OCR
RECOGNISING ACHIEVEMENT

ADVANCED GCE

MATHEMATICS (MEI) 4777

Numerical Computation

Candidates answer on the answer booklet.

OCR supplied materials:
- 8 page answer booklet (sent with general stationery)
- MEI Examination Formulae and Tables (MF2)
- Graph paper

Other materials required:
- Scientific or graphical calculator
- Computer with appropriate software and printing facilities

Friday 24 June 2011
Afternoon

Duration: 2 hours 30 minutes

INSTRUCTIONS TO CANDIDATES

- Write your name, centre number and candidate number in the spaces provided on the answer booklet. Please write clearly and in capital letters.
- Use black ink. Pencil may be used for graphs and diagrams only.
- Read each question carefully. Make sure you know what you have to do before starting your answer.
- Answer any **three** questions.
- Additional sheets, including computer print-outs, should be fastened securely to the Answer Booklet.
- Do **not** write in the bar codes.

COMPUTING RESOURCES

- Candidates will require access to a computer with a spreadsheet program and suitable printing facilities throughout the examination.

INFORMATION FOR CANDIDATES

- The number of marks is given in brackets **[ ]** at the end of each question or part question.
- In each of the questions you are required to write spreadsheet routines to carry out various numerical analysis processes.
- You will not receive credit for using any numerical analysis functions which are provided within the spreadsheet. For example, many spreadsheets provide a solver routine; you will not receive credit for using this routine when asked to write your own procedure for solving an equation.
  You may use the following built-in mathematical functions: square root, sin, cos, tan, arcsin, arccos, arctan, ln, exp.
- For each question you attempt, you should submit print-outs showing the spreadsheet routine you have written and the output it generates. It will be necessary to print out the formulae in the cells as well as the values in the cells.
  You are not expected to print out and submit everything your routine produces, but you are required to submit sufficient evidence to convince the examiner that a correct procedure has been used.
- You are advised that an answer may receive **no marks** unless you show sufficient detail of the working to indicate that a correct method is being used.
- The total number of marks for this paper is **72**.
- This document consists of **4** pages. Any blank pages are indicated.

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1 In this question, the notation $\exp(t)$ is used to denote e^t.

(i) Show, graphically or otherwise, that the equation $x = \exp(-x^2)$ has exactly one root, α.

Use a spreadsheet to show that the iteration $x_{r+1} = \exp(-x_r^2)$, with a suitable starting value, converges slowly to α. Confirm your findings by considering the derivative of $\exp(-x^2)$. **[9]**

(ii) Obtain the relaxed iteration $x_{r+1} = (1-\lambda)\, x_r + \lambda \exp(-x_r^2)$.

On a spreadsheet investigate the speed of convergence of the relaxed iteration for various values of λ. Hence find, correct to 1 decimal place, the value of λ that gives fastest convergence. **[6]**

(iii) Show that, theoretically, the best value of λ is given by

$$\lambda = \frac{1}{1 + 2\alpha \exp(-\alpha^2)}.$$

Evaluate this expression. **[3]**

(iv) On a spreadsheet, carry out the iteration $x_{r+1} = (1-\lambda_r)\, x_r + \lambda_r \exp(-x_r^2)$ where

$$\lambda_r = \frac{1}{1 + 2x_r \exp(-x_r^2)}.$$

Show that the convergence of this iteration is faster than first order. **[6]**

2 **(i)** Obtain from first principles the Gaussian two-point rule for numerical integration:

$$\int_{-h}^{h} f(x)\,dx \approx h\left(f\left(-\frac{h}{\sqrt{3}}\right) + f\left(\frac{h}{\sqrt{3}}\right)\right).$$

Find the error when this rule is used to evaluate $\int_{-h}^{h} x^3\,dx$ and $\int_{-h}^{h} x^4\,dx$. Hence state the orders of the local and global errors in the rule. **[10]**

(ii) Use the Gaussian two-point rule to find, correct to 6 decimal places, the value of the integral

$$I = \int_0^1 \sqrt{2 + \sin x}\,dx.$$

You should begin with $h = 0.5$ and then take $h = 0.25, 0.125, \ldots$ as necessary.
Show, by considering ratios of differences, that the global error is as stated in part **(i)**. **[9]**

(iii) Modify your routine so that it calculates values of the integral

$$J = \int_0^1 (2 + \sin x)^k\,dx$$

for any specified k. Find, correct to 2 decimal places, the value of k for which $J = 3$. **[5]**

3 The differential equation $\frac{dy}{dx} = f(x, y)$ with initial conditions $x = x_0$, $y = y_0$, is to be solved by using the Runge-Kutta methods given below.

