Numerical Linear Algebra Homework Project 3: Eigenvalues and Eigenvectors

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Problem 1

(1) We want to reduce the symmetric matrix A

$$A = \begin{bmatrix} 4 & -1 & -1 & 0 \\ -1 & 4 & 0 & -1 \\ -1 & 0 & 4 & -1 \\ 0 & -1 & -1 & 4 \end{bmatrix} \tag{1}$$

to a tridiagonal form using Housholder similarity transformations. The matrix A can be expressed in the following, compact way:

$$A = \left[\begin{array}{c|c} a_{11} & \mathbf{x}^T \\ \hline \mathbf{x} & \hat{A}_1 \end{array}\right]. \tag{2}$$

Let us define the vector $\mathbf{u}_1$

$$\mathbf{u}_1 = \mathbf{x} + \text{sgn}(x_1)\|\mathbf{x}\|_2 \mathbf{e}_1 \tag{3}$$

thanks to which we can define the matrix $\hat{R}_1$

$$\hat{R}_1 = \mathbb{1}_3 - \frac{2}{\|\mathbf{u}_1\|_2^2}\mathbf{u}_1\mathbf{u}_1^T \tag{4}$$

and a new matrix R_1, as follows:

$$R_1 = \left[\begin{array}{c|c} 1 & \mathbf{0}^T \\ \hline \mathbf{0} & \hat{R}_1 \end{array}\right]. \tag{5}$$

We will not explicitly construct the matrix R_1, as we know that the product $R_1 A$ will assume the following form:

$$R_1 A = \left[\begin{array}{c|c} a_{11} & \mathbf{x}^T \\ \hline -\text{sgn}(x_1)\|\mathbf{x}\|_2 & \\ 0 & \hat{R}_1\hat{A}_1 \\ 0 & \end{array}\right], \tag{6}$$

where the first column is obtained by construction and the matrix $\hat{R}_1\hat{A}_1$ can be obtained by considering the matrix $\hat{A}_1$ written by columns as $\hat{A}_1 = \Big[(\hat{A}_1)_1, (\hat{A}_1)_2, (\hat{A}_1)_3\Big]$. Hence $\hat{R}_1\hat{A}_1 = \Big[(\hat{R}_1\hat{A}_1)_1, (\hat{R}_1\hat{A}_1)_2, (\hat{R}_1\hat{A}_1)_3\Big]$, where we know that a single column can be computed as:

$$(\hat{R}_1\hat{A}_1)_i = (\hat{A}_1)_i - \frac{2}{\|\mathbf{u}_1\|_2^2}\mathbf{u}_1\mathbf{u}_1^T(\hat{A}_1)_i. \tag{7}$$

By expliciting all the terms, we obtain:

$$R_1 A = \begin{bmatrix} 4 & -1 & -1 & 0 \\ \sqrt{2} & -2\sqrt{2} & -2\sqrt{2} & \sqrt{2} \\ 0 & -2\sqrt{2} & 2\sqrt{2} & 0 \\ 0 & -1 & -1 & 4 \end{bmatrix}. \tag{8}$$

Since we want to obtain a tridiagonal matrix, we have to compute the matrix $R_1 A R_1$, namely:

$$R_1 A R_1 = \left[\begin{array}{c|ccc} a_{11} & \|\mathbf{x}\|_2 & 0 & 0 \\ \hline \|\mathbf{x}\|_2 & & & \\ 0 & & \hat{R}_1\hat{A}_1\hat{R}_1 & \\ 0 & & & \end{array}\right]. \tag{9}$$

Knowing that $\hat{R}_1\hat{A}_1\hat{R}_1 = (\hat{R}_1\hat{A}_1\hat{R}_1)^T = (\hat{R}_1)^T(\hat{R}_1\hat{A}_1)^T = \hat{R}_1(\hat{R}_1\hat{A}_1)^T$, we can apply $\hat{R}_1$ to $(\hat{R}_1\hat{A}_1)^T$ by columns:

$$\left[\hat{R}_1\hat{A}_1\hat{R}_1\right]_i = \left[(\hat{R}_1\hat{A}_1)^T\right]_i - \frac{2}{\|\mathbf{u}_1\|_2^2}\mathbf{u}_1\mathbf{u}_1^T\left[(\hat{R}_1\hat{A}_1)^T\right]_i, \tag{10}$$

obtaining the following form for the matrix $R_1 A R_1$:

$$R_1 A R_1 = \begin{bmatrix} 4 & \sqrt{2} & 0 & 0 \\ \sqrt{2} & 4 & 0 & \sqrt{2} \\ 0 & 0 & 4 & 0 \\ 0 & \sqrt{2} & 0 & 4 \end{bmatrix}. \tag{11}$$

