PHAS0012 Open Book Exam

Computing for Mathematical Physics

Tuesday 24th March 2020 12:00 - 2:30 pm

150 minutes

This is an open book exam and you may refer to any of your previous work, notes or course material to help you complete the exam.

Note that working with, receiving help from, or offering help to, another student on this exam constitutes, and will be treated as, academic misconduct. We will be using several methods to check submissions for potential plagiarism and misconduct.

You should use *Mathematica* version 12 to complete this exam.

Be sure to have a text cell at the top of your *Mathematica* notebook containing your student number. DO NOT put your name in your answer notebook.

Take care to save your work at frequent intervals - <u>work lost because it was not saved cannot be marked.</u>

At the end of the examination, you will need to upload your notebook to Moodle. Time after the end of the exam will be allowed for this.

You should delete all output from the notebook prior to submitting it (from the menu bar: `Cell->Delete All Output`**).**

Prior to marking, the notebook will be run under a fresh kernel, so you should ensure your notebook works properly when evaluated under a fresh kernel (from the menu bar: `Evaluation->Quit Kernel->Local` **followed by** `Evaluation->Evaluate Notebook`**).**

[Dr J. Bhamrah]

Answer ALL SIX questions in Section A and ALL THREE questions from Section B.

The numbers in square brackets show the provisional allocation of maximum marks per question or part of question.

[Part marks]

Section A

(Answer ALL SIX questions from this section)

1. Using `Around`, or otherwise, plot a graph of the points $(0.0, 0.19 \pm .01)$, $(1.0, 0.76 \pm 0.1)$, $(2.0, 5.4 \pm 0.5)$, $(3.0, 9.0 \pm 1)$, $(4.0, 25. \pm 2)$ and $(5.0, 76 \pm 3)$, and superpose a plot of $\sinh(x)$ for $0 < x < 5$. Ensure that the whole graph, including all the error bars, is visible. **[7]**

2. Find the values of a, b and c which provide the best fit of $a + bx + cx^2$ to $\cos(x)$ over the range $0 < x < \pi/2$ by integrating $\left(a + bx + cx^2 - \cos(x)\right)^2$ over the required range and using `FindMinimum` to find the optimal values of a, b and c. Also give the result of expanding $\cos(x)$ about $x = 0$ up to the term in x^2 using `Series`. **[7]**

3. Use `ElementData[n,"AbsoluteMeltingPoint"]` to construct a list of ordered pairs {element number, melting point} for all the elements from 1 to 92. Plot the associated points, labelling the axes appropriately. You should see no consistent pattern, as the bonding between the atoms varies in character from column to column in the Periodic Table.

   By using `ElementData[n,"Series"]` generate another table of the form {series, element number, melting point}, select the elements from the series `"AlkaliMetal"`, and generate a line plot of their melting points as a function of atomic number. You may find `Select`, `Map` and `Rest` useful. **[7]**

[Part marks]

4. Nonlinear differential equations are usually not analytically soluble, but there are exceptions such as the separable equation $\mathrm{d}x/\mathrm{d}t = \sin(x)$. Solve this equation analytically for the initial conditions $x(0) = 0$, $x(0) = 1/2$ and $x(0) = 1$, and plot all three solutions on the same graph, with appropriate legends. **[6]**

5. Create three vectors $\overrightarrow{a}_1 = (a11, a12, a13)$ and similarly for $\overrightarrow{a}_2$ and $\overrightarrow{a}_3$. From these create $\overrightarrow{b}_1 = \overrightarrow{a}_2 \times \overrightarrow{a}_3/(\overrightarrow{a}_1.\overrightarrow{a}_2 \times \overrightarrow{a}_3)$. Also form $\overrightarrow{b}_2$ and $\overrightarrow{b}_3$ by cyclically permuting the indices. Confirm that $\overrightarrow{a}_1.\overrightarrow{b}_1 = 1$ and $\overrightarrow{a}_1.\overrightarrow{b}_2 = 0$, $\overrightarrow{a}_1.\overrightarrow{b}_3 = 0$: you may need to use `Simplify`. Confirm that if this is generalised to four dimensions by appending 0 to all the $\overrightarrow{a}_i$ and $\overrightarrow{b}_i$, and defining $\overrightarrow{b}_4 = (0, 0, 0, 1)$, the scalar product of $\overrightarrow{a}_1$ with all four $\overrightarrow{b}_i$ has the same behaviour. **[6]**

6. Write a function which will accept one argument and which has the following properties:

   (a) it will return "`Error`" if the argument is not an integer between 1000 and 9999 inclusive

   (b) it will return "`Correct`" if the last digit is equal to the sum of the first three digits modulo 10;

   (c) it will return "`CheckSum Failed`" otherwise.

   Check that your function works correctly (this will require at least 3 checks). You may find the `IntegerDigits`, `Most` and `Mod` functions useful. **[7]**

Section B

(Answer ALL THREE questions from this section.) **[Part marks]**

7. Gerald North set up a model for average sea-level temperature. With some simplifications the evolution over time of the edge of an ice cap, x_s, may be modelled by

$$\frac{dx_s}{dt} = (1 - x_s)\left(Q - 335 + 3\left(\frac{x_s - 0.89}{0.09}\right)^2\right) \qquad (7.1)$$

where Q is the incoming solar energy in $\mathrm{W\,m^{-2}}$ and the time t is measured in centuries. Note that $x_s = 1$ corresponds to the icecap vanishing and $x_s < 1$ corresponding to a growing icecap.

(a) Solve the ordinary differential equation (7.1) numerically for $Q = 333$ and $0 < t < 1$ with the initial condition $x_s(0) = 0$, and plot a graph of your result.

