

**Problem 1.** Let  $f : \mathbb{R} \rightarrow \mathbb{R}$  be a  $C^\infty$  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  $f(x-2h)$ ,  $f(x)$ ,  $f(x+h)$ ,  $f(x+3h)$  such that the local truncation error is  $O(h^3)$ , i.e., such that

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

*Hint:* Expand  $f(x-2h)$ ,  $f(x+h)$ ,  $f(x+3h)$  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

$$\int_0^2 f(x) dx = c_0 f(0) + c_1 f(1) + c_2 f(2)$$

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

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

$$\langle P, Q \rangle = \int_a^b P(x) Q(x) w(x) dx .$$

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

$$\int_0^\infty x^k e^{-x} dx = k! .$$

- (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,  $\text{proj}_{B_0+2B_1} P$ , of the polynomial  $P(x) = x^2 + 3$  onto the “straight line”

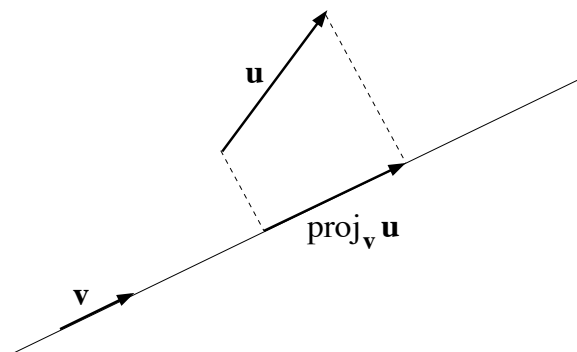
$$\ell := \{t(B_0 + 2B_1) \mid t \in \mathbb{R}\}$$

in the 3-dimensional inner product linear space  $V_2(0, \infty; e^{-x})$ . 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

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

– see the picture below.



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

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

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

**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  $P_0, P_1, \dots, P_n$  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

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

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

$$\operatorname{erf}(1)_{\text{exact}} = 0.8427007929497148693412206350826092592960669979663029084599 \dots .$$