

Numerical Linear Algebra - EXAM

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Declaration:

I have prepared the assignment myself and I have only used the sources declared in comments to the program

[Programming Assignment Instructions \(qr-method.pdf\)](#)

Numerical Linear Algebra
 Dense Algebraic Eigenvalue Problems
 Subspace iterations, the QR-iteration

1.4.14 Algorithm(The QR-Method)

Compute the spectrum of a matrix $\mathbf{A} \in \mathbb{C}^{n \times n}$ by

- ① Use $n - 2$ Householder transformations to transform \mathbf{A} to Hessenberg form

$$\mathbf{H} = \mathbf{Q}\mathbf{A}\mathbf{Q}^*.$$
- ② QR-iteration: let $\mathbf{H}_0 = \mathbf{H}$ and perform until convergence

$$\Omega_{1,2}^{(k)} \times \cdots \times \Omega_{n-1,n}^{(k)} \mathbf{R} = \mathbf{H}_k$$

$$\mathbf{H}_{k+1} = \mathbf{R}\Omega_{1,2}^{(k)} \times \cdots \times \Omega_{n-1,n}^{(k)}.$$
- ③ Store Householder vectors as well as r and c for each Givens rotation if the eigenvectors are desired in the end.

Image source: Lecture Notes

```
In [1]: 1 # Import Libraries
        2
        3 import numpy as np
        4 import cmath
        5 import matplotlib.pyplot as plt
        6 from scipy.linalg import hessenberg
        7 from scipy.io import mmread
```

```
In [2]: 1 # Set Global Variables
2
3 MAX_ITER = 1000 # maximum number of iterations for testing
4 RTOL = 1e-6 # relative tolerance for convergence, i.e., when subsequent iterates are smaller than RTOL, stop iteration
5 ATOL = 1e-18 # same as numpy: absolute(a - b) <= (atol + rtol * absolute(b))
6 np.set_printoptions(precision=3, linewidth=300, suppress=True)
```

```
In [3]: 1 # Generate Test Data
2
3 def generate_random_matrix(dtype, n):
4     if dtype == 'float':
5         A = np.random.rand(n,n)
6     elif dtype == 'complex':
7         A = np.random.rand(n,n) + np.random.rand(n,n)*1j
8     return A
9
10 RANDOM_REAL_MATRICES = []
11 RANDOM_COMPLEX_MATRICES = []
12
13 for n in [3,5,10]:
14     A = generate_random_matrix(dtype='float', n=n)
15     RANDOM_REAL_MATRICES.append(A)
16
17     A_ = generate_random_matrix(dtype='complex', n=n)
18     RANDOM_COMPLEX_MATRICES.append(A_)
19
20 # symmetric real
21 A = np.random.randint(-3,3,(10,10))
22 A = (A.T + A).astype('float')
23
24 # diagonal dominant
25 B = A - np.triu(A,1)*0.99 - np.tril(A,-1)*0.99
26
27 # unbalanced
28 C = np.tril(np.ones((10,10),dtype='float'),0)
29
30 # Numerical example from https://people.inf.ethz.ch/arbenz/ewp/Lnotes/chapter4.pdf p.81 4.5.1
31 # Eigenvalues = {1 ± 2i, 3, 4, 5 ± 6i}
32
33 D = np.array([[7, 3, 4, -11, -9, -2],
34               [-6, 4, -5, 7, 1, 12],
35               [-1, -9, 2, 2, 9, 1],
36               [-8, 0, -1, 5, 0, 8],
37               [-4, 3, -5, 7, 2, 10],
38               [6, 1, 4, -11, -7, -1]], dtype='float')
39
40 SPECIAL_REAL_MATRICES = [A, B, C, D]
```

Householder Transformation to Upper Hessenberg

Similarity Transformation

Two matrices A and B are similar if there exists an *invertible* matrix S such that $A = S^{-1}BS$.

Similar matrices have the same eigenvalues. Proof: $Av = \lambda v \Leftrightarrow B(S^{-1}v) = \lambda(S^{-1}v)$.

If S can be chosen to be a unitary matrix then A and B are *unitarily equivalent*.

Similarity transformation to Hessenberg form preserves eigenvalues.

The iterates A_0, A_1, \dots from the QR algorithm are also similar matrices since $A_{k+1} = R_k Q_k = Q_k^{-1}(Q_k R_k)Q_k = Q_k^{-1}A_k Q_k$. Therefore, A_0, A_1, \dots , have the same eigenvalues.

Householder Reflector

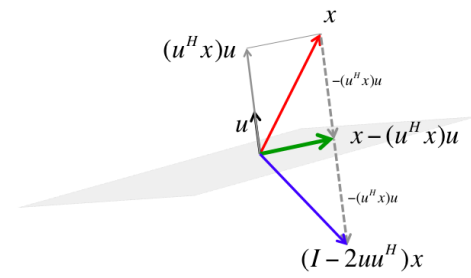


Image source: <https://www.cs.utexas.edu/users/flame/laff/alaff/chapter03-householder-transformation.html> (<https://www.cs.utexas.edu/users/flame/laff/alaff/chapter03-householder-transformation.html>).

Hessenberg Reduction

$$A = \begin{bmatrix} * & * & * & * & * & * \\ * & * & * & * & * & * \\ * & * & * & * & * & * \\ * & * & * & * & * & * \\ * & * & * & * & * & * \\ * & * & * & * & * & * \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 0 \\ 0 & \hat{P}_1 \end{bmatrix} A = \begin{bmatrix} * & * & * & * & * & * \\ * & * & * & * & * & * \\ 0 & * & * & * & * & * \\ 0 & * & * & * & * & * \\ 0 & * & * & * & * & * \\ 0 & * & * & * & * & * \end{bmatrix} \Rightarrow \begin{bmatrix} 1 & 0 \\ 0 & \hat{P}_1 \end{bmatrix} A \begin{bmatrix} 1 & 0 \\ 0 & \hat{P}_1 \end{bmatrix}^{-1} = \begin{bmatrix} * & * & * & * & * & * \\ * & * & * & * & * & * \\ 0 & * & * & * & * & * \\ 0 & * & * & * & * & * \\ 0 & * & * & * & * & * \\ 0 & * & * & * & * & * \end{bmatrix} \Rightarrow P_4 \cdots P_1 A P_1^{-1} \cdots P_4^{-1} = \begin{bmatrix} * & * & * & * & * & * \\ * & * & * & * & * & * \\ 0 & * & * & * & * & * \\ 0 & 0 & * & * & * & * \\ 0 & 0 & 0 & * & * & * \\ 0 & 0 & 0 & 0 & * & * \end{bmatrix}$$

Therefore, compute a Householder matrix $\hat{P}_1 \in \mathbb{C}^{(n-1) \times (n-1)}$ that maps the **red** column vector to the first unit coordinate vector and consider

$$P_1 = \begin{bmatrix} 1 & 0 \\ 0 & \hat{P}_1 \end{bmatrix}.$$

Summary: The algorithm computes a Hessenberg matrix that is similar to A in finitely many steps.

cost: ca. $\frac{10}{3}n^3$ flops

Modified based on image source: https://www3.math.tu-berlin.de/Vorlesungen/SoSe11/NumMath2/Materials/hessenberg_eng.pdf (https://www3.math.tu-berlin.de/Vorlesungen/SoSe11/NumMath2/Materials/hessenberg_eng.pdf).

```

In [42]: 1 def Householder(a):
2
3         """      Compute the Householder refelector H for a given vector a
4         H = I - 2 u @ u.T ;  a' = H @ a
5         Input      -----
6         a: 1D np.array with real or complex entries, size n
7         Return     -----
8         H: 2D np.array with real or complex entries, size nxn
9         """
10
11 #      Initial try: naive implementation for real vectors
12
13 #      n = len(a)
14 #      e = np.zeros(n)
15 #      e[0] = np.sign(a[0])
16 #      v = a + np.linalg.norm(a,2) * e
17 #      H = np.eye(n) - 2* np.outer(v,v) / np.dot(v,v)
18
19
20 #      Improved version: for both real and complex vectors; element update rather than entire vector
21
22 n = len(a)
23 v = a.copy()
24
25 if np.sign(a[0]) >= 0: #sign of the first element to avoid cancellation
26     sign = 1
27 else:
28     sign = -1
29
30 # for real matrix: v @ v.T (transpose)
31
32 if a.dtype != 'complex':
33     v[0] = a[0] + sign * np.linalg.norm(a,2)
34     if np.linalg.norm(v,2) != 0:
35         u = v / np.linalg.norm(v,2)
36     else:
37         u = v
38     H = np.eye(n) - 2 * np.outer(u,u)
39
40
41 # for complex matrix: v @ v.conjugate.T, phase cancellation so that the first subdiagonal element should be real
42 # (Source: https://arxiv.org/pdf/math-ph/0609050.pdf p.19)
43
44 else: # a.dtype == 'complex':
45
46     theta = cmath.phase(a[0])
47     v[0] = a[0] + sign * np.linalg.norm(a,2) * np.exp(theta*1j)
48
49     if np.linalg.norm(v,2) != 0:
50         u = v / np.linalg.norm(v,2)
51     else:
52         u = v

```

```

53
54     H = np.exp(-theta*1j)*(np.eye(n) - 2* np.outer(u,u.conjugate()))
55
56     #print(">>> check if H v = e1:", np.round(H.dot(a),3))
57     #print('>>> check if H is Hermitian:',np.allclose(H@H.conjugate().T, np.eye(n))) # H @ H.conjugate().T = I
58
59     return H
60
61
62
63 def Hessenberg(A,eigvec=False, inplace=True):
64
65     """ Reduce a general square matrix to an upper Hesseberg matrix by similarity transformation
66     Input -----
67         A: 2D np.array with real or complex entries, shape is n x n (i.e. square matrix)
68         eigvec : bool, indicating whether eigenvectors are required; default is False
69         inplace: bool, indicating whether to update A in place; default is True
70     Return -----
71         H: 2D np.array with real or complex entries, same shape as A
72         S: similarity transformation matrix such that H = S @ A @ S.T, if eigvec is True; otherwise S = identity matrix
73     """
74
75     # check if input is a square matrix
76     if len(A.shape)!=2 or A.shape[0]!=A.shape[1]:
77         raise ValueError('Input matrix is of shape {}. Expected square matrix.'.format(A.shape))
78
79     n = A.shape[0]
80
81     # if input matrix is 2x2 or smaller: already in Hessenberg
82     if n <= 2:
83         return A, np.eye(n)
84
85     S = np.eye(n, dtype=A.dtype)
86
87     if not inplace:
88         A_ = A.copy()
89     else:
90         A_ = A
91
92     for i in range(n-1): # (n-2) Householder transformations are needed
93         a = A_[i+1:,i] # a = column vectors below diagonal, size (n-i-1), i = 0,...,n-2
94         H_ = Householder(a)
95
96         P = np.eye(n, dtype = A_.dtype) # Force P to have the same data type as input matrix
97         P[i+1:,i+1:] = H_
98         #print(">>> check if P is Hermitian and orthogonal:",np.allclose(P@P.conjugate().T, np.eye(n)))
99
100        if A_.dtype != 'complex':
101            A_ = P @ A_ @ P.T
102        else:
103            A_ = P @ A_ @ P.conjugate().T
104