By identifying the submatrix $\hat{R}_1\hat{A}_1\hat{R}_1$ as

$$\hat{R}_1\hat{A}_1\hat{R}_1 = \begin{bmatrix} 4 & 0 & \sqrt{2} \\ 0 & 4 & 0 \\ \sqrt{2} & 0 & 4 \end{bmatrix} = \begin{bmatrix} (\hat{R}_1\hat{A}_1\hat{R}_1)_{11} & \mathbf{y}^T \\ \mathbf{y} & \hat{A}_2 \end{bmatrix}, \tag{12}$$

we can build the vector $\mathbf{u}_2$ as

$$\mathbf{u}_2 = \mathbf{y} + \operatorname{sgn}(y_1)\|\mathbf{y}\|_2\mathbf{e}_1^{(2)}, \tag{13}$$

with $\mathbf{e}_1^{(2)} = (1,0)^T$, which will allow us to define the matrix $\hat{R}_2$

$$\hat{R}_2 = \mathbb{1}_2 - \frac{2}{\|\mathbf{u}_2\|_2^2}\mathbf{u}_2\mathbf{u}_2^T. \tag{14}$$

Using the same logic, we obtain the i-th column of the matrix $\hat{R}_2\hat{A}_2$, namely:

$$(\hat{R}_2\hat{A}_2)_i = (\hat{A}_2)_i - \frac{2}{\|\mathbf{u}_2\|_2^2}\mathbf{u}_2\mathbf{u}_2^T(\hat{A}_2)_i, \tag{15}$$

and, by expliciting all the terms we obtain:

$$\hat{R}_2\hat{A}_2 = \begin{bmatrix} 0 & -4 \\ -4 & 0 \end{bmatrix}. \tag{16}$$

As before, we can compute $\hat{R}_2\hat{A}_2\hat{R}_2$ by columns, and the final form of the matrix will be:

$$R_2 R_1 A R_1 R_2 = \begin{bmatrix} 4 & \sqrt{2} & 0 & 0 \\ \sqrt{2} & 4 & -\sqrt{2} & 0 \\ 0 & -\sqrt{2} & 4 & 0 \\ 0 & 0 & 0 & 4 \end{bmatrix}. \tag{17}$$

As we can see, we have reduced the initial matrix A to a tridiagonal form.

(2) In the following we report the script where we implement the QR diagonalization of a matrix A, defined as:

$$A = \begin{bmatrix} 4 & 3 & 2 & 1 \\ 3 & 4 & 3 & 2 \\ 2 & 3 & 4 & 3 \\ 1 & 2 & 3 & 4 \end{bmatrix}. \tag{18}$$

```
import numpy as np
import matplotlib.pyplot as plt

# Set the initial values
tol = 1e-5
counter = 0
t = 1 # Initial exponent for the tolerance

# Set the number of significant digits
np.set_printoptions(precision=15, suppress=True)

# Construct the matrix A
A = np.array([[4,3,2,1],[3,4,3,2],[2,3,4,3],[1,2,3,4]])
# Compute the exact eigenvalues
exact_eigenvalues = np.linalg.eigvals(A)

# Initialize an empty list to store the number of iterations at each t
t_counter_list = []

# Cycle until the stopping criterion is not satisfied
while np.amax(np.abs(A - np.diag(np.diag(A)))) >= tol:
 # Obtain the QR factorization of A and perform the QR iteration
 Q, R = np.linalg.qr(A)
 A = R@Q

 # Obtain the current approximation of the eigenvalues
 computed_eigvals = np.diag(A)

 # Compute and store the maximum absolute error on the eigenvalues
 abs_error = max(np.abs(exact_eigenvalues - computed_eigvals))

 counter += 1

 if abs_error < 10**(-t):
   t_counter_list.append(counter)
   t += 1

 if counter in [1,5,10,15]:
   print(f'k={counter}')
   print(A)
   print('--------------------------')
print(f'Final k = {counter}')
print(A)
```

```
computed_eigvals = np.diag(A)

print('------------------------')
print(f'Exact eigenvalues = {format(exact_eigenvalues)}')
print(f'Computed eigenvalues = {format(computed_eigvals)}')
diff_eigvals = np.abs(exact_eigenvalues - computed_eigvals)
print(f'Absolute error = {format(diff_eigvals)}')
```

