DKE Numerical Mathematics
Resit June 2015

Part I

During this part of the exam, you may *only* use the formula sheet provided, and an electronic calculator. You may *not* use a textbook or your own notes.

1. **[10 points]** For this question, perform *all* computations rounding to 3 significant figures after *every* arithmetic operation.

   Let $f(x) = 2x^3 - 5x^2 - x + 7$. Write f and f' in Horner's nested form, and evaluate f both at $x = 1.33$. Use one step of Newton's method starting at $x = 1.33$ to estimate the root of f.

2. **[10 Points]** Compute the divided differences $f[x_i, \ldots, x_j]$, $0 \leq i \leq j \leq 3$ for the data:

i	0	1	2	3
x_i	1.0	2.0	1.5	3.0
$f(x_i)$	0.842	0.455	0.665	0.0470

   Write down the nested form of the interpolating cubic polynomial. Estimate the value of y when $x = 2.5$.

3. **[12 Points]** Consider the data

i	0	1	2	3	4
x_i	0.0	0.25	0.5	0.75	1.0
$f(x_i)$	0.000	0.031	0.128	0.295	0.543

   Estimate $f'(x_i)$ for $i = 0, 1, 2, 3, 4$ using the most appropriate three-point difference formula in each case. Use Simpson's rule to estimate

$$\int_0^1 \sqrt{1 + f'(x)^2}\, dx.$$

4. **[8 points]** Compute the solution of the initial-value problem

$$\dot{y} = t - \sin(y), \quad y(0.0) = 1.5000$$

   at time $t = 0.5$ using one step of the 4^{th}-order Runge-Kutta method.

   Compare your results with the exact answer $y(0.5) = 1.145994875$ (9dp). What would you expect the error to be if you were to use *two* steps of the method to estimate $y(0.5)$?

5. **[10 points]** Compute the trigonometric polynomial best approximating the data (x_j, y_j) below in the least-squares sense, computing terms up to $\cos(2x)$, $\sin(x)$. (Values of $\cos(x_j)$ are also given; note $1/\sqrt{2} = 0.707107$ (6dp).)

j	0	1	2	3	4	5	6	7
x_j	$-\pi$	$-\frac{3}{4}\pi$	$-\frac{1}{2}\pi$	$-\frac{1}{4}\pi$	0	$\frac{1}{4}\pi$	$\frac{1}{2}\pi$	$\frac{3}{4}\pi$
y_j	−0.88	−0.50	0.76	0.98	0.88	0.86	0.76	0.18
$\cos(x_j)$	−1	$-1/\sqrt{2}$	0	$1/\sqrt{2}$	1	$1/\sqrt{2}$	0	$-1/\sqrt{2}$

   Use your result to approximate y when $x = \pi/3$; note $\sin(\pi/3) = \sqrt{3}/2 = 0.866025$ (6dp).

Part II

During this part of the exam, you may *only* use the formula sheet provided, and the version of Matlab installed on the Department's computers. You may *not* use the internet, any other software, or your own laptop.

6. **[10 points]** Use the secant method to estimate the root of f in $[2,3]$ to an accuracy of 10^{-6}, where
$$f(x) = x^2 + 5 - e^x.$$

7. **[14 points]** Consider the cubic spline $s(x)$ interpolating the data

x	1	2	3	4	5
y	1.143	0.444	0.519	1.430	2.471

   using the boundary conditions $s''(0) = 0.0$ and $s'(5) = 0.800$.

   Write down and solve a system of linear equations from which you can determine the coefficients c_j of the quadratic terms. Determine the polynomial giving the values of s for $2 \le x \le 3$. Estimate the value of y when $x = 2.7$.

8. **[8 Points]** If you were to compute the solution of the differential equation $\dot{x} = t - \sin(x)$ at $t = 0$, $x = 1.5$ using the adaptive Bogavine-Shampine method with an error of 0.0001, would a step size of 0.1 be adequate?

9. **[10 Points]** Let P_n be the Legendre polynomials, and
$$f(x) = \sin(e^x).$$

   Find the coefficients $c_0, c_1, \ldots, c_6$ of Legendre polynomials of least-squares approximation to f by a polynomial g of degree 6.

   Compute the least-squares error
$$E = \int_{-1}^{+1} \big(f(x) - g(x)\big)^2 \, dx$$

   for the function g you have found.

   Evaluate the Legendre polynomials $P_k(x)$ at $x = 0.3$ for $k = 0, 1, \ldots, 6$, and hence evaluate $g(x)$.

10. **[8 Points]** In a chemical reaction system, the concentrations of *substrate* S and *product* P satisfy
$$\frac{d[S]}{dt} = k_b[P] - 2k_f[S]^2; \quad \frac{d[P]}{dt} = k_f[S]^2 - (k_b + k_d)[P].$$

    Show how to express this system as a system of two first-order differential equations. Compute the solution over the time interval $[0, 10]$, using rate constants $k_f = 0.1$, $k_b = 0.05$ and $k_d = 0.01$, starting with initial conditions $[S] = 10$ and $[P] = 0$. Sketch a plot of $[P]$ against t and describe the solution. Estimate the time at which you should stop the reaction to maximise $[P]$.