1 Inner Product and Quadrature

Exercise 1

(a) For $f, g \in C([0,1])$, show that

$$\langle f, g \rangle = \int_0^1 x^{-1/2} f(x) g(x)\, dx$$

is well defined.

We need to prove that $\langle f, g \rangle = \int_0^1 \frac{f(x)g(x)}{\sqrt{x}} dx$ is continuous on $C([0,1])$ so that the integral is calculable, and also this integral needs to converge so that its value is finite. C([0,1]) is the set of all continuous functions on the closed interval x in [0,1]

- First, we can see that both f(x), g(x) and 1/sqrt(x) are continuous in (0, 1]. At x = 0, 1/sqrt(x) is undefined, so this is an improper integral => f(x)g(x)/sqrt(x) is continuous on (0, 1] and thus this improper integral is defined.

- Second, we need to prove that $\left| \int_0^1 \frac{f(x)g(x)}{\sqrt{x}} dx \right| < \infty$. Let

$\arg\min_{x\in[0,1]} f(x) = a, \arg\max_{x\in[0,1]} f(x) = b, \arg\min_{x\in[0,1]} g(x) = m, \arg\max_{x\in[0,1]} g(x) = n$ (Since f(x) and g(x) is continuous) => $\frac{f(x)g(x)}{\sqrt{x}} \in [\frac{am}{\sqrt{x}_{\min}}, \frac{bn}{\sqrt{x}_{\max}}] => \left| \int_0^1 \frac{f(x)g(x)}{\sqrt{x}} dx \right| \approx \frac{am+bn}{\sqrt{x}_{\min}\sqrt{x}_{\max}} \times (1-0)$ (Trapezoid area)

$=> \left| \int_0^1 \frac{f(x)g(x)}{\sqrt{x}} dx \right| <= \frac{2bn}{\sqrt{x}_{\min}\sqrt{x}_{\max}} = M$ (Trapezoidal area of equal bases)

M is a finite number => $\langle f, g \rangle = \int_0^1 \frac{f(x)g(x)}{\sqrt{x}} dx$ is well defined

(b) Show that $\langle \cdot, \cdot \rangle$ defines an inner product on $C([0,1], \mathbb{R})$.

We need to prove the following properties:

1) $\langle f, g \rangle = \langle g, f \rangle$

$\langle f, g \rangle = \int_0^1 \frac{f(x)g(x)}{\sqrt{x}} dx = \int_0^1 \frac{g(x)f(x)}{\sqrt{x}} dx = \langle g, f \rangle$ (proven)

2) $\langle f, f \rangle \geq 0$

$\langle f, f \rangle = \int_0^1 \frac{f(x)f(x)}{\sqrt{x}} dx = \int_0^1 \frac{f(x)^2}{\sqrt{x}} dx$. We see that both $f(x)^2$ and $\sqrt{x}$ are positive on [0,1]

$$=> \frac{f(x)^2}{\sqrt{x}} \geq 0 => \int_0^1 \frac{f(x)^2}{\sqrt{x}} dx \geq 0 => \langle f, f \rangle \geq 0 \text{ (proven)}$$

3) $\langle f, f \rangle = 0 <=> f = 0$

$$\langle f, f \rangle = 0 => \int_0^1 \frac{f(x) f(x)}{\sqrt{x}} dx = \int_0^1 \frac{f(x)^2}{\sqrt{x}} = 0 => f = 0 \text{ (Since } f(x)^2 \geq 0)$$

$$f = 0 => \langle f, f \rangle = \int_0^1 \frac{0 \times 0}{\sqrt{x}} dx = \int_0^1 0 dx = 0$$

$$=> \langle f, f \rangle = 0 <=> f = 0 \text{ (proven)}$$

4) $\langle f, f \rangle > 0 <=> f \neq 0$

We have $\langle f, f \rangle \geq 0$ from (2) and $\langle f, f \rangle = 0 <=> f = 0$ from (3)

=> $\langle f, f \rangle > 0 <=> f \neq 0$ (proven)

