

1 Undetermined Coefficients [25%]

States u_i are given at three nodes in a non-uniform, one-dimensional grid, as shown below. Using the method of undetermined coefficients, derive the most accurate formula for du/dx at node 2, and give the order of accuracy, with respect to h , of your formula.

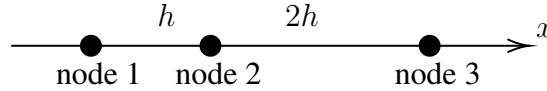


Figure 1: Undetermined coefficients non-uniform, one-dimensional grid.

First I will consider forward, backward, and central differences

Forward Difference:

$$\sum_{i=2}^3 a_i u_i = a_2 u_2 + a_3 u_3$$

$$u_3 \approx u_2 + 2hu' + \frac{1}{2}(2h)^2 u'' + \frac{1}{6}(2h)^3 u'''$$

$$\frac{du}{dx}|_2 = a_2 u_2 + a_3 \left(u_2 + 2hu' + \frac{1}{2}(2h)^2 u'' + \frac{1}{6}(2h)^3 u''' \right)$$

This gives the following systems of equations,

$$a_2 + a_3 = 0, \quad 2ha_3 = 1 \text{ Solving gives, } a_3 = \frac{1}{2h}, \quad a_2 = -\frac{1}{2h}$$

$$\frac{du}{dx}|_2 \approx \frac{1}{2h}(u_3 - u_2)$$

$$a_3 2h^2 u'' \rightarrow \frac{1}{2h} 2h^2 u'' \rightarrow hu'', \quad \mathcal{O}(h) \rightarrow \text{First-Order}$$

Backward Difference:

$$\sum_{i=1}^2 a_i u_i = a_1 u_1 + a_2 u_2$$

$$u_1 \approx u_2 + (-h)u' + \frac{1}{2}(-h)^2 u'' + \frac{1}{6}(-h)^3 u'''$$

$$\frac{du}{dx}|_2 = a_1 \left(u_2 + (-h)u' + \frac{1}{2}(-h)^2 u'' + \frac{1}{6}(-h)^3 u''' \right) + a_2 u_2$$

$$a_1 + a_2 = 0, \quad -ha_1 = 1, \text{ Solving gives, } a_1 = -\frac{1}{h}, \quad a_2 = \frac{1}{h}$$

$$\frac{du}{dx}|_2 \approx \frac{1}{h}(u_2 - u_1)$$

$$a_1 \frac{h^2}{2} u'' \rightarrow -\frac{1}{h} \frac{h^2}{2} u'' \rightarrow -\frac{h}{2} u'', \quad \mathcal{O}(h) \rightarrow \text{First-Order}$$

Central Difference:

$$\sum_{i=1}^3 = a_1 u_1 + a_2 u_2 + a_3 u_3$$

Using the expressions for u_1 and u_3 from forward and backward gives,

$$\begin{aligned} & a_1(u_2 - hu' + \frac{1}{2}h^2u'' - \frac{1}{6}h^3u''') + \dots \\ & a_2u_2 + \dots \\ & a_3(u_2 + 2hu' + 2h^2u'' + \frac{4}{3}h^3u''') \end{aligned}$$

This gives the following systems of equations,

$$\begin{aligned} a_1 + a_2 + a_3 &= 0 \\ -ha_1 + 2ha_3 &= 1 \\ \frac{1}{2}h^2a_1 + 2h^2a_3 &= 0 \end{aligned}$$

Solving for a_1 , a_2 , a_3 gives,

$$a_1 = -\frac{2}{3h}, \quad a_2 = \frac{1}{2h}, \quad a_3 = \frac{1}{6h}$$

This gives that the approximation is,

$$\left. \frac{du}{dx} \right|_2 \approx \frac{1}{6h} (u_3 + 3u_2 - 4u_1)$$

Finding the order of accuracy can be done by,

$$\begin{aligned} & \left(a_1 \frac{1}{2}h^2 + a_3 2h^2 \right) u'' \\ & \left(-\frac{2}{3h} \frac{1}{2}h^2 + \frac{1}{6h} 2h^2 \right) u'' \\ & \left(-\frac{1}{3}h + \frac{1}{3}h \right) u'' = 0u'' \end{aligned}$$

