MATH661 Project 3 - Operator approximation in Sturm-Liouville eigenbasis

Posted: 11/30/22

Due: 12/02/22 11:55PM (First Draft), 12/07/22, 5:00PM (Final Draft)

- Julia SpecialFunctions package installation (only needs to be invoked once, will be used in this assignment)

This serves both as your final project and final examination. The topic you are exploring is the use of problem-specific bases. In the project, an academic analytical cyclindrical function basis is used to exemplify the idea, but in practice bases are extracted from the problem itself. The monograph by Patera and Rozza in the `MATH661/bibliography` directory presents a full treatment. This final examination is meant to be completed in 3-9 hours. Read through the Introduction prior to December 2, add the `SpecialFunctions` package to your Julia environment, and complete a first draft during the regularly scheduled Final Examination time of on Saturday, Dec. 2. Comments on the first draft will be returned by 3:00PM on Monday Dec. 5. Address the comments and submit a second, final draft during the reading day, Dec. 7.

1 Introduction

1.1 Sturm-Liouville eigenfunctions

It is traditional to introduce the main concepts in operator approximation using the monomial basis $\mathcal{M}=\{1,t,t^2,\ldots\}$ in which integration and differentiation operations are simple to carry out. However, in numerical work algorithm conditioning, stability, and accuracy are more important than easy-to-use analytical formulas. This final project brings together all main course concepts to construct approximation procedures for problems that are naturally stated in the eigenfunctions of a Sturm-Liouville problem for an orthogonal, curvilinear coordinate system.

1.1.1 Regular Sturm-Liouville problems

The regular Sturm-Liouville problem (SLP) is to find $y\colon [a,b]\rightarrow\mathbb{R}$, twice differentiable that satisfies

$$L(y)=\frac{\mathrm{d}}{\mathrm{d}x}[w(x)\,y']+[q(x)+\lambda p(x)]y=0, \tag{1}$$

with the two-point boundary value conditions $V(y) = 0$

$$A_1\, y(a) + B_1 y'(a) = 0,$$

$$A_2\, y(b) + B_2 y'(b) = 0.$$

The functions p, q are continuous and w is differentiable. The SLP is linear in operator L and boundary conditions V. When $w(x) > 0$ and $p(x) > 0$ the SLP is said to be regular. A singular SLP results when $w(x) = 0$ for some $x \in [a, b]$.

1.1.2 Physical conservation laws

The ubiquity of SLPs is due to physics being naturally expressed through a small set of conservation laws, e.g., mass, momentum, energy, and electrical charge in classical physics (additional quantum conservation laws arise from quantum mechanics). Consider the familiar statement from mechanics

$$\boldsymbol{F} = m\boldsymbol{a},$$

more properly written as

$$\frac{\mathrm{d}}{\mathrm{d}t}(\boldsymbol{H}) = \boldsymbol{F},$$

stating that the rate of change of a point mass's momentum $\boldsymbol{H}$ is due to the sum of applied forces $\boldsymbol{F}$. In the absence of any external forces the momentum is conserved

$$\frac{\mathrm{d}}{\mathrm{d}t}(\boldsymbol{H}) = 0 \Rightarrow \boldsymbol{H} = \text{constant}.$$

