MATH523 , Homework 6
Due December 7, 2017 in class

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1. [8 pts] *Milne's rule* in $[0,1]$ is the following quadrature

$$M(f;0,1)=\frac{1}{90}(7f(0)+32f(1/4)+12f(1/2)+32f(3/4)+7f(1)).$$

   ~~(a)~~ Show that Milne's rule is the Newton-Cotes formula of order 4.

   ~~(b)~~ Use the appropriate k to compute the constant C of the following error: $E(f;0,1)=Cf^{(k)}(\xi)/k!$.

   ~~(c)~~ State the composite Milne's rule $M_n(f;a,b)$ and derive an expression for the error $E_n(f;a,b)$ in terms of powers of the meshsize h and derivatives of f.

   (d) Show that the composite Milne's rule $M_n(f;a,b)$ is the second step $T_n^{(2)}(f;a,b)$ in Romberg integration, where $T_n^{(0)}(f;a,b)$ is the composite Trapezoidal formula with n panels. Use this to rederive the error formula found in (c).

2. [8 pts] Write a MATLAB function `q = trapezoid (f,a,b,n)` to implement the composite *trapezoid rule* $T_n(f;a,b)$ for a function f on the interval `[a,b]` with `n` panels. The function `f` is to be given in a separate m-file `f.m`, and `feval(f,x)` is to be used for evaluation of `f(x)` in `trapezoid`.

   ~~(a)~~ Apply `trapezoid` with `n=2, 4, 8, 16, 32, 64, 128` to the following integrals

$$\frac{2}{\sqrt{\pi}}\int_0^1 e^{-x^2}dx=\texttt{erf(1)},\qquad \int_{-1}^1|x-0.1|dx,\qquad \int_0^1 x^{1/2}dx.$$

   (b) Compare your results with the exact answer (`erf` is a built-in function), namely compute the errors $E_n(f;a,b)$. Determine the rate of convergence in each case, and do a `loglog` plot of $E_n(f;a,b)$ versus n. Discuss how the slope of the plots relates to the rate of convergence and how the latter relates to theory and the regularity of f.

~~3.~~ [8 pts] *Adaptive Quadrature:* Two quadratures rules of different order, or the same rule with two panels, can be combined to estimate the quadrature error and decide whether it meets an accuracy goal or not, and thus bisect the panel and recompute

   ~~(a)~~ Write a recursive MATLAB function `[Q,n] = adapt_quad(f,a,b,tol)`, which computes an approximate integral `Q` satisfying `|I-Q|`$\leq$`tol` for a continuous function f on `[a,b]`. To this end, use the *Simpson*'s rule with 1 and 2 panels to estimate the error of the latter.

   ~~(b)~~ Use `adapt_quad` to obtain *adaptive* approximations of the integrals of Problem 2(a) with `tol=`10^{-2}.

~~4.~~ [10 pts] Define $S_n(x) = \dfrac{1}{n+1} T'_{n+1}(x),\ n \geq 0$, with $T_{n+1}(x)$ the Chebyshev polynomial of degree $n+1$. The polynomials $S_n(x)$ are called the *Chebyshev polynomials of the second kind*.

~~(a)~~ Show that $\{S_n(x) \mid n \geq 0\}$ is an orthogonal family on $[-1, 1]$ with respect to the weight function $w(x) = \sqrt{1-x^2}$.

~~(b)~~ Show that the family $\{S_n(x)\}$ satisfies the same triple recursion relation as the family $\{T_n(x)\}$.

~~(c)~~ Given $f \in C[-1, 1]$, solve the problem

$$\min \int_{-1}^{1} \sqrt{1-x^2}[f(x) - p_n(x)]^2 \, dx,$$

where $p_n(x)$ is allowed to range over all polynomials of degree $\leq n$.

~~(d)~~ For the integral

$$I = \int_{-1}^{1} \sqrt{1-x^2} f(x) \, dx$$

with weight $w(x) = \sqrt{1-x^2}$, find explicit formulae for the nodes and weights of Gaussian quadrature formula. Also give the error formula.

~~5.~~ [10 pts] *Lobatto's Rule*: This is a Gaussian rule for integrating $I(f) = \int_{-1}^{1} f(x)dx$ except that it includes ± 1 as two preassigned abscissas. It has the form

$$I(f) \approx L_n(f) = w_0 f(-1) + \sum_{i=1}^{n} w_i f(x_i) + w_{n+1} f(1), \tag{1}$$

with abscissas x_i and weights w_i chosen to maximize the order of the integration method. Counting degrees of freedom we expect the formula to be exact for polynomials of degree $\leq 2n+1$. This problem explains how to determine the abscissas and weights for $n = 2$. The argument is general in that it applies for all n as well as for Gauss-Konrod.