Need to go higher,

$$\begin{aligned} & \left(a_1 \left(-\frac{1}{6} \right) h^3 + a_3 \left(\frac{4}{3} \right) h^3 \right) u''' \\ & \left(\frac{2}{3h} \frac{1}{6}h^3 + \frac{1}{6h} \frac{4}{3}h^3 \right) \\ & \rightarrow \left(\frac{h^2}{9} + \frac{2}{9}h^2 \right) u''' \rightarrow \frac{h^2}{2}u''' \end{aligned}$$

Thus, a central order difference is more accurate $\mathcal{O}(h^2)$, meaning that it is second-order accurate and is more accurate than forward or backward differences (with them being first-order). The expression for du/dx at node 2 is given below.

$$\left. \frac{du}{dx} \right|_2 \approx \frac{1}{6h} (u_3 + 3u_2 - 4u_1)$$

2 Gram Schmidt [25%]

Using the function inner product $(f, g) = \int_0^1 f g \, dx$, apply the Gram-Schmidt algorithm to orthonormalize the following two one-dimensional functions.

$$f_1 = x^4, \quad f_2 = 2x.$$

Then, project the function $g = x^2$ onto the space spanned by these two functions.

First is to orthogonalize the basis function,

$$\begin{aligned} u_1 &= f_1 = \boxed{x^4} \\ u_2 &= f_2 - \frac{(u_1, f_2)}{(u_1, u_1)} u_1 \\ &= 2x - \frac{\int_0^1 x^4 \cdot 2x \, dx}{\int_0^1 x^4 \cdot x^4 \, dx} x^4 = 2x - \frac{\int_0^1 2x^5 \, dx}{\int_0^1 x^8 \, dx} x^4 \\ &= 2x - \frac{1/3}{1/9} x^4 = \boxed{2x - 3x^4} \end{aligned}$$

Then next is to normalize the orthonormal functions,

$$\begin{aligned} u_{1,norm} &= \frac{u_1}{\sqrt{(u_1, u_1)}} = \frac{x^4}{\sqrt{\int_0^1 x^8 \, dx}} = \frac{x^4}{1/3} \\ u_{2,norm} &= \frac{u_2}{\sqrt{(u_2, u_2)}} = \frac{(2x - 3x^4)}{\sqrt{\int_0^1 (2x - 3x^4)^2 \, dx}} = \frac{2x - 3x^4}{1/\sqrt{3}} \end{aligned}$$

$$\boxed{u_{1,norm} = 3x^4, \quad u_{2,norm} = \sqrt{3} (2x - 3x^4)}$$

The projection of the vector can be expressed as

$$\text{proj}_{u_i}(g) = \frac{(u_i, g)}{(u_i, u_i)} u_i$$

Performing the projection of the orthonormal vector gives,

$$\begin{aligned} \text{proj}_{u_1}(g) &= \frac{(u_1, g)}{(u_1, u_1)} u_1 = \frac{\int_0^1 x^4 \cdot x^2 \, dx}{\int_0^1 x^4 \cdot x^4 \, dx} x^4 = \frac{\int_0^1 x^6 \, dx}{\int_0^1 x^8 \, dx} x^4 = \boxed{\frac{9x^4}{7}} \\ \text{proj}_{u_2}(g) &= \frac{(u_2, g)}{(u_2, u_2)} u_2 = \frac{\int_0^1 (2x - 3x^4) \cdot x^2 \, dx}{\int_0^1 (2x - 3x^4) \cdot (2x - 3x^4) \, dx} (2x - 3x^4) \end{aligned}$$

