frac{-\sin x}{\cos x} \right] dx = -\int \left[\frac{du}{u} \right] = -\ln|u| + C_2 = -\ln|\cos x| + C_2$$

For v3

$$v_3 = \int \frac{W_3}{W} dx = -\int 1 dx = -x + C_3$$

Hence the solution is

$$y = v_1 * y_1 + v_2 * y_2 + v_3 y_3$$

$$y = [\ln|\sec(x) + \tan(x)| + C_1] * [1] + [-\ln|\cos x| + C_2] * [\cos x] + [-x + C_3] * [\sin x]$$

$$y = C_1 + C_2 \cos x + C_3 \sin x + \ln|\sec(x) + \tan(x)| - \ln|\cos x| * \cos x - x * [\sin x]$$

Helpful links

http://en.wikipedia.org/wiki/Euler%27s_formula

Example 1 Pg103 "Advanced engineering mathematics" 2nd edition

Also pg80 for wronskian (pg 83 for example 1 euler chauchy)

http://au.answers.yahoo.com/question/index?qid=20110221094122AAsWBNO

http://answers.yahoo.com/question/index?qid=20080901053216AA5k9KZ

Question 3

The following Poisson equation is often used for describing a screened electric potential around a changed spherical particles in an liquid electrolyte

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\phi}{dr}\right) = k^2\phi \quad for \ a \le r \le \infty$$

Where r is the distance away from the center of the particle, a is the particle radius, phi is the local electic potential, and k controls the screening effect. If k=0, no screening and the equation becomes 1d laplace equation. Solve for the local electric potential and compare your results for various k values

<u>Answer</u>

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\phi}{dr}\right) = k^2\phi$$

∇ · denotes divergence

The solution ϕ of this second-order differential equation must satisfy the following first-order differential equation:

$$r^2 \frac{d\phi}{dr} = \frac{k^2}{2} \phi^2$$

This differential equation can be rewritten as

$$\frac{d\phi}{dr} = \frac{k^2}{2r^2} \ \phi^2$$

Separation of variables

$$\int \frac{1}{\phi^2} d\phi = \frac{k^2}{2} \int \frac{1}{r^2} dr$$

$$\frac{1}{\phi} = \frac{k^2}{2} \frac{1}{r} + C_1 = \frac{k^2 + 2rC_1}{2r}$$

$$\phi(r) = \frac{2r}{k^2 + 2rC_1}$$

To compare different k values just plug this equation into matlab and evaluate and plot

Useful link:

http://hyperphysics.phy-astr.gsu.edu/hbase/electric/laplace.html

http://en.wikipedia.org/wiki/Electric potential

http://mathworld.wolfram.com/SphericalCoordinates.html

http://teacher.pas.rochester.edu/PHY217/LectureNotes/Chapter3/LectureNotesChapter3.html

 $http://www.phengkimving.com/calc_of_one_real_var/16_diffl_eq/16_01_first_ord_eq/16_01_02_var_sep_eq.htm$

Question 4

Find the general solution of

$$y'' + xy' + 2y = 0$$
 near $x_0 = 0$

<u>Answer</u>

Sounds like we can use a sum of infinite series method, because you said "near", which we did in class

First we note that the equation does not have constant coefficients. Next we see that x = 0 is an ordinary point of the equation. Existence and uniqueness theory guarantees that this IVP has a unique solution.

There is a solution of the form

$$y = \sum_{n=0}^{\infty} c_n x^n$$

$$y' = \sum_{n=1}^{\infty} nc_n x^{n-1}$$

$$y'' = \sum_{n=2}^{\infty} n(n-1)c_n x^{n-2} = \sum_{n=0}^{\infty} (n+2)(n+1)c_{n+2} x^n$$

Substituting in the differential equation we get

$$y'' + xy' + 2y = 0 = \sum_{n=0}^{\infty} (n+2)(n+1)c_{n+2}x^n + x\sum_{n=1}^{\infty} nc_nx^{n-1} + 2\sum_{n=0}^{\infty} c_nx^n = 0$$

$$\sum_{n=0}^{\infty} (n+2)(n+1)c_{n+2}x^n + \sum_{n=1}^{\infty} nc_nx^n + \sum_{n=0}^{\infty} 2c_nx^n = 0$$

Note: $\sum_{n=1}^{\infty} nc_n x^n = \sum_{n=0}^{\infty} nc_n x^n$

therefore

$$\sum_{n=0}^{\infty} [(n+2)(n+1)c_{n+2} + (n+2)c_n]x^n = 0$$

This equation is true if the coefficient of x'' is 0:

$$(n+2)(n+1)c_{n+2} + (n+2)c_n = 0$$

$$eq1 c_{n+2} = \frac{-(n+2)}{(n+1)(n+2)}c_n n = 0,1,2,3....$$

We solve this recursion relation by putting n=0,1,2,3 successively in equation 1

Put n=0:

$$c_2 = \frac{-2}{1*2}c_0$$

Put n=1:

$$c_3 = \frac{-3}{2*3}c_1$$

Put n=2:

$$c_4 = \frac{-4}{3*4}c_2 = \frac{8}{1*2*3*4}c_0 = \frac{8}{4!}c_0$$

Put n=3:

$$c_5 = \frac{-5}{4 * 5} c_3 = \frac{15}{2 * 3 * 4 * 5} c_1 = \frac{15}{5!} c_1$$