5) $\langle af + bg, h \rangle = a\langle f, h \rangle + b\langle g, h \rangle$

$$\langle af + bg, h \rangle = \int_0^1 \frac{(af(x) + bg(x))h(x)}{\sqrt{x}} dx = \int_0^1 \frac{af(x)h(x) + bg(x)h(x)}{\sqrt{x}} dx$$

$$=> \langle af + bg, h \rangle = \int_0^1 \frac{af(x)h(x)}{\sqrt{x}} + \frac{bg(x)h(x)}{\sqrt{x}} dx = \int_0^1 \frac{af(x)h(x)}{\sqrt{x}} dx + \int_0^1 \frac{bg(x)h(x)}{\sqrt{x}} dx \text{ (sum rule of integration)}$$

$$=> \langle af + bg, h \rangle = a\int_0^1 \frac{f(x)h(x)}{\sqrt{x}} dx + b\int_0^1 \frac{g(x)h(x)}{\sqrt{x}} dx = a\langle f, h \rangle + b\langle g, h \rangle \text{ (proven)}$$

(c) Construct a corresponding second order orthonormal basis.

We will use the Gram's Schmidt method to construct the 2nd order orthonormal basis by the Kronecker Delta, where the basis is $\{p_0, p_1, p_2\} : \langle p_i, p_j \rangle = \delta_{ij} = \begin{cases} 1 \text{ if } i = j \\ 0 \text{ if } i \neq j \end{cases}$

$\begin{cases} p_0 = a_0 \\ p_1 = a_1 x + b_1 \\ p_2 = a_2 x^2 + b_2 x + c_2 \end{cases}$ and we have six equations to solve it.

1) $\langle p_0, p_0 \rangle = 1 => \langle p_0, p_o \rangle = \int_0^1 \frac{a_0^2}{\sqrt{x}} dx = 1 => 2a_0^2 = 1 => a_0 = \frac{1}{\sqrt{2}}$

2) $\langle p_0, p_1 \rangle = 0$

$$\langle p_0, p_1 \rangle = \int_0^1 \frac{a_0(a_1 x + b_1)}{\sqrt{x}} dx = \frac{1}{\sqrt{2}} \int_0^1 \frac{a_1 x + b_1}{\sqrt{x}} dx$$

$$=> \langle p_0, p_1 \rangle = \frac{a_1}{\sqrt{2}} \int_0^1 \sqrt{x} dx + \frac{b_1}{\sqrt{2}} \int_0^1 \frac{1}{\sqrt{x}} dx = \frac{a_1}{\sqrt{2}} \times \frac{2}{3} + \frac{b_1}{\sqrt{2}} \times 2 => a_1 \frac{\sqrt{2}}{3} + b_1\sqrt{2} = 0$$

3) $\langle p_1, p_1 \rangle = 1$

$$\langle p_1, p_1 \rangle = \int_0^1 \frac{\left(a_1 x + b_1\right)^2}{\sqrt{x}} dx = a_1^2 \int_0^1 x\sqrt{x} dx + 2a_1 b_1 \int_0^1 \sqrt{x} dx + b_1^2 \int_0^1 \frac{1}{\sqrt{x}} dx$$

$$=> \langle p_1, p_1 \rangle = \frac{2}{5} a_1^2 + \frac{4}{3} a_1 b_1 + 2b_1^2 = 1$$

From (2) and (3) => $a_1 = \frac{3\sqrt{10}}{4}$ and $b_1 = -\frac{\sqrt{10}}{4}$

4) $\langle p_0, p_2 \rangle = 0$

$$\langle p_0, p_2 \rangle = \int_0^1 \frac{a_0\left(a_2 x^2 + b_2 x + c_2\right)}{\sqrt{x}} dx = \frac{\sqrt{2}}{15}\left(3a_2 + 5b_2 + 15c_2\right) = \frac{\sqrt{2}}{5} a_2 + \frac{\sqrt{2}}{3} b_2 + \sqrt{2} c_2 = 0$$

5) $\langle p_1, p_2 \rangle = 0$

$$\langle p_1, p_2 \rangle = \int_0^1 \frac{\left(a_1 x + b_1\right)\left(a_2 x^2 + b_2 x + c_2\right)}{\sqrt{x}} dx => a_2\left(\frac{4\sqrt{10}}{35}\right) + b_2\left(\frac{2\sqrt{10}}{15}\right) = 0$$

6) $\langle p_2, p_2 \rangle = 1$

$$\langle p_2, p_2 \rangle = \int_0^1 \frac{\left(a_2 x^2 + b_2 x + c_2\right)^2}{\sqrt{x}} dx => \frac{2}{9} a_2^2 + \frac{2}{5} b_2^2 + 2c_2^2 + \frac{4}{7} a_2 b_2 + \frac{4}{5} a_2 c_2 + \frac{4}{3} b_2 c_2 = 1$$

