CS4210 Assignment 1 Due: 9/5/14 (Fri) at 6pm

You must work either on your own or with one partner. You may discuss background issues and general solution strategies with others, but the solutions you submit must be the work of just you (and your partner). If you work with a partner, you and your partner must first register as a group in CMS and then submit your work as a group. Each problem is worth 5 points. One point may be deducted for poor style.

Topics: Matlab warm-up. Using Taylor series. Vectorization. Approximation. Heuristics.

1 Padé Approximation of e^x

A very useful class of approximants for the exponential function e^z are the diagonal Padé functions defined by

$$R_{qq}(z) = \left(\sum_{k=0}^{q} \frac{(2q-k)!q!}{(2q)!k!(q-k)!} z^{k}\right) \left/ \left(\sum_{k=0}^{q} \frac{(2q-k)!q!}{(2q)!k!(q-k)!} (-z)^{k}\right).$$

Implement a function

function y = DiagPade(x,q)

% x is a column n-vector

% y is a column n-vector with the property that y(k) = Rqq(x(k)), k=1:n

Your implementation should be vectorized. To force issues, you are not allowed to use the built-in function factorial and you are not allowed to use the exponentiation operator. Avoid redundant computation. Read §1.5.1 in CVL for guidance. You may also wish to check out the CVL code PadeCoeff. A test script P1 is available on the course website. Submit DiagPade to CMS.

2 Second Derivative Approximation

By adding this

$$f(a+h) = f(a) + hf^{(1)}(a) + \frac{h^2}{2}f^{(2)}(a) + \frac{h^3}{6}f^{(3)}(a) + \frac{h^4}{24}f^{(4)}(a) + \frac{h^5}{120}f^{(5)}(a) + \frac{h^6}{720}f^{(6)}(\eta_+)$$

to this

$$f(a-h) = f(a) - hf^{(1)}(a) + \frac{h^2}{2}f^{(2)}(a) - \frac{h^3}{6}f^{(3)}(a) + \frac{h^4}{24}f^{(4)}(a) - \frac{h^5}{120}f^{(5)}(a) + \frac{h^6}{720}f^{(6)}(\eta_-)$$

and rearranging we conclude that

$$f^{(2)}(a) = \frac{f(a-h) - 2f(a) + f(a+h)}{h^2} - \frac{h^2}{12}f^{(4)}(a) + O(h^4)$$
(1)

Replacing h with 2h we also have

$$f^{(2)}(a) = \frac{f(a-2h) - 2f(a) + f(a+2h)}{4h^2} - \frac{4h^2}{12}f^{(4)}(a) + O(h^4)$$
(2)

By combining (1) and (2) obtain a higher order approximation of the form

$$f^{2}(a) = \frac{\alpha_{1}f(a-2h) + \alpha_{2}f(a-h) + \alpha_{3}f(a) + \alpha_{4}f(a+h) + \alpha_{5}f(a+2h)}{h^{2}} + O(h^{4})$$
(3)

After you figure out the α 's, implement a function of the form

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function y2p = SecondDerivative(f,a,h)
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% f is a handle to a function f(x) that has six continuous derivatives.

% y2p is an estimate of f''(a)

Your implementation should make use of (3). It should also include a comment that indicates how to choose h so as to minimize the overall error. To do this you need to understand §1.5.2 in CVL. The $O(h^4)$ term in (3) actually has the form $ch^4 f^{(6)}(\eta)$ where c is a constant and $a - 2h \le \eta \le a + 2h$. You can figure out c by applying SecondDerivative to $f(x) = x^6$. Why? If one has an estimate M_6 of $f^{(6)}$ in the vicinity of a, then it is reasonable to choose h so as to minimizes $ch^4M_6 + eps/h$. Submit SecondDerivative to CMS.

3 MyErf

The Taylor series for the error function erf(x) is

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \sum_{k=0}^{\infty} \frac{(-1)^k x^{2k+1}}{k! (2k+1)}$$
(4)

Write a function of the form

function y = MyErf(x)
% x is a column n-vector
% y is a column n-vector with the property that y(i) = erf(x(i)), i=1:n.

Your implementation should make use of (4), adding in terms until they no longer change the running sum. Your code should be vectorized meaning that the running sum should be a vector of scalar running sums. Submit MyErf to CMS. A test script P3 is available.