Method A	Method B
$k_1 = h\,f(x_r, y_r)$	$k_1 = h\,f(x_r, y_r)$
$k_2 = h\,f(x_r + \frac{1}{2}h, y_r + \frac{1}{2}k_1)$	$k_2 = h\,f(x_r + h, y_r + k_1)$
$y_{r+1} = y_r + k_2$	$y_{r+1} = y_r + \frac{1}{2}(k_1 + k_2)$
$x_{r+1} = x_r + h$	$x_{r+1} = x_r + h$

(i) Set up a spreadsheet to obtain a numerical solution by each method to the differential equation

$$\frac{dy}{dx} = \sqrt{1 + x + y}, \text{ with } y = 0 \text{ when } x = 0.$$

For $h = 0.2, 0.1, 0.05, 0.025$, find the estimates given by each method for y when $x = 2$. By considering ratios of differences show that each method is second order. Show that the errors in one method are substantially less than the errors in the other. **[20]**

(ii) Obtain a graph of the solution curve.

Determine, correct to 2 decimal places, the value of x on the solution curve for which $y = 2x$. **[4]**

[Question 4 is printed overleaf.]

4 The variables x and y are thought to be related by an equation of the form

$$y = ax + bx^2 + cx^3, \qquad (*)$$

for some constants a, b and c.

The following experimental data are available. The x values are exact but the y values contain experimental error.

x	–3	–2	–1	0	1	2	3
y	–35.25	–8.01	2.51	–0.09	–4.07	–5.06	0.65

(i) Use a spreadsheet to obtain a sketch of the data points and use it to explain why (*) looks like a reasonable fit. **[4]**

(ii) Show that one of the normal equations for finding the least squares estimates of a, b and c is

$$\sum xy = a\sum x^2 + b\sum x^3 + c\sum x^4.$$

Write down the other two normal equations. **[5]**

(iii) Find

- the least squares estimates of a, b and c,
- the fitted values of y,
- the sum of the residuals,
- the sum of the squares of the residuals. **[12]**

(iv) Obtain a sketch of the fitted curve and the data points. Comment briefly on the fit of the curve to the data. **[3]**

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GCE

Mathematics (MEI)

Advanced GCE

Unit **4777:** Numerical Computation

Mark Scheme for June 2011

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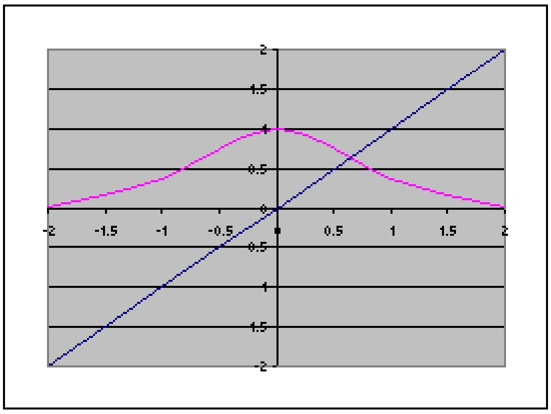
1(i)



r	x_r	
		[G2]
0	0.7	
1	0.612626	
2	0.687075	
3	0.623708	
4	0.677726	
5	0.631718	
6	0.670946	**[M1A1]**
7	0.637521	
8	0.666022	

- slow convergence

Derivative of $\exp(-x^2)$ is $-2x \exp(-x^2)$. Value at 0.6 (0.7) about -0.83 (-0.86). **[M1A1A1]**
Less than 1 in magnitude so converges, but not close to zero so slow. **[E1E1]**
[subtotal 9]

(ii) Multiply both sides by λ, then add (1 - λ) x to both sides. **[M1A1]**

λ	x_0	x_1	x_2	x_3	x_4	x_5	x_6	
0.4	0.7	0.6651	0.6561	0.6537	0.6531	0.6530	0.6529	
0.5	0.7	0.6563	0.6532	0.6529	0.6529	0.6529	0.6529	
0.6	0.7	0.6476	0.6535	0.6529	0.6529	0.6529	0.6529	**[M1A1A1]**

λ = 0.5 (to 1 dp) seems fastest **[A1]**
[subtotal 6]

(iii) Differentiate RHS, set to zero at x = α and solve for λ **[M1A1]**

Best λ evaluates to about 0.53978 **[B1]**
[subtotal 3]

(iv)

r	0	1	2	3	4	
x_r	0.7	0.652966	0.652919	0.652919	0.652919	
λ_r	0.538307	0.539778	0.53978	0.53978	0.53978	**[M1A1A1]**
Δx_r		-0.04703	-4.8E-05	-1.2E-10	0	
$\Delta x_{r+1}/\Delta x_r$			0.001011	2.47E-06	0	**[M1A1]**