Computing the integral on matlab gives,

$$= \frac{\int_0^1 x^2 (2x - 3x^4) \, dx}{\int_0^1 (2x - 3x^4)^2 \, dx} (2x - 3x^4) = \boxed{\frac{3x}{7} - \frac{9x^4}{14}}$$

Again, expressing in vector form the projection of g onto the orthonormal vector function \vec{u} gives,

$$\boxed{\text{proj}_{u_1}(g) = \frac{9x^4}{7}, \quad \text{proj}_{u_2}(g) = \frac{3x}{7} - \frac{9x^4}{14}}$$

Checking that these are orthogonal taking the inner product of (u_1, u_2) gives that the inner product is zero. Re-affirming that these are indeed orthogonal to each other. My matlab code can be found attached at the end of the assignment.

3 Gauss Seidel [25%]

Consider the successively over-relaxed, left-to-right Gauss-Seidel iterative smoother applied to a standard, second-order, central-difference discretization of the 1D Poisson equation ($-u_{xx} = f$) on $x \in [0, 1]$ with homogeneous Dirichlet boundary conditions. The grid is uniform and contains N intervals.

- a. Write an expression for the iteration matrix, $\underline{\underline{S}}$, for this smoother, using the decomposition $\underline{\underline{A}} = \underline{\underline{L}} + \underline{\underline{D}} + \underline{\underline{U}}$, where $\underline{\underline{A}}u = \underline{\underline{f}}$ is the discretized system, as in the notes. Note that ω is a successive over-relaxation factor, applied immediately on each node update.

Since I will be implementing a second-order central-difference discretization of 1D Poisson's equation with homogeneous Dirichlet boundary conditions. The expression $\underline{\underline{A}}u = \underline{\underline{f}}$

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ -1 & 2 & 1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 & 0 \\ \vdots & \vdots & & \ddots & \ddots & \ddots & \\ 0 & 0 & \cdots & 0 & -1 & 2 & -1 \\ 0 & 0 & \cdots & 0 & 0 & 0 & 1 \end{bmatrix}}_{\underline{\underline{A}}} \underbrace{\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ \vdots \\ u_n \\ u_{n+1} \end{bmatrix}}_{\underline{\underline{u}}} = \underbrace{\begin{bmatrix} 0 \\ h^2 f_2 \\ h^2 f_3 \\ \vdots \\ \vdots \\ h^2 f_n \\ 0 \end{bmatrix}}_{\underline{\underline{f}}}$$

Re-writing $\underline{\underline{A}}$ in terms of $\underline{\underline{L}}$, $\underline{\underline{D}}$, $\underline{\underline{U}}$ gives,

$$\underline{\underline{L}} = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ -1 & 0 & 0 & \cdots & 0 \\ 0 & \ddots & 0 & 0 & 0 \\ 0 & \cdots & -1 & 0 & 0 \\ 0 & \cdots & 0 & 0 & 0 \end{bmatrix}, \quad \underline{\underline{D}} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 2 & 0 & \cdots & 0 \\ 0 & 0 & \ddots & \cdots & 0 \\ 0 & \cdots & 0 & 2 & 0 \\ 0 & \cdots & 0 & 0 & 1 \end{bmatrix}, \quad \underline{\underline{U}} = \begin{bmatrix} 0 & -1 & 0 & \cdots & 0 \\ 0 & 0 & \ddots & \cdots & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & \cdots & 0 & 0 & -1 \\ 0 & \cdots & 0 & 0 & 0 \end{bmatrix}$$

The smoothing iteration matrix is then given by,

$$\underline{\underline{S}} = -(\underline{\underline{D}} + \underline{\underline{L}})^{-1} \underline{\underline{U}}$$

