MATH 4073 Homework 6 Due Thu, 10/22/13

Problem 1. Let $f : \mathbb{R} \to \mathbb{R}$ be a C^∞ function (i.e., a function that is differentiable infinitely many times), and suppose that $x \in \mathbb{R}$ and $h > 0$ are some fixed numbers. Derive a formula to approximate $f'(x)$ that uses only $f(x-2\,h)$, $f(x)$, $f(x+h)$, $f(x+3\,h)$ such that the local truncation error is $O(h^3)$, i.e., such that

$$f'(x) = \big[\text{your expression approximating } f'(x)\big] + O(h^3) \; .$$

Hint: Expand $f(x-2\,h)$, $f(x+h)$, $f(x+3\,h)$ in a Taylor series about x up to h^3, as in

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2!}f''(x)h^2 + \frac{1}{3!}f'''(x)h^3 + O(h^4) \; ,$$

and from these expressions eliminate the terms containing $f''(x)$ and $f'''(x)$.

Problem 2. The quadrature formula

$$\int_0^2 f(x)\,\mathrm{d}x = c_0 f(0) + c_1 f(1) + c_2 f(2)$$

is exact for all polynomials of degree less than or equal to 2. Determine c_0, c_1, and c_2.

Hint: Note that this quadrature formula must be exact for the polynomials $f(x) = 1$, $f(x) = x$, and $f(x) = x^2$. Use this fact to write a system of three (linear) equations for c_0, c_1, and c_2.

Problem 3. Bhagyashri defined a family of polynomials, which she modestly denoted by B_0, B_1, B_2, …, that satisfy the following conditions:

(i) the polynomial B_k is of degree k;

(ii) the polynomials B_k are *monic*, i.e., the coefficient in front of the term with the highest power of x in B_k (in our case, this is the coefficient of x^k) is equal to 1;

(iii) the polynomials B_0, B_1, B_2, …, B_n form an orthogonal basis in the space of polynomials $V_n(0,\infty; w(x) = \mathrm{e}^{-x})$.

Recall that $V_n(a,b;w(x))$ stands for the linear space of polynomials of degree no greater than n endowed with the inner product

$$\langle P, Q\rangle = \int_a^b P(x)\,Q(x)\,w(x)\,\mathrm{d}x \; .$$

In the solution of this problem the following identity will be handy (where $0! := 1$):

$$\int_0^\infty x^k\,\mathrm{e}^{-x}\,\mathrm{d}x = k! \; .$$

(a) Clearly, $B_0(x) = 1$ for each $x \in [0, \infty)$. Find the only monic polynomial B_1 of degree 1 that is orthogonal to B_0.

(b) Find the only monic quadratic polynomial B_2 that is orthogonal to both B_0 and B_1.

(c) Show that the polynomial $P(x) = x^2 + 3$ can be represented as a linear combination of the polynomials B_0, B_1 and B_2 as follows: $P = B_2 + 4B_1 + 5B_0$.

(d) Show directly that $\langle B_0, B_0 \rangle = 1$, $\langle B_1, B_1 \rangle = 1$, $\langle B_2, B_2 \rangle = 4$.

(e) Find the orthogonal projection, $\mathrm{proj}_{B_0+2B_1} P$, of the polynomial $P(x) = x^2 + 3$ onto the "straight line"

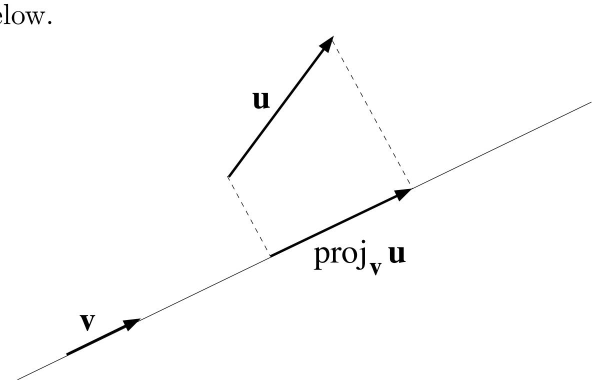
$$\ell := \{t(B_0 + 2B_1) \mid t \in \mathbb{R}\}$$

in the 3-dimensional inner product linear space $V_2(0, \infty; \mathrm{e}^{-x})$. If you have solved part (c), then finding this orthogonal projection should be easy.