The solution is

$$y = c_0 + c_1 x + c_2 x^2 + c_3 x^3 + c_4 x^4 + c_5 x^5 + \dots +$$

$$= c_0 \left(1 - \frac{2}{2!} x^2 + \frac{8}{4!} x^4 + \dots + \right) + c_1 \left(x - \frac{3}{3!} x^3 + \frac{15}{5!} x^5 + \dots + \right)$$

Helpful link

P1199 stewart calculus

Also class notes on 9/21/2011 pg4-5

http://calculusplus.cuny.edu/ODE Series%20Solutions1.html

Question 5

Find the general solution of the ODE

$$y'' - \frac{1+x}{x}y' + \frac{1}{x}y = 0$$

<u>Answer</u>

X=0 is a regular singular point

Let

$$y = \sum_{n=0}^{\infty} a_n x^n$$

$$y' = \sum_{n=0}^{\infty} a_n n x^{n-1}$$

$$y'' = \sum_{n=0}^{\infty} a_n n (n-1) x^{n-2}$$

Substituting to ODE eq we obtain

$$\sum_{n=0}^{\infty} \left[a_n n(n-1) x^{n-2} - \frac{1+x}{x} a_n n x^{n-1} + a_n x^{n-1} \right] = 0$$

$$\sum_{n=0}^{\infty} \left[a_n n(n-1) x^{n-2} - \frac{1}{x} a_n n x^{n-1} - a_n n x^{n-1} + a_n x^{n-1} \right] = 0$$

$$\sum_{n=0}^{\infty} \left[a_n n(n-2) x^{n-2} + (1-n) a_n x^{n-1} \right] = 0$$

For our a's we get:

$$a_1 = a_0$$

$$a_3 = \frac{1}{3} a_2$$

$$a_4 = \frac{1}{4*3} a_2$$

$$a_5 = \frac{1}{5 * 4 * 3} a_2$$

Therefore

$$y(x) = a_0 + a_0 x + a_2 \left[x^2 + \frac{1}{3} x^3 + \frac{1}{4 \cdot 3} x^4 + \frac{1}{5 \cdot 4 \cdot 3} x^5 + \frac{1}{6 \cdot 5 \cdot 4 \cdot 3} x^6 + \dots + \right]$$

Question 6

Show that the differential equation

$$y'' + \sqrt{x}y = 0$$
 for $x \ge 0$

Has an irregular singular point at x=0. Show that the simple transformation $x=t^2$ can transform the equation to

$$t\ddot{y} - \dot{y} + 4t^4y = 0$$

With a regular singular point at t=0

<u>Answer</u>

Transform the equation

$$y'' + \sqrt{x} \ y = 0 \quad for \quad x \ge 0$$
$$P(x) = 0$$
$$Q(x) = \sqrt{x}$$

Because

$$\sqrt{0}$$
 is undefined

Because of this the function is not analytic at the point x=0

This means that the ode has an irregular singular point at x=0

Now we need to transform the equation by

$$x = t^{2}$$

$$dx = 2t dt$$

$$y'' = \frac{d\left[\frac{dy}{dx}\right]}{dx} = \frac{d\left[\frac{dy}{2t dt}\right]}{2t dt} = \frac{1}{2t} * \frac{d\left[(2t)^{-1} \frac{dy}{dt}\right]}{2t dt} = (2t)^{-2} \ddot{y} - (2t)^{-3} * 2 * \dot{y}$$

In conclusion

$$y'' + \sqrt{x}y = 0$$

$$(2t)^{-2} \ \ddot{y} - (2t)^{-3} * 2 * \dot{y} + ty = 0$$

$$t \ddot{y} - \dot{y} + 4t^{4}y = 0$$

$$\ddot{y} - \frac{1}{t}\dot{y} + 4t^{3}y = 0$$

As said in the problem statement the transformed equation has a regular singular point at t=0

Useful link:

Redo this problem after looking at pg405 of advanced engineering math 2nd edition

http://www.physicsforums.com/archive/index.php/t-321945.html

http://en.wikipedia.org/wiki/Analytic_function

http://mathworld.wolfram.com/MaclaurinSeries.html

http://www.mathcs.citadel.edu/~chenm/335.dir/03fal.dir/lect5 2.pdf (recurence relations)

Chapter 7.7 in haberman

Pg 6 in series solution handout