Doing so and creating a general expression for the matrix I get that $\underline{\underline{S}}$ can be expressed to be,

$$\underline{\underline{S}} = \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots & \cdots & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & \cdots & \cdots & 0 & 0 \\ 0 & 0 & \frac{1}{4} & \frac{1}{2} & \ddots & \cdots & 0 & 0 \\ 0 & 0 & \frac{1}{8} & \frac{1}{4} & \ddots & \ddots & 0 & 0 \\ 0 & 0 & \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \frac{1}{2^{n-1}} & \cdots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \frac{1}{2^n} & \frac{1}{2^{n-1}} & \cdots & \frac{1}{8} & \frac{1}{4} & \frac{1}{2} \\ 0 & 0 & \cdots & \cdots & 0 & 0 & 0 & 0 \end{bmatrix}$$

Looking to the matrix above, it takes the form that the first two columns are completely zero and that the first/last rows are fully zero as well. Then along the lower matrix it follows a pattern of decreasing by factors of two from the value of the index above it. Meaning the values decrease in $\frac{1}{2}, \frac{1}{2^2}, \frac{1}{2^3}, \frac{1}{2^4}, \dots, \frac{1}{2^{n-1}}, \frac{1}{2^n}$ along the rows of the matrix along the diagonal.

- b. In the complex number plane, plot the eigenvalues of the iteration matrix, $\underline{\underline{S}}$, for this smoother, using $N = 32$ and an over-relaxation factor of $\omega = 1.5$.

Plotting the eigenvalues of the iteration matrix by the formula,

$$\lambda(\underline{\underline{S}}_\omega) = \omega\lambda(\underline{\underline{S}}) + (1 - \omega)$$

Gives the plot shown below in Figure 2,

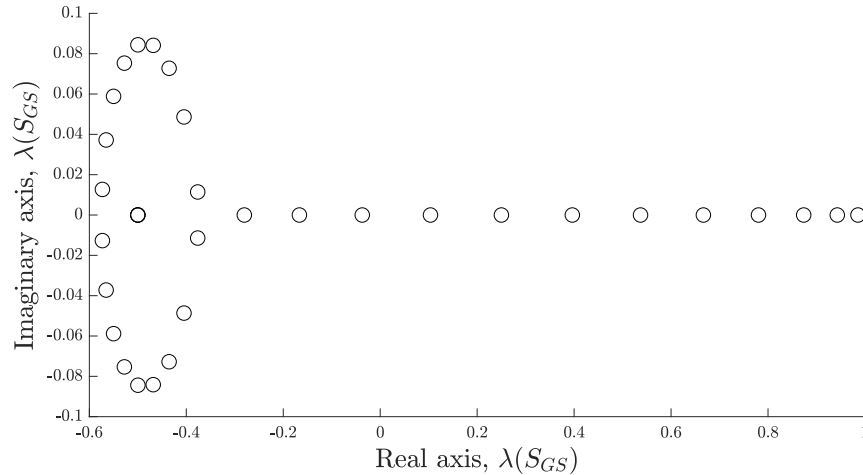


Figure 2: Eigenvalues in the complex number plane.

- c. Make a plot of the magnitude of the largest magnitude eigenvalue of $\underline{\underline{S}}$ versus ω , and identify the optimal over-relaxation factor. Use $N = 32$.

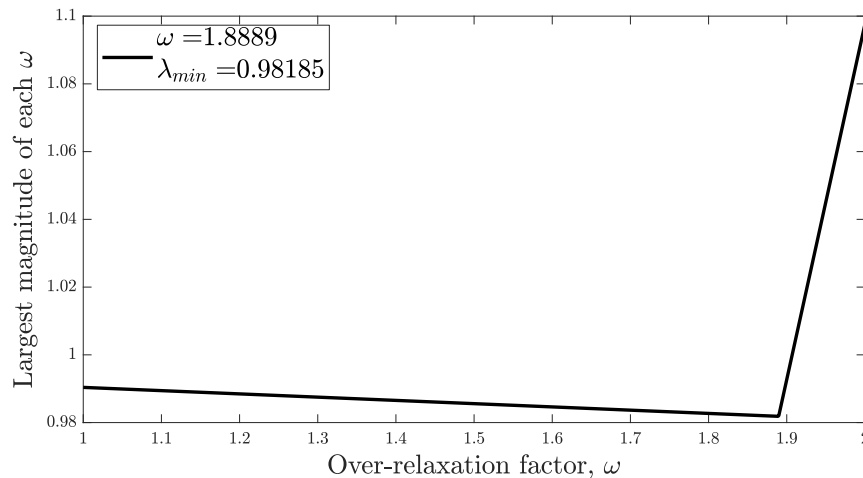


Figure 3: Determining the optimal over-relaxation factor.