Here we report the intermediate A_k matrices for $k = 1, 10, 15, 15$ and the final one with $k = 21$ and the exact and computed eigenvalues, with the absolute errors.

```
k=1
[[ 9.733333333333334  2.834948829502994  0.878364340955178 -0.231869447880085]
 [ 2.834948829502991  3.783908045977011  1.539932953851869 -0.60279905751826 ]
 [ 0.878364340955178  1.539932953851869  1.515016685205784 -0.509164636937078]
 [-0.231869447880084 -0.602799057518259 -0.509164636937078  0.967741935483871]]
-------------------------
k=5
[[11.098895703904493  0.030845371708295  0.000040119600318 -0.000003286456335]
 [ 0.030845371708295  3.414318666854397  0.006815571252927 -0.000792986818634]
 [ 0.000040119600319  0.006815571252927  0.884533164554776 -0.070136316449804]
 [-0.000003286456334 -0.000792986818633 -0.070136316449804  0.602252464686331]]
-------------------------
k=10
[[11.099019512653443  0.000084962498578  0.00000000014034  0.000000000001383]
 [ 0.000084962498578  3.414213563282151  0.000008722995681  0.000000121056837]
 [ 0.00000000014034   0.000008722995681  0.900746172772326  0.008590655965716]
 [ 0.000000000001382  0.000000121056836  0.008590655965716  0.586020751292075]]
-------------------------
k=15
[[11.099019513592774  0.000000234022501  0. -0.000000000000001]
 [ 0.000000234022501  3.414213562373102  0.000000011163285 -0.000000000018006]
 [ 0.                 0.000000011163285  0.900977321539928 -0.000998767899781]
 [-0.                -0.000000000018005 -0.000998767899781  0.585789602494192]]
-------------------------
Final k = 26
[[11.099019513592783  0.000000000000546 -0.  0.000000000000001]
 [ 0.000000000000546  3.414213562373094  0.000000000000005  0.000000000000001]
 [ 0.                 0.000000000000005  0.900980486163497  0.000008764600757]
 [ 0.                 0.                 0.000008764600758  0.585786437870623]]
-------------------------
Exact eigenvalues =
[11.099019513592786  3.414213562373094  0.900980486407215  0.585786437626905]
Computed eigenvalues =
[11.099019513592783  3.414213562373094  0.900980486163497  0.585786437870623]
Absolute error =
[0.000000000000004 0.                0.000000000243718 0.000000000243717]
```

We can observe the decreasing of the off-diagonal entries and the convergence of the diagonal terms to the eigenvalues computed using the function np.linalg.eigvals, which we consider as exact. The maximum absolute error on the eigenvalues is of the order of 10^{-8}.

In the following script we implement the QR diagonalization of the matrix A using the Rayleigh quotient shift and deflation.

```
# Initialize values
t = 9
tol_list = 10.**(-np.array(range(1,t)))
counter_list = []

# Construct the matrix A
A = np.array([[4,3,2,1],[3,4,3,2],[2,3,4,3],[1,2,3,4]])
# Compute the exact eigenvalues
exact_eigenvalues = np.linalg.eigvals(A)
exact_eigenvalues_copy = exact_eigenvalues.copy()

# Cycle on the list of tolerances
for tol in tol_list:
  counter = 0
  A = np.array([[4,3,2,1],[3,4,3,2],[2,3,4,3],[1,2,3,4]])
  exact_eigenvalues = exact_eigenvalues_copy.copy()
  dim = np.shape(A)[0]

  # Perform QR iteration until the matrix is reduced to a single value by
  ↪  deflation
  while dim > 0:
    approx_lambda = A[dim-1,dim-1]
    eig_error = abs(exact_eigenvalues-approx_lambda)
    # If the error on an eigenvalue is less than the tolerance, perform
    ↪  deflation
    if min(eig_error) < tol:
       index = np.argmin(eig_error)
       exact_eigenvalues = np.delete(exact_eigenvalues,index)
       A = A[:dim-1,:dim-1]
       dim = dim - 1
       continue

    # Compute the shift and perform QR iteration
    shift = A[dim-1,dim-1]
    Q, R = np.linalg.qr(A - shift * np.eye(dim))
    A = R@Q + shift * np.eye(dim)
    counter = counter + 1

  counter_list.append(counter)
```

