PH2130 Mathematical Methods
Lab 3

This script should keep you busy for the next two weeks. You should aim to create a tidy and well-structured *Mathematica* Notebook. Do include plentiful annotations to show that you know what you are doing, where you have experimented, and what you have learned. You should then find your notebooks useful to you later on when you are working on other problems.

A. Partial differentiation

In the first part of this exercise you will gain practice in using *Mathematica* for the evaluation of partial derivatives. Most of the exercises will be taken from problem sheets you worked on last year. You should recall how you evaluated the derivatives and the tedious calculation sometimes required. Here you will see how easy it is to get *Mathematica* to do the 'donkey work' for you. But do appreciate that *Mathematica* can be no substitute for knowing *how* to do the calculation.

1. Given that $f(x,y,x) = ye^z + 2x\cos z - x^2yz$, find $\frac{\partial f}{\partial x}, \frac{\partial^2 f}{\partial x\partial y}, \frac{\partial^3 f}{\partial x\partial y\partial z}, \frac{\partial^2 f}{\partial x^2}, \frac{\partial^3 f}{\partial y\partial z^2}$.

You should investigate some of the features of Mathematica's D[..] function, using the Help facility, to find an easy way of performing multiple differentiation.

2. For (i) $f(x,y) = xy - \ln xy$ and (ii) $f(x,y) = \sin xy + y$, find f_x and f_y and f_{xx}.

Recall that f_x is a compact notation indicating partial differentiation with respect to x.

3. If $f(x,y) = ye^{x/y}$, find the slopes f_x and f_y when $x = 0$, $y = 0$.

Here you should be aware of Mathematica's substitution syntax … /. …

4. Find the slopes in the *x* and *y*- directions (i.e. f_x and f_y) of each of the following (*k* is a constant):

$x^2+y^3,\ kx^3y^2,\ x^2\sin y,\ k\cos xy,\ \left(x^2+1\right)\ln y,\ x\ln xy,\ xye^{-x^2},$

$e^{x^2y},\ \left(x^2-k^2y^2e^{xy}\right),\ \ln(x+ky),\ y\ln(kx-y),\ \frac{y}{x}\ln(kx-y), \frac{\sinh\left(x^2+y^2\right)}{x^2}.$

Remember that Mathematica uses the syntax Log[…] to denote the natural logarithm.

5. For the above expressions, evaluate $\frac{\partial^2 f}{\partial x\partial y}, \frac{\partial^3 f}{\partial x\partial y\partial z}, \frac{\partial^2 f}{\partial x^2}, \frac{\partial^3 f}{\partial y\partial z^2}$.

You will find it convenient to use the Windows 'cut and paste' facilities to do this speedily and painlessly.

6. Show that $f(r,\theta) = r^3\sin 4\theta$ satisfies the partial differential equation

$$f_{\theta\theta} + 3r^2 f_{rr} - rf_r + f = 0.$$

7. Show that $V = r^n \cos n\theta$ and $V = r^{-n-1} \cos n\theta$ both satisfy Laplace's equation in polar coordinates in two dimensions:

$$V_{rr} + \frac{1}{r}V_r + \frac{1}{r^2}V_{\theta\theta} = 0 .$$

8. If $u(x, y) = \ln\sqrt{x^2 + y^2}$, show that $u(x, y)$ satisfies Laplace's equation in Cartesian coordinates in two dimensions: $u_{xx} + u_{yy} = 0$.

9. Show that $\Psi = A\sin(\omega t + kx)$ and $\Psi = (kx + \omega t)^2 e^{-(kx+\omega t)}$ each satisfies the wave equation

$$\frac{\partial^2 \Psi}{\partial t^2} = \left(\frac{\omega}{k}\right)^2 \frac{\partial^2 \Psi}{\partial x^2} .$$

You should be able to identify the speed of propagation of the waves; if not, have a look at your lecture notes.

10. Show that $U = (A\sin kx + B\cos kx)e^{-k^2 Dt}$ satisfies the diffusion equation

$$\frac{\partial^2 U}{\partial x^2} = \frac{1}{D}\frac{\partial U}{\partial t} .$$

Plot this for suitably chosen *A* and *B*.

11. Show that $\Psi(x,t) = Ae^{i(px-Et)/\hbar}$ satisfies Schrödinger's equation for a free particle

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} = i\hbar\frac{\partial \Psi}{\partial t}$$

if $E = p^2 / 2m$. What does *p* represent in the expression for Ψ?

12. If $u = \frac{x}{y} + \frac{y}{z}$, where $x = 2t,\ y = 1/t,\ z = t^2$, find $\partial u / \partial t$ in terms of *t*.
This is a nice example of the tidy use of Mathematica.

13. If $x = e^u \cos v$ and $y = e^u \sin v$, show that $\partial x / \partial v = -y$ and $\partial y / \partial v = x$. Find $\left(\frac{\partial x}{\partial u}\right)\left(\frac{\partial u}{\partial x}\right)$.

