Computational Mathematics/Information Technology

Worksheet 8

Numerical Integration.

We can programme Excel to do numerical integrations. However we will use Derive again, as it has a feature that will be useful in a later example. We will use four features of Derive that we have not used before: defining functions, summation, the IF statement and high precision calculations.

Problem 1

This is just to check things are working, we will sum n^2 from 1 to 5 and check we get the same answer as the summation formula

$$\sum_{n=1}^{N} n^2 = \frac{1}{6}N(N+1)(2N+1)$$

First we define a function $f(x) = x^2$ in derive:

- Click on Declare \rightarrow Function definition...
- A pop-up menu appears. On the top line type f(x) and on the second x^2 . Click OK.
- Now enter f(i) in the editing box at the bottom and hit Return.
- With f(i) still highlighted click on Calculus → Sum... and in the pop-up menu you want variable to be i, the sum to be definite and the limits 1 and 5. Click OK.
- Go Simplify \rightarrow Basic, or click on the = button at the top, and you should get a number.

The sum is

Is this the same as the answer from the formula?

Problem 2 Now we will attempts to estimate

$$\int_0^1 \frac{1}{1+x^2} \, dx$$

- Define the function g(x) to be 1/(1 + x²) as above, or type g(x) :=1/(1+x²) in the box at the bottom (the colon is important).
- Of course Derive can integrate this directly, as I hope you can. First check that Derive gets $\pi/4$. Enter g(x), then do Calculus \rightarrow Integrate. Enter the limits 0 and 1, and Simplify. The answer $\pi/4$ should be given.
- We divide the interval into n sub-intervals. We will use

$$\int_0^1 \frac{1}{1+x^2} \, dx \approx \sum_{i=0}^{N-1} \frac{g(i/N) + g((i+1)/N)}{2N}$$

First let us define N to be 1. Use Declare \rightarrow Variable Value, or just type n:=1

- Enter (g(i/n)+g((i+1)/n))/(2*n)
- Click on Then Calculus \rightarrow Sum..., and set Lower limit to be 0 and Upper limit n-1 and Simplify. You should now have a displayed summation.
- Highlight it and Simplify. Your answer should be 3/4.
- Now redefine n to be 2 by typing n:=2. Highlight the summation again and Simplify. The answer should be 31/40.

• Repeat this for n set to 4 and 8. The fractions are now getting a bit large, and probably do not give you any feel for the convergence, so instead of Simplifying we will Approximate these fractions make a table of sums and the errors for N given below. Find the error by subtracting $\pi/4$ from your answer. Give the answers to 7 decimal places.

N	Estimate of integral	Error of estimate	$\mathrm{Error} \times N^2$
1	0.7500000		
2	0.7750000		
4			
8			
16			
32			
64			
256			
1024			
4096			

• Fill in the last column of the table. Does it tend to a constant? If so what is it?

Problem 3

The above is typical behaviour of the trapezium rule. Sometimes you get surprises, as I did when I first tried a different function intending to use it in the lectures. My intention was to use an integral I could do, but you were unlikely to be able to manage (yet). The first integral I thought of was

$$\int_0^\infty \frac{1}{1+x^6} \, dx = \frac{\pi}{3}$$

(If you can get this result without using contour integration techniques there may be a prize.)

Integrals to infinity are difficult numerically, so I transformed it using a change of variable $x = \tan(\pi t/2)$ to give

$$\int_0^1 \frac{1 + \tan^2(\pi t/2)}{1 + \tan^6(\pi t/2)} \, dt = \frac{2}{3}$$

- Confirm on paper that the given change of variable changes the first integral to the second integral.
- Define h(x) to be $(1+\tan(\pi x/2)^2)/(1+\tan(\pi x/2)^6)$. You can use the π from the buttons at the bottom right.
- We have to be careful here as x = 1 will give and undefined quantity. Confirm that

$$\lim_{t \to 1} \frac{1 + \tan^2(\pi t/2)}{1 + \tan^6(\pi t/2)} = 0$$

You can do this by hand, or see if you can work out how to get Derive to do it for you.