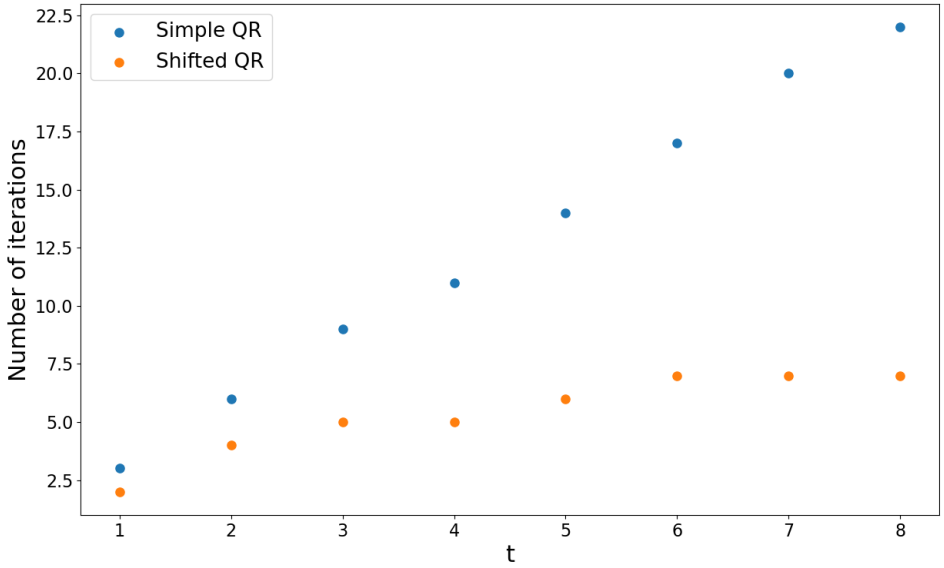

Figure 1: Number of iterations needed to achieve a maximum absolute error less than 10^{-t} on the eigenvalues computed by using standard and shifted QR iteration algorithm.

As we see from Fig. 1 the number of iterations required to achieve a maximum absolute error less than 10^{-t} on eigenvalues appears to grow linearly with t in the case of the simple QR iteration algorithm. On the other hand, in the case of the shifted QR iteration algorithm, implemented by using the Rayleigh shift, the same error appears to grow sublinearly with t, meaning that this last algorithm reaches the required tolerance with a smaller number of iterations, thus being faster.

Problem 2

We want to find approximations to the eigenvalues and eigenfunctions of the one-dimensional Laplace operator $L[u] := -\frac{d^2u}{dx^2}$ on the unit interval $[0,1]$ with boundary conditions $u(0) = u(1) = 0$. Let us define as λ_i an eigenvalue of L and as u_i the corresponding eigenfunction. Approximations to the eigenvalues and eigenfunctions can be obtained by discretizing the interval $[0,1]$ through $N+2$ evenly spaced points: $x_i = ih$ where $i = 0, 1, ..., N+1$ and $h = 1/(N+1)$. The second derivative operator can then be approximated by centered finite differences:

$$-\frac{d^2u}{dx^2}(x_i) \approx \frac{-u(x_{i-1} + 2u(x_i) - 2u(x_{i+1}))}{h^2} \tag{19}$$

and therefore the continuous (differential) eigenproblem can be approximated by the discrete (algebraic) eigenvalue problem

$$h^{-2}T_N\mathbf{u} = \lambda\mathbf{u}, \tag{20}$$

where we have set

$$T_N = \begin{bmatrix} 2 & -1 & & 0 \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ 0 & & -1 & 2 \end{bmatrix}, \text{ and } \mathbf{u} = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{bmatrix}, \tag{21}$$

with $u_i := u(x_i)$. Recall that the eigenvalues and eigenfunctions of L are $\lambda_j = j^2\pi^2$ and $u_j(x) = \alpha \sin(j\pi x)$ for any nonzero constant α, which we can take to be 1, and j positive integer. On the other hand, the $N \times N$ matrix T_N has eigenvalues $\mu_j = 2(1 - \cos\frac{\pi j}{N+1})$ for $j = 1, \dots, N$, corresponding to the eigenvectors $\mathbf{u}_j$, where $\mathbf{u}_j(k) = \sqrt{\frac{2}{N+1}} \sin\left(\frac{jk\pi}{N+1}\right)$ is the kth entry in $\mathbf{u}_j$.

