PHAS1449
Computing for Mathematical Physics

Exam

Tuesday 20th March 2018

2:30pm - 5:00pm

During this examination, the only program which you may run is *Mathematica*, and the only files you may use are your own file for answers to the questions and *Mathematica*'s own help files. The use of any other program or file will be taken as a breach of examination regulations. You should use *Mathematica* version 11.1 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.

If you need scrap paper to help to organise your thoughts, this will be provided.

Take care to save your work at frequent intervals.

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`**).**

In addition to uploading your notebook to Moodle, please also email a copy to dr.j.bhamrah@gmail.com

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 Jasvir Bhamrah]

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

The numbers in square brackets in the right-hand margin indicate a provisional allocation of maximum possible marks for different parts of each question.

Section A

(Answer ALL SIX questions from this section)

1. Plot a single graph showing the two functions $1 - e^{-x}$ and $x - \frac{x^2}{2} + \frac{x^3}{6} - \frac{x^4}{24}$ in different colours over the range $0 \leq x \leq 5$. Ensure that the graph shows the whole range of both functions and includes a legend to distinguish the two functions. **[6]**

2. Use `Solve` to find the solutions to the equation $ax^3 + bx^2 + cx + d = 0$. Denoting these solutions by s_i, confirm that $ax^3 + bx^2 + cx + d = a(x - s_1)(x - s_2)(x - s_3)$. Use `Replace` to generate a list of solutions to the first equation for the values $a = 5, b = 4, c = 3, d = 0$. **[7]**

3. The expression `PolyhedronData["Archimedean"]` will return a list of names of the Archimedean solids. `PolyhedronData["name","VertexCount"]` will return the number of vertices on the solid called `name` and `PolyhedronData["name"]` will return an image of that solid.

   (a) Generate a list of all the Archimedean solids in the form {{`number of vertices,name`},....} sorted in increasing order of number of vertices. **[4]**

   (b) Show the images of the four solids which each have 60 vertices. If possible, do so without specifying the polyhedra by name. **[3]**

4. Analytically solve the third-order nonlinear differential equation

$$2\left(\frac{\mathrm{d}y}{\mathrm{d}x}\right)\left(\frac{\mathrm{d}^3y}{\mathrm{d}x^3}\right) - 3\left(\frac{\mathrm{d}^2y}{\mathrm{d}x^2}\right)^2 = 0$$

   (a) with boundary conditions $y = 1, \mathrm{d}y/\mathrm{d}x = -1$ and $\mathrm{d}^2y/\mathrm{d}x^2 = 2$ at $x = 1$. **[3]**

   (b) Find the value of your function $y(x)$ from part (a) as x approaches zero. **[1]**

   (c) By substitution into the differential equation, confirm that the expression $y = (ax + b)/(cx + d)$ is a solution, independent of any boundary conditions. You may find a pure function or the `Function`[] expression useful, and you may need to `Simplify` your result. **[3]**

5. If A is a matrix such that $\mathrm{A}^2 = 0$, A is called nilpotent; if $\mathrm{A}^2 = \mathrm{I}$ where I is a unit matrix, A is called unipotent; if $\mathrm{A}^2 = \mathrm{A}$, A is called idempotent. Use *Mathematica* to determine the natures of the matrices **[6]**

$$B = \begin{pmatrix} -5 & -8 & 0 \\ 3 & 5 & 0 \\ 1 & 2 & -1 \end{pmatrix}, \qquad C = \begin{pmatrix} 5 & -3 & 2 \\ 15 & -9 & 6 \\ 10 & -6 & 4 \end{pmatrix}, \qquad D = \begin{pmatrix} 2 & 3 & -4 \\ 0 & 1 & 0 \\ 1/2 & 3/2 & -1 \end{pmatrix}$$

6. Write a function which will accept any number of arguments, with the following properties:

   (a) If there is one argument which is an integer, it will return that integer with its sign changed;

   (b) In all other cases, including no arguments, one non-integer argument, or more than one argument, it will return "`Error`". **[3]**

   Check that your function works correctly (this will require at least four checks). **[4]**

Section B

(Answer ALL THREE questions from this Section)

7. Otto Rössler constructed the following set of coupled differential equations which illustrates some chaotic features:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -(y+z),$$
$$\frac{\mathrm{d}y}{\mathrm{d}t} = x + ay,$$
$$\frac{\mathrm{d}z}{\mathrm{d}t} = b + xz - cz$$

This question investigates some of these features.