From (4),(5) and (6) => $a_2 = \frac{105}{8\sqrt{2}}, \; b_2 = -\frac{45}{4\sqrt{2}}, \; c_2 = \frac{9}{8\sqrt{2}}$

=> The second order orthonormal basis is:

$$\begin{cases} p_0 = \frac{1}{\sqrt{2}} \\ p_1 = \frac{3\sqrt{10}}{4} x - \frac{\sqrt{10}}{4} \\ p_2 = \frac{105}{8\sqrt{2}} x^2 - \frac{45}{4\sqrt{2}} x + \frac{9}{8\sqrt{2}} \end{cases}$$ (answer). The roots are: $$\begin{cases} p_0\text{: no roots} \\ p_1 : x_0 = \frac{1}{3} \\ p_2 : x_0 = \frac{15 + 2\sqrt{30}}{35} \text{ and } x_1 = \frac{15 - 2\sqrt{30}}{35} \end{cases}$$

=> The normalized polynomials:

$$\begin{cases} p_0 = \frac{1}{\sqrt{2}} \\ p_1 = x - \frac{1}{3} \\ p_2 = \left(x - \frac{15 + 2\sqrt{30}}{35}\right)\left(x - \frac{15 - 2\sqrt{30}}{35}\right) \end{cases} => \begin{cases} p_0 = \frac{1}{\sqrt{2}} \\ p_1 = x - \frac{1}{3} \\ p_2 = x^2 - \frac{6}{7} x + \frac{3}{35} \end{cases} \quad (answer)$$

(d) Find the two-point Gauss rule for this inner product.

Let x_0 ,...., x_n be the roots of an orthonormal polynomial of degree n. Then:

$$\int_a^b w(x) f(x)dx \approx A_i f(x_i)$$

$$A_i = \int_a^b w(x)\varphi_i(x)dx, \ \ \varphi_i(x) = \prod_{j=0, j\neq i}^{n} \frac{x-x_j}{x_i - x_j}$$

In this case, we have $w(x) = \dfrac{1}{\sqrt{x}}$ and $n=1$. We have:

$$A_0 = \int_0^1 \frac{1}{\sqrt{x}} \frac{x-x_1}{x_0 - x_1} dx = \frac{6x_1 - 2}{3x_1 - 3x_0}$$
$$A_1 = \int_0^1 \frac{1}{\sqrt{x}} \frac{x-x_0}{x_1 - x_0} dx = \frac{6x_0 - 2}{3x_0 - 3x_1}$$

Now x_0 and x_1 be the roots of an orthonormal polynomial of degree 2. We have:

$$p_2 = \frac{105}{8\sqrt{2}}x^2 - \frac{45}{4\sqrt{2}}x + \frac{9}{8\sqrt{2}} = 0 \Rightarrow x_0 = \frac{15+2\sqrt{30}}{35} \text{ and } x_1 = \frac{15-2\sqrt{30}}{35}$$

=> $A_0 = \dfrac{6x_1 - 2}{3x_1 - 3x_0} = \dfrac{18-\sqrt{30}}{18}$, $A_1 = \dfrac{6x_0 - 2}{3x_0 - 3x_1} = \dfrac{18+\sqrt{30}}{18}$ (answer)

The two-point Gauss quadrature is:

$$\langle f, g\rangle = \int_0^1 \frac{f(x)g(x)}{\sqrt{x}} dx \approx A_0 f(x_i)g(x_i) + A_1 f(x_i)g(x_i) = \frac{18-\sqrt{30}}{18} f(x_i)g(x_i) + \frac{18+\sqrt{30}}{18} f(x_i)g(x_i)$$

Observation: we see that

$$\int_a^b w(x)dx = \int_0^1 \frac{1}{\sqrt{x}} dx = 2 \text{ and } A_0 + A_1 = \frac{18+\sqrt{30}}{18} + \frac{18-\sqrt{30}}{18} = 2 \Rightarrow A_0 + A_1 = \int_a^b w(x)dx$$

(e) For $f \in C^4([0,1], \mathbb{R})$, prove the error bound of the error $R(f) \leq c_2 M_4(f)$, where $M_4(f) = \max_{t\in[0,1]} |f^{(4)}(t)|$. Find an estimate for c_2 using MATLAB.