(1) Since we are considering $j \ll N$ and $N \gg 1$ we can consider the Taylor expansion of $\cos\left(\frac{\pi j}{N+1}\right)$, which leads us to approximate the smallest eigenvalues of $h^{-2}T_N$ as follows:

$$2h^{-2}\left(1 - \cos\frac{\pi j}{N+1}\right) = 2h^{-2}\left(\frac{(\pi jh)^2}{2!} - \frac{(\pi jh)^4}{4!} + O(h^6)\right) = \pi^2 j^2\left(1 - \frac{(\pi jh)^2}{12} + O(h^4)\right), \tag{22}$$

where we used that $h = 1/N + 1$.

For the largest eigenvalue of T_N, we have that $j = N$, therefore we can not truncate anymore the Taylor expansion of $\cos\frac{\pi j}{N+1}$ if we want a good approximation. We can compute the $N-th$ eigenvalue of T_N in the limit of $N \gg 1$ (namely $h \ll 1$) with the following manipulations:

$$\mu_N = 2\left(1 - \cos\frac{\pi N}{N+1}\right) = 2(1 - \cos(\pi - \pi h)) = 2(1 + \cos\pi h) = 4 - \pi^2 h^2 + O(h^4). \tag{23}$$

Therefore, we have

$$h^{-2}\mu_N = \frac{4}{h^2} - \pi^2 + O(h^2) = 4(N+1)^2 - \pi^2 + O(N^{-2}), \tag{24}$$

which is not a good approximation of $\lambda_N = \pi^2 N^2$.

(2) We want to compare the eigenvectors $\mathbf{u}_j$ of T_N with the eigenfunctions of L, up to the normalization constant, that we will set to 1 for both. If we recall that $x_k = kh \; \forall k = 1, \dots, N$, we can observe that the $k - th$ component of the eigenvector $\mathbf{u}_j$ is equal to the $j - th$ eigenfunction $u_j(x)$ computed in correspondence of the value $x = x_k$:

$$u_j(x_k) = \sin(j\pi x_k) = \sin(j\pi kh) = \sin\left(\frac{j\pi k}{N+1}\right) = \mathbf{u}_j(k). \tag{25}$$

(3) Now we compute the spectral condition number of T_N, defined as $k_2(T_N) = \frac{h^{-2}\mu_N}{h^{-2}\mu_1}$, in the limit of $N \gg 1$. We recall that the eigenvalues of T_N are

$$\mu_j = 2\left(1 - \cos\frac{\pi j}{N+1}\right) = 2\left(1 - \cos\pi jh\right). \tag{26}$$

By considering the Taylor expansion of the cosine, we can compute the numerator and the denominator of $k_2(T_N)$. In particular, to compute the numerator we can use the expression reported in Eq. (22), where $j = 1$, while for the denominator we use the expression reported in Eq. (23).

$$k_2(T_N) = \frac{h^{-2}\mu_N}{h^{-2}\mu_1} = \frac{4h^{-2} - \pi^2 + \frac{1}{12}\pi^4 h^2 + O(h^4)}{\pi^2(1 - \frac{1}{12}\pi^2 h^2 + O(h^4))}. \tag{27}$$

Here, in the denominator, we can use the expansion $(1 + x)^\alpha = 1 + \alpha x + O(x^2)$, finding $(1 - \frac{1}{12}\pi^2 h^2 + O(h^4))^{-1} = 1 + \frac{1}{12}\pi^2 h^2 + O(h^4)$. Therefore, we find

$$\begin{aligned} k_2(T_N) &= \left(\frac{4h^{-2}}{\pi^2} - 1 + \frac{1}{12}\pi^4 h^2 + O(h^4)\right)\left(1 + \frac{1}{12}\pi^2 h^2 + O(h^4)\right) \\ &= \frac{4h^{-2}}{\pi^2} - 1 + \frac{1}{12}\pi^4 h^2 + \frac{4h^{-2}}{\pi^2}\frac{1}{12}\pi^2 h^2 - \frac{1}{12}\pi^2 h^2 + O(h^4) \\ &= \frac{4h^{-2}}{\pi^2} - \frac{2}{3} + O(h^2) = \frac{4(N+1)^2}{\pi^2} - \frac{2}{3} + O(N^{-2}). \end{aligned} \tag{28}$$

(4-5) Here we report the plot of the eigenvalues and eigenvectors of T_N, with $N = 21$.