Looking above to Figure 3, the optimal over-relaxation value occurs when the magnitude of the eigenvalues reach a minimum. This is because we need $\lambda(\underline{\underline{S}}) < 1$ for convergence and further from 1 for fast convergence. This minimum value can be found on the Figure to be $\lambda_{\min} = 0.98185$, at this minimum amplification factor the over-relaxation factor is found to be an optimal of $\omega = 1.8889$. Any value of ω greater than this value will risk deteriorating the convergence rates. Matlab code can be found attached at the end of my assignment.

4 Mesh Connectivity [25%]

Section 1.7.5 of the notes introduces matrices $\underline{\underline{E}}$ and $\underline{\underline{N}}$ for describing connections between elements and nodes of a mesh. Assume that both matrices are made unique by using a counter-clockwise ordering of nodes/elements and by beginning each row with the smallest index. Element/node numbering starts at 1 and no numbers are skipped. Assume triangular elements.

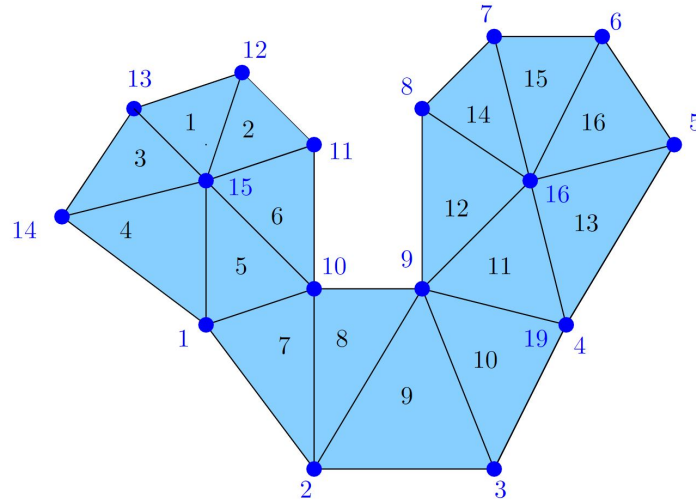


Figure 4: Triangular mesh grid.

- a. For the mesh shown above, write down the matrices $\underline{\underline{E}}$ and $\underline{\underline{N}}$.

$$\underline{\underline{E}} = \begin{bmatrix} 12 & 13 & 15 \\ 11 & 12 & 15 \\ 13 & 14 & 15 \\ 1 & 15 & 14 \\ 1 & 10 & 15 \\ 10 & 11 & 15 \\ 1 & 2 & 10 \\ 2 & 9 & 10 \\ 2 & 3 & 9 \\ 3 & 4 & 9 \\ 4 & 16 & 9 \\ 8 & 9 & 16 \\ 4 & 5 & 16 \\ 7 & 8 & 16 \\ 6 & 7 & 16 \\ 5 & 6 & 16 \end{bmatrix}, \quad \underline{\underline{N}} = \begin{bmatrix} 4 & 5 & 7 \\ 7 & 8 & 9 \\ 9 & 10 \\ 10 & 11 & 13 \\ 13 & 16 \\ 15 & 16 \\ 14 & 15 \\ 12 & 14 \\ 8 & 9 & 10 & 11 & 12 \\ 5 & 6 & 7 & 8 \\ 2 & 6 \\ 1 & 2 \\ 1 & 3 \\ 3 & 4 \\ 1 & 2 & 3 & 4 & 5 & 6 \\ 11 & 12 & 13 & 14 & 15 & 16 \end{bmatrix}$$

Shown above are the matrices for $\underline{\underline{E}}$ and $\underline{\underline{N}}$ for the irregular mesh as indicated in Section 1.7.5 of the course notes.