Ratio of differences tending (rapidly) to zero so (much) faster than first order **[E1]**
[subtotal 6]
[TOTAL 24]

2(i)	set up RHS as	$a(f(-\alpha) + f(\alpha))$	(by symmetry)	*(award same marks*	**[M1A1]**
	$f(x) = 1$:	$2h = 2a$	hence $a = h$	*for solution without*	**[M1A1]**
	$f(x) = x$:	$0 = 0$		*symmetry assumed)*	**[A1]**
	$f(x) = x^2$	$2h^3/3 = 2a\alpha^2$	hence $\alpha = h/\text{sqrt}(3)$		**[A1]**
	$f(x) = x^3$	$0 = 0$	so no error		**[A1]**
	$f(x) = x^4$	$2h^5/5 = 2a\alpha^4 = 2h^5/9$	so local error of order h^5, global error h^4		**[A1E1E1]**
		error is $8h^5/45$			***[subtotal 10]***

(ii)

h	m	m-h/sqrt3	m+h/sqrt3	f(m-h/sqrt3)	f(m+h/sqrt3)	integral	diffs	
0.5	0.5	0.211325	0.788675	1.486525	1.646032	1.566278	*ratios*	**[M1A1]**
0.25	0.25	0.105662	0.394338	1.451022	1.544084			
0.25	0.75	0.605662	0.894338	1.602906	1.667272	1.566321	4.29E-05	**[M1A1]**
0.125	0.125	0.052831	0.197169	1.432762	1.481855			
0.125	0.375	0.302831	0.447169	1.515989	1.55962			
0.125	0.625	0.552831	0.697169	1.589056	1.625438			
0.125	0.875	0.802831	0.947169	1.649038	1.676832	1.566324	2.73E-06	**[A1]**
0.0625	0.0625	0.026416	0.098584	1.423521	1.448594		*0.06371*	
0.0625	0.1875	0.151416	0.223584	1.466573	1.490546			
0.0625	0.3125	0.276416	0.348584	1.507617	1.530218			
0.0625	0.4375	0.401416	0.473584	1.546196	1.567188			
0.0625	0.5625	0.526416	0.598584	1.581909	1.601085			
0.0625	0.6875	0.651416	0.723584	1.614408	1.631587			
0.0625	0.8125	0.776416	0.848584	1.643389	1.658417			
0.0625	0.9375	0.901416	0.973584	1.668594	1.681341	1.566324	1.71E-07	**[A1]**
							0.06275	

Ratio of differences very close to the theoretical 0.0625 for fourth order **[M1A1E1]**

[subtotal 9]

(iii) e.g.:

k	h	m	m-h/sqrt3	m+h/sqrt3	f(m-h/sqrt3)	f(m+h/sqrt3)	integral	
1.22	0.5	0.5	0.211325	0.788675	2.630873	3.373721	3.002297	
	0.25	0.25	0.105662	0.394338	2.480189	2.886405		
	0.25	0.75	0.605662	0.894338	3.162099	3.480932	3.002406	
	0.125	0.125	0.052831	0.197169	2.404721	2.610753		
	0.125	0.375	0.302831	0.447169	2.759934	2.95778		
	0.125	0.625	0.552831	0.697169	3.095848	3.271659		
	0.125	0.875	0.802831	0.947169	3.388775	3.529836	3.002413	
	0.0625	0.0625	0.026416	0.098584	2.367053	2.470074		
	0.0625	0.1875	0.151416	0.223584	2.545548	2.648271		
	0.0625	0.3125	0.276416	0.348584	2.72289	2.823568		
	0.0625	0.4375	0.401416	0.473584	2.896046	2.992924		
	0.0625	0.5625	0.526416	0.598584	3.061986	3.153343		
	0.0625	0.6875	0.651416	0.723584	3.21775	3.301937		
	0.0625	0.8125	0.776416	0.848584	3.360519	3.435994		
	0.0625	0.9375	0.901416	0.973584	3.487672	3.553039	3.002413	**[M3A2]**

k	1.2	1.3	1.21	1.23	1.22
I	2.948	3.229	2.975	3.030	3.002

[subtotal 5]

[TOTAL 24]