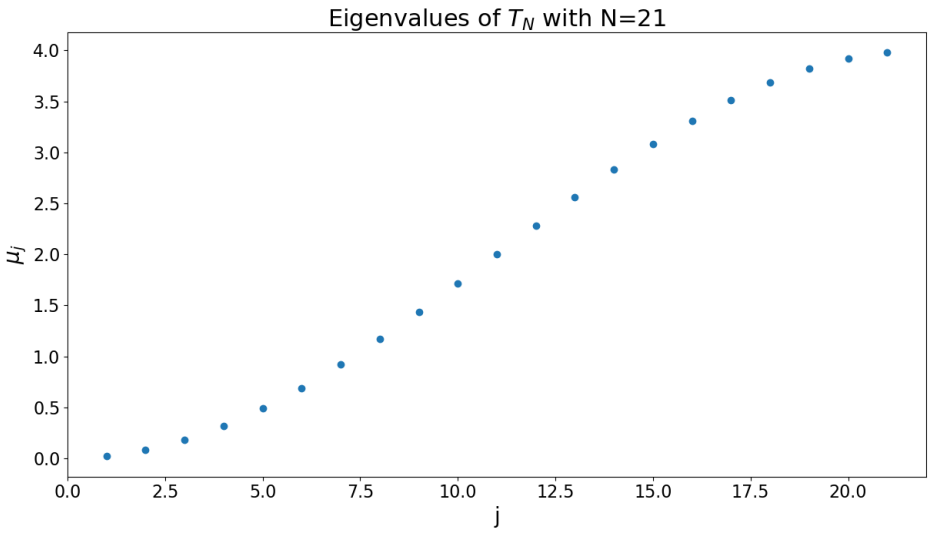

Figure 2: Eigenvalues of T_N, with $N = 21$.

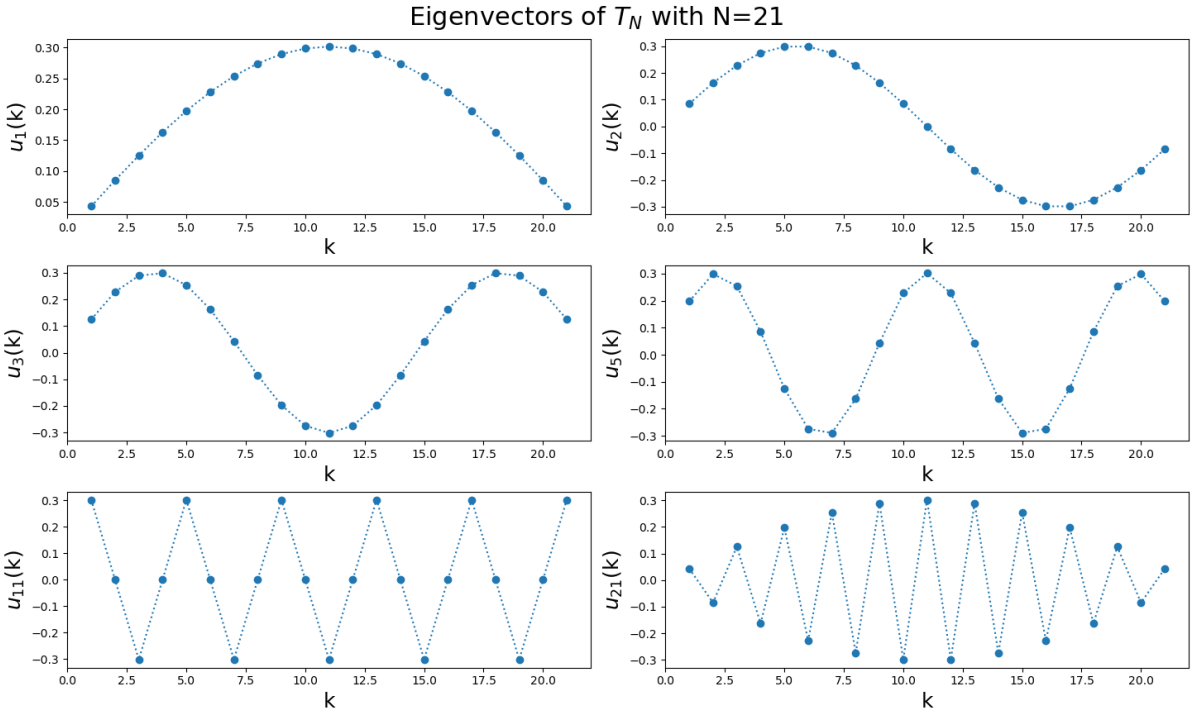

Figure 3: Eigenvectors of T_N for different values of j, with j being the number that identifies the j-th eigenvector.