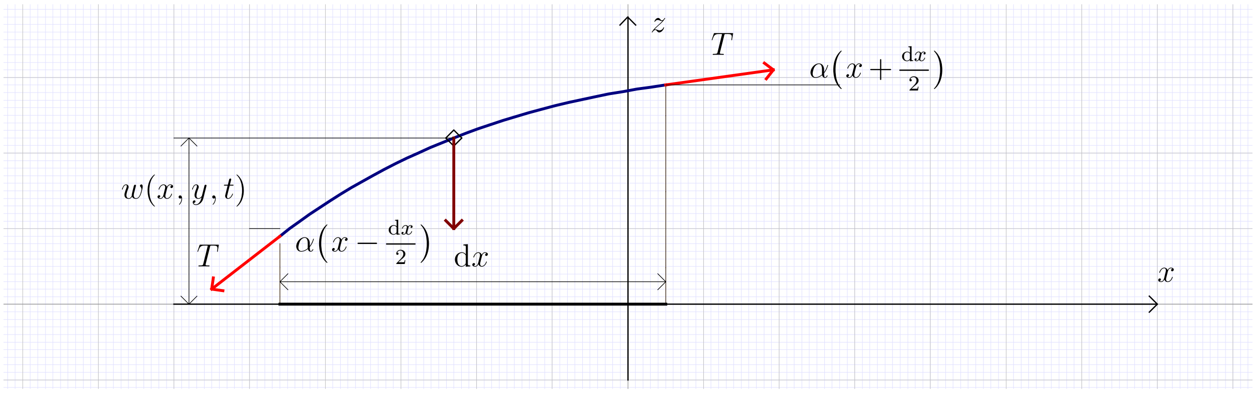
When applied to continua, conservation laws lead to PDEs, for example the motion of a drumhead membrane. An infinitesimal portion of membrane of area $\mathrm{d}A = \mathrm{d}x\,\mathrm{d}y$ has mass $\mathrm{d}m = \rho \mathrm{d}A$ and is brought out of its equilibrium position by small displacement $w(x, y, t)$ along the z-axis, such that the tangent makes angle $\alpha \cong \sin\, \alpha \cong \tan\, \alpha = \partial w / \partial x$. The membrane is stretched from its equilibrium position by tension T, and the resultant force on the infinitesimal portion is

$$T\left[\frac{\partial w}{\partial x}\left(x + \frac{\mathrm{d}x}{2}\right) - \frac{\partial w}{\partial x}\left(x - \frac{\mathrm{d}x}{2}\right)\right] \cong T\,\frac{\partial^2 w}{\partial x^2}.$$

A similar argument along the y-axis then gives the wave equation

$$w_{tt} = c^2\, \mathrm{div}\, (\mathrm{grad}\, w) = c^2\, \nabla \cdot (\nabla w) = c^2 (w_{xx} + w_{yy}),$$

with $w_{xx} = \partial^2 w / \partial x^2$, etc., and $c^2 = T / \rho$.



For a square-shaped drumhead with edge-length a that is pinned along its perimeter, separation of variables $w(x,y,t)=X(x)Y(y)T(t)$ then leads to

$$\frac{1}{c^2}\frac{T''}{T}=\frac{X''}{X}+\frac{Y''}{Y}=-\frac{\omega^2}{c^2}$$

and three SLPs, e.g., along x

$$X''+n^2X=0, X(0)=X(a)=0.$$

The eigenfunctions in this case are the familiar trig-functions $\sin(n\pi x/a)$. These eigenfunctions play a fundamental role in problems stated in Cartesian coordinates, as exemplified by Fourier transforms.

1.1.3 Differential operators in curvilinear coordinates

Consider now a circular-shaped of radius $r=a$ drum pinned along its perimeter, in which case it is convenient to carry out separation of variables in polar coordinates $w(r,\theta,t)=R(r)\Theta(\theta)T(t)$. The wave equation in polar coordinates

$$w_{tt}=c^2\nabla\cdot(\nabla w)=c^2\left[w_{rr}+\frac{1}{r}w_r+\frac{1}{r^2}w_{\theta\theta}\right],$$

then leads to

$$\frac{1}{c^2}\frac{T''}{T}=\frac{R''}{R}+\frac{1}{r}\frac{R'}{R}+\frac{1}{r^2}\frac{\Theta''}{\Theta}=-\frac{\omega^2}{c^2},$$

and assuming rotational symmetry around the z-axis, $\Theta''=0$, gives two ODEs

$$T''+\omega^2T=0\Rightarrow T(t)=A\cos(\omega t)+B\sin(\omega t),$$

for which initial conditions are given, and the SLP

$$R''+\frac{1}{r}R'+k^2R=0, R(0)\text{ finite}, R(a)=0, k^2=\frac{\omega^2}{c^2}. \tag{2}$$

The ODE has general solution

$$R(r) = A\,J_0(kr) + B\,Y_0(kr),$$

and imposing boundary conditions leads to $B = 0$ (to maintain finite $R(0)$) and

$$J_0(ka) = 0, \tag{3}$$

with a denumerable set of solutions k_n, $n = 1, 2, \ldots$, the eigenvalues of the SLP, $k_1 < k_2 < \cdots$. The corressponding eigenfunctions are $y_n(r) = J_0(k_n r)$, and can be evaluated in Julia through the `besselj0()` function. SLP eigenfunctions are orthogonal with respect to the scalar product

$$(f, g) = \int_0^a p(r)\, f(r)\, g(r) \mathrm{d}r,$$

i.e.

$$m \neq n \Rightarrow \int_0^a p(r)\, J_0(k_m r)\, J_0(k_n r) \mathrm{d}r = 0.$$

The Bessel function has an asymptotic approximation

$$J_0(x) \cong \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{\pi}{4}\right),$$

useful in initial approximation of the eigenvalues from (3). Another useful result is

$$\frac{\mathrm{d}}{\mathrm{d}x} J_0(x) = -J_1(x),$$

evaluated by the `besselj1()` Julia function.

