CAAM 453/553 · NUMERICAL ANALYSIS I

Problem Set 5

Posted Friday 30 October 2009. Due Monday 9 November 2009.
CAAM 453 students should complete 4 problems (including problem 1).
CAAM 553 students should complete 5 problems (including problems 1 and 6).
Students are welcome to attempt more problems if they wish.

General note: Unless specified otherwise, it is acceptable to use Mathematica, Maple, or MATLAB's Symbolic Toolbox to evaluate the occasionally tedious integrals on this problem set. If you do so, please include your output to demonstrate how you calculated these integrals.

1. [25 points]

   Consider approximations to $\sqrt{x}$ for $x \in [0,1]$.

   (a) Find the line that best approximates $\sqrt{x}$ in the minimax (L^∞) sense, and report the error. [Kincaid & Cheney]

   (b) Find the line that best approximates $\sqrt{x}$ in the least-square (L^2) sense, and report the error.

   (c) For a general interval $[a,b]$, prove that for all $f \in C[a,b]$,

   $$\min_{p\in\mathcal{P}_n} \|f-p\|_{L^2} \le \sqrt{b-a}\,\min_{p\in\mathcal{P}_n} \|f-p\|_{L^\infty}.$$

   Confirm that your solutions to (a) and (b) are consistent with this bound.

   (d) Let $[a,b]$ be any fixed interval. Given any $\varepsilon > 0$, show that there exists some $f \in C[a,b]$ such that $\|f\|_{L^2} \le \varepsilon$, while $\|f\|_{L^\infty} \ge 1/\varepsilon$. (This implies that there exists *no* constant M such that $\|f\|_{L^\infty} \le M\|f\|_{L^2}$ for all $f \in C[a,b]$.) [Süli and Mayers, problem 8.1]

2. [25 points]

   Clenshaw–Curtis quadrature approximates the integral of a function by the integral of the degree-N polynomial that interpolates it at $N+1$ Chebyshev points. A MATLAB routine for computing the nodes and weights of this rule for the interval $[a,b] = [-1,1]$, called `clencurt.m`, is linked from the course website. (This implementation is from Trefethen's *Spectral Methods in MATLAB* book.)

   (a) Use Clenshaw–Curtis quadrature (with nodes and weights from `clencurt.m`) to approximate $\int_{-1}^{1} f(x)\,dx$ for each of:

   $$f(x) = e^{-x^2}, \qquad f(x) = (1+25x^2)^{-1}, \qquad f(x) = |x|.$$

   In particular, for each f, produce a `semilogy` plot showing the degree of interpolating polynomial N versus the error between the Clenshaw–Curtis approximation and the true integral (whose values can be computed in MATLAB via `sqrt(pi)*erf(1)`, `2*atan(5)/5`, and `1`), for $N = 1,\dots,50$.

   (b) Why do you think the three different functions in part (a) produce such different results?

   (c) For the first function, $f(x) = e^{-x^2}$, use MATLAB's `tic` and `toc` commands to time how long it takes compute the Clenshaw-Curtis approximation for $N = 20$ (include the time for computing the nodes and weights). Compare this value to the time required to integrate this same f using MATLAB's all-purpose adaptive quadrature routine, `quad`, with precision `1e-15`.

3. [25 points]

You may use the following facts without proof: For positive integers N and n,

$$\sum_{k=1}^{N} \sin\left(\frac{2\pi nk}{N}\right) = 0$$

and

$$\sum_{k=1}^{N} \cos\left(\frac{2\pi nk}{N}\right) = \begin{cases} N & \text{if } n/N \text{ is an integer;} \\ 0 & \text{otherwise.} \end{cases}$$

(a) Write down the composite trapezoid rule for approximating

$$\int_a^b f(x)\,\mathrm{d}x$$

with function evaluations at $x_k = a + kh$ for $h = (b-a)/N$ and $k = 0, \ldots, N$.

(b) Suppose we wish to approximate

$$\int_0^{2\pi} f(x)\,\mathrm{d}x,$$

where f is a 2π-periodic function (that is, $f(x) = f(x+2\pi)$ for all $x \in \mathbb{R}$). Show that in this case the composite trapezoid rule reduces to

$$\frac{2\pi}{N}\sum_{k=1}^{N} f\left(\frac{2\pi k}{N}\right).$$

For the rest of the problem, suppose f is a 2π-periodic function with Fourier series

$$f(x) = \frac{c_0}{\sqrt{2\pi}} + \sum_{n=1}^{\infty} c_{-n}\frac{1}{\sqrt{\pi}}\cos(nx) + \sum_{n=1}^{\infty} c_n \frac{1}{\sqrt{\pi}}\sin(nx)$$

for constants $c_0, c_{-1}, c_1, \ldots$.