```

```
105     #The first subdiagonal element should have only a real part; enforced here
106     A_[i+1,i] = A_[i+1,i].real
107     #A_ = np.triu(A_, -1)
108
109     if eigvec:
110         S = P @ S
111
112     return A_, S
113
```

In [5]:

```

1  ### Testing Hessenberg() on Real Matrices
2  #from scipy.linalg import hessenberg
3
4  print('\n\n')
5  print("=====")
6  print('Testing Hessenberg() function on randomly generated REAL matrices')
7  print("=====")
8
9  #for n in [3,5,10,100]:
10 #   A = np.random.rand(n,n)
11
12 for A in RANDOM_REAL_MATRICES:
13     print('\nReal >>> Input shape = {}'.format(A.shape))
14     Hessenberg_A, S = Hessenberg(A,eigvec=True, inplace=False)
15     scipy_hess_A = hessenberg(A)
16     print('\nscipy.linalg.hessenberg and my Hessenberg close?',np.allclose(scipy_hess_A,Hessenberg_A))
17     if not np.allclose(scipy_hess_A,Hessenberg_A):
18         print('scipy.linalg.hessenberg and my Hessenberg close in abs() except signs?',
19               np.allclose(np.abs(scipy_hess_A),np.abs(Hessenberg_A)))
20     print('\nReconstructed matrix S.T@H@S close to input?',np.allclose(A, S.T@Hessenberg_A@S))
21
22 #   n = A.shape[0]
23 #   if n <=5:
24 #       print('\ninput matrix=\n', A)
25 #       print('\nreconstructed matrix=\n',S.T@Hessenberg_A@S)
26 #       print('\nscipy.linalg.hessenberg=\n',scipy_hess_A)
27 #       print('\nmy Hessenberg=\n',Hessenberg_A)
28
29
30 print('\n\n')
31 print("=====")
32 print('Testing Hessenberg() function on special REAL matrices')
33 print("=====")
34
35 for A in SPECIAL_REAL_MATRICES:
36     print('\nReal >>> Input shape = {}'.format(A.shape))
37     Hessenberg_A, S = Hessenberg(A,eigvec=True, inplace=False)
38     scipy_hess_A = hessenberg(A)
39     print('\nscipy.linalg.hessenberg and my Hessenberg close?',np.allclose(scipy_hess_A,Hessenberg_A))
40     if not np.allclose(scipy_hess_A,Hessenberg_A):
41         print('scipy.linalg.hessenberg and my Hessenberg close in abs() except signs?',
42               np.allclose(np.abs(scipy_hess_A),np.abs(Hessenberg_A)))
43     print('\nReconstructed matrix S.T@H@S close to input?',np.allclose(A, S.T@Hessenberg_A@S))
44
45 print('\ninput matrix=\n', A)
46 print('\nreconstructed matrix=\n',S.T@Hessenberg_A@S)
47 print('\nscipy.linalg.hessenberg=\n',scipy_hess_A)
48 print('\nmy Hessenberg=\n',Hessenberg_A)
49

```



```
=====
Testing Hessenberg() function on randomly generated REAL matrices
=====

Real >>> Input shape = (3, 3)

scipy.linalg.hessenberg and my Hessenberg close? False
scipy.linalg.hessenberg and my Hessenberg close in abs() except signs? True

Reconstructed matrix S.T@H@S close to input? True

Real >>> Input shape = (5, 5)

scipy.linalg.hessenberg and my Hessenberg close? False
scipy.linalg.hessenberg and my Hessenberg close in abs() except signs? True

Reconstructed matrix S.T@H@S close to input? True

Real >>> Input shape = (10, 10)

scipy.linalg.hessenberg and my Hessenberg close? False
scipy.linalg.hessenberg and my Hessenberg close in abs() except signs? True

Reconstructed matrix S.T@H@S close to input? True


=====
Testing Hessenberg() function on special REAL matrices
=====

Real >>> Input shape = (10, 10)

scipy.linalg.hessenberg and my Hessenberg close? False
scipy.linalg.hessenberg and my Hessenberg close in abs() except signs? True

Reconstructed matrix S.T@H@S close to input? True

Real >>> Input shape = (10, 10)

scipy.linalg.hessenberg and my Hessenberg close? False
scipy.linalg.hessenberg and my Hessenberg close in abs() except signs? True

Reconstructed matrix S.T@H@S close to input? True

Real >>> Input shape = (10, 10)

scipy.linalg.hessenberg and my Hessenberg close? False
scipy.linalg.hessenberg and my Hessenberg close in abs() except signs? True
```

```
Reconstructed matrix S.T@H@S close to input? True
```

```
Real >>> Input shape = (6, 6)
```

```
scipy.linalg.hessenberg and my Hessenberg close? False
```

```
scipy.linalg.hessenberg and my Hessenberg close in abs() except signs? True
```

```
Reconstructed matrix S.T@H@S close to input? True
```

```
input matrix=
```

```
[[ 7.  3.  4. -11. -9. -2.]  
 [-6.  4. -5.  7.  1. 12.]  
 [-1. -9.  2.  2.  9.  1.]  
 [-8.  0. -1.  5.  0.  8.]  
 [-4.  3. -5.  7.  2. 10.]  
 [ 6.  1.  4. -11. -7. -1.]]
```

```
reconstructed matrix=
```

```
[[ 7.  3.  4. -11. -9. -2.]  
 [-6.  4. -5.  7.  1. 12.]  
 [-1. -9.  2.  2.  9.  1.]  
 [-8. -0. -1.  5. -0.  8.]  
 [-4.  3. -5.  7.  2. 10.]  
 [ 6.  1.  4. -11. -7. -1.]]
```

```
scipy.linalg.hessenberg=
```

```
[[ 7.      7.276  5.812 -0.14   9.015  7.936]  
 [12.369  4.131 18.969 -1.207 10.683  2.416]  
 [ 0.     -7.16   2.448 -0.566 -4.181 -3.251]  
 [ 0.      0.    -8.599  2.915 -3.417  5.723]  
 [ 0.      0.      0.    1.046 -2.835 -10.979]  
 [ 0.      0.      0.      0.    1.414  5.342]]
```

```
my Hessenberg=
```

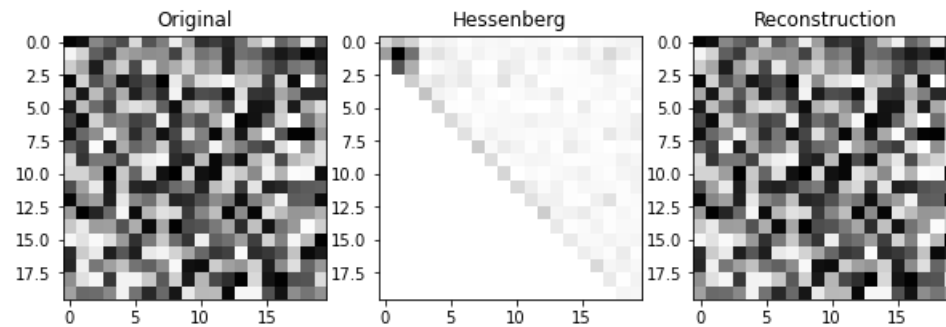
```
[[ 7.      7.276  5.812 -0.14   9.015 -7.936]  
 [12.369  4.131 18.969 -1.207 10.683 -2.416]  
 [ 0.     -7.16   2.448 -0.566 -4.181  3.251]  
 [-0.      0.    -8.599  2.915 -3.417 -5.723]  
 [-0.     -0.     -0.    1.046 -2.835 10.979]  
 [-0.     -0.      0.     -0.    -1.414  5.342]]
```

```

In [6]: 1 # Visualiation of Tranforming Matrix A to Hessenberg form via Householder Reflection
2
3 f, (ax0, ax1, ax2) = plt.subplots(1,3,figsize=(10,20))
4
5 n = 20
6 A = np.random.rand(n,n)
7 H, S = Hessenberg(A,eigvec=True, inplace=False)
8 recon = S.T @ H @ S
9
10 im = ax0.imshow(-abs(A),cmap='gray')
11 ax0.set_title('Original')
12 ax1.imshow(-abs(H),cmap='gray')
13 ax1.set_title('Hessenberg')
14 ax2.imshow(-abs(recon),cmap='gray')
15 ax2.set_title('Reconstruction')
16
17 print("Illustration of Transformation to Hessenberg Form ")
18

```

Illustration of Transformation to Hessenberg Form



Observations:

- Hessenberg() function seems to be working for real matrices


```

In [7]: 1  ### Testing Hessenberg() on Random Complex Matrices
2
3  print('\n\n')
4  print("=====")
5  print('Testing Hessenberg() function on randomly generated COMPLEX matrices')
6  print("=====")
7
8  #for n in [3,5,10,100]:
9  #    A = np.random.rand(n,n)+np.random.rand(n,n)*1j
10
11  for A in RANDOM_COMPLEX_MATRICES:
12      print('\n\nComplex >>> Input shape = {}'.format(A.shape))
13      Hessenberg_A, S = Hessenberg(A,eigvec=True,inplace=False)
14      scipy_hess_A = hessenberg(A)
15      print('\nscipy.linalg.hessenberg and my Hessenberg close?',np.allclose(scipy_hess_A,Hessenberg_A))
16      if not np.allclose(scipy_hess_A,Hessenberg_A):
17          #print('scipy.linalg.hessenberg and my Hessenberg close in abs() except signs?',np.allclose(np.abs(scipy_hess_A),np.abs(Hessenberg_A)))
18          print('scipy.linalg.hessenberg and my Hessenberg close in absolute values of re() and im()?',
19                np.allclose(np.abs(np.real(scipy_hess_A)),np.abs(np.real(Hessenberg_A))),
20                np.allclose(np.abs(np.imag(scipy_hess_A)),np.abs(np.imag(Hessenberg_A))))
21          #print(np.real(scipy_hess_A),'\n',np.real(Hessenberg_A),'\n\n',np.imag(scipy_hess_A),'\n',np.imag(Hessenberg_A))
22      print('\nReconstructed matrix S.T@H@S close to input?',np.allclose(A, S.conjugate().T@Hessenberg_A@S))
23
24  #    n = A.shape[0]
25  #    if n <=5:
26  #        print('\ninput matrix=\n', A)
27  #        print('\nreconstructed matrix=\n',S.conjugate().T@Hessenberg_A@S)
28  #        print('\nscipy.linalg.hessenberg=\n',scipy_hess_A)
29  #        print('\nmy Hessenberg=\n',Hessenberg_A)
30
31