3(i) Method A

h	x	y	k1	k2	new y		
0.2	0	0	0.2	0.219089	0.219089		
	0.2	0.219089	0.238251	0.255986	0.475075		
	0.4	0.475075	0.273867	0.290655	0.76573	*setup:*	**[M2]**
	0.6	0.76573	0.307619	0.3237	1.089429		
	0.8	1.089429	0.339966	0.355495	1.444924	*first run:*	**[A2]**
	1	1.444924	0.37121	0.386292	1.831216		
	1.2	1.831216	0.401558	0.416269	2.247484		
	1.4	2.247484	0.431161	0.445559	2.693043		
	1.6	2.693043	0.460132	0.474262	3.167305		
	1.8	3.167305	0.488561	0.502457	3.669763		
	2	3.669763					

h	y(2)	diffs	ratio of diffs			
0.2	3.669763					
0.1	3.671640	0.001877			*further runs:*	**[A1A1A1]**
0.05	3.672112	0.000473	0.251926			
0.025	3.672231	0.000119	0.250918	≈ 0.25 so 2nd order	*diffs + ratios:*	**[M1A1]**
						[subtotal 9]

Method B

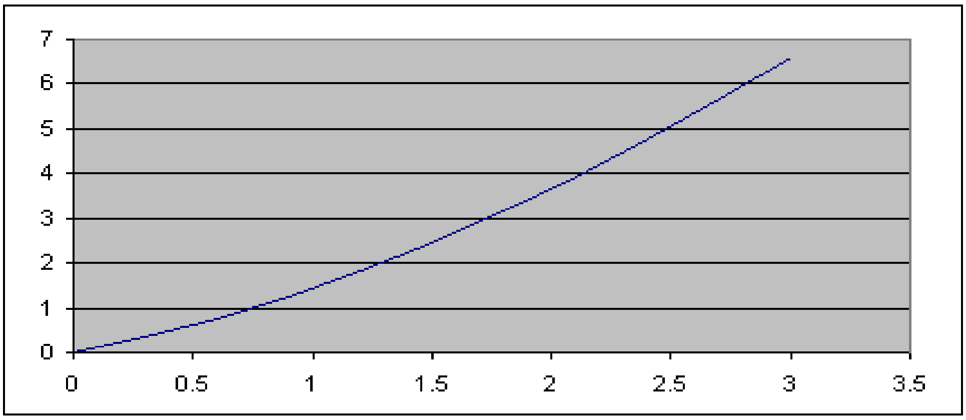
h	x	y	k1	k2	new y		
0.2	0	0	0.2	0.236643	0.218322		
	0.2	0.218322	0.238187	0.272507	0.473669		
	0.4	0.473669	0.273764	0.306427	0.763764	*setup:*	**[M2]**
	0.6	0.763764	0.307491	0.338896	1.086957		
	0.8	1.086957	0.339821	0.370231	1.441983	*first run:*	**[A2]**
	1	1.441983	0.371052	0.400651	1.827835		
	1.2	1.827835	0.401389	0.430313	2.243686		
	1.4	2.243686	0.430984	0.459333	2.688844		
	1.6	2.688844	0.45995	0.487803	3.162721		
	1.8	3.162721	0.488374	0.515794	3.664805		
	2	3.664805					

h	y(2)	diffs	ratio of diffs			
0.2	3.664805					
0.1	3.670336	0.005531			*further runs:*	**[A1A1A1]**
0.05	3.671778	0.001442	0.260722			
0.025	3.672146	0.000368	0.255408	≈ 0.25 so 2nd order	*diffs + ratios:*	**[M1A1]**

Differences (and hence errors) in Method B about 3 times those in method A **[M1E1]**

[subtotal 11]

(ii)



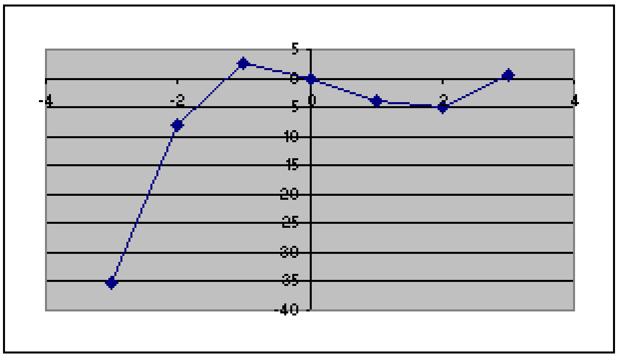
[G2]

Trial and error: y = 2x at x = 2.45 (accept 2.44 or 2.46) **[M1A1]**

[subtotal 4]

[TOTAL 24]

4(i)



[G2]

Two tps: could be cubic [E1]

Almost passes through origin [E1]

[subtotal 4]

(ii)