(a) Solve this set of differential equations *numerically*, over the range $0 \leq t \leq 200$, with the initial conditions (at $t = 0$) $x = y = z = 1$ and the parameters $a = 0.2$, $b = 0.2$, $c = 2.3$. Plot your solution for x over the same range of t . **[7]**

(b) A good way of illustrating the regularity of the behaviour is through a three-dimensional parametric plot showing x, y and z with t as the parameter. Display your results from (a) in this form, but just show the range $100 \leq t \leq 200$ to miss out the early-time behaviour. You should see a single closed loop – a period-one cycle. **[4]**

(c) Repeat parts (a) and (b), including both plots and ensuring that the whole ranges of x and y are displayed, with the same initial conditions but with the parameters $a = 0.2$, $b = 0.2$, $c = 3.3$. Your plot for x should be shown for the same time interval as that for part (a) and your parametric plot of x and y for the same interval as that for part (b). **[3]**

(d) Investigate the effect of initial conditions by repeating part (c) with the same parameters $a = 0.2$, $b = 0.2$, $c = 3.3$, but with new initial conditions (at $t = 0$) $x = y = z = 1.01$. **[1]**

(e) Finally, investigate a chaotic region, with the parameters $a = 0.2$, $b = 0.2$, $c = 6.6$. Compare the results of the two sets of initial conditions (at $t = 0$) where $x = y = z = 1.01$ and $x = y = z = 1.0$, and comment on what you see. **[5]**

8. The constant $6/\pi^2$ occurs in several places in the theory of prime numbers. This question will numerically investigate two of these occasions.

   (a) Write a function, `coprime`, which will take two integer arguments and return `True` or `False` depending on whether or not the integers have a common factor (other than 1). Pairs of integers which have no common factors are called *coprime*.
   Base your function on `FactorInteger`, which returns a list of factors in the form {...{`integerfactor, power`},...}. Compare your function with the *Mathematica* function, `CoprimeQ`, on the pairs (5,7) and (6,8). **[6]**

   (b) The probability that two randomly chosen integers are coprime is $6/\pi^2$. Use `RandomInteger` to generate a list of 10 pairs of integers in the range 1 to 100,000, and find the number of coprime pairs using your function, `coprime` from part (a). **[4]**

   (c) Repeat (b) with 10,000 pairs of integers (take care not to display or print the lists you generate) and hence estimate the probability that a pair is coprime. Compare the result with the numerical value of $6/\pi^2$. **[2]**

   (d) Write a function `squarefree` of one integer argument which returns `True` or `False` depending on whether the argument has any factors which are perfect squares: an integer with no square factors is referred to as *squarefree*. Your function must not use the *Mathematica* function `SquareFreeQ`, but you should compare your function with `SquareFreeQ` for the integers 8, 10 and 12. You may find `FactorInteger` useful. **[5]**

   (e) The probability that a randomly chosen integer is squarefree is $6/\pi^2$. Calculate how many of 10,000 randomly selected integers between 1 and 100,000 are squarefree, and compare the resulting probability estimate with $6/\pi^2$. **[3]**

9. The Hermite polynomials $H_n(x)$ are defined by the recurrence relation

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x)$$

with $H_0(x) = 1$ and $H_1(x) = 2x$.

(a) Set up a recursive function definition of $H_n(x)$ in *Mathematica* and use it to show that $H_3(x) = 8x^3 - 12x$, and find an expression for $H_{10}(x)$. **[5]**

(b) The Hermite polynomials satisfy the differential equation

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}H_n(x) - 2x\frac{\mathrm{d}}{\mathrm{d}x}H_n(x) + 2nH_n(x) = 0.$$

Confirm that your form of $H_{10}(x)$ satisfies this equation. **[3]**

(c) Expansions in Hermite polynomials can be used to approximate other functions. A function of x may be approximated as

$$f(x) = \sum_{n=0}^{n_{\max}} a_n H_n(x),$$

where the coefficients in the expansion are given by

$$a_n = \frac{1}{n!2^n\sqrt{\pi}} \int_{-\infty}^{\infty} f(x)H_n(x)\exp\left(-x^2\right)\, \mathrm{d}x.$$

Using `Table`, evaluate and store in memory the coefficients a_n for $n_{\max} = 12$ for the function $f(x) = \sin(x)$. You may use the built-in function `HermiteH[n,x]` for this part of the question and for the remainder of the question.

Using these stored coefficients, create a suitable plot to compare the approximations to this function for $n_{\max} = 6$ and $n_{\max} = 12$. **[6]**

(d) A quantitative measure of the accuracy of the expansion for a given $n_{\max}$ over the range $a \leq x \leq b$ is given by:

$$\int_a^b \left(\sin(x) - \sum_{n=0}^{n_{\max}} a_n H_n(x)\right)^2 \mathrm{d}x.$$

Evaluate this expression numerically over the range $-\pi \leq x \leq \pi$ for $n_{\max} = 5$ and 6. By considering $H_5(x)$, $H_5(-x)$, $H_6(x)$, $H_6(-x)$, $\sin(x)$, and $\sin(-x)$, comment on why there is no difference in the accuracy of the expansion for $n_{\max} = 5$ and $n_{\max} = 6$. **[6]**

END OF PAPER