In the following length units are chosen such that the drumhead has radius $a = 1$.

2 Track 1 & 2 common problems

1. Use Newton's method to find the first $n = 64$ eigenvalues by solving (3) numerically to six-digit accuracy (relative error $\varepsilon < 10^{-6}$). Plot the eigenvalues. Plot the $j = 1, 2, 4, 8, 16, 32$ eigenfunctions $y_j(r)$. Comment on the basis functions by comparison, say, to the monomial basis $\{1, r, r^2, \ldots\}$.

   Solution:

   We will apply Newton's method to find n solutions of the equation $J_0(k) = 0$. Figure 1 shows the plot of $J_0(x)$, which looks roughly like oscillating sinusodal function that decays gradually.

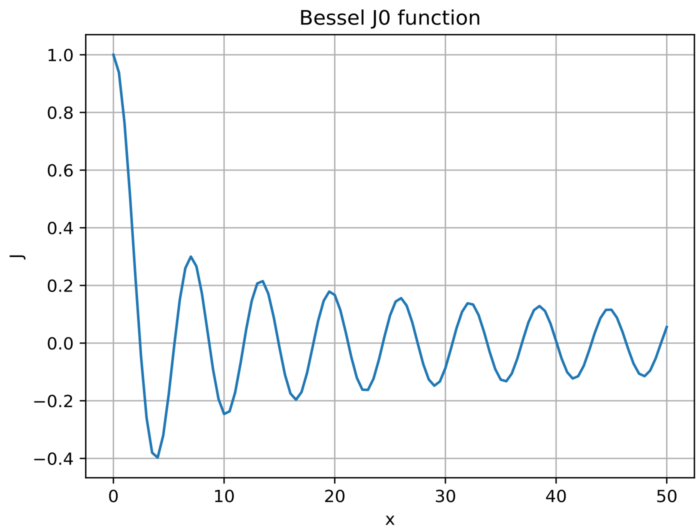


Figure 1. Plot of Bessel J_0 function. It has infinitely many solutions. Use Insert->Image->Insert image to include figure in document

The Newton's algorithm can make use of `besselj0()` for the objective function and `-besselj1()` for its derivative function. We can implement the Newton's method algorithm to find the first root in 6-digit accuracy as follows. Figure 1 suggests that the inital value $x_0 = 1$ would be a moderate choice.

Algorithm Newton

Input : x_0, f, f', tolerance ϵ,
max iteration N
Output: root k
for $i = 1$ to N
  $y = f(x_0)$
  $y' = f'(x_0)$
  $x_1 = x_0 - y / y'$
  if $(x_1 - x_0 < \epsilon)$
    return x_1
  $x_0 = x_1$
end

```
∴ function Newton(x, f, df, tol,
  max_it=1000)
    for i=1:max_it
      y=f(x)
      dy=df(x)
      x1 = x - y/dy
      if abs(x1-x) <= tol
        return x1
      end
      x = x1
    end
  end;
```

```
∴ function dbesselj0(x) return
  -besselj1(x) end;
```

```
∴
```

```
∴ x0=1;tol=1e-6; k0=Newton(x0,besselj0,dbesselj0,tol)
```

2.404825557695773

```
∴
```

Again, Figure 1 suggests that the ditance between successive roots are roughly around 3. We can find the next root successively by applying the Newton's method again with initial value k_0+2, where k_0 is the previous root found. The left plot of Figure 2 shows the plot of first $n=64$ eigenvalues obtained. The right figure of Figure 2 shows that the distance between successive eigenvalues converges to a value around π.