```

```

=====
Testing Hessenberg() function on randomly generated COMPLEX matrices
=====

```

Complex >>> Input shape = (3, 3)

scipy.linalg.hessenberg and my Hessenberg close? False
scipy.linalg.hessenberg and my Hessenberg close in absolute values of re() and im()? True True

Reconstructed matrix S.T@H@S close to input? True

Complex >>> Input shape = (5, 5)

scipy.linalg.hessenberg and my Hessenberg close? False

```
scipy.linalg.hessenberg and my Hessenberg close in absolute values of re() and im()? True True
```

```
Reconstructed matrix S.T@H@S close to input? True
```

```
Complex >>> Input shape = (10, 10)
```

```
scipy.linalg.hessenberg and my Hessenberg close? False
```

```
scipy.linalg.hessenberg and my Hessenberg close in absolute values of re() and im()? True True
```

```
Reconstructed matrix S.T@H@S close to input? True
```

Observations:

- Hessenberg() function works for complex matrices as well
- Modified for the optional output of the similarity transformation matrix S

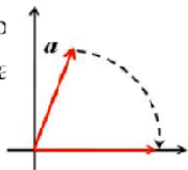
Givens Rotation

Given rotations introduce zeros on

Given vector $[a_1 \ a_2]^T$, choose scale that

$$\begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \alpha \\ 0 \end{bmatrix}$$

with $c^2 + s^2 = 1$, or equivalently, $\alpha = \sqrt{a_1^2 + a_2^2}$



$$G(i, k, \theta) = \begin{bmatrix} 1 & \cdots & 0 & \cdots & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & & \vdots & & \vdots \\ 0 & \cdots & c & \cdots & s & \cdots & 0 \\ \vdots & & \vdots & \ddots & \vdots & & \vdots \\ 0 & \cdots & -s & \cdots & c & \cdots & 0 \\ \vdots & & \vdots & & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \cdots & 0 & \cdots & 1 \end{bmatrix}$$

$$G_{1,m}A = \begin{bmatrix} * & \cdots & \cdots & * \\ \vdots & \ddots & \ddots & \vdots \\ * & \cdots & \cdots & * \\ 0 & * & \cdots & * \end{bmatrix}$$

$$G_1A = \begin{bmatrix} * & \cdots & \cdots & * \\ 0 & * & \ddots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ 0 & * & \cdots & * \end{bmatrix}$$

$$G_1 := G_{1,2} \cdots G_{1,m}$$

Modified from Image Source: <https://www.slideserve.com/pekelo/scientific-computing-chapter-3-linear-least-squares> (<https://www.slideserve.com/pekelo/scientific-computing-chapter-3-linear-least-squares>), <https://de.wikipedia.org/wiki/Givens-Rotation> (<https://de.wikipedia.org/wiki/Givens-Rotation>).

If x_j and x_k are real numbers:

$$\bullet \begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} x_j \\ x_k \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix}, \text{ where } r = \sqrt{x_j^2 + x_k^2}, c = x_j/r \text{ and } s = x_k/r$$

If x_j and x_k are complex numbers:

$$\bullet \begin{bmatrix} c & s \\ -\bar{s} & c \end{bmatrix} \begin{bmatrix} x_j \\ x_k \end{bmatrix} = \begin{bmatrix} r \\ 0 \end{bmatrix}, \text{ where}$$

- $c = x_j^* / \sqrt{|x_j|^2 + |x_k|^2} = \cos\theta_a e^{-i\theta_j}$
- $s = x_k^* / \sqrt{|x_j|^2 + |x_k|^2} = \sin\theta_a e^{-i\theta_k}$
- $\theta_a = \arctan(|x_k|/|x_j|) = \arctan(\operatorname{Re}(x_k)/\cos\theta_k \times \cos\theta_j/\operatorname{Re}(x_j))$

Source: <https://amir.sdsu.edu/Wen17A.pdf> (<https://amir.sdsu.edu/Wen17A.pdf>), page 2, equations (7) and (8)

```

In [9]: 1 def Givens(x_j,x_k):
2
3         """ Find the Givens rotation matrix such that  $G @ [x_j, x_k] = [*, 0]$ 
4         Input -----
5             x_j: jth row/column element from a np.array with real or complex entries
6             x_k: kth row/column element from a np.array with real or complex entries
7
8         Return -----
9             G: 2x2 rotation matrix in np.array with real or complex entries
10        """
11
12
13        if x_k == 0. or x_k.real == 0: #x_k== 0+0*1j : # including the case x_j=0 and x_k=0
14            c = 1.
15            s = 0.
16
17        elif x_j == 0. or x_j.real == 0: #x_j == 0+0*1j : # i.e. x_k!=0
18            c = 0.
19            s = 1.
20
21        else: # f, g both non-zero
22            theta_j = cmath.phase(x_j)
23            theta_k = cmath.phase(x_k)
24            theta_a = np.arctan(x_k.real/np.cos(theta_k)*np.cos(theta_j)/x_j.real) #div by zero excluded from condition above
25            c = np.cos(theta_a)*np.exp(-1j*theta_j)
26            s = np.sin(theta_a)*np.exp(-1j*theta_k)
27
28        if x_j.dtype == 'complex' or x_k.dtype == 'complex':
29            G = np.array([[c,s],[-s.conjugate(),c.conjugate()]]).astype('complex')
30
31        else:
32            G = np.array([[c,s],[-s,c]]).astype('float')
33
34        return G
35
36
37
38        # Previous unsuccessful attempts
39        # (Source: https://www.netlib.org/lapack/lawnspdf/Lawn148.pdf, p.5) -> implementation does not work for complex matrices.
40
41    #def __Givens__(f,g):
42    #    if g == 0:
43    #        c = 1
44    #        s = 0
45    #        r = f
46    #    elif f == 0: # g!=0
47    #        c = 0
48    #        s = np.sign(g.conjugate())
49    #        r = np.abs(g)
50    #    else: # f, g both non-zero
51    #        d = np.sqrt(np.abs(f)**2 + np.abs(g)**2 )
52    #        c = np.abs(f) / d

```



```

53 #         s = np.sign(f) * (g.conjugate()) / d
54 #         r = np.sign(f) * d
55 #     G = np.array([[c,s],[-s.conjugate(),c]])
56 #     return G
57
58
59 #def Givens_real(x_j, x_k):
60 #     """Avoiding squaring of small numbers
61 #     TODO: Need to adapt for complex numbers
62 #     """
63 #     # if the subdiagonal is already zero or close enough to zero, just return identity matrix
64 #     if abs(x_j) > abs(x_k) and x_j!=0:
65 #         tan = x_k / x_j
66 #         c = 1/np.sqrt(1+np.square(tan))
67 #         s = tan*c
68 #     else:
69 #         cotan = x_j / x_k
70 #         s = 1/np.sqrt(1+np.square(cotan))
71 #         c = cotan*s
72 #     G = np.array([[c,s],[-s,c]])
73 #     return G
74
75
76 #def QR_Givens_naive(H):
77 #     '''Input: matrix H in Hessenberg form
78 #     Matrix multiplication directly
79 #     '''
80 #     n = H.shape[0]
81 #     G = np.eye(n)
82 #     for i in range(n-1): # apply (n-1) Givens rotations to zero-out the sub-diagonal elements in Hessenberg matrix
83 #         G_ = np.eye(n)
84 #         G_[i:i+2, i:i+2] = Givens(H[i,i],H[i+1,i])
85 #         G = G_ @ G
86 #     R = G @ H
87 #     Q = G.conjugate().T
88 #     return Q, R
89
90 # [Gn ... G2 G1].T [Gn ... G2 G1] H = H;
91
92
93 #def QR_Givens_rows(H,eigvec=False):
94 #     '''Row-wise application of Givens rotation (2 rows at a time) rather than whole matrix multiplication
95 #     Input: H = numpy array, Hessenberg matrix
96 #     eigvec = Bool, indicating whether eigenvectors is required; if True, store and output all Givens matrices
97 #     Return: Updated H_new overwritten on H_old // no explicit calculation of Q and R matrices
98 #     '''
99 #     n = H.shape[0]
100 #     G_store = []
101 #     G_iter = np.eye(n,dtype=H.dtype)
102 #
103 #     for i in range(n-1):
104 #         G = Givens(H[i,i],H[i+1,i])

```

```

105 #         new_rows = G @ H[i:i+2, :]
106 #         H[i:i+2, :] = new_rows
107 #         G_store.append(G)
108 #
109 #         # if eigenvectors are required
110 #         if eigvec:
111 #             G_ = np.eye(n, dtype=H.dtype)
112 #             G_[i:i+2, i:i+2] = G
113 #             G_iter = G_ @ G_iter
114 #
115 #         for i in range(n-1):
116 #             G = G_store.pop(0) #same order as above G1, G2, ...
117 #
118 #             if G.dtype != 'complex':
119 #                 new_cols = H[:, i:i+2] @ G.T
120 #             else:
121 #                 new_cols = H[:, i:i+2] @ G.conjugate().T
122 #
123 #             H[:, i:i+2] = new_cols
124 #
125 #         return H, G_iter
126
127
128
129 def select_idx(i,n,tridiagonal):
130
131     """ Find the start and end indices for element-wise application of Givens Rotation
132     Input -----
133         i: ith row/column of current application
134         n: total number of rows / columns
135         tridiagonal: bool, indicating whether the matrix is tridiagonal
136     Return -----
137         row_start: start index for row operations
138         col_end: end index for column operations
139     """
140
141     if tridiagonal: # only operates on 3 elements per row / column
142         row_start = max(0,i-1) # for post multiplication of G.T
143         col_end = i+3
144
145     else:
146         row_start = 0
147         col_end = n
148
149     return row_start, col_end
150
151
152
153 def QR_Givens(H, eigvec=False, inplace=True, tridiagonal=False):
154
155     """ Perform QR decomposition on a Hessenberg matrix by applying Givens Rotation
156         (element-wise rather than whole matrix multiplication)