14. Show that $\partial^2 / \partial x\partial y$ yields the same result as $\partial^2 / \partial y\partial x$ when operating on functions of *x* and *y*. You should invent some on functions of *x* and *y* to try this out on. *The independence of the order of differentiation is an important result which you will make use of in Thermodynamics.*

B. Defining your own functions

In the second part of the exercise you will learn how to define your own functions in Mathematica. This will then be extended, in the next section, to the definition of the Laplacian operator and the investigatin of some solutions of Laplace's equations.

The Mathematica syntax for defining a function is demonstrated in this simple example

```
square[x_] := x^2
```

which will square whatever argument you give it. Thus typing `square[2]` will return 4, while `square[a+b]` will return $a^2 + 2ab + b^2$.

In this example `square` is the name you have chosen for your function. Remember it is preferable *not* to start the function name with a capital letter to avoid any potential conflict with *Mathematica*'s built-in functions you might not be aware of.

As expected, the argument of the function is contained in square brackets. However note that the argument is written with an underscore: `x_` . This indicates that the *x* here is a *dummy* variable; the function will operate on any argument you give it, not just on *x*. On the right hand side, however, in the function definition, you just use *x*.

Finally, note that the equality symbol used here is the Pascal/Algol assignment ‘`:=`’. This tells Mathematica to evaluate the right hand side each time ‘on demand’ rather than ‘once and for all’. Otherwise the same answer would be returned every time the function was called, regardless of the new argument. (*Don't worry if you don't understand this; just be sure to use* `:=` *when defining a function*)

Try a few examples of defining your own functions.

A function can take more than one argument; the syntax is a natural extension:

```
dist[x_, y_] := Sqrt[x^2 + y^2]
```

What could this be used for?

Define your own function to give the roots of a quadratic equation from its three coefficients. Some forethought and planning will pay dividends here.

C. The laplacian operator

You should recall from the lectures that the laplacian operator ∇^2 is given, in rectangular cartesian coordinates, by

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} .$$

Laplace's equation for Ψ is written simply as $\nabla^2\Psi = 0$.

You can define your own laplacian operator in *Mathematica* by:

```
laplacianxyz[f_] := D[f,{x,2}] + D[f,{y,2}] + D[f,{z,2}]
```

The name `laplacianxyz` has been chosen to indicate that it expects the cartesian coordinates *x*, *y*, and *z* to operate on. Be sure you are happy with this definition.

Using your own defined laplacian operator, check whether the following functions obey Laplace's equation:

1. $\Psi(x, y) = 2xy$, 2. $\Psi(x, y) = x^3 - 3xy^2$, 3. $\Psi(x, y) = x^4 - 6x^2y^2$, 4. $\Psi(x, y) = e^x \sin(y)$, 5. $\Psi(x, y) = \sin x \sinh y$, 6. $\Psi(x, y) = \arctan(y/x)$, 7. $\Psi(x, y, z) = 1/\sqrt{x^2 + y^2 + z^2}$.
In places you will find it useful/necessary to use Mathematica's 'Simplify' commands.

Verify that $\Psi(x, y) = a \ln(x^2 + y^2) + b$ satisfies Laplace's equation, and determine *a* and *b* so that Ψ satisfies the boundary conditions $\Psi = 0$ on the circle $x^2 + y^2 = 1$, and $\Psi = 5$ on the circle $x^2 + y^2 = 9$. *Think carefully before doing the second part; you don't want to end up with something messy. And be sure to explain in your Mathematica notebook what you are doing.*

D. The d'alembertian operator

The wave equation treats space and time on an equal footing (almost). Using the laplacian operator allows the wave equation

$$\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\frac{\partial^2\Psi}{\partial z^2}-\frac{1}{v^2}\frac{\partial^2\Psi}{\partial t^2}=0$$

to be written in the much more compact form

$$\nabla^2\Psi-\frac{1}{v^2}\frac{\partial^2\Psi}{\partial t^2}=0\,.$$

But this can be taken one step further, by combining the space and time differentiation into a single symbol. In this way the d'alembertian operator is defined as

$$\Box^2 = \nabla^2-\frac{1}{v^2}\frac{\partial^2}{\partial t^2}\,.$$

And then the wave equation takes on the remarkably compact form

$$\Box^2\Psi = 0.$$

Define your own d'alembertian operator in *Mathematica*. Using this operator, verify that the following functions obey the wave equation for a suitable choice of v:

1. $\Psi(x,t)=x^2+4t^2$, 2. $\Psi(x,t)=x^3+3xt^2$, 3. $\Psi(x,t)=\sin 2vt\,\sin 2x$,
4. $\Psi(x,t)=\cos 4t\,\sin x$, 5. $\Psi(x,t)=\cos vt\,\sin x$, 6. $\Psi(x,t)=\sin\omega vt\,\sin\omega x$.

E. Diffusion

You must think how to answer the next questions. Explain clearly what you are doing.

Verify that the following functions are solutions of the diffusion equation for a suitable value of D:

1. $\Psi(x,t)=e^{-t}\cos x$, 2. $\Psi(x,t)=e^{-2t}\cos x$, 3. $\Psi(x,t)=e^{-t}\sin 3x$,
4. $\Psi(x,t)=e^{-4t}\cos kx$, 5. $\Psi(x,t)=e^{-16t}\cos 2x$, 6. $\Psi(x,t)=e^{-k^2Dt}\sin kx$.