(6) In the following we report the script implementing the inverse power method to find the smallest eigenvalue of $h^{-2}T_N$.

```
import numpy as np
import scipy

# Set initial parameters
```

```
N = 500
tol = 1e-8
initial_guess = np.random.random(N)
initial_guess = initial_guess/np.linalg.norm(initial_guess, ord=2)
count = 0
diff = 10 * tol

# Build T_N
T_N = scipy.sparse.diags([-1,2,-1],[-1,0,1],shape=(N,N)).toarray()

# Cholesky factorization of h^(-2)T_N
L, low = scipy.linalg.cho_factor(T_N)
L = (N+1) * L

vect_old = initial_guess

# Cycle until the difference in the 2-norm between two successive
↪  (approximated) eigenvectors is less than the chosen tolerance
while diff >= tol:
  # Compute and normalize the new vector by using the Choleski factorization
  ↪  of T_N
  vect_new = scipy.linalg.cho_solve((L, low),vect_old)
  vect_new = vect_new/np.linalg.norm(vect_new, ord=2)
  diff = np.linalg.norm(vect_new - vect_old, ord=2)
  count += 1
  vect_old = vect_new

# Compute the approximated eigenvalue
approx_eig = vect_new @ T_N @ vect_new * (N+1)**2

print(f'Iterations performed = {count}')
exact_eigval_T_N = 2 * (N+1)**2 * (1-np.cos(np.pi/(N+1)))
print(f'Absolute error eigenvalue) = {abs(approx_eig - exact_eigval_T_N)}')
index = np.array(range(1,N+1))
exact_eigvect = np.sqrt(2/(N+1)) * np.sin(index*np.pi/(N+1))
print(f'2-norm error eigenvector = {np.linalg.norm(vect_new - exact_eigvect,
↪  ord=2)}')
```

The output of this code is the following:

```
Iterations performed = 10
Absolute error eigenvalue = 1.531041959879076e-11
2-norm error eigenvector = 3.2570943203952573e-09
```

As we can see, 10 iterations are required to obtain the chosen tolerance on the computed eigenvector. Finally, we report the plot of the computed eigenvector.

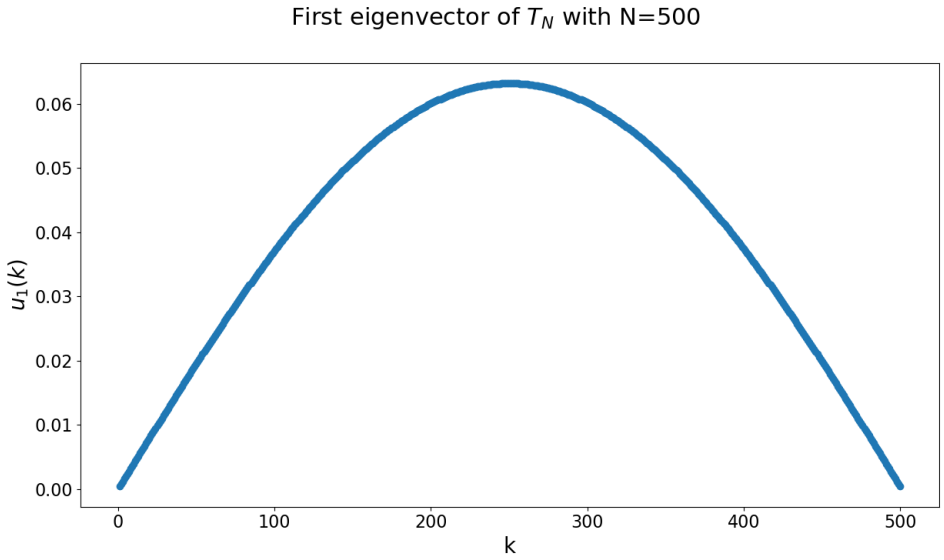

Figure 4: First eigenvector of T_N, with $N = 500$ computed by using the inverse power method.