Hint: If $\mathbf{u}$ and $\mathbf{v}$ are vectors in the inner product linear space V, then the orthogonal projection of the vector $\mathbf{u}$ onto the straight line in the direction of $\mathbf{v}$ is the vector

$$\mathrm{proj}_{\mathbf{v}} \mathbf{u} = \frac{\langle \mathbf{u}, \mathbf{v} \rangle}{\langle \mathbf{v}, \mathbf{v} \rangle} \mathbf{v}$$

– see the picture below.



(f) Finally, let $\widetilde{B}_k := \mu_k B_k$, where $\mu_k > 0$ is a constant (depending on k) such that the norm,

$$\|\widetilde{B}_k\| := \sqrt{\langle \widetilde{B}_k, \widetilde{B}_k \rangle}\ ,$$

of the polynomial $\widetilde{B}_k$ is 1. Find the explicit expressions for $\widetilde{B}_0(x)$, $\widetilde{B}_1(x)$, and $\widetilde{B}_2(x)$.

Problem 4. The Legendre polynomials are a family of monic polynomials

$$P_0(x) = 1\ , \quad P_1(x) = x\ , \quad P_2(x) = x^2 - \frac{1}{3}\ , \quad P_3(x) = x^3 - \frac{3}{5}x\ , \dots\ ,$$

such that P_0, P_1, ..., P_n form an orthogonal basis of the linear space $V_n(-1, 1; w(x) \equiv 1)$ (i.e., the vector space of all polynomials of degree $\leq n$ endowed with the weight function $w(x) = 1$ for all $x \in [-1, 1]$).

The goal of this problem is to find a Gaussian quadrature formula with degree of precision 5 based on the general formalism developed in class. The notations used are the same as in the handout "Theoretical foundations of Gaussian quadrature".

(a) Find the roots x_1, x_2, and x_3, of the polynomial P_3. Order them so that $x_1 < x_2 < x_3$.

Remark: Recall that the general theory (Lemma 1 on page 7 of the handout) guarantees that P_3 has three *real* roots, all of them in the interval $(-1, 1)$.

(b) Write down the polynomials L_1, L_2, L_3.

Hint: Here is what I obtained for L_2: $L_2(x) = -\frac{5}{3}x^2 + 1$ (but you have to derive this).

(c) Find the weights w_1, w_2, w_3.

Hint: I obtained $w_3 = \frac{5}{9}$.

(d) Write down the quadrature formula coming from parts (a), (b), (c).

(e) Show that the quadrature formula obtained in (d) is *exact* for all monomials x^k if k is an odd positive integer.

Hint: This can be done without doing any computations!

(f) Show that the quadrature formula obtained in (d) is exact for the polynomial $f(x) = 1$.

(g) Show that the quadrature formula obtained in (d) is exact for the polynomial $f(x) = x^2$.

(h) Show that the quadrature formula obtained in (d) is exact for the polynomial $f(x) = x^4$.

(i) Show that the quadrature formula obtained in (d) is *not* exact for the polynomial $f(x) = x^6$. Does this agree with the theoretical prediction about the degree of precision of the method you developed?

(j) Now let us apply the beautiful quadrature formula you derived in (d) to a concrete problem. The so-called *error function* is defined as

$$\operatorname{erf}(z) := \frac{2}{\sqrt{\pi}} \int_0^z \mathrm{e}^{-x^2}\,\mathrm{d}x \ .$$

It is important for engineering applications; it is related to the c.d.f. $\Phi(z)$ of the standard normal distribution by $\operatorname{erf}(z) = 2\Phi(\sqrt{2}\,z) - 1$. (To solve this problem, you do not need to know what these words mean.)

You have to find the value of $\operatorname{erf}(1)$. Since the limits of the integral in the definition of $\operatorname{erf}(1)$ are 0 and 1 but in the quadrature formula the integral was from -1 to 1, first find an appropriate *linear* change of variables $y = \eta(x)$ such that $\eta(0) = -1$ and $\eta(1) = 1$. Change the integration variable from x to $y = \eta(x)$.

Remark: You can also find infinitely many nonlinear changes of variables that satisfy these two conditions, but why make things more complicated?

(k) Apply the Gaussian quadrature formula found in (d) to compute the numerical value of $\operatorname{erf}(1)$. Find the absolute and the relative error if you know that the exact value of $\operatorname{erf}(1)$ is

$$\operatorname{erf}(1)_{\text{exact}} = 0.842700792949714869341220635082609259296066997966302908459\ldots\ .$$