Repeat the solution and the plot for $x_s(0) = 1$. **[4]**

(b) Consider the steady state equation, obtained by setting the time derivative to zero.

i. Find the numerical solution of the equation for the case $Q = 333$. **[2]**

ii. Find the percentage difference between the smallest steady-state result and the first solution obtained in part (a) at $t = 1$. **[2]**

(c) The intermediate solution in part (b) giving $x_s = 0.963485$ corresponds to an unstable state of the system, whereas the other two solutions are stable.

i. By numerically solving the differential equation for $0 < t < 10$ for initial values of x_s just greater and just less than this intermediate value, confirm that the system evolves to the other, stable, states. **[2]**

THIS QUESTION CONTINUES ON THE NEXT PAGE

ii. One way of capturing the unstable state is to propagate backwards in time: find the numerical solution for x_s for t running from 0 to -10 with an initial value of $x_s = 0.9$. Find the percentage difference between the solution at $t = -10$ and your intermediate solution in part (b). **[2]**

(d) We can investigate the effect of climate change by altering Q to represent the effect of emissions on the balance between incoming solar energy and outgoing energy.

Modify your differential equation in part (a) to allow Q to be a function of time,

$$Q(t) = \begin{cases} 333 & \text{if } t < 5 \\ 336 & \text{if } t \geq 5 \end{cases}$$

and solve for $0 < t < 10$ with $x_s = 0.8$ at $t = 0$.

Comment on your result. **[4]**

(e) If we take action on climate change, we may be able to alleviate some of the damage we are doing.

Modify your calculations in part (d) to investigate what happens if the same increase in Q again happens instantaneously at $t = 5$, but Q then reverts to 333 after a further 0.5, 1 or 2 centuries.

Plot all three results on one graph, with appropriate legends, and comment on your result. **[4]**

8. Newton's method of finding a root of a function works by repeatedly using the gradient to move towards zero.

   (a) Write a function which will accept two arguments: the name of a function, f, and an estimate of the zero, x_i. Your function should return $x_o = x_i - f(x_i)/f'(x_i)$, where the prime denotes differentiation. Check your function by defining another function which will return $x - 1$ and confirm that your first function immediately returns the value 1 for the position of the root of this second function when given 1 or 0 as the starting value. **[4]**

   (b) Use `FindRoot` to locate the zero of `ExpIntegralEi`, starting from the point $x = 1$ and store the value as a variable for later use. **[2]**

   (c) Use `Nest` and your first function, with a starting value of 0.5, to estimate the position of the zero of `ExpIntegralEi` by `Nest`ing your function three times. What is the numerical difference between this result and the result from (b)? **[3]**

   (d) Use `FixedPoint` and your first function, with a starting value of 0.5, to find the position of the zero of `ExpIntegralEi` to machine precision. Confirm that your result agrees with that from (b). **[3]**

   (e) Produce a diagram illustrating the convergence of three iterations of Newton's method to the root of $\sin(x)$ at $x = 0$, starting from $x = 1$. Your diagram should show the sin function over the range $-1 < x < 1$, and straight-line segments for each iteration joining $(x_i, \sin(x_i))$, $(x_o, 0)$ and $(x_o, \sin(x_o))$. You may find `Graphics` and `Line` useful. **[6]**

   (f) Repeat part (e) for the tan function, using the same plotting range and starting value. **[2]**

9. Laguerre polynomials $L_n(x)$ occur in quantum mechanics in the theory of the hydrogen atom. They are solutions of the differential equation

$$x\frac{d^2f}{dx^2} + (1-x)\frac{df}{dx} + nf = 0 \tag{9.1}$$

for integer n, and satisfy the recurrence relation

$$(n+1)L_{n+1}(x) = (2n+1-x)L_n(x) - nL_{n-1}(x)$$

(a) Show by substitution that the two lowest Laguerre polynomials, $L_0(x) = 1$ and $L_1(x) = 1 - x$, are solutions of equation 9.1 for the appropriate values of n. **[3]**

(b) Use the recurrence relation to generate the polynomials L_2 through to L_6, starting from L_0 and L_1. Print the results in simplified form. **[4]**

(c) The Laguerre polynomials have the property

$$\int_0^x L_m(y)L_n(x-y)dy = L_{m+n}(x) - L_{m+n+1}(x).$$

Confirm this for the special case $m = 2$, $n = 3$. **[2]**

(d) The Laguerre polynomials are orthonormal with a weighting function $\exp(-x)$, that is

$$\int_0^\infty L_m(x)L_n(x)\exp(-x)dx = \delta_{nm}.$$

Verify that in this sense L_6 is normalised (the integral with $m = n = 6$ equals 1) and L_5 and L_6 are orthogonal (the integral with $m = 5$ and $n = 6$ equals 0) **[2]**

THIS QUESTION CONTINUES ON THE NEXT PAGE

(e) The Laguerre polynomials may be used to expand other functions, thus

$$f(x) = \sum_{n=0}^{\infty} b_n L_n(x),$$

with

$$b_n = \int_0^{\infty} f(x) L_n(x) \exp(-x) \mathrm{d}x.$$

Generate the coefficients b_0 to b_6 in the expansion of $\cos(x)$, and plot the expansion and $\cos(x)$ over the range $0 < x < \pi$ on the same graph. **[4]**

(f) One measure of the goodness-of-fit of a function $g(x)$ to a target function $f(x)$ is

$$\int (f(x) - g(x))^2 \mathrm{d}x.$$

Evaluate this quantity for the Laguerre polynomial expansion of $\cos(x)$, integrating over the range $0 < x < \pi$, taking $1, 2, \ldots, 7$ terms in the expansion.

Plot the results for $1, 2, \ldots, 7$ terms in the expansion as a line plot of the goodness-of-fit versus the number of terms in the expansion. **[5]**