$Q = \Sigma (y - ax - bx^2 - cx^3)^2$				[M1]
$\partial Q/\partial a = 0$ gives	$\Sigma xy =$	$a \Sigma x^2 + b \Sigma x^3 + c \Sigma x^4$	as given	[M1A1]
other equations:	$\Sigma x^2y =$	$a \Sigma x^3 + b \Sigma x^4 + c \Sigma x^5$		[B1]
	$\Sigma x^3y =$	$a \Sigma x^4 + b \Sigma x^5 + c \Sigma x^6$		[B1]
				[subtotal 5]

(iii)

$\Sigma x^3 = 0 \quad \Sigma x^5 = 0$

x	y	x^2	x^4	x^6	xy	x^2y	x^3y	
-3	-35.25	9	81	729	105.75	-317.25	951.75	
-2	-8.01	4	16	64	16.02	-32.04	64.08	
-1	2.51	1	1	1	-2.51	2.51	-2.51	
0	-0.09	0	0	0	0	0	0	
1	-4.07	1	1	1	-4.07	-4.07	-4.07	
2	-5.06	4	16	64	-10.12	-20.24	-40.48	
3	0.65	9	81	729	1.95	5.85	17.55	*totals*
		28	**196**	**1588**	**107.02**	**-365.24**	**986.32**	[M1A3]

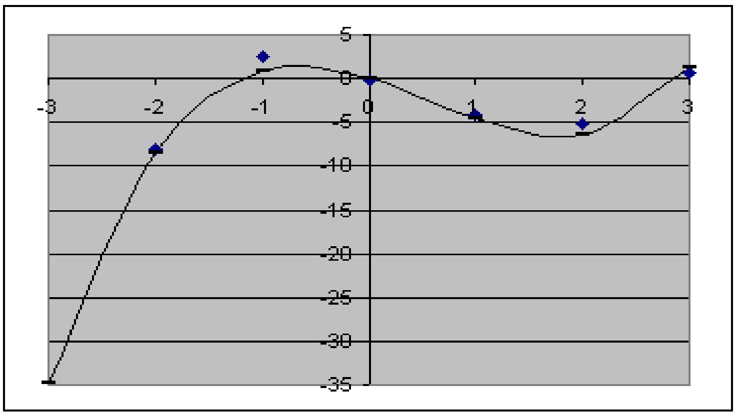
Normal equations:	107.02 =	28 a	+	196 c	
	-365.24 =		196 b		
	986.32 =	196 a	+	1588 c	*set up & solve*
hence:	a = -3.86425		b = -1.86347	c = 1.098056	[M1A3]

x	y	y-fitted	res	res^2
-3	-35.25	-34.826	0.424014	0.179788
-2	-8.01	-8.50983	-0.49983	0.24983
-1	2.51	0.902721	-1.60728	2.583345
0	-0.09	0	0.09	0.0081
1	-4.07	-4.62966	-0.55966	0.313219
2	-5.06	-6.39793	-1.33793	1.790044
3	0.65	1.283537	0.633537	0.40137
			-2.85714	**5.525696**

[M1A1A1A1]

[subtotal 12]

(iv)



[G2]

Comment on goodness of fit [E1]

[subtotal 3]

[TOTAL 24]

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4777: Numerical Computation

General Comments

As usual, there was only a small entry for this paper. About half the candidates produced three good or very good solutions. Of the remainder almost all were able to demonstrate a decent ability to do numerical work on a spreadsheet.

Candidates' organisation of their work remains something of a problem. Solutions should not consist just of print-outs of numbers: the formulae used should be printed too. And it is only common sense that solutions should be labelled and properly ordered. If candidates do not indicate what a sheet of numbers represents or even which question they are from, there is every chance that correct work will go unrewarded.

Comments on Individual Questions

1 **Solution of an equation by relaxation**
This was a popular question, attracting some excellent solutions. Those candidates who did not score high marks generally fell down on the algebra rather than the numerical work.

2 **Gaussian integration**
This was the least popular question, but again there was very good work seen. A mistake, perhaps arising from unfamiliarity, was failing to realise that when a Gaussian rule is applied to an integral over the interval [0, 1] the formula needs to be adjusted so that it is centred on 0.5 rather than 0.

3 **Runge-Kutta methods**
This question was generally very well done, with candidates showing a good grasp of technique (implementing the given algorithms on a spreadsheet) and an understanding of principle (comparing the accuracy of the two methods).

4 **Least squares approximation**
Again, this question attracted some very good solutions – though there were a couple of candidates who made very limited progress. Obtaining the given normal equation was a challenge to one or two, but writing down the normal equations proved easy enough. The numerical work was often successful, though a couple of candidates wanted the sum of the residuals to be zero. (In this case there is no constant term in the fitted equation so the sum of the residuals will *not* be zero.)