~~(a)~~ Use Hermite interpolation to show that any polynomial $p \in \Pi_5$ can be written as

$$p(x) = \sum_{i=0}^{3} p(x_i) h_i(x) + \sum_{j=1}^{2} p'(x_j) g_j(x),$$

where h_i and g_j are polynomials of degree 5 that satisfy

$$h_i(x_j) = \delta_{ij}, \quad h'_i(x_j) = 0, \quad g_i(x_j) = 0, \quad g'_i(x_j) = \delta_{ij},$$

where $\delta_{ij} = 1$ if $i = j$ and zero otherwise. Here, the conditions on h', g' are only imposed at the interior nodes $j = 1, 2$.

~~(b)~~ Show that for suitable $\alpha, \beta \in \mathbb{R}$,

$$\begin{aligned} g_1(x) &= \alpha(1-x^2)(x-x_1)(x-x_2)^2, \\ g_2(x) &= \beta(1-x^2)(x-x_1)^2(x-x_2). \end{aligned}$$

~~(c)~~ Show that a sufficient condition for $L_2(f)$ to be of the form (1) is

$$\int_{-1}^{1} g_j(x)dx = 0, \quad j = 1, 2. \tag{2}$$

~~(d)~~ Prove that a sufficient condition for (2) to hold is that $q(x) = (x-x_1)(x-x_2)$ be orthogonal to all linear polynomials with respect to the weight $w(x) = 1 - x^2$.

~~(e)~~ Compute the first three orthogonal polynomials q_0, q_1, q_2 with respect to $w(x) = 1 - x^2$.

~~(f)~~ Use q_2 to demonstrate that the abscissas are $x_1 = -1/\sqrt{5}, x_2 = 1/\sqrt{5}$.

~~(g)~~ Compute the weights w_0, w_1, w_2, w_3.

~~(h)~~ If $f \in \mathcal{C}^{(6)}[-1, 1]$, then show the error formula

$$I(f) - L_2(f) = -\frac{f^{(6)}(\xi)}{6!} \int_{-1}^{1} (1-x^2)(1/5 - x^2)^2 dx.$$

~~6.~~ [8 pts] *Monte-Carlo Integral:* Consider a two-dimensional Gaussian density function

$$p(x, y) = \frac{1}{2\pi} e^{-(x^2+y^2)/2}.$$

The Box-Muller algorithm generates a two-dimensional independent random variables (η_1, η_2) with density function above as follows: Draw a two-dimensional independent uniform random variable (ψ_1, ψ_2) from [0,1] with MATLAB function **rand** and let

$$\begin{aligned} \eta_1 &= \sqrt{-2\psi_1}\cos(2\pi\psi_2) \\ \eta_2 &= \sqrt{-2\psi_1}\sin(2\pi\psi_2). \end{aligned}$$

Note that these formula can be derived by directly inverting cdf's (you don't have to ~~proof~~ this).

~~(a)~~ Generate $n = 10^6$ pairs of Gaussian random variables with the Box-Muller algorithm and determine h such that 10% of the samples are in the rectangular box

$$B = \{(x, y) | |x| \leq h/2, |y| \leq h/2\}$$

Now, use **quad2** to obtain an estimate of

quad2d

$$\int_B p(x, y)dxdy.$$

From this exercise, conclude that

$$\Omega(B)/n \approx \int_B p(x, y)dxdy,$$

where $\Omega(B)$ is the number random samples in B.

Var[X] = E[X^2]-E[X]^2

~~(b)~~ Let x be a one-dimensional Gaussian random variable with mean 0 and variance 1. Note that

$$E(x^{2p}) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} x^{2p} e^{-x^2/2} dx = 1 \cdot 3 \cdot 5 \cdots (2p-1).$$

For $p = 1, 2, 5$, compute $Var(x^{2p})$ and find the minimum sample size n to achieve an accuracy of 1% for the sampling moments

$$\frac{1}{n} \sum_{j=1}^{n} X_j^{2p} \tag{3}$$

to approximate $E(x^{2p})$. *Hint: Use the Monte-Carlo error estimate with one-standard deviation.*

~~(c)~~ Now, generate the random samples (use (b) as a guideline for sample size) with the Box-Muller to estimate $E(x^{2p})$ with (3) for $p = 1, 2, 5$. Compute the error and check whether they are within 1% of the accuracy? Why more samples are required for large p?

~~7.~~ [8 pts] Consider a quadrature rule of the form,

$$\int_0^1 x^\alpha f(x) dx \approx A f(0) + B \int_0^1 f(x) dx, \quad \alpha > -1, \alpha \neq 0.$$

~~(a)~~ Determine A and B such that the formula above has degree of exactness 1.

~~(b)~~ Let $E(f)$ be the error functional of the rule determined in (a). Show that the Peano Kernel $K_1(t) \geq 0$ if $\alpha < 0$ and $K_1(t) \leq 0$ if $\alpha > 0$.

~~(c)~~ As a consequence to the result of (b), determine e_2 in $E(f) = e_2 f''(\tau)$ for some $\tau \in (a, b)$.