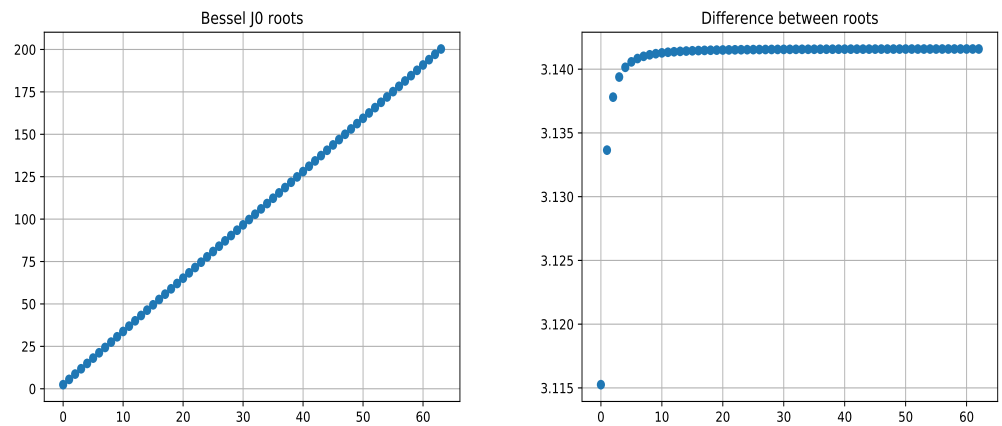
- 

Figure 2. Plot of $n=64$ roots J_0 function (Left) and the difference between successive roots (Right).

```
∴ k = [k0];n=64;diff=[];
∴ for i=2:n
    global k,diff
    k=[k; Newton(k[i-1]+2,besselj0,dbesselj0,tol)]
    diff=[diff; k[i]-k[i-1]]
  end
∴ clf();plot(k,"o");grid("on");
∴ title("Bessel␣J0␣roots");savefig(FigPrefix*"F01root.eps");
∴ clf();plot(diff,"o");grid("on");
∴ title("Difference␣between␣roots");savefig(FigPrefix*"F01rootdiff.eps");
∴
```

$y_n(r) = J_0(k_n\, r)$ is a solution to the equation (2), thus y_n is an eigenfunction corresponds to eigenvalue $\lambda = k_n^2$. Figure 3 plots the $j=1,2,4,8,16,32$ eigenfunctions $y_j(r)$. Compared to the monomial basis set, Bessel functions have a regulation that they are orthogonal respect to a scalar product. It differs in their periodicity, amplitude and topologies. The Bessel eigenfunctions will construct linearly independent basis while the monomial basis are likely to form linearly dependent basis No, the monomials do form a basis, hence by definition they're linearly independent. The problem is that the condition number increases, which you can interpret as a "distance" to being linearly dependent. This is due to the magnitude of monomial basis values becomes large as the number of basis grows making the lower-degree values marginal compared to the largest value.

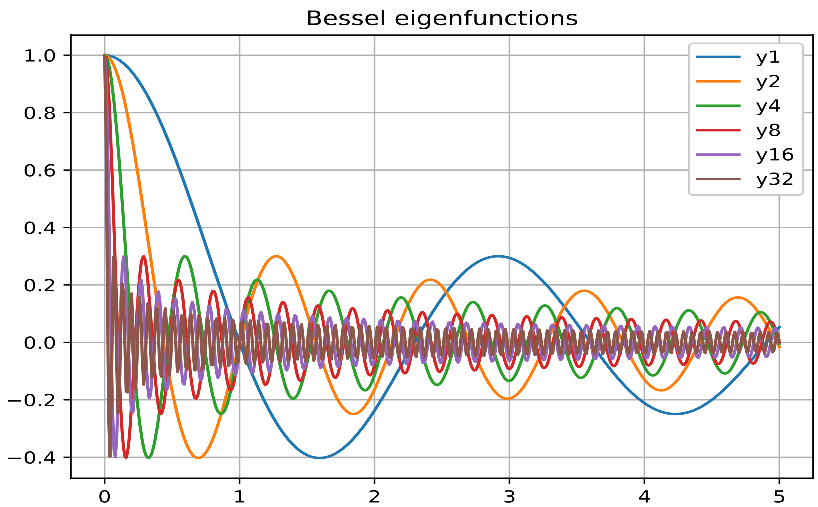


Figure 3. Plot of eignefunctions $y_n(r) = J_0(k_n r)$ for $n = 1, 2, 4, 8, 16, 32$. Scale to the same subinterval, similar to presenting $\sin(x), \sin(2x), \ldots$ on the interval 0 to 2pi]