(7) Below we report the script implementing the shift-and-invert method to find the fifth eigenvalue of $h^{-2}T_N$. In this case, it is not possible to use the Cholesky factorization since the matrix $h^{-2}T_N - 25\pi^2\mathbb{1}_N$ is not positive-definite.

```
import numpy as np
import scipy

# Set initial parameters
N = 500
lambda_5 = 25*np.pi**2
initial_guess = np.random.random(N)
initial_guess = initial_guess/np.linalg.norm(initial_guess, ord=2)
count = 0

# Build T_N
T_N = scipy.sparse.diags([-1,2,-1],[-1,0,1],shape=(N,N)).toarray()

tol = 1e-12 * np.linalg.norm((N+1)**2 * T_N, ord = np.inf)
diff = 10 * tol

# LU factorization of h^(-2)T_N
lu, piv = scipy.linalg.lu_factor(T_N*(N+1)**2 - lambda_5 * np.eye(N))

vect_old = initial_guess

# Cycle until the stopping criterion is satisfied - condition on the
↪  residual
while diff >= tol:
  # Compute and normalize the new vector by using the LU factorization to
  ↪  solve a linear system
  vect_new = scipy.linalg.lu_solve((lu, piv), vect_old)
  vect_new = vect_new/np.linalg.norm(vect_new, ord=2)
```

```
    # Compute the approximated eigenvalue
    approx_eig = vect_new @ T_N @ vect_new * (N+1)**2
    diff = np.linalg.norm(( T_N * (N+1)**2 - approx_eig * np.eye(N) ) @
    ↪  vect_new, ord=np.inf)
    count += 1
    vect_old = vect_new

print(f'Iterations performed = {count}')
exact_eigval_T_N = 2 * (N+1)**2 * (1-np.cos(5*np.pi/(N+1)))
print(f'Absolute error eigenvalue = {abs(approx_eig - exact_eigval_T_N)}')
index = np.array(range(1,N+1))
exact_eigvect = np.sqrt(2/(N+1)) * np.sin(index*np.pi*5/(N+1))
print(f'2-norm error eigenvector = {np.linalg.norm(vect_new - exact_eigvect,
↪  ord=2)}')
```

The output of this code is the following:

```
Iterations performed = 2
Absolute error eigenvalue = 1.0032863428932615e-11
2-norm error eigenvector = 5.021569614559994e-08
```

In this case, 2 iterations are required to obtain an accurate approximation of the fifth eigenvector. Finally, we report the plot of the computed eigenvector.

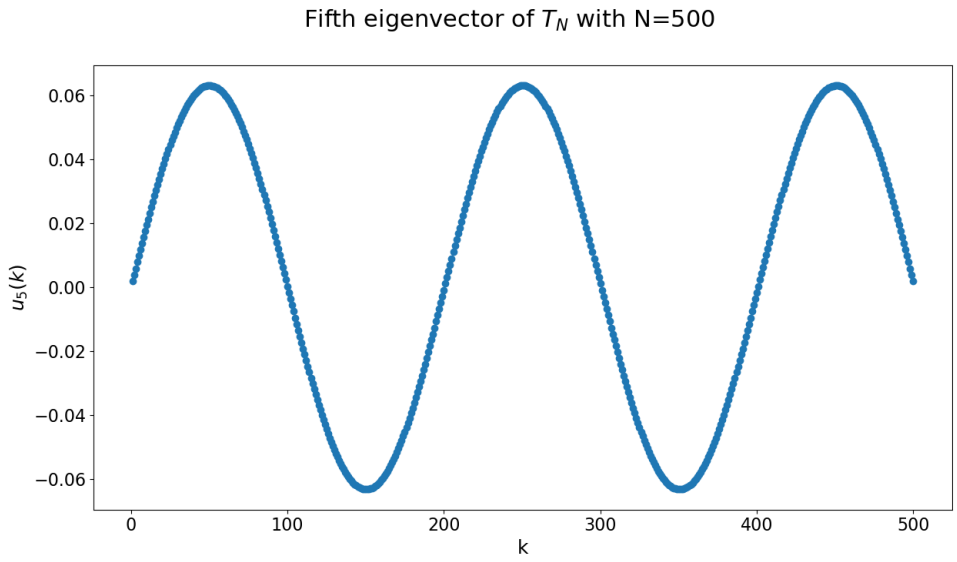

Figure 5: Fifth eigenvector of T_N, with $N = 500$ computed by using the inverse shift-and-invert algorithm.