- We will redefine g(x) to be h(x) for x < 1 and 0 for x ≥ 1. Define g(x) := If (x<1,h(x),0). This takes the x<1 bit and checks it is true. If so it returns the next argument as the answer, i.e. h(x). Otherwise it returns the third argument, i.e. 0.
- We can reuse the summation from before, and only use approximate values. Fill in the following table:

N	Estimate of integral	Error of estimate
1		
2		
4		
8		
16		
32		

• You should have found that you have converged as far as the given accuracy. Derive is capable of approximating results to a very high accuracy, far more than is useful in the physical world. Use Simplify → Approximate and increase the number of decimal places to 20 to recalculate this. Now continue this, but instead count the number of 6s, ensuring you have enough accuracy for your approximation. If you see only 6s, then increase the number of decimal places until you get something else at the end.

N	Number of leading 6s in estimate
4	
8	
16	
32	
64	
128	
256	

• From this you should see that the appropriate measure of the error that grows with N is the number of correct decimal places. It should be clear that the the number of correct decimal places is approximately proportional to N. Hence the error is approximately $a \times 10^{-\alpha N}$ for some value of α just under 1/2. The error decays exponentially.

This convergence is very rare for any problem like this, and is due to a special feature of this function – that the odd derivatives evaluated at x = 0 and x = 1 are all zero.

As an indication of why these numbers of decimal places are not useful in the physical world: If you used a unit of length which gives the size of our galaxy to be 1, then to give the size of an atom you would only need around 32 decimal places.

Minitab

Open files

Open Minitab which is under Programs \rightarrow - M to N \rightarrow Minitab.

Retrieve the Excel Workbook from the course web page.

Save this data file in your home directory — do not try and work directly with it.

Open this Excel saved workbook.

The Excel workbook contains two sheets, the second sheet, "math-act", containing the results from a first year progress test separated into two groups and the first sheet, "combined" containing the combined data in ascending order.

Copy data

To copy the marks from the first sheet in Excel to column 1 (C1) of Minitab:

- Highlight A1:A108 in the "combined" sheet of the Excel workbook and copy.
- In Minitab with row1–col1 active Paste the data using the right mouse option or Paste from the pull down Edit menu.
- In the "label" row immediately under C1 name the column "Total".

Repeat the above process to copy the Math and ActSci data from the "math-act" sheet of the Excel Workbook to respectively C2 and C3 of Minitab. Label the data as "Maths" and "Act Sci".

Descriptive Statistics

Minitab allows us to calculate a set of simple statistics for a given data set and displays the results on the Session window.

- Select **Stat** from the top menu and **Basic Statistics** from the sub menu followed by **Display Descriptive Statistics**.
- Set Variable set equal to C1 C2 C3 by typing these directly into the window, or use the names you have given the data, or highlight each variable in turn and press the Select button. (A double click also works.)
- Select **Statistics** and tick: mean; SE of mean; standard deviation; variance; coefficient of variation; Min; Max; First quartile; Median; Third quartile; inter-quartile range; N non missing.

Select OK OK to close all sub-windows.

• The basic statistics should now be visible in the **Session Window**

Enter the results:

Data	N	Mean	SE	StDev	Var	CoefVar	Min	Q_1	Med	Q_3	Max	IQR
Total												
Math												
ActSci												

Box Plots

Simple box plots can be used to compare the three sets of data, indicating central tendency using the median and spread using quartiles, whiskers and outliers. To plot a box plot for each of the three sets of data on the same graphs with the boxes horizontal carry out the following:

- Select **Graph** from the top menu followed by **Box Plot**.
- Select Multiple Y Simple. OK
- Select all three data sets as the **Graph variables**.
- By default Minitab creates vertical box plots, here we produce horizontal box plots by:

Selecting Scale and ticking transpose. OK. OK.

This should give a graph containing three box plots placed horizontally. Some of the data used to create the plots can be displayed by pointing into the relevant box or by simply reading from the x-axis.