(c) Integrate each term of this Fourier series to obtain a simple formula for $\int_0^{2\pi} f(x)\,\mathrm{d}x$.

(d) Write down a descriptive bound for the difference between the true integral found in part (c) and the approximation obtained from the composite trapezoid rule applied to the function f with the above Fourier series.

(e) If f and its first p derivatives are continuous and 2π-periodic, then there exists a constant γ such that $|c_{|n|}| \le \gamma/|n|^p$ for all integers n. Compare the performance of the composite trapezoid rule applied to such an f with the usual composite trapezoid error bound that holds for functions that are in C^2, but not necessarily 2π-periodic.

(f) Produce a `loglog` plot comparing the error in the trapezoid rule approximations to the 2π-periodic problem

$$\int_0^{2\pi} \exp(\sin(x))\,\mathrm{d}x = 7.95492652101284527451322\ldots$$

and the smooth but not 2π-periodic problem

$$\int_0^{2\pi} \exp(\sin(x/\pi))\,\mathrm{d}x = 13.3094551602297896414536\ldots.$$

4. [25 points]

The gamma function is defined as

$$\Gamma(x) = \int_0^\infty t^{x-1}\mathrm{e}^{-t}\,\mathrm{d}t.$$

(a) Use the composite Simpson's rule to evaluate $\Gamma(5)$, $\Gamma(10)$, and $\Gamma(.5)$ to five digits of accuracy. You may use MATLAB's built-in `gamma` function to verify your answer. Please report the number of integrand evaluations required. In particular, show how to reliably compute $\Gamma(.5)$ using fewer than 1000 function evaluations.

Now, repeat your computations using the 8-point Gauss–Laguerre quadrature rule. (This Gaussian quadrature rule has nodes at the roots of the degree-8 Laguerre polynomial, an orthogonal polynomial over $[0,\infty)$ with respect to the weight function $w(x) = \mathrm{e}^{-x}$.)

(b) Find the necessary quadrature nodes and weights in a mathematical table, or by searching on the web, or by computing them yourself via either the method in the previous problem or symbolic packages such as Mathematica or Maple. Please cite your source for this data.

(c) Compute $\Gamma(5)$, $\Gamma(10)$, and $\Gamma(.5)$ using this 8-point Gauss–Laguerre rule. Each of these integrals will only require eight $f(t)$ evaluations.

(d) How does the accuracy of Gauss–Laguerre quadrature compare to that obtained by the composite Simpson's rule? Give pros and cons of each method.

5. [25 points]

Monte Carlo methods provide an alternative to interpolatory quadrature schemes. Given $f \in C[a,b]$, from a probabilistic perspective one can interpret the integral of f as its *expected value*:

$$\int_0^1 f(x)\,\mathrm{d}x =: \mathsf{E}[f].$$

The expected value $\mathsf{E}[f]$ is just another name for the *mean*, which can be estimated by averaging values of f sampled at uniformly distributed random points in $[a,b]$. Hence, the N-point *Monte Carlo* estimate of the integral is given by

$$\int_0^1 f(x)\,\mathrm{d}x \approx \frac{b-a}{N}\sum_{k=1}^{N} f(\xi_j),$$

where $\xi_1,\ldots,\xi_N$ are N independent samples of a uniform random variable over $[a,b]$, as can be generated using MATLAB's `rand` command. The Central Limit Theorem suggests that this estimate will converge to the exact integral at a rate of $N^{-1/2}$. (For details, see R. E. Caflisch, "Monte Carlo and quasi-Monte Carlo methods," *Acta Numerica*, 1998.)

(a) Consider the function $f(x) = \sin(x)$ over $x \in [0,2]$. Produce a `loglog` plot comparing N versus error for the N-point Monte Carlo method and the trapezoid rule based on N function evaluations, for various values of N. (Take your largest N to be at least 10^5.) Which method is superior?