2. Identify in (2) the functions w, r, p from the general formulation of a SLP (1). Verify eigenfunction orthogonality numerically through the approximation

$$(y_m, y_n) = \int_0^1 p(r)\, y_m(r)\, y_n(r)\, \mathrm{d}r \cong \boldsymbol{y}_m^T \boldsymbol{P} \boldsymbol{y}_n \tag{4}$$

where $\boldsymbol{y}_m$ is a sampling of the eigenfunction at nodes $\boldsymbol{r} = [r_i] \in \mathbb{R}^N$

$$h = 1/N, r_i = i h, i = 1, \ldots, N,$$

and the scalar product weight $p(r)$ determines the diagonal matrix $\boldsymbol{P} = \operatorname{diag}(p(\boldsymbol{r}))$. The approximation (4) is a (right) Darboux sum, or approximation of the integral by a piecewise constant function. Plot the orthogonality error $\|\boldsymbol{Y}^T \boldsymbol{P} \boldsymbol{Y}\|$ with increasing $N = 2^q$, $q = 3, \ldots, 12$ in log coordinates.

Solution:

Rewrite (1) as

$$w(x) y'' + w'(x) y' + (q(x) + \lambda p(x)) y = 0,$$

and compare it with (2),

$$R'' + \frac{1}{r} R' + k^2 R = 0.$$

$w'/w = 1/r$ leads to $w(r) = Ar$. Set $\lambda = k^2$ then we also get $q(r) = 0$, $p(r) = Ar$. We can set $A = 1$ to get $p(r) = w(r) = r$.

- `Darboux(m,k,q)` function returns the approximation $\widehat{(y_m,\ y_k)} \cong \boldsymbol{y}_m^T \boldsymbol{P} \boldsymbol{y}_k$ value derived from $N = 2^q$ equidistant samples on [0,1].

```
∴ function Darboux(m,k,q)
            N=2 ^q; r = (1:N)/N
            return sum(y.(r,m) .* r .* y.(r,k))
  end;
```

```
∴
```

- `orthoErr` returns the norm of the vector $\{\widehat{(y_m,\ y_k)}\}_{m=k+1,\ldots,n,k=1,\ldots,n}$

```
∴ function orthoErr(q, Apprx)
     e=[];for k=1:(n-1)
     e=[e; Apprx.((k+1):n,k,q)]
     end
     return(norm(e))
  end;
```

```
∴
```

Figure 4 plots the orthogonality errors for $q = 3, \ldots, 12$. We can observe that the norm of the error starts to decrease linearly in log scale when q is larger then 5, implying the exponential convergence of the error. This confirms that the Darboux sum performs better if we make partition dense.

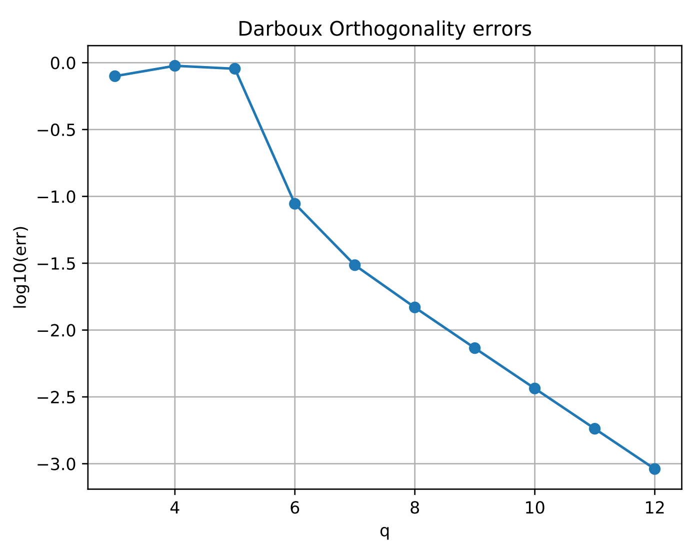
- 

Figure 4. Orthogonality errors based on the Darboux sum with increasing $N = 2^q$, $q = 3, \ldots, 12$ in log coordinates. Estimate an order of convergence.