With reference to your previous results, check that the ends of the boxes are at Q_1 and Q_3 with the median in the correct place. Check with reference to the data that the position of any outliers and the extreme ends of the arms are shown correctly.

Frequency Histogram

Minitab allows three types of histogram, frequency, percentage and density. This task creates a simple frequency histogram for each of the three sets of data using the default "equal intervals". It then asks you to place these graphs together with the box plot in a single layout.

- Select **Graph** from the top menu followed by **Histogram**.
- Select **Simple** type. OK
- Set Graph variables to C1 C2 C3. Select Scale
- Select the **y-scale type** tag and select **Frequency**. OK. OK

This gives a default Histogram for each of the three data sets of the selected type with equal sub-intervals over a slightly extended range.

To produce a layout of the four graphs created so far:

- With one of the histograms active (*click inside one of the histograms windows if not active*) Select **Editor** from the top menu followed by **Layout tools**.
- The layout tool is fairly easy to follow. Select two rows and two columns and position your three Histograms and Box Plot in the boxes on the right using the ">" button. Select **Finish**

To print out or save the layout:

- Make the layout active
- Select **File** from the top menu
- Select Print Graph or Save Graph As. You can choose the format yourself.

Percentage and Density Histograms

This tasks requires you to construct a percentage and a density histogram using unequal class intervals (sub intervals) for the data in C1.

Close all the existing graph windows using the \times in the right hand corner of each window and select NO to save.

- Select Graph, Histogram Simple, OK
- Enter just C1 as the Graph variable
- Select Scale, Y-Scale type, Percent. OK. OK.
- Repeat the above but select **Density** as the Y-Scale type.

You should now have two histograms that are the same shape, only the Y-scales are different in value. This is to be expected as the sub-intervals on which the histograms are based are all of equal length. In such a case is it irrelevant as to whether it is the height or area of each rectangle that is proportional to the frequency.

You are now required to change the x-scale of these graphs to create histograms with unequal class intervals. The two histograms should then appear different, as the percentage histogram is based on height whereas the density histogram is based on area.

With the percentage histogram active:

- Select Editor from the top menu, Select Item, X-Scale. (an alternative to this is to point to the x-axis, until you get the message X-scale, and left click)
- Select Editor from the top menu, Select Edit X Scale. (alternatively point to the selected x-axis and right-click; select option)

- We wish to change the sub-intervals (*class intervals*) on which the histogram is based, this is referred to as "binning". Click the **Binning** tag.
- We can specify the start and ends of the intervals on which the rectangles are constructed, cut-points or alternatively specify the midpoints.
 Select: Cut-point. Select: Midpoint/Cutpoint positions. It is now possible to enter the cut-points in the window.
- Enter the values: 0 30 50 60 70 80 85 90 95 100 leaving a space between each. OK.

The histogram will now be converted into one with the given class intervals.

Repeat the above process on the density histogram.

It is now possible to see the difference in shape between the two histograms due to the subintervals not being equal.

Layout

Use **Layout tools** (*see above*) to form a layout of your two histograms, setting the Layout tool to have two rows and one column. Print or save your layout.

Assessment Exercises Worksheet 8

Numerical Integration and Minitab

Surname:..... Forename.....

Group No¹.

For the Actuarial Science students this sheet is to be handed in at the associated lab session. For Maths students it should be handed in at the second of the two associated lab sessions. Late submission is only allowed with the permission of the lab tutor.

Numerical Integration.

- 1. From Problem 1, what is the sum?
- 2. From Problem 2 complete the table

N	Estimate of integral	$\mathrm{Error} \times N^2$
1	0.7500000	
2	0.7750000	
4		
16		
64		
256		
1024		
4096		

3. For problem 3 complete the tables

				N	Number of leading
N	Estimate of integral	Error of estimate			6s in estimate
1				4	
2				8	
4				16	
8				32	
16				64	
32			1	128	
·	L	,	2	256	

Minitab.

Complete the following table based on the data on marks:

Data	N	Min	Q_1	Med	Q_3	Max
Total						
Math						
Act Sci						

¹Actuarial Science Students only