```

```

157     No explicit computation of Q and R matrices; output updated Hessenberg matrix directly
158
159     Input -----
160     H: 2D np.array with real or complex entries, in the form of an upper Hessenberg matrix of shape n x n (square matrix)
161     eigvec : bool, indicating whether eigenvectors are required; default is False
162     inplace: bool, indicating whether to update H in place; default is True
163     tridiagonal: bool, indicating whether H is tridiagonal; default is False
164
165     Return -----
166     H_new: 2D np.array with real or complex entries, in the form of an *updated* Hessenberg matrix, effectively R@Q
167
168     G_iter: 2D np.array, the accumulated Givens rotation matrix, effectively Q.T;
169             if eigvec is False, not explicitly calculated and output identity matrix
170
171     R = G @ H_old : applying Givens rotation G = Gn @ ... @ G2 @ G1 column by column to reduce Hessenberg to upper triangular
172     H_old = G.T @ R => Q = G.T
173     H_new = R @ Q = G @ H_old @ G.T : update Hessenberg matrix (no explicit calculation )
174     G_iter = G = Gn @ ... @ G2 @ G1 : this is effectively the Givens rotation per round of QR iteration
175
176
177     n = H.shape[0]
178     G_store = []
179     G_iter = np.eye(n,dtype=H.dtype)
180
181     if inplace:
182         H_old = H
183     else:
184         H_old = H.copy()
185
186     for i in range(n-1):
187
188         _, col_end = select_idx(i,n,tridiagonal)
189
190         G = Givens(H_old[i,i],H_old[i+1,i])
191
192         # Premultiplication by a rotation in the (i, i+1)-plane only involves rows i and i+1 and leaves other rows unaffected
193         # Furthermore, only consider non-zero entries in these two rows, to avoid unnecessary multiplication by zero
194         H_old[i:i+2,i:col_end] = G @ H_old[i:i+2, i:col_end]
195
196         G_store.append(G)
197
198         # if eigenvectors are required
199         if eigvec:
200             G_ = np.eye(n,dtype=H.dtype)
201             G_[i:i+2,i:i+2] = G
202             G_iter = G_ @ G_iter
203
204         # H_old is now effectively R; next is to obtain H_new = R @ Q where Q = G1.T G2.T ... Gn-1.T
205
206         H_new = H_old
207
208         for i in range(n-1):

```

```
209     row_start, _ = select_idx(i,n,tridiagonal)
210
211     G = G_store.pop(0) #same order as above G1, G2, ...
212
213     if G.dtype != 'complex':
214         G_T = G.T
215     else:
216         G_T = G.conjugate().T
217
218     # Similar to above, postmultiplication by a rotation in the (i, i+1)-plane affects only columns i and i+1.
219     H_new[row_start:i+2, i:i+2] = H_new[row_start:i+2, i:i+2] @ G_T
220
221     # H_new is the updated version, effectively R @ Q
222
223     return H_new, G_iter
224
225
```

```

In [10]: 1  ### Testing QR_Givens() on Random Complex Matrices
2
3  print('\n\n')
4  print("=====")
5  print('Testing QR_Givens() function on randomly generated COMPLEX matrices')
6  print("=====")
7
8  for A in RANDOM_COMPLEX_MATRICES:
9      print('\n\nComplex >>> Input shape = {}'.format(A.shape))
10     H, S = Hessenberg(A,eigvec=True)
11     #print('A =\n',A)
12     #print('H =\n',H)
13
14     H_new, G = QR_Givens(H,eigvec=True, tridiagonal=False)
15     Q = G.T
16     print('\nQR_Givens: H_new=\n',H_new)
17     print('Q.conjugate().T @ Q = np.eye(n)? ',np.allclose(Q.conjugate().T@Q,np.eye(A.shape[0], dtype='complex'))))
18
19
20
21
22  ### Testing QR_Givens() on Random REAL Matrices
23
24  print('\n\n')
25  print("=====")
26  print('Testing QR_Givens() function on randomly generated REAL matrices')
27  print("=====")
28
29  for A in RANDOM_REAL_MATRICES:
30      print('\n\nComplex >>> Input shape = {}'.format(A.shape))
31      H, S = Hessenberg(A,eigvec=True)
32      #print('A =\n',A)
33      #print('H =\n',H)
34
35      H_new, G = QR_Givens(H,eigvec=True, tridiagonal=False)
36      Q = G.T
37      print('\nQR_Givens: H_new=\n',H_new)
38      print('Q.T @ Q = np.eye(n)? ',np.allclose(Q.T@Q,np.eye(A.shape[0])))
39
40
41
42
43  ### Testing QR_Givens() on Random Complex Matrices
44
45  print('\n\n')
46  print("=====")
47  print('Testing QR_Givens() function on SPECIAL real matrices')
48  print("=====")
49
50  for A in SPECIAL_REAL_MATRICES:
51      print('\n\nSpecial >>> Input shape = {}'.format(A.shape))
52      H, S = Hessenberg(A,eigvec=True)

```

```

53     #print('A =\n',A)
54     #print('H =\n',H)
55
56     H_new, G = QR_Givens(H,eigvec=True, tridiagonal=True)
57     Q = G.T
58     print('\nQR_Givens: H_new=\n',H_new)
59     print('Q.T @ Q = np.eye(n)? ',np.allclose(Q.T@Q,np.eye(A.shape[0])))
60
61

```

```

=====
Testing QR_Givens() function on randomly generated COMPLEX matrices
=====

```

Complex >>> Input shape = (3, 3)

```

QR_Givens: H_new=
[[ 1.547+1.438j  0.288-0.896j  0.856-0.45j ]
 [-0.677-0.j    0.402-0.333j -0.096-0.059j]
 [ 0.   -0.j    0.033+0.081j  0.035-0.13j ]]
Q.conjugate().T @ Q = np.eye(n)? True

```

Complex >>> Input shape = (5, 5)

```

QR_Givens: H_new=
[[ 2.081+2.091j -0.111-0.981j -0.224+0.181j  0.197-0.359j  0.353+0.104j]
 [-0.733+0.j    0.077+0.777j -0.204-0.177j  0.066-0.478j  0.475-0.164j]
 [ 0.   +0.j    0.443+0.j    -0.144-0.247j  0.003-0.088j -0.344-0.207j]
 [ 0.   -0.j    0.   +0.j    -0.531+0.j    -0.36 +0.057j  0.07 -0.j ]
 [ 0.   +0.j    -0.   -0.j    -0.   +0.j    -0.028-0.168j -0.084+0.72j ]]
Q.conjugate().T @ Q = np.eye(n)? True

```

Complex >>> Input shape = (10, 10)

```

QR_Givens: H_new=
[[ 3.65 +4.147j  0.258-2.361j  0.102-0.964j -0.403+0.485j -0.269+0.468j  0.414-0.241j -0.411+0.212j -0.569+0.084j -0.183+0.146j  0.93 -0.711j]
 [-3.069+0.j    0.917+1.403j -0.566+0.44j -0.148-0.674j -0.009-0.237j  0.248-0.012j  0.636+0.266j -0.573-0.708j -0.088-0.47j  0.143-0.05j ]
 [ 0.   -0.j    1.104+0.j    0.308+0.162j  0.013+0.298j -0.18 -0.073j  0.28 -0.22j  0.25 +0.09j -0.267+0.112j -0.58 +0.029j -0.013+0.73j ]
 [ 0.   -0.j    -0.   +0.j    -0.919+0.j    -0.82 +0.018j -0.095+0.488j -0.094-0.097j -0.3 -0.09j  0.142+0.034j -0.155+0.269j -0.201+0.37j ]
 [-0.   +0.j    -0.   -0.j    -0.   +0.j    -1.11 +0.j    0.597-0.219j -0.144-0.066j -0.284+0.373j  0.225+0.256j  0.543-0.28j -0.295-0.441j]
 [ 0.   +0.j    0.   -0.j    0.   +0.j    0.   +0.j    0.944+0.j    -0.159+0.048j -0.151+0.444j -0.093+0.103j -0.303-0.007j -0.208-0.099j]
 [-0.   -0.j    0.   +0.j    -0.   -0.j    -0.   +0.j    -0.902+0.j    0.404-0.188j  0.246+0.019j  0.21 +0.029j  0.01 +0.087j]
 [-0.   +0.j    0.   +0.j    -0.   +0.j    0.   +0.j    -0.   -0.j    0.374+0.j    -0.331-0.035j  0.31 +0.259j -0.207+0.306j]
 [ 0.   -0.j    -0.   +0.j    -0.   +0.j    -0.   +0.j    0.   -0.j    0.   +0.j    -0.   +0.j    0.192+0.j    -0.513+0.064j  0.271+0.081j]
 [-0.   -0.j    -0.   +0.j    -0.   -0.j    0.   -0.j    -0.   -0.j    -0.   +0.j    -0.   +0.j    -0.358-0.263j  0.055+0.222j]]

```

```
Q.conjugate().T @ Q = np.eye(n)? True
```

```
=====
Testing QR_Givens() function on randomly generated REAL matrices
=====
```

```
Complex >>> Input shape = (3, 3)
```

```
QR_Givens: H_new=
[[ 0.737 -0.473  0.06 ]
 [-0.434  0.349 -0.381]
 [-0.      0.354 -0.068]]
Q.T @ Q = np.eye(n)? True
```

```
Complex >>> Input shape = (5, 5)
```

```
QR_Givens: H_new=
[[ 1.076 -0.96  -0.065  0.577  0.089]
 [-1.481  0.692 -0.924  0.368 -0.17 ]
 [-0.     -0.127  0.072 -0.04  0.321]
 [-0.      0.     0.397  0.182  0.204]
 [-0.      0.     -0.     0.007  0.067]]
Q.T @ Q = np.eye(n)? True
```

```
Complex >>> Input shape = (10, 10)
```

```
QR_Givens: H_new=
[[ 4.074 -1.492 -0.118  0.082 -0.496  0.335 -0.538 -0.027  0.089 -0.36 ]
 [-2.145  0.537 -0.244 -0.342  0.093  0.94  0.018 -0.45  0.525  0.518]
 [ 0.     -0.744  0.267 -0.053  0.355 -0.016 -0.17  0.18  0.29  0.151]
 [ 0.     -0.     0.833 -0.195 -0.594  0.055 -0.081  0.06  0.106 -0.032]
 [ 0.     -0.     -0.     0.819 -0.141  0.032  0.097 -0.36 -0.42  0.214]
 [ 0.      0.      0.      0.      0.436  0.083  0.155  0.411  0.196 -0.435]
 [ 0.      0.     -0.     -0.      0.     -0.222 -0.5  -0.007 -0.165  0.215]
 [-0.      0.     -0.      0.     -0.     -0.     -0.158  0.406 -0.208 -0.423]
 [ 0.     -0.      0.     -0.      0.      0.      0.      0.045  0.247  0.277]
 [ 0.     -0.     -0.     -0.     -0.      0.      0.      0.     -0.193 -0.362]]
Q.T @ Q = np.eye(n)? True
```

```
=====
Testing QR_Givens() function on SPECIAL real matrices
=====
```

```
Special >>> Input shape = (10, 10)
```

```

QR_Givens: H_new=
[[-2.853  9.49  0.  0. -0.  0.  0. -0.  0.  0. ]
 [ 9.49 -1.212 -3.894 -0.  0.  0.  0.  0. -0.  0. ]
 [-0. -3.894 -9.049 6.26  0. -0. -0. -0. -0.  0. ]
 [ 0. -0.  6.26 4.223 5.993 -0.  0. -0. -0. -0. ]
 [-0.  0.  0. 5.993 -7.009 4.185 0. -0. -0. -0. ]
 [ 0.  0. -0. -0. 4.185 -3.363 -5.347 -0.  0. -0. ]
 [ 0.  0. -0.  0.  0. -5.347 5.205 -3.516 -0. -0. ]
 [-0.  0. -0. -0. -0.  0. -3.516 -2.659 3.083  0. ]
 [ 0. -0. -0. -0. -0.  0.  0. 3.083 -0.084 0.12 ]
 [ 0.  0.  0. -0. -0. -0. -0.  0.  0.12 -1.199]]
Q.T @ Q = np.eye(n)? True