3 Track 1 problems

3. Increase the accuracy of scalar product evaluation by replacing (4) by:

   a) midpoint integration;

   b) trapezoid integration;

   c) Simpson integration.

For each of the above, plot the orthogonality error

Solution:

Here we compare the approximation of $(y_m, y_n) = \int_0^1 p(r)\, y_m(r)\, y_n(r)\, \mathrm{d}r = 0$ for $m \neq n$. Set $f(r) = p(r)\, y_m(r)\, y_n(r)$.

a) midpoint integretion

The midpoint integration approximates the integration as

$$\int_0^1 f(t)\, \mathrm{d}t \approx \sum_{i=1}^{n} f(m_i) h,$$

where $h = \frac{1}{N}$, $m_i = r_i - \frac{h}{2} = \frac{2i-1}{2N}$. This was derived from the constant approximation of the function $f(t)$.

```
∴ function f(r, m,k)
          return y(r,m) * r * y(r,k)
  end;
```

```
∴ function Midpoint(m,k,q)
          N=2 ^q; r = (2 .*(1:N) .-1)/(2*N)
          return sum(f.(r,m,k))/N
  end;
```

```
∴
```

b) trapezoid integration;

The trapezoid integration approximates the integration as

$$\int_0^1 f(t)\, \mathrm{d}t \approx \frac{h}{2}\left(f(r_0) + f(r_N) + \sum_{i=1}^{N-1} 2 f(r_i) \right)$$

where $h = \frac{1}{N}$, $r_i = i h$. This was derived from the linear approximation of the function $f(t)$.

```
∴ function Trapezoid(m,k,q)
              N=2 ^q; r = (1:(N-1))/N;
              return (f(1,m,k)+2*sum(f.(r,m,k)))/(2*N)
  end;
```

```
∴
```

c) Simpson integration.

The Simpson integration approximate the integration as

$$\int_0^1 f(t)\,\mathrm{d}t \approx \frac{h}{3}\left(f(r_0) + 4\sum_{i=1}^{N/2} f(r_{2i-1}) + 2\sum_{i=1}^{N/2-1} f(r_{2i}) + f(r_N) \right),$$

where $h = \frac{1}{N}$, $r_i = ih$. This was derived from the quadratic approximation of the function $f(t)$.

```
∴ function Simpson(m,k,q)
              N=2 ^q; M=2 ^(q-1);
              r1=2 .*(1:M).-1;r2=2 .*(1:(M-1))
              return (f(1,m,k)+4*sum(f.(r1,m,k)) +
  2*sum(f.(r2,m,k)))/(3*N)
  end;
```

```
∴
```

The approximation (a), (b), (c) improves the approximation repectively from constant to linear to quadratic approximation.

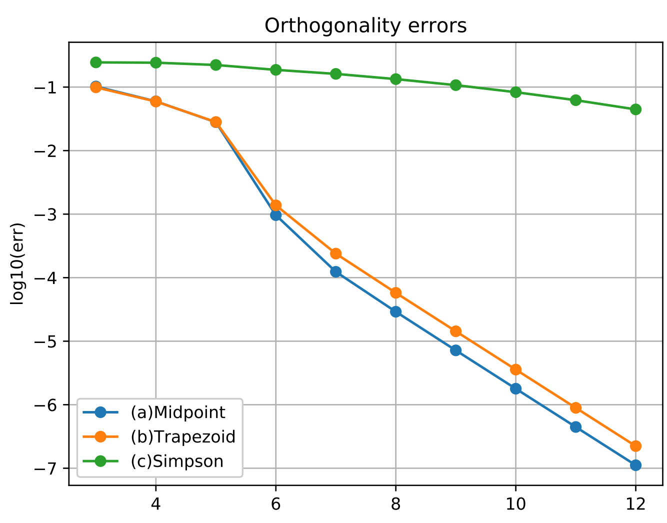
○ 

Figure 5. Orthogonality errors based on the Darboux sum with increasing $N = 2^q$, $q = 3, \ldots, 12$ in log coordinates. Very good. Are you obtaining the expected orders of convergence?

4 Track 2 problems

1. Increase the accuracy of scalar product evaluation by replacing (4) by:

    a)

    b) trapezoid integration;

    c) Simpson integration.

    For each of the above, plot the orthogonality error

2.