MATH 651: Numerical Analysis II

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Homework assignment 3 – due 10/24/2017

Problem 1 (Numerical differentiation). We proved in class that the symmetric two-point finite difference operator

$$D_\varepsilon^{\pm} f(x_0) = \frac{f(x_0+\varepsilon) - f(x_0-\varepsilon)}{2\varepsilon}$$

converges to the exact derivative $f'(x_0)$ like

$$|f'(x_0) - D_\varepsilon^{\pm} f(x_0)| \le C\varepsilon^2$$

as $\varepsilon \to 0$.

One may ask if it is possible to get better convergence orders if one is willing to use more function evaluations. For example, one could postulate an operator

$$D_\varepsilon^{[\alpha_{-1},\alpha_0,\alpha_1]} f(x_0) = \frac{\alpha_{-1} f(x_0-\varepsilon) + \alpha_0 f(x_0) + \alpha_1 f(x_0+\varepsilon)}{\beta\varepsilon}$$

and then hope that one can choose $\alpha_{-1}, \alpha_0, \alpha_1$ and β in such a way that

$$|f'(x_0) - D_\varepsilon^{[\alpha_{-1},\alpha_0,\alpha_1]} f(x_0)| \le C\varepsilon^3$$

as $\varepsilon \to 0$, or possibly of even higher order.

- **(a)** Relatively simple considerations show that $D_\varepsilon^{[\alpha_{-1},\alpha_0,\alpha_1]}$ can only be a reasonable operator if $\alpha_{-1}+\alpha_0+\alpha_1 = 0$ and $-\alpha_{-1}+\alpha_1 = \beta$. Show why these equations have to hold by considering what happens if you apply the operator to a function f that is (i) constant, and (ii) linear.
- **(b)** Having so reduced the number of unknowns to two (for example $\alpha_{\pm 1}$), see if you can choose these leftover unknowns so that you get at least third order convergence. To this end, you will have to do Taylor expansions as we did in class and see whether you can choose the unknowns in such a way that as many Taylor terms as possible cancel. Alternatively, you could ask that the operator is exact when applied to functions that are constant, linear, quadratic, ..., until you have enough equations to determine all coefficients. You may assume that $f \in C^\infty$.
- **(c)** Repeat this kind of exercise for a finite difference operator

  $$D_\varepsilon^{[\alpha_{-2},\alpha_{-1},\alpha_0,\alpha_1,\alpha_2]} f(x_0) = \frac{\alpha_{-2} f(x_0-2\varepsilon) + \alpha_{-1} f(x_0-\varepsilon) + \alpha_0 f(x_0) + \alpha_1 f(x_0+\varepsilon) + \alpha_2 f(x_0+2\varepsilon)}{\beta\varepsilon}$$

  and see what kind of convergence order you can achieve by choosing the coefficients in appropriate ways.
- **(d)** Using the function $f(x) = e^x$ and $x_0 = 0$, demonstrate numerically that the theoretical convergence order you have derived above indeed holds for both the three-point and the five-point stencil in practice as well.

(30 points)

Problem 2 (Numerical differentiation). As part of the previous homework assignment, you have found a root of the function $f(x) = xe^x - 1$. (As a complete aside, this means that you computed $W(1)$ where $W(x)$ is the *Lambert W function*.)

Let us repeat a similar exercise except that we now want to find the *minimum* of that function. To this end, we need to solve the problem $g(x) = f'(x) = 0$ for which we can use a Newton method that computes $x_{k+1} = x_k - \frac{g(x_k}{g'(x_k)}$. Here, this equates to iterating $x_{k+1} = x_k - \frac{f'(x_k}{f''(x_k)}$.

(a) Use Newton's method to compute the root x^* to at least six digits of accuracy, starting with $x_0 = -0.5$ and using exact derivatives of f.

(b) Let us pretend that $f(x)$ was an expensive function for which we do not have a formula, and that we can only compute f' and f'' in Newton's method by a finite difference approximation using the symmetric first and second derivative operators. Using these, compute approximate roots $x^{\varepsilon,*}$ for a variety of values ϵ to at least six digits of accuracy. Demonstrate numerically that $x^{\varepsilon,*} \to x^*$ as $\varepsilon \to 0$ and plot the error $|x^{\varepsilon,*} - x^*|$ as a function of ε for a number of values $\varepsilon = 1, \ldots, 10^{-6}$.

(30 points)

Problem 3 (Numerical integration). Let's go back to the function $f(x) = \sin \frac{1}{x}$ and assume that we want to compute the integral $J = \int_{0.05}^{1} f(x)\ dx$. The value of the integral is about 0.50283962, but you should find a numerical approximation to it.

(a) Using a subdivision of the interval $[0.05, 1]$ into K equally sized intervals I_k, approximate the integral above using the

(i) midpoint rule,
(ii) trapezoidal rule,
(iii) Simpson rule,
(iv) 2-point Gauss rule,
(v) 3-point Gauss rule.

For each of these methods, generate a plot that shows the error between the exact integral value and your numerical approximation as a function of the number of function evaluations you need. (The number of function evaluations will be K, $K+1$, $2K+1$, $2K$, and $3K$ for the methods above.)

For each of the methods, also state how many function evaluations you need to achieve an accuracy of 10^{-6}.

(b) In the derivation of the convergence rates for the various methods, always came to a point where we could state the error as

$$|e| \leq \sum_{k=1}^{K} \frac{1}{p!} \|f^{(p)}\|_{\infty,I_k} h_k^{p+1}.$$

Here, p is the convergence order of the respective method. (Remember that we lose one power of h in the summation, to obtain $|e| = \mathcal{O}(h)$ if the h_k are all roughly of the same size.)

This representation of the total suggests a strategy like the one we explored for interpolation: To choose intervals so that h_k is only small if $f^{(p)}$ is large. To this end, we should start with a relatively coarse mesh and then for each interval compute some sort of criterion η_k that indicates how large the error is – for example

$$\eta_k = \frac{1}{p!} \left| f^{(p)} \left(\frac{x_k - x_{k-1}}{2} \right) \right| h_k^{p+1},$$

where (i) we assume that we can evaluate *derivatives* of f exactly, and (ii) we approximate the ∞-norm of the derivative by just evaluating it at the midpoint of the interval. We would then "refine" the interval with the largest η_k by replacing it with its two halves, recompute our current approximation of the interval, and repeat the process.

Try this strategy with the trapezoidal rule. In each iteration of the algorithm, evaluate the error between the numerical approximation of the integral and the exact value. Produce a plot that shows the error as a function of the number of function evaluations you need and compare the results with the data obtained in part (a).

How many function evaluations do you now need to achieve an accuracy of 10^{-6}?

(40 points)