- b. Write a pseudo-code for efficiently determining $\underline{\underline{E}}$ given $\underline{\underline{N}}$. For this part, the rows of the $\underline{\underline{E}}$ matrix need not satisfy the ordering requirement.

Pseudo-Code

```

1: Create  $\underline{\underline{E}} = []$ 
2: for i = 1:length( $\underline{\underline{N}}$ )  Loop through all the nodes in  $\underline{\underline{N}}$ 
3:   for j = 1:max(size( $\underline{\underline{N}}$ (i,:)))  Loop through all the elements for a given node
4:      $\underline{\underline{E}}(\underline{\underline{N}}(i, j), \text{end}) = i$   Place the node value at the end of the the  $i^{\text{th}}$  column in  $\underline{\underline{E}}$ 
5:   end
6: end

```

This is the code in theory that should be implemented to be efficiently implemented meaning that it scales $\mathcal{O}(\text{size}(\underline{\underline{N}}))$. However, placing these values into the $\underline{\underline{E}}$ matrix is unique to each given coding programming language (i.e. C++ would use `.pushback()`) so in application, with Matlab at least, I would pre-allocate $\underline{\underline{E}}$ to be a matrix of nan and have several if, elseif statements to determine the ending index for a given iteration if the last index is nan and replace with the current node value from the iteration through $\underline{\underline{N}}$.

- c. How many edges (total, interior and boundary) are in the above mesh? Write a pseudo-code for efficiently determining the number of edges in a mesh given $\underline{\underline{E}}$.

Total: 31
 Interior: 17
 Boundary: 14

Pseudo-Code

```

1: Create  $\underline{\underline{N}}$  to have empty indices of nan
2: counter = 0  Initialize counter to be zero
3: for j = 1:max(size( $\underline{\underline{N}}$ ))  Loop through all the nodes
4:   for i = 1:max(size( $\underline{\underline{N}}$ (j, :)))  Loop through each element adjacent to a node
5:     if isnan( $\underline{\underline{N}}$ (j, i)) == 1  For easy implementation check if value is nan, because
                             if so it has been used before and should be skipped
6:       [row, col] = find( $\underline{\underline{N}}$  ==  $\underline{\underline{N}}$ (j,i))  Find the indices of the node
7:        $\underline{\underline{N}}(\text{row}(\text{end}), \text{col}(\text{end})) = \text{nan}$   Replace with nan to indicate it's been used
8:       counter += 1  Increment the counter
9:     end if, end for(i), end for(j)
10: counter -= 1  Since the final pass is inevitable without heavy modification, increment down after the full pass

```

In the pseudo-code shown above, it scales $\mathcal{O}(N)$ making it as efficient as possible in determining the number of edges. Actual code implementation can be found attached at the end of my assignment.

Matlab Code

Algorithm 1: Matlab code for Gram Schmidt orthonormalization.

```

1 %-----
2 clear all; clc; close all
3 %-----
4 syms x
5 f1 = x^4; f2 = 2*x;
6
7 u1 = f1;
8 u2 = f2 - int(u1*f2, x, 0, 1)/int(u1*u1, x, 0, 1) * u1;
9
10 int(u1*u2, x, 0, 1)
11 tolatex('u1norm', u1/sqrt(int(u1*u1, x, 0, 1)))
12 tolatex('u2norm', u2/sqrt(int(u2*u2, x, 0, 1)))
13
14 g = x^2;
15 proju1g = int(u1*g, x, 0, 1) / int(u1*u1, x, 0, 1)* u1;
16 proju2g = int(u2*g, x, 0, 1) / int(u2*u2, x, 0, 1)* u2;