```

Special >>> Input shape = (10, 10)

```

QR_Givens: H_new=
[[ 0.077  2.979 -0.  0.  0.  0. -0. -0. -0.  0. ]
 [ 2.979 -1.097 -3.511  0.  0.  0. -0.  0. -0.  0. ]
 [ 0. -3.511 -0.763 -1.662  0.  0.  0.  0. -0. -0. ]
 [ 0. -0. -1.662 -4.181 0.311  0.  0.  0. -0.  0. ]
 [ 0.  0.  0. 0.311 1.002 -2.148 -0.  0.  0. -0. ]
 [ 0.  0.  0. -0. -2.148 0.85 3.502  0. -0.  0. ]
 [-0. -0.  0.  0. -0. 3.502 -3.55 0.921  0.  0. ]
 [-0.  0.  0. -0. -0.  0. 0.921 -4.319 -0.008  0. ]
 [-0. -0. -0. -0.  0.  0. -0. -0.008 -6.019 -0. ]
 [ 0.  0. -0.  0.  0.  0.  0.  0. -0.  0. ]]
Q.T @ Q = np.eye(n)? True

```

Special >>> Input shape = (10, 10)

```

QR_Givens: H_new=
[[ 5.5  2.872 -0.  0.  0.  0.  0.  0.  0.  0. ]
 [-2.872 0.5 1.265 -0. -0.  0. -0.  0. -0.  0. ]
 [-0. -1.265 0.5 -0.806 -0. -0. -0.  0.  0. -0. ]
 [ 0.  0. 0.806 0.5 0.577 -0.  0. -0.  0. -0. ]
 [ 0. -0. -0. -0.577 0.5 -0.435 0.  0.  0. -0. ]
 [-0.  0.  0. -0. 0.435 0.5 -0.334 -0.  0. -0. ]
 [ 0. -0.  0.  0. -0. 0.334 0.5 -0.256 -0. -0. ]
 [-0.  0. -0.  0.  0. -0. 0.256 0.5 -0.188  0. ]
 [ 0. -0.  0. -0. -0. -0.  0. 0.188 0.5 -0.121]
 [ 0.  0. -0.  0.  0. -0.  0.  0. 0.121 0.5 ]]
Q.T @ Q = np.eye(n)? True

```

Special >>> Input shape = (6, 6)

```

QR_Givens: H_new=
[[ 13.248 -12.062 -17.543 -0.14  9.015 -7.936]
 [ 7.268  1.573  0.487  5.827 10.683 -2.416]

```



```
[ 0.      -7.658   1.654   1.797   5.373   3.251]
[ -0.       0.     -1.01  -3.139  -3.496   9.98 ]
[ -0.      -0.     -0.     4.939  -1.009   4.566]
[ -0.      -0.       0.    -0.     -1.99   6.674]]
Q.T @ Q = np.eye(n)? True
```

C:\ProgramData\Anaconda3\lib\site-packages\ipykernel_launcher.py:32: ComplexWarning: Casting complex values to real discards the imaginary part

Observation:

- Function QR_Givens() seems to be working for both real and complex matrices as expected
- **Where does the complex warning come from??**

QR Iteration

Some Background Information

Source: <https://scicomp.stackexchange.com/questions/30407/how-does-the-qr-algorithm-applied-to-a-real-matrix-returns-complex-eigenvalues>
(<https://scicomp.stackexchange.com/questions/30407/how-does-the-qr-algorithm-applied-to-a-real-matrix-returns-complex-eigenvalues>)

- QR algorithm converges to the real Schur decomposition: a unitary matrix Q and a matrix R in block upper triangular form such that $A = QRQ^T$
- The key point is the *block upper triangular* form, which means here R_{ii} are real blocks of
 - EITHER **size 1x1** (R_{ii} is a (real) eigenvalue of A)
 - OR **size 2x2** (R_{ii} has a pair of complex conjugate eigenvalues).

```

In [11]: 1 #def QR_Iteration_Eigenvalues_naive(A, max_iter, tol):
2 #   # step 1: tranform A to Hessenberg
3 #   H, _ = Hessenberg(A)
4 #   # step 2: QR iteration
5 #   H_old = H
6 #   for i in range(max_iter):
7 #       Q, R = QR_Givens_naive(H_old)
8 #       H_new = R @ Q
9 #       # TODO: test for convergence
10 #       if np.linalg.norm(H_new - H) < tol:
11 #           print('break at i=',i,np.linalg.norm(H_new - H),H_new)
12 #           break
13 #       H_old = H_new
14 #   R = H_new
15 #   return np.diag(R) # this is wrong
16
17
18 def diagonal_block(R):
19
20     """    Read eigenvalues from the diagonal block matrix R, either in 1x1 block (i.e. real eigenvalue)
21           or in 2x2 block (i.e. complex conjugate pair)
22     Input  -----
23           R: 2D np.array with real or complex entries, in the form of a block upper triangular matrix
24     Return -----
25           eigenvalues: 1D np.array with real or complex entries
26     """
27
28     eigenvalues = []
29
30     for i in range(len(R)):
31         if i < len(eigenvalues): # if current diagonal values has already been used in previous step, skip
32             continue
33
34         if i == len(R)-1 or np.abs(R[i+1,i]) < ATOL: # if subdiagonal element is sufficiently small, treat as zero OR if last row
35             eigenvalues.append(R[i,i])
36
37         else:
38             # solving eigenvalues from characteristic polynomial lam^2 - (R[i,i]+R[i+1,i+1])*lam + (R[i,i]*R[i+1,i+1] - R[i,i+1]*R[i+1,i]) = 0
39             b = - (R[i,i]+R[i+1,i+1])
40             c = R[i,i]*R[i+1,i+1] - R[i,i+1]*R[i+1,i]
41
42             lam_1 = -b/2
43             sign = np.sign(lam_1)
44
45             if b**2 - 4*c >= 0:
46                 lam_2 = np.sqrt(b**2-4*c)/2
47                 eigenvalues.append(lam_1 + sign*lam_2)
48                 eigenvalues.append(lam_1 - sign*lam_2)
49             else:
50                 lam_2 = np.sqrt(-(b**2-4*c))/2
51                 eigenvalues.append(lam_1 + sign*lam_2*1j)
52                 eigenvalues.append(lam_1 - sign*lam_2*1j)

```

```

53
54     return np.array(eigenvalues)
55
56
57
58 def QR_Iteration_Eigenvalues(A, max_iter, tol):
59
60     """    Perform QR iteration to obtain eigenvalues
61     Input  -----
62           A: 2D np.array with real or complex entries
63           max_iter: int, maximum number of iterations to be performed
64           tol: float, relative tolerance between eigenvalues by successive iterations
65     Return -----
66           eigvals_new: 1D np.array with real or complex entries
67           i: total number of iterations
68     """
69
70
71     # step 1: tranform A to Hessenberg
72     H, _ = Hessenberg(A) # default: eigvec=False, inplace=True
73
74     # step 2: QR iteration
75     H_old = H #.copy()
76     eigvals_old = diagonal_block(H)
77
78     for i in range(max_iter):
79         H_new, _ = QR_Givens(H_old) # updating H_old in-place # default QR_Givens(H,eigvec=False, inplace=True, tridiagonal=False)
80
81         eigvals_new = diagonal_block(H_new)
82         #print('>>>\n', H_new, '\n\n', np.diag(H_new), '\n')
83
84         # Test for convergence: relative tol = 1- w / w' for each eigenvalue
85         if np.allclose(eigvals_new, eigvals_old, rtol=tol):
86             print('Iteration terminates at i={} with tol={} reached'.format(i,tol))
87             break
88
89         if i == max_iter-1:
90             err = np.max(abs((eigvals_new - eigvals_old)) / abs(eigvals_old))
91             idx = np.argwhere(np.isclose(eigvals_new, eigvals_old, rtol=tol)==False).tolist()
92             print('max_iter={} reached, max error={} vs tol={}; index of non-convergence={}'.format(max_iter, err, tol, idx))
93
94         eigvals_old = eigvals_new.copy() # need to save a copy for comparison in the next iteration
95         # H_old = H_new # this is not needed as H_old is updated inplace
96
97     return eigvals_new, i
98
99
100

```

```

In [12]: 1 # Testing
2
3 def sort_(eigenvalues):
4
5     """    Sort eigenvalues in descending order by magitude;
6             following Numpy's extended sort order: Real: [R, nan]; Complex: [R + Rj, R + nanj, nan + Rj, nan + nanj]
7     Input    -----
8             eigenvalues: 1D np.array with real or complex entries
9     Return   -----
10            eigenvalues_sorted: 1D np.array with real or complex entries, sorted in descending order
11    """
12    eigenvalues_sorted = np.flip(np.sort(eigenvalues))
13
14    return eigenvalues_sorted
15
16 # if eigenvalues.dtype != 'complex':
17 #     eigenvalues_sorted = np.sort(eigenvalues) #np.flip(sorted(eigenvalues,key=abs))
18 # else:
19 #     eigenvalues_sorted = np.sort_complex(eigenvalues)
20 #     return eigenvalues_sorted
21
22
23
24 def test_eigenvalues_function(A,function):
25
26     """    Perform eigenvalue testing on selected function; eigenvalues are compared with results from np.linalg.eig()
27     Input    -----
28             A: input matrix, 2D np.array with real or complex entries
29             function: name of the function being tested
30     Return   -----
31             None; test results will be printed
32     """
33
34     print("----- Testing for function: {}() -----".format(function.__name__))
35     w,v = np.linalg.eig(A)
36     w_sorted = sort_(w)
37     eigenvalues,i = function(A,max_iter=MAX_ITER, tol=RTOL)
38     eigenvalues_sorted = sort_(eigenvalues)
39     print()
40     print('my eigenvalues: {}'.format(eigenvalues_sorted))
41     print('np.linalg.eig: {}'.format(w_sorted)) #sort in descending order of magnitudes
42
43     if np.allclose(w_sorted,eigenvalues_sorted):
44         print('\nnp.linalg.eig and my eigenvalues close? True \n')
45     else:
46         print('\nnp.linalg.eig and my eigenvalues close? False \n')
47         print('\nmy eigenvalues - np.linalg.eig =\n', eigenvalues_sorted - w_sorted,'\n')
48
49     print('\n')
50
51
52 def test_eigenvalues(eigenvalues,w, verbose=True):