First, $f \in C([0,1])$ means that f to the 4[th] derivative is continuous on $x \in [0,1]$. We need to prove the error bound $R(f) \leq c_2 M_4(f)$. The quadrature error is given by:

$$R(f) = \frac{f^{(2n)}(\xi(x))}{(2n)!} \langle p_n(x), p_n(x)\rangle$$

We haveL 2n = 4 => n = 2. Thus the quadrature error in this case is:

$R(f)=\dfrac{f^{(4)}(\xi(x))}{4!}\langle p_2(x),p_2(x)\rangle \le c_2 M_4(f)$, where

$c_2=\dfrac{\langle p_2(x),p_2(x)\rangle}{4!}$ and $M_4(f)=\max_{x\in[0,1]}\left|f^{(4)}(\xi(x))\right|$ (proven)

The Matlab code for errorBound.m is

```
clc;
format long
% The two roots of the polynomial p2
root0 = (15 + 2*sqrt(30))/35;
root1 = (15 - 2*sqrt(30))/35;
l1w = @(x) (1./sqrt(x)).*(x - root0)/(root1 - root0);
% A1
alpha1=quadl(l1w,0,1);
disp("The weighted term A1 is: " + alpha1);
l2w = @(x) (1./sqrt(x)).*(x - root1)/(root0 - root1);
alpha2=quadl(l2w,0,1);
disp("The weighted term A2 is: " + alpha2);
pi2w = @(x)(1./sqrt(x)).*((x.^2)-(6/7).*x + 3/35).*((x.^2)-(6/7).*x
+ 3/35);
% Estimate for c2
c2 = quadl(pi2w,0,1)/24;
disp("The estimate for c2 is: " + c2);
```

```
The weighted term A1 is: 1.3043
The weighted term A2 is: 0.69571
Estimation of c2 is: 0.00048377
fx >>
```

The estimate of c_2 computed by Matlab is therefore around 4.837711261601187e-04

2 Monte Carlo

Consider for positive real numbers a, b, c the solid ellipsoid

(1) $$K=\{(x,y,z)\in\mathbb{R}^3 \mid \frac{x^2}{a^2}+\frac{y^2}{b^2}+\frac{z^2}{c^2}\le 1\}.$$

Exercise 2

(a) Let I denote the interval $[-1,1]$. Show that K is contained in the hypercube

$$C=\{(au,bv,cw)\mid(u,v,w)\in C_B\},\quad C_B=I^3=I\times I\times I.$$

First, we have $I\in[-1,1], I^3=C_B=I\times I\times I$ which is a cube with side length 2 =>

$C=\{(au,bv,cw)\mid(u,v,w)\in C_B\}$ is a stretched box of the cube C_B by a,b,c times in u,v,w directions

So we need to show that the solid ellipsoid is contained inside this stretched box C.

Pick $(x_0, y_0, z_0) \in K \Rightarrow \frac{x_0^2}{a^2} + \frac{y_0^2}{b^2} + \frac{z_0^2}{c^2} \le 1 \Rightarrow \left(\frac{x_0^2}{a^2} + \frac{y_0^2}{b^2} + \frac{z_0^2}{c^2}\right)a^2 \le a^2$

$\Rightarrow x_0^2 + \left(\frac{y_0^2}{b^2} + \frac{z_0^2}{c^2}\right)a^2 \le a^2 \Rightarrow x_0^2 \le a^2 - \left(\frac{y_0^2}{b^2} + \frac{z_0^2}{c^2}\right)a^2 \Rightarrow x_0^2 \le \left(1 - \frac{y_0^2}{b^2} - \frac{z_0^2}{c^2}\right)a^2$

We see that $\frac{y_0^2}{b^2} + \frac{z_0^2}{c^2} \ge 0 \Rightarrow 0 \le 1 - \frac{y_0^2}{b^2} - \frac{z_0^2}{c^2} \le 1 \Rightarrow x_0^2 \le \left(1 - \frac{y_0^2}{b^2} - \frac{z_0^2}{c^2}\right)a^2 \Rightarrow x_0^2 \le a^2 \Rightarrow -a \le x_0 \le a$