The rest of this problem concerns approximation of a 10-dimensional integral,

$$\int_a^b\int_a^b\int_a^b\int_a^b\int_a^b\int_a^b\int_a^b\int_a^b\int_a^b\int_a^b f\big(x_1,x_2,x_3,x_4,x_5,x_6,x_7,x_8,x_9,x_{10}\big)\,\mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_3\mathrm{d}x_4\mathrm{d}x_5\mathrm{d}x_6\mathrm{d}x_7\mathrm{d}x_8\mathrm{d}x_9\mathrm{d}x_{10},$$

a type of problem that arises in mathematical physics and financial modeling.

(b) Write a MATLAB code based on nested trapezoid rules to evaluate this ten-dimensional integral. If each trapezoid rule uses n function evaluations, then the total procedure should require n^{10} function evaluations.

(c) Use your code from part (b) to approximate the integral for $a = 0$, $b = 2$, and

$$f(x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}) = \sin(x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8 x_9 x_{10})$$

for several small values of n (e.g., $n = 3, 4, 5$). Produce a table showing your estimate for the integral, as well as the total error. (The exact integral is approximately 174.467318369179.)

(d) Compare your result from (c) to the Monte Carlo approximation

$$\frac{(b-a)^{10}}{N} \sum_{k=1}^{N} f(\xi_1, \xi_2, \xi_3, \xi_4, \xi_5, \xi_6, \xi_7, \xi_8, \xi_9, \xi_{10})$$

for $f(\xi_1, \xi_2, \xi_3, \xi_4, \xi_5, \xi_6, \xi_7, \xi_8, \xi_9, \xi_{10}) = \sin(\xi_1\xi_2\xi_3\xi_4\xi_5\xi_6\xi_7\xi_8\xi_9\xi_{10})$ on $[a, b] = [0, 2]$. Use the same number of total function evaluations that you used for the trapezoid rule in part (c): i.e., take $N = 10^n$ for the same values of n used in part (c).

Here $\xi_1, \ldots, \xi_{10}$ denote independent, identically distributed random variables uniformly distributed over $[a, b] = [0, 2]$.

(e) Which approach is superior for the 10-dimensional integral? (Include a rough explanation.)

6. [25 points]

The *three-eighths rule* is a 4-point interpolatory quadrature method that exactly integrates cubic polynomials. It is defined by the formula

$$I(f) = \frac{3h}{8}(f(a) + 3f(a+h) + 3f(a+2h) + f(b)),$$

where $h = (b-a)/3$. Apply the Peano Kernel Theorem to show that there exists $\xi \in [a, b]$ such that

$$E(f) \equiv \int_a^b f(x)\,\mathrm{d}x - I(f) = -\frac{3}{80}h^5 f^{(4)}(\xi).$$

A key part of this argument is that $K(t)$ does not change sign on $[a, b]$. You do not need to prove this (it is quite tedious), but please do include a plot verifying this fact.

Supplemental Problem

S1. Compute

$$\lim_{\varepsilon \to 0} \int_\varepsilon^1 x^{-1} \cos(x^{-1} \log x)\,\mathrm{d}x$$

to as many digits as possible.

[Trefethen]

S2. (a) Does the standard error bound derived in class for the composite trapezoid rule give any insight about the performance of that method applied to the Fresnel integral

$$\int_0^1 \frac{\sin(x)}{\sqrt{x}}\,\mathrm{d}x\,?$$

(b) One can compute this Fresnel integral by expanding $\sin(x)$ in a Taylor series about $x = 0$ to obtain

$$\int_0^{\varepsilon} \Big(\frac{x - \frac{1}{3!}x^3 + \cdots}{\sqrt{x}}\Big)\,\mathrm{d}x + \int_{\varepsilon}^1 \frac{\sin(x)}{\sqrt{x}}\,\mathrm{d}x.$$

To approximate this quantity, one can truncate the Taylor series after m terms and compute the resulting approximation to the first integral exactly; approximate the second integral using the composite trapezoid rule. Estimate the accuracy of this procedure as a function of m, ε, and the number of subintervals used in the composite trapezoid rule for the second integral.

(c) Construct a function $g(x)$ such that the integral in part (a) can be effectively computed via

$$\int_0^1 \Big(\frac{\sin(x)}{\sqrt{x}} - g(x)\Big)\,\mathrm{d}x + \int_0^1 g(x)\,\mathrm{d}x,$$

where the first integral can be computed accurately with the composite trapezoid rule and the second integral can be computed exactly without need for numerical quadrature.

[Bulirsch and Stoer]