```

```
53
54 """    Comparing two sets of eigenvalues
55 Input  -----
56         eigenvalues: 1D np.array with real or complex entries, eigenvalues from my function
57         w: eigenvalues from np.linalg.eig(), basis for comparison
58         verbose: bool, indicating whether to print the difference between the two sets of eigenvalues
59 Return -----
60         None; test results will be printed
61 """
62
63 eigenvalues_sorted = sort_(eigenvalues)
64 w_sorted = sort_(w)
65
66 if verbose:
67     print()
68     print('my eigenvalues: {}'.format(eigenvalues_sorted))
69     print('np.linalg.eig: {}'.format(w_sorted)) #sort in descending order of magnitudes
70
71 if np.allclose(w_sorted,eigenvalues_sorted):
72     print('\nnp.linalg.eig and my eigenvalues close? True \n')
73 else:
74     print('\nnp.linalg.eig and my eigenvalues close? False \n')
75     if verbose:
76         print('my eigenvalues - np.linalg.eig =\n', eigenvalues_sorted - w_sorted,'\n')
77         print('max abs diff = ',np.abs(eigenvalues_sorted - w_sorted).max(),'\n')
78     print('\n')
79
```

```

In [43]: 1  ### Testing QR_Iteration_Eigenvalues() on Random Complex Matrices
2
3  print('\n\n')
4  print("=====")
5  print('Testing QR_Iteration_Eigenvalues() function on randomly generated COMPLEX matrices')
6  print("=====")
7
8  for A in RANDOM_COMPLEX_MATRICES:
9      print('\nComplex >>> Input shape = {}\n'.format(A.shape))
10     test_eigenvalues_function(A, QR_Iteration_Eigenvalues)
11
12
13
14  ### Testing QR_Iteration_Eigenvalues() on Random Real Matrices
15
16  print('\n\n')
17  print("=====")
18  print('Testing QR_Iteration_Eigenvalues() function on randomly generated REAL matrices')
19  print("=====")
20
21  for A in RANDOM_REAL_MATRICES:
22      print('\nReal >>> Input shape = {}\n'.format(A.shape))
23      test_eigenvalues_function(A, QR_Iteration_Eigenvalues)
24
25
26
27  ### Testing QR_Iteration_Eigenvalues() on Special Matrices
28
29  print('\n\n')
30  print("=====")
31  print('Testing QR_Iteration_Eigenvalues() function on SPECIAL real matrices')
32  print("=====")
33
34  for A in SPECIAL_REAL_MATRICES:
35      print('\nSpecial >>> Input shape = {}\n'.format(A.shape))
36      test_eigenvalues_function(A, QR_Iteration_Eigenvalues)
37
38
39

```

```

=====
Testing QR_Iteration_Eigenvalues() function on randomly generated COMPLEX matrices
=====

```

```
Complex >>> Input shape = (3, 3)
```

```

----- Testing for function: QR_Iteration_Eigenvalues() -----
Iteration terminates at i=11 with tol=1e-06 reached

```

```

my eigenvalues: [ 1.71 +1.655j  0.288-0.519j -0.015-0.161j]
np.linalg.eig:  [ 1.71 +1.655j  0.288-0.519j -0.015-0.161j]

np.linalg.eig and my eigenvalues close? True

```

Complex >>> Input shape = (5, 5)

```

----- Testing for function: QR_Iteration_Eigenvalues() -----
Iteration terminates at i=935 with tol=1e-06 reached

```

```

my eigenvalues: [ 2.251+2.287j  0.132+0.508j -0.182+0.806j -0.189-0.474j -0.442+0.271j]
np.linalg.eig:  [ 2.251+2.287j  0.132+0.508j -0.182+0.806j -0.189-0.474j -0.442+0.271j]

np.linalg.eig and my eigenvalues close? True

```

Complex >>> Input shape = (10, 10)

```

----- Testing for function: QR_Iteration_Eigenvalues() -----
Iteration terminates at i=74 with tol=1e-06 reached

```

```

my eigenvalues: [ 4.624+5.231j  1.242-0.661j  0.321-0.067j  0.194+0.373j  0.193-1.047j  0.058+1.069j -0.285+0.567j -0.419-0.316j -0.705-0.182j -1.116+0.655j]
np.linalg.eig:  [ 4.624+5.231j  1.242-0.661j  0.321-0.067j  0.194+0.373j  0.193-1.047j  0.058+1.069j -0.285+0.567j -0.419-0.316j -0.705-0.182j -1.116+0.655j]

np.linalg.eig and my eigenvalues close? True

```

```

=====
Testing QR_Iteration_Eigenvalues() function on randomly generated REAL matrices
=====

```

Real >>> Input shape = (3, 3)

```

----- Testing for function: QR_Iteration_Eigenvalues() -----
Iteration terminates at i=35 with tol=1e-06 reached

```

```

my eigenvalues: [0.992+0.j      0.013+0.295j 0.013-0.295j]
np.linalg.eig:  [0.992+0.j      0.013+0.295j 0.013-0.295j]

np.linalg.eig and my eigenvalues close? True

```

Real >>> Input shape = (5, 5)

----- Testing for function: QR_Iteration_Eigenvalues() -----
Iteration terminates at i=28 with tol=1e-06 reached

```
my eigenvalues: [ 2.116+0.j      0.207+0.229j  0.207-0.229j  0.073+0.j      -0.515+0.j      ]
np.linalg.eig:  [ 2.116+0.j      0.207+0.229j  0.207-0.229j  0.073+0.j      -0.515+0.j      ]
```

np.linalg.eig and my eigenvalues close? True

Real >>> Input shape = (10, 10)

----- Testing for function: QR_Iteration_Eigenvalues() -----

C:\ProgramData\Anaconda3\lib\site-packages\ipykernel_launcher.py:32: ComplexWarning: Casting complex values to real discards the imaginary part

Iteration terminates at i=558 with tol=1e-06 reached

```
my eigenvalues: [ 4.82 +0.j      0.579+0.149j  0.579-0.149j  0.377+0.j      0.146+0.j      -0.24 +0.j      -0.352+0.944j -0.352-0.944j -0.571+0.117j -0.571-0.117j]
np.linalg.eig:  [ 4.82 +0.j      0.579+0.149j  0.579-0.149j  0.377+0.j      0.146+0.j      -0.24 +0.j      -0.352+0.944j -0.352-0.944j -0.571+0.117j -0.571-0.117j]
```

np.linalg.eig and my eigenvalues close? True

=====

Testing QR_Iteration_Eigenvalues() function on SPECIAL real matrices

=====

Special >>> Input shape = (10, 10)

----- Testing for function: QR_Iteration_Eigenvalues() -----
Iteration terminates at i=194 with tol=1e-06 reached

```
my eigenvalues: [ 9.684  8.685  7.302  1.666 -1.201 -3.008 -5.856 -8.817 -11.764 -14.69 ]
np.linalg.eig:  [ 9.684  8.685  7.302  1.666 -1.201 -3.008 -5.856 -8.817 -11.764 -14.69 ]
```

np.linalg.eig and my eigenvalues close? True

Special >>> Input shape = (10, 10)

----- Testing for function: QR_Iteration_Eigenvalues() -----
Iteration terminates at i=644 with tol=1e-06 reached

```
my eigenvalues: [ 4.03  3.972  0.064  0.    -0.064 -3.97  -4.03  -5.954 -6.018 -6.03 ]
np.linalg.eig:  [ 4.03  3.972  0.064  0.    -0.064 -3.97  -4.03  -5.953 -6.018 -6.03 ]
```

np.linalg.eig and my eigenvalues close? False

```
my eigenvalues - np.linalg.eig =
[-0. -0. -0. -0.  0. -0.  0. -0.  0.  0.]
```

Special >>> Input shape = (10, 10)

----- Testing for function: QR_Iteration_Eigenvalues() -----
Iteration terminates at i=780 with tol=1e-06 reached

```
my eigenvalues: [1.026+0.009j 1.026-0.009j 1.016+0.022j 1.016-0.022j 0.999+0.027j 0.999-0.027j 0.984+0.021j 0.984-0.021j 0.975+0.008j 0.975-0.008j]
np.linalg.eig:  [1. 1. 1. 1. 1. 1. 1. 1. 1. 1.]
```

np.linalg.eig and my eigenvalues close? False

```
my eigenvalues - np.linalg.eig =
[ 0.026+0.009j  0.026-0.009j  0.016+0.022j  0.016-0.022j -0.001+0.027j -0.001-0.027j -0.016+0.021j -0.016-0.021j -0.025+0.008j -0.025-0.008j]
```

Special >>> Input shape = (6, 6)

----- Testing for function: QR_Iteration_Eigenvalues() -----
Iteration terminates at i=52 with tol=1e-06 reached

```
my eigenvalues: [5.+6.j 5.-6.j 4.+0.j 3.+0.j 1.+2.j 1.-2.j]
np.linalg.eig:  [5.+6.j 5.-6.j 4.+0.j 3.+0.j 1.+2.j 1.-2.j]
```

np.linalg.eig and my eigenvalues close? True

Observations:

- Function `QR_Iteration_Eigenvalues()` seems to be working as expected with both real and complex matrices, with real eigenvalues or complex conjugate pairs
- Underperformance in special matrices: diagonal dominant and unbalanced
 - *real symmetric* `A = np.random.randint(-3,3,(10,10)) A = (A.T + A).astype('float')`
 - *diagonal dominant* `B = A - np.triu(A,1)0.99 - np.tril(A,-1)0.99`
 - *unbalanced* `C = np.tril(np.ones((10,10),dtype='float'),0)`

```
In [14]: 1  ### Testing QR_Iteration_Eigenvalues() on COMPLEX Matrices with only pure imaginary parts
          2
          3 print('\n\n')
          4 print("=====")
          5 print('Testing QR_Iteration_Eigenvalues() function on SPECIAL complex matrices (Im Only)')
          6 print("=====")
          7
          8 A = np.random.rand(5,5) * 1j
          9 print('\nSpecial >>> Input shape = {}'.format(A.shape))
         10 test_eigenvalues_function(A,QR_Iteration_Eigenvalues)
         11
```

```
=====
Testing QR_Iteration_Eigenvalues() function on SPECIAL complex matrices (Im Only)
=====

Special >>> Input shape = (5, 5)

----- Testing for function: QR_Iteration_Eigenvalues() -----
Iteration terminates at i=23 with tol=1e-06 reached

my eigenvalues: [ 0.561+0.013j  0.   -0.296j  0.   +0.978j  0.   -2.01j  -0.561+0.013j]
np.linalg.eig:  [ 0.752+0.172j  0.   +2.607j  0.   -0.248j  0.   -0.023j  -0.752+0.172j]

np.linalg.eig and my eigenvalues close? False

my eigenvalues - np.linalg.eig =
[-0.192-0.159j  0.   -2.903j  0.   +1.225j  0.   -1.986j  0.192-0.159j]
```

Observations:

- Does not seem to work for matrices with pure imaginary parts ... **#TODO**

Wilkinson Shift

1.4.22 Definition(Wilkinson shift)

Let

$$\mathbf{M} = \begin{pmatrix} h_{n-1,n-1}^{(k)} & h_{n-1,n}^{(k)} \\ h_{n,n-1}^{(k)} & h_{nn}^{(k)} \end{pmatrix}.$$

Then, for σ_k use the eigenvalue of \mathbf{M} which is closer to $h_{nn}^{(k)}$.

