1 Math 406: Ass. 1: Due Friday 20 Sept.

1. **Least squares fitting - $m-$th degree polynomial through N points.**

   (a) Find a system of equations for the coefficients of an $m-$th degree polynomial that fits a function f at given data points $(x_k, f(x_k)), k = 1, \ldots, N$ in the least squares sense. Write the equations in matrix form. What is the size of the matrix ?

   (b) Solve the system of equations using Matlab for $x_k = \{0, 0.2, 0.3, 0.4, 0.6, 0.7\}$, $f(x) = \sin x$, and $m = 3$ and 5. Evaluate the resulting polynomial at $x = 0.5$. Compare the answers to the "*exact*" value of $\sin x$. Use the MATLAB function "polyfit" to check the results.

2. **Finite Difference Tables:** Let S_N^k denote the sum of the k th powers of the first N integers i.e.:

   $$S_N^k = \sum_{i=1}^{N} i^k$$

   Write a simple MATLAB program to evaluate these sums for a specified value of k for values of N from $1 \ldots k+3$. Now write MATLAB code to form the forward difference table (since the sample points are uniform). Notice that for each value of k the difference table terminates - why does this happen? For the special case $k = 3$ extract the differences from your table and use the Gregory-Newton finite difference formula to derive the formula:

   $$S_N^3 = \sum_{i=1}^{N} i^3 = \frac{1}{4} N^2 (N+1)^2$$

3. **Newton's Divided Difference formula and numerical differentiation**

   Use Newton's divided difference formula to derive an approximate expression for the derivatives f'_{k-1}, f'_k, and f'_{k+1} of a function f that is approximated by a quadratic polynomial that interpolates f at the three points (x_{k-1}, f_{k-1}), $(x_k,\, f_k)$ and (x_{k+1}, f_{k+1}).

4. **The pchip function in MATLAB:** Piecewise Cubic Hermite interpolation assumes the following representation of a given function $f(x)$ in terms of the cubic basis functions $h_i^{(0)}$ and $h_i^{(1)}$:

   $$f(x) \approx h(x) = \sum_{i=0}^{N} f(x_i) h_i^{(0)}(x) + \sum_{i=0}^{N} f^{'}(x_i) h_i^{(1)}(x)$$

   where $h_i^{(0)}$ and $h_i^{(1)}$ are assumed to have the properties

   $$\left.\begin{array}{ll} h_i^{(0)}(x_j) = \delta_{ij} & \frac{d}{dx} h_i^{(1)}(x_j) = \delta_{ij} \\ \frac{d}{dx} h_i^{(0)}(x_j) = 0 & h_i^{(1)}(x_j) = 0 \end{array}\right\} \qquad (1)$$

(a) Show that the expressions for these basis functions are given by

$$\begin{aligned}
h_i^{(0)}(x) &= \frac{[\Delta x_i + 2\,(x - x_i)]\,(x_{i+1} - x)^2}{(\Delta x_i)^3} \\
h_{i+1}^{(0)}(x) &= \frac{[\Delta x_i + 2\,(x_{i+1} - x)]\,(x - x_i)^2}{(\Delta x_i)^3} \\
h_i^{(1)}(x) &= \frac{(x - x_i)(x_{i+1} - x)^2}{(\Delta x_i)^2} \\
h_{i+1}^{(1)}(x) &= -\frac{(x_{i+1} - x)(x - x_i)^2}{(\Delta x_i)^2}
\end{aligned}$$

(b) In order to specify the interpolant it is necessary to supply both the function values $f(x_i)$ and the derivatives $f'(x_i)$ at the interpolation points. Write a matlab function $\texttt{hermite}(x, y, yp, xi)$ that will evaluate the Piecewise Cubic Hermite interpolant of a function sampled at the points given by the vector x and whose values and derivatives are given by y and yp respectively. Let xi be the set of desired sample points. For the function $f(x) = \sin(3x)e^{-x^3}$ on the interval $[0, 1]$ plot the Piecewise Cubic Hermite interpolant and the function f. Compare the value of the Piecewise Cubic Hermite interpolant with the function at $x = 3/8$ by sampling the function and its derivative at only 4 uniformly distributed points and completing the table

$f(3/8)$	
$h(3/8)$	

(c) It is often not possible to provide the derivatives $f'(x_i)$ at the interpolation points. Use the formulae for the approximate derivatives determined in problem 3 to approximate the required derivatives $f'(x_i)$ by the derivatives of a local quadratic polynomial. For the left endpoint of the interval use the formula for the derivative at x_{k-1}, for the interior nodes use the formula for the approximate derivative at x_k, and for the right endpoint use the formula for the approximate derivative at x_{k+1}.

(d) The pchip routine in MATLAB (see the reference * below) uses the following scheme to approximate the derivatives at the interpolation points. The slope at each interior node is taken to be the following weighted mean of the slopes of the piecewise linear interpolant either side of the interior point:

$$f'(x_i) = \begin{cases} \frac{f[x_{i-1},x_i]f[x_i,x_{i+1}]}{\alpha f[x_i,x_{i+1}]+(1-\alpha)f[x_{i-1},x_i]} & \text{if } f[x_{i-1}, x_i]f[x_i, x_{i+1}] > 0 \\ 0 \text{ otherwise} \end{cases}$$

where $\alpha = (\Delta x_{i-1} + 2\Delta x_i)/3(\Delta x_{i-1} + \Delta x_i)$ and $\Delta x_i = x_{i+1} - x_i$. Impose the quadratic one-sided derivative conditions at the two end points. Now construct a pchip routine of your own to interpolate a function given only nodal values, constructing the weighted derivative approximations at the nodes and then calling your `hermite` routine.

(e) For the function $f(x) = \sin(3x)e^{-x^3}$ on the interval $[0, 1]$ plot f, the the results of your `hermite` code using the quadratic derivatives defined in part (c), and those of your `pchip` code described in (d) by sampling the function at 4 uniformly distributed points and provide a similar plot for 8 uniformly distributed points. Complete the following table:

	$N = 4$	$N = 8$
$f(3/8)$		
$h_{quadratic\ f'}(3/8)$		
$pchip(3/8)$		

(*) Reference: F.N Fritsch and J. Butland, "A method for constructing local monotone piecewise cubic interpolants", SIAM J. Sci. Stat. Comput. Vol 5, No 2, 1984.