```

Algorithm 2: Matlab implementation to determine over-relaxation factor for Gauss Seidel.

```

1 %-----
2 clear all; clc; close all
3 set(groot,'defaulttextinterpreter','latex');
4 set(groot, 'defaultAxesTickLabelInterpreter','latex');
5 set(groot, 'defaultLegendInterpreter','latex');
6 %-----
7 % Part b
8 N = 32; omega = 1.5;
9 D = eye(N+1); L = zeros(N+1); U = L;
10
11 for i = 1:N-1
12     L(i+1, i) = -1; % Fill the left-matrix
13 end
14 for i = 2:N
15     U(i, i+1) = -1;% Fill the right-matrix
16     D(i,i) = 2; % Fill the rest of the diagonals
17 end
18
19 Sgs = -inv(D + L)*U; % Solve for the iterative matrix
20 lambdas = omega.*eig(Sgs) + (1-omega);
21
22 figure()
23 scatter(real(lambdas), imag(lambdas), 75, 'ko')
24 xlabel('Real axis, $\lambda(S_{GS})$', 'fontsize', 16)
25 ylabel('Imaginary axis, $\lambda(S_{GS})$', 'fontsize', 16)
26 set(gcf, 'Color', 'w', 'Position', [200 200 800 400]);
27 export_fig('q3_eigens.eps')
28 %-----
29 % Part c
30 num = 1000;
31 omegas = linspace(1, 2, num);
32 eigval = eig(Sgs);
33
34 data = zeros(num, 1);
35 for i = 1:num
36     vals = omegas(i).*eigval + (1-omegas(i));
37     norms = sqrt(real(vals).^2 + imag(vals).^2);
38     data(i) = max(norms);
39 end
40
41 idx = find(data == min(data));
42
43 figure()
44 plot(omegas, data, 'k', 'linewidth', 2)
45 xlabel('Over-relaxation factor, $\omega$', 'fontsize', 16)
46 ylabel('Largest magnitude of each $\omega$', 'fontsize', 16)
47 legend(['$\omega = $', num2str(omegas(idx)), newline, '$\lambda_{\min} = $', num2str(min(data))],
         'location', 'best', 'fontsize', 16)
48 set(gcf, 'Color', 'w', 'Position', [200 200 800 400]);
49 export_fig('q3_omegas.eps')

```


Algorithm 3: Matlab implementation for determining number of edges on a mesh.

```

1  %-----
2  clear all; clc; close all
3  set(groot,'defaulttextinterpreter','latex');
4  set(groot, 'defaultAxesTickLabelInterpreter','latex');
5  set(groot, 'defaultLegendInterpreter','latex');
6  %-----
7  N = [4, 5, 7, nan, nan, nan; 7, 8, 9, nan, nan, nan;
8      9, 10, nan, nan, nan, nan; 10,11,13, nan, nan, nan;
9      13,16, nan, nan, nan, nan; 15,16, nan, nan, nan, nan;
10     14,15, nan, nan, nan, nan; 12,14, nan, nan, nan, nan;
11     8:12, nan; 5:8, nan, nan;
12     2,6, nan, nan, nan, nan; 1,2, nan, nan, nan, nan;
13     1,3, nan, nan, nan, nan; 3,4, nan, nan, nan, nan;
14     1:6; 11:16];
15  E = [12, 13, 15; 11, 12, 15; 13, 14, 15; 1, 15, 14; 1, 10, 15;
16      10, 11, 15; 1, 2 , 10; 2, 9 , 10; 2, 3 , 9; 3, 4 , 9;
17      4, 16, 9; 8, 9 , 16; 4, 5 , 16; 7, 8 , 16; 6, 7 , 16; 5, 6 , 16];
18
19  counter = 0;
20  for j = 1:max(size(N))
21      for i = 1:max(size(N(j, :)))
22          if isnan(N(j, i)) ~= 1
23              [row, col] = find(N == N(j, i));
24              N(row(end), col(end)) = nan;
25              counter = counter + 1;
26          end
27      end
28  end
29  counter = counter - 1;

```