1.4.23 Remark

The Wilkinson shift is reliable and the $h_{n,n-1}$ and h_{nn} converge to zero and the smallest eigenvalue by magnitude, respectively. They converge at least quadratically and cubically in the symmetric case [GvL83, Section 8.2].

Source: NLA Lecture Notes

```

In [15]: 1
2 def Wilkinson_shift(H):
3
4     """    Using the bottom right 2x2 block of Hessenberg matrix to determine if eigenvalues are real or complex (b^2-4ac)
5             Calculate the Wilkinson's shift according to Lecture Notes 1.4.22 Definition (Wilkinson shift)
6     Input   -----
7             H: 2D np.array with real or complex entries, in the form of an upper Hessenberg matrix
8     Return  -----
9             datatype: 'complex' or 'float'
10            lam1 or lam2: shift to be performed
11     """
12
13     n = H.shape[0]
14
15     # find the current index where the subdiagonal is non-zero
16     # (if the subdiagonal is zero, it means the shift has worked and converged to an eigenvalue)
17     while abs(H[n-1,n-2]) < ATOL: #global variable ATOL = 1e-18, proxy for zero
18         n -= 1
19
20     # M is the bottom right 2x2 block with nonzero subdiagonal (equivalent to the idea of deflation)
21     M = H[n-2:n,n-2:n]
22
23     # characteristic polynomial x^2 + bx + c = 0
24     b = -(M[0,0] + M[1,1])
25     c = (M[0,0]*M[1,1] - M[1,0]*M[0,1])
26
27     # if real eigenvalues - return the one closer to A[n,n]'
28     if b**2 >= 4*c:
29         lam1 = (-b + np.sqrt(b**2-4*c))/2
30         lam2 = (-b - np.sqrt(b**2-4*c))/2
31         datatype = 'float'
32
33     # if complex eigenvalues - return Re(x) and Im(x)
34     else:
35         re_ = -b/2
36         im_ = np.sqrt(4*c-b**2)/2
37         lam1 = re_+1j*im_
38         lam2 = re_+1j*im_
39         datatype = 'complex'
40
41     if abs(lam1-M[1,1]) < abs(lam2-M[1,1]):
42         return (datatype, lam1)
43
44     else:
45         return (datatype, lam2)
46
47
48
49 def QR_Iteration_WilkinsonShift(A, max_iter, tol):
50
51     """    Perform QR iteration with Wilkinson's shift to obtain eigenvalues
52     Input   -----

```

```

53     A: 2D np.array with real or complex entries
54     max_iter: int, maximum number of iterations to be performed
55     tol: float, relative tolerance between eigenvalues by successive iterations
56     Return -----
57     eigvals_new: 1D np.array with real or complex entries
58     i: total number of iterations
59     """
60
61     n = A.shape[0]
62
63     # step 1: transform A to Hessenberg
64     H, _ = Hessenberg(A)
65
66     # step 2: QR iteration
67     H_old = H.copy()
68     eigvals_old = diagonal_block(H)
69
70     for i in range(max_iter):
71
72         datatype, lam = Wilkinson_shift(H_old)
73         # print(">>> Wilkinson_shift = {}".format(lam))
74
75         # H_old = H_old - lam * np.eye(n)
76         for j in range(n):
77             H_old[j,j] -= lam
78
79         #H_new, _ = QR_Givens(H_old) + lam * np.eye(n) # updating H_old in-place # default QR_Givens(H,eigvec=False, inplace=True, tridiagonal=False)
80         H_new, _ = QR_Givens(H_old)
81         for j in range(n):
82             H_new[j,j] += lam
83
84         eigvals_new = diagonal_block(H_new)
85         H_old = H_new
86
87         # Test for convergence: relative tol = 1- w / w' for each eigenvalue
88         if np.allclose(eigvals_new, eigvals_old, rtol=tol):
89             print('Iteration terminates at i={} with tol={} reached'.format(i,tol))
90             break
91
92         if i == max_iter-1:
93             err = np.max(abs((eigvals_new - eigvals_old)) / abs(eigvals_old))
94             idx = np.argwhere(np.isclose(eigvals_new, eigvals_old, rtol=tol)==False).tolist()
95             print('max_iter={} reached, max error={} vs tol={}; index of non-convergence={}'.format(max_iter, err, tol, idx))
96
97         eigvals_old = eigvals_new
98
99     return eigvals_new, i
100
101
102

```



```

In [16]: 1  ### Testing QR_Iteration_WilkinsonShift() on Random Complex Matrices
2
3  print('\n\n')
4  print("=====")
5  print('Testing QR_Iteration_WilkinsonShift() function on randomly generated COMPLEX matrices')
6  print("=====")
7
8  for A in RANDOM_COMPLEX_MATRICES:
9      print('\nComplex >>> Input shape = {}'.format(A.shape))
10     test_eigenvalues_function(A, QR_Iteration_Eigenvalues)
11     test_eigenvalues_function(A, QR_Iteration_WilkinsonShift)
12
13
14  ### Testing QR_Iteration_WilkinsonShift() on Random Real Matrices
15
16  print('\n\n')
17  print("=====")
18  print('Testing QR_Iteration_WilkinsonShift() function on randomly generated REAL matrices')
19  print("=====")
20
21  for A in RANDOM_REAL_MATRICES:
22      print('\nReal >>> Input shape = {}'.format(A.shape))
23      test_eigenvalues_function(A, QR_Iteration_Eigenvalues)
24      test_eigenvalues_function(A, QR_Iteration_WilkinsonShift)
25
26
27  ### Testing QR_Iteration_WilkinsonShift() on Special Matrices
28
29  print('\n\n')
30  print("=====")
31  print('Testing QR_Iteration_WilkinsonShift() function on SPECIAL real matrices')
32  print("=====")
33
34  for A in SPECIAL_REAL_MATRICES:
35      print('\nSpecial >>> Input shape = {}'.format(A.shape))
36      test_eigenvalues_function(A, QR_Iteration_Eigenvalues)
37      test_eigenvalues_function(A, QR_Iteration_WilkinsonShift)
38
39
40

```

```

=====
Testing QR_Iteration_WilkinsonShift() function on randomly generated COMPLEX matrices
=====

```

```
Complex >>> Input shape = (3, 3)
```

```

----- Testing for function: QR_Iteration_Eigenvalues() -----
Iteration terminates at i=11 with tol=1e-06 reached

```

```
my eigenvalues: [ 1.71 +1.655j  0.288-0.519j -0.015-0.161j]
np.linalg.eig: [ 1.71 +1.655j  0.288-0.519j -0.015-0.161j]

np.linalg.eig and my eigenvalues close? True
```

```
----- Testing for function: QR_Iteration_WilkinsonShift() -----
Iteration terminates at i=5 with tol=1e-06 reached
```

```
my eigenvalues: [ 1.71 +1.655j  0.288-0.519j -0.015-0.161j]
np.linalg.eig: [ 1.71 +1.655j  0.288-0.519j -0.015-0.161j]

np.linalg.eig and my eigenvalues close? True
```

Complex >>> Input shape = (5, 5)

```
----- Testing for function: QR_Iteration_Eigenvalues() -----
Iteration terminates at i=935 with tol=1e-06 reached
```

```
my eigenvalues: [ 2.251+2.287j  0.132+0.508j -0.182+0.806j -0.189-0.474j -0.442+0.271j]
np.linalg.eig: [ 2.251+2.287j  0.132+0.508j -0.182+0.806j -0.189-0.474j -0.442+0.271j]

np.linalg.eig and my eigenvalues close? True
```

```
----- Testing for function: QR_Iteration_WilkinsonShift() -----
Iteration terminates at i=12 with tol=1e-06 reached
```

```
my eigenvalues: [ 2.251+2.287j  0.132+0.508j -0.182+0.806j -0.189-0.474j -0.442+0.271j]
np.linalg.eig: [ 2.251+2.287j  0.132+0.508j -0.182+0.806j -0.189-0.474j -0.442+0.271j]

np.linalg.eig and my eigenvalues close? True
```

