Math 116 Numerical PDEs: Homework 3—debriefing

January 30, 2012

Debugging is becoming important now: devise simple checks for your codes for which you know the answer. Have a think about the convergence rate you expect. Does your code even converge? Also print out numbers and look at them, or make plots of intermediate variables. You'll find making your main program a script is easier to debug since the variables stay around afterwards (not true for function).

Generally it will help you to make you code modular*, so that you have a single main script which defines the integrand, and calls functions which supply the nodes and weights, for different schemes. You can set a flag at the script start, then use an* `if ... else ... end` *type construction to call the various functions. This will help with HW4.*

1. [3+2 pts] See Brad's pics, except note $e^{-1/z}$ is *essential singularity*, the worst kind. Also note that $e^{-1/z}$ is C^∞ smooth on $(0, \infty)$, the positive real axis. Taylor plotted an interesting log vertical scale which makes it look anti-symmetric about 0.

2. [3 pts] See Jeff solution, except, note A isn't Vandermonde, but A^T is, and transpose preserves the property of a matrix being nonsingular.

3. [7 pts: 4+ 3] For a) Always think what convergence rate you expect from lecture, so if it comes out wrong, or doesn't converge, you know to debug.

   (a) Use log-log plot to see algebraic as straight line, slope -2. See Taylor who did it for general $[a, b]$. The exact integral is $\tan^{-1} 2$.

   (b) Note you should be expecting exponential convergence, since from HW2 we found (initially) exponential convergence for interpolation via Newton Cotes. However, it seems linear, and soon by $n = 38$ the ill-conditioning of linear system makes it break down anyway. So min acheivable error is around 10^{-3}.

   Amazing thing: by $n = 35$ the condition number of the Vandermonde matrix is 10^{16} so the weights are complete garbage, $O(1)$ errors! However, since $A\mathbf{w} = \mathbf{b}$ is solved in backwards stable way, the weights produced still integrate the monomials up to degree n sort-of accurately. How accurately is a subtle issue; suffice it to say that you cannot avoid rounding errors here, which is controlled by the large weights of typ size 10^6.

4. [7 pts: 3+2+2]

   (a) Real analytic function. Exponential convergence with $\alpha \approx 0.96$. We can compute the expected rate exactly! Looking in Trefethen's ATAP book, Thm 19.3, we have that Gaussian quadrature error should converge as ρ^{-2n}, where ρ is the sum of semimajor and semiminor axes of an ellipse with foci ± 1. This "Bernstein" ellipse is the image of the circle radius ρ under the map $z \to (z + z^{-1})/2$. See Ch. 8 of ATAP.

   Thus, the ellipse touching $\pm i/2$, the poles of our f, has $\rho = (1 + \sqrt{5})/2$, the golden ratio, by solving a quadratic. Then $\alpha = 2\log(\rho) = 0.9624\ldots$. Jeff measured this correct to 3 digits!

   (b) Exact up to degree $2n + 1$ explains the sudden jump down to ε_{mach} at $n = 10$.

   (c) $|x|^3$ is C^2 smooth, and not analytic (not analytic at zero). One expects 4th-order algebraic convergence; people reported orders around 3 to 3.5, but you should take the tail only.

Also see p.36 Trefethen, Spectral Methods book, p. 130.

5. [4 pts] This caused trouble! Brad has a solution using my 2nd hinted method. You need to check q_{j+1} is orthog to *all* previous members in the set: $q_j, q_{j-1}, \ldots, 1$. This is what *mutually* orthog means. This is why Gram-Schmidt is generally $O(n^2)$ to build a set of size n, as we did in lecture, but since polynomials are special you beat that down to $O(n)$ with this amazing 3-term recurrence.

   Here's a solution using the first hinted method. We use induction. Assume q_j down to q_0 exist and are mutually orthog, for some $j > 0$, and that for $i = 0, \ldots, j$ that $\text{Span}\{q_m\}_{m=0}^{i} = \mathbb{P}_i$. Apply standard G-S to the new element xq_j (which is in $\mathbb{P}_{j+1}$ so lin. indep.) to get q_{j+1}:

$$q_{j+1}(x) = xq_j(x) - \frac{(xq_j, q_j)}{(q_j, q_j)} q_j(x) - \frac{(xq_j, q_{j-1})}{(q_{j-1}, q_{j-1})} q_{j-1}(x) - \cdots - \frac{(xq_j, q_0)}{(q_0, q_0)} q_0(x)$$

   That's the usual G-S formula. Now all the terms $j-2$ down to 0 vanish by orthog since, eg, $(xq_j, q_{j-2}) = (q_j, xq_{j-2})$ and $q_j \perp \mathbb{P}_{j-1}$. Note the trick of "moving the x over in the inner product". And the 1st and 2nd terms in the above are as given in the question. So, the only thing left to show is that the top of the β term is as given, ie $(xq_j, q_{j-1}) = (q_j, q_j)$. But this follows by using our trick, and noticing that by the previous G-S, $q_j = xq_{j-1} +$ (stuff in $\mathbb{P}_{j-1}$). Again, the stuff here vanishes by the orthogonality assumed in the induction.

   See G. W. Stewart, Afternotes on Numerical Analysis, book.

6. [2+3+2 = 7 pts]

   See Jeff's plots here (but warning about interpretation of c).

   (a) It is super-exponential, which is typical of entire functions (distance to nearest singularity would give a fixed exponential rate, but here this distance is ∞ so the rate keeps growing). The function of n that is e^{-n^2} is an example of super-exponential convergence to zero.

   (b) The exact answer is $\sqrt{2}\pi$ which comes from a half-angle substitution! (I didn't expect you to get this). Finding the poles? Solve for when denominator blows up, when $\cos(x/2) = i$, If lazy use Matlab's `acos(1i)*2` which has Im part $a = 1.762\ldots$. This predicts the exponential rate α. Note that if you take the (open) strip to have exactly this half-width, you can't then find a bound $M\infty$ for the sup norm of f in the strip, since f blows up on the top and bottom of the strip. So, the theorem cannot give you the constant. It's not even obvious why the slope is so well predicted, then, since the theorem can only predict arbitrary close to the slope, but not the slope itself. However, espilon-close is good enough.

   (c) It is C^∞ (because $e^{-1/x}$ on is on $x > 0$), but not real analytic, since there's an essential singularity at 0. Convergence gets continually steeper on a log-log plot, hence is super-algebraic. (Note that it gets continually *flatter* on a semilogy plot, so is worse than exponential for any rate $\alpha > 0$.). Taylor did a nice empirical fit to $e^{-2.3\sqrt{n}}$ which is indeed super-algebraic but not exponential. I wonder if you can find some theory on this?