Similarly, we can prove that $-b \le y_0 \le b$ and $-c \le z_0 \le c$ The stretched box C of the cube C_B has the dimension of $[-a, a] \times [-b, b] \times [-c, c]$ and we have proof from above that $-a \le x_0 \le a$ and $-b \le y_0 \le b$ and $-c \le z_0 \le c$

=> All points in the solid ellipsoid are contained in the hypercube C (proven)

(b) Show that the volume of K is approximated by

$$\text{vol}_K \approx 8abc\frac{N_B}{N},$$

where N_B is the number of points in C_B sampled from the unit ball

$$B = \{(u, v, w) \in \mathbb{R}^3 \mid u^2 + v^2 + w^2 \le 1\}.$$

First, we can write the volume of K is as:

$$\text{vol}_K = \text{vol}_C \frac{\text{vol}_K}{\text{vol}_C} = 2a \times 2b \times 2c \frac{\frac{4}{3}\pi abc}{2a \times 2b \times 2c} = 8abc\frac{\frac{4}{3}\pi abc}{8abc} = 8abc\frac{\frac{4}{3}\pi}{8}$$

Considering the ratio of the volume of unit ball over volume of cube with sides 2

$$\frac{\text{vol}_{Unit\,Sphere}}{\text{vol}_{C_B}} = \frac{\frac{4}{3}\pi 1 \times 1 \times 1}{2 \times 2 \times 2} = \frac{\frac{4}{3}\pi}{8} \Rightarrow \text{vol}_K = 8abc\frac{\frac{4}{3}\pi}{8} = 8abc\frac{\text{vol}_{Unit\,Sphere}}{\text{vol}_{C_B}}$$

Let N be the number of uniformly distributed points generated inside the cube C_B of side length 2 and N_B be the number of points of those generated points that lie inside the unit sphere. By the central limit theorem, as the sample size N approaches to infinity, the ratio $\frac{N_B}{N}$ starts to approach the ratio $\frac{\text{vol}_{Unit\,Sphere}}{\text{vol}_{C_B}} \Rightarrow \lim_{N\to\infty}\text{vol}_K = 8abc\frac{\text{vol}_{Unit\,Sphere}}{\text{vol}_{C_B}} \cong 8abc\frac{N_B}{N}$. Therefore, the volume of the ellipsoid can be approximated by the formula $\text{vol}_K \approx 8abc\frac{N_B}{N}$.

This formula can also be correct even if the points are not uniformly distributed.

(c) Using the Monte Carlo method, write a MATLAB program that computes an approximation of the volume vol_K of the ellipsoid corresponding to $a = 1$, $b = 2$, and $c = 3$, and adds the computation of $\mathrm{vol}_K/8$.

The Matlab code for MonteCarlo.m is

```
clc;
format long
a = 1; b = 2; c = 3;
volC = 8*a*b*c;
N = input("Enter the number of uniformly distributed points: ");
X = rand(N,3).*2 - 1 ;
[numPoints, vectorSize] = size(X);
countInsideSphere = 0;
lie_inside_sphere = @(u, v, w) u^2 + v ^2 + w^2 <= 1;
for i=1:numPoints
    point = X(i,:);
    if lie_inside_sphere(point(1),point(2),point(3))
        countInsideSphere = countInsideSphere + 1;
    end
end
disp("Number of uniformly generated points inside the cube of side
2: " + numPoints);
disp("Number of points inside the unit sphere: " +
countInsideSphere);
ratio = countInsideSphere/numPoints;
disp("The ratio of '(4/3pi)/8'(0.523599) approximated by the Monte
Carlo method: " + ratio);
volKtrue = volC * (4/3 * pi)/8;
disp("True volume of ellipsoid K: " + volKtrue)
volKapprox = volC * ratio;
disp("Approximated volume of ellipsoid K by Monte Carlo method: " +
volKapprox)
piApprox = ratio*8/(4/3);
disp("Approximation of pi: " + piApprox)
```

Inputting 100000 uniformaly distributed points, we get the results as follows:

```
Enter the number of uniformly distributed points: 100000
Number of uniformly generated points inside the cube of side 2: 100000
Number of points inside the unit sphere: 52355
The ratio of '(4/3pi)/8'(0.523599) approximated by the Monte Carlo method: 0.52355
True volume of ellipsoid K: 25.1327
Approximated volume of ellipsoid K by Monte Carlo method: 25.1304
Approximation of pi: 3.1413
fx >>
```