Complex >>> Input shape = (10, 10)

```
----- Testing for function: QR_Iteration_Eigenvalues() -----
Iteration terminates at i=74 with tol=1e-06 reached
```

```
my eigenvalues: [ 4.624+5.231j  1.242-0.661j  0.321-0.067j  0.194+0.373j  0.193-1.047j  0.058+1.069j -0.285+0.567j -0.419-0.316j -0.705-0.182j -1.116+0.655j]
np.linalg.eig: [ 4.624+5.231j  1.242-0.661j  0.321-0.067j  0.194+0.373j  0.193-1.047j  0.058+1.069j -0.285+0.567j -0.419-0.316j -0.705-0.182j -1.116+0.655j]
```



```
np.linalg.eig and my eigenvalues close? True
```

```
----- Testing for function: QR_Iteration_WilkinsonShift() -----
Iteration terminates at i=40 with tol=1e-06 reached
```

```
my eigenvalues: [ 4.624+5.231j  1.242-0.661j  0.321-0.067j  0.194+0.373j  0.193-1.047j  0.058+1.069j -0.285+0.567j -0.419-0.316j -0.705-0.182j -1.116+0.655j]
np.linalg.eig: [ 4.624+5.231j  1.242-0.661j  0.321-0.067j  0.194+0.373j  0.193-1.047j  0.058+1.069j -0.285+0.567j -0.419-0.316j -0.705-0.182j -1.116+0.655j]
```

```
np.linalg.eig and my eigenvalues close? True
```

```
=====
Testing QR_Iteration_WilkinsonShift() function on randomly generated REAL matrices
=====
```

```
Real >>> Input shape = (3, 3)
```

```
----- Testing for function: QR_Iteration_Eigenvalues() -----
Iteration terminates at i=35 with tol=1e-06 reached
```

```
my eigenvalues: [0.992+0.j      0.013+0.295j 0.013-0.295j]
np.linalg.eig: [0.992+0.j      0.013+0.295j 0.013-0.295j]
```

```
np.linalg.eig and my eigenvalues close? True
```

```
----- Testing for function: QR_Iteration_WilkinsonShift() -----
Iteration terminates at i=36 with tol=1e-06 reached
```

```
my eigenvalues: [0.992+0.j      0.013+0.295j 0.013-0.295j]
np.linalg.eig: [0.992+0.j      0.013+0.295j 0.013-0.295j]
```

```
np.linalg.eig and my eigenvalues close? True
```

```
Real >>> Input shape = (5, 5)
```

```
----- Testing for function: QR_Iteration_Eigenvalues() -----
Iteration terminates at i=28 with tol=1e-06 reached
```

```
my eigenvalues: [ 2.116+0.j      0.207+0.229j 0.207-0.229j  0.073+0.j      -0.515+0.j      ]
```

```
np.linalg.eig: [ 2.116+0.j      0.207+0.229j  0.207-0.229j  0.073+0.j      -0.515+0.j      ]
```

```
np.linalg.eig and my eigenvalues close? True
```

```
----- Testing for function: QR_Iteration_WilkinsonShift() -----
Iteration terminates at i=14 with tol=1e-06 reached
```

```
my eigenvalues: [ 2.116+0.j      0.207+0.229j  0.207-0.229j  0.073+0.j      -0.515+0.j      ]
np.linalg.eig: [ 2.116+0.j      0.207+0.229j  0.207-0.229j  0.073+0.j      -0.515+0.j      ]
```

```
np.linalg.eig and my eigenvalues close? True
```

```
Real >>> Input shape = (10, 10)
```

```
----- Testing for function: QR_Iteration_Eigenvalues() -----
```

```
C:\ProgramData\Anaconda3\lib\site-packages\ipykernel_launcher.py:32: ComplexWarning: Casting complex values to real discards the imaginary part
C:\ProgramData\Anaconda3\lib\site-packages\ipykernel_launcher.py:75: ComplexWarning: Casting complex values to real discards the imaginary part
C:\ProgramData\Anaconda3\lib\site-packages\ipykernel_launcher.py:80: ComplexWarning: Casting complex values to real discards the imaginary part
```

```
Iteration terminates at i=558 with tol=1e-06 reached
```

```
my eigenvalues: [ 4.82 +0.j      0.579+0.149j  0.579-0.149j  0.377+0.j      0.146+0.j      -0.24 +0.j      -0.352+0.944j -0.352-0.944j -0.571+0.117j -0.571-0.117j]
np.linalg.eig: [ 4.82 +0.j      0.579+0.149j  0.579-0.149j  0.377+0.j      0.146+0.j      -0.24 +0.j      -0.352+0.944j -0.352-0.944j -0.571+0.117j -0.571-0.117j]
```

```
np.linalg.eig and my eigenvalues close? True
```

```
----- Testing for function: QR_Iteration_WilkinsonShift() -----
Iteration terminates at i=465 with tol=1e-06 reached
```

```
my eigenvalues: [ 4.82 +0.j      0.579+0.149j  0.579-0.149j  0.377+0.j      0.146+0.j      -0.24 +0.j      -0.352+0.944j -0.352-0.944j -0.571+0.117j -0.571-0.117j]
np.linalg.eig: [ 4.82 +0.j      0.579+0.149j  0.579-0.149j  0.377+0.j      0.146+0.j      -0.24 +0.j      -0.352+0.944j -0.352-0.944j -0.571+0.117j -0.571-0.117j]
```

```
np.linalg.eig and my eigenvalues close? True
```

```
=====
Testing QR_Iteration_WilkinsonShift() function on SPECIAL real matrices
```

=====

Special >>> Input shape = (10, 10)

----- Testing for function: QR_Iteration_Eigenvalues() -----

Iteration terminates at i=194 with tol=1e-06 reached

my eigenvalues: [9.684 8.685 7.302 1.666 -1.201 -3.008 -5.856 -8.817 -11.764 -14.69]

np.linalg.eig: [9.684 8.685 7.302 1.666 -1.201 -3.008 -5.856 -8.817 -11.764 -14.69]

np.linalg.eig and my eigenvalues close? True

----- Testing for function: QR_Iteration_WilkinsonShift() -----

Iteration terminates at i=52 with tol=1e-06 reached

my eigenvalues: [9.684 8.685 7.302 1.666 -1.201 -3.008 -5.856 -8.817 -11.764 -14.69]

np.linalg.eig: [9.684 8.685 7.302 1.666 -1.201 -3.008 -5.856 -8.817 -11.764 -14.69]

np.linalg.eig and my eigenvalues close? True

Special >>> Input shape = (10, 10)

----- Testing for function: QR_Iteration_Eigenvalues() -----

Iteration terminates at i=644 with tol=1e-06 reached

my eigenvalues: [4.03 3.972 0.064 0. -0.064 -3.97 -4.03 -5.954 -6.018 -6.03]

np.linalg.eig: [4.03 3.972 0.064 0. -0.064 -3.97 -4.03 -5.953 -6.018 -6.03]

np.linalg.eig and my eigenvalues close? False

my eigenvalues - np.linalg.eig =

[-0. -0. -0. -0. 0. -0. 0. -0. 0. 0.]

----- Testing for function: QR_Iteration_WilkinsonShift() -----

Iteration terminates at i=30 with tol=1e-06 reached

my eigenvalues: [4.03 3.972 0.064 0. -0.064 -3.97 -4.03 -5.953 -6.018 -6.03]

np.linalg.eig: [4.03 3.972 0.064 0. -0.064 -3.97 -4.03 -5.953 -6.018 -6.03]

np.linalg.eig and my eigenvalues close? True

```
Special >>> Input shape = (10, 10)
```

```
----- Testing for function: QR_Iteration_Eigenvalues() -----  
Iteration terminates at i=780 with tol=1e-06 reached
```

```
my eigenvalues: [1.026+0.009j 1.026-0.009j 1.016+0.022j 1.016-0.022j 0.999+0.027j 0.999-0.027j 0.984+0.021j 0.984-0.021j 0.975+0.008j 0.975-0.008j]  
np.linalg.eig: [1. 1. 1. 1. 1. 1. 1. 1. 1. 1.]
```

```
np.linalg.eig and my eigenvalues close? False
```

```
my eigenvalues - np.linalg.eig =  
[ 0.026+0.009j 0.026-0.009j 0.016+0.022j 0.016-0.022j -0.001+0.027j -0.001-0.027j -0.016+0.021j -0.016-0.021j -0.025+0.008j -0.025-0.008j]
```

```
----- Testing for function: QR_Iteration_WilkinsonShift() -----  
Iteration terminates at i=605 with tol=1e-06 reached
```

```
my eigenvalues: [1.026+0.j 1.02 +0.015j 1.02 -0.015j 1.007+0.024j 1.007-0.024j 0.992+0.023j 0.992-0.023j 0.98 +0.014j 0.98 -0.014j 0.976+0.j ]  
np.linalg.eig: [1. 1. 1. 1. 1. 1. 1. 1. 1. 1.]
```

```
np.linalg.eig and my eigenvalues close? False
```

```
my eigenvalues - np.linalg.eig =  
[ 0.026+0.j 0.02 +0.015j 0.02 -0.015j 0.007+0.024j 0.007-0.024j -0.008+0.023j -0.008-0.023j -0.02 +0.014j -0.02 -0.014j -0.024+0.j ]
```

```
Special >>> Input shape = (6, 6)
```

```
----- Testing for function: QR_Iteration_Eigenvalues() -----  
Iteration terminates at i=52 with tol=1e-06 reached
```

```
my eigenvalues: [5.+6.j 5.-6.j 4.+0.j 3.+0.j 1.+2.j 1.-2.j]  
np.linalg.eig: [5.+6.j 5.-6.j 4.+0.j 3.+0.j 1.+2.j 1.-2.j]
```

```
np.linalg.eig and my eigenvalues close? True
```

```
----- Testing for function: QR_Iteration_WilkinsonShift() -----  
Iteration terminates at i=16 with tol=1e-06 reached
```

```
my eigenvalues: [5.+6.j 5.-6.j 4.+0.j 3.+0.j 1.+2.j 1.-2.j]  
np.linalg.eig: [5.+6.j 5.-6.j 4.+0.j 3.+0.j 1.+2.j 1.-2.j]
```

```
np.linalg.eig and my eigenvalues close? True
```

**Observations:**

- Function `QR_iteration_WilkinsonShift()` seems to be working as expected with both real and complex matrices, with real eigenvalues or complex conjugate pairs
- Same issue with special matrices -> diagonal dominant with ones in lower triangular

Visualization of Convergence Comparison with Wilkinson's Shift

```

In [17]: 1 # TAKES QUITE A WHILE - RERUN ONLY IF NEEDED!
2
3 size = [5,25,50,75,100]
4 no_shift = []
5 Wilkinson = []
6
7 for n in size:
8     A = np.random.rand(n,n)+1j*np.random.rand(n,n)
9     print('\n\nRandom Complex >>> Input shape = ',A.shape)
10    eig,_ = np.linalg.eig(A)
11    print('\nQR Iteration without shift:')
12    eig_, i_ = QR_Iteration_Eigenvalues(A, max_iter = 10000, tol=RTOL)
13    print('\nQR Iteration with WILKINSON shift:')
14    eig_w, i_w = QR_Iteration_WilkinsonShift(A,max_iter = 10000, tol=RTOL)
15    no_shift.append(i_)
16    Wilkinson.append(i_w)
17    #print('np.linalg.eig:           ', sort_(eig))
18    #print('QR_Iteration:           ', sort_(eig_))
19    #print('QR_Iteration_WilkinsonShift:', sort_(eig_w))
20
21 plt.plot(size, no_shift,marker='o',color='red',linestyle='dashed',label='Without Shift')
22 plt.plot(size, Wilkinson,marker='x',color='blue',linestyle='dotted',label='Wilkinson Shift')
23 plt.title('Comparison of QR Iteration Convergence')
24 plt.xlabel('Size of Input Matrix')
25 plt.ylabel('Num of Iterations')
26 plt.legend()
27 plt.show()
28

```

Random Complex >>> Input shape = (5, 5)

QR Iteration without shift:

Iteration terminates at i=559 with tol=1e-06 reached

QR Iteration with WILKINSON shift:

Iteration terminates at i=18 with tol=1e-06 reached

Random Complex >>> Input shape = (25, 25)

QR Iteration without shift:

Iteration terminates at i=3283 with tol=1e-06 reached

QR Iteration with WILKINSON shift:

Iteration terminates at i=312 with tol=1e-06 reached

Random Complex >>> Input shape = (50, 50)

QR Iteration without shift:

Iteration terminates at i=8193 with tol=1e-06 reached

QR Iteration with WILKINSON shift:

Iteration terminates at i=1132 with tol=1e-06 reached

Random Complex >>> Input shape = (75, 75)

QR Iteration without shift:

max_iter=10000 reached, max error=0.00947315121975121 vs tol=1e-06; index of non-convergence=[[16], [17], [36], [38]]

QR Iteration with WILKINSON shift:

Iteration terminates at i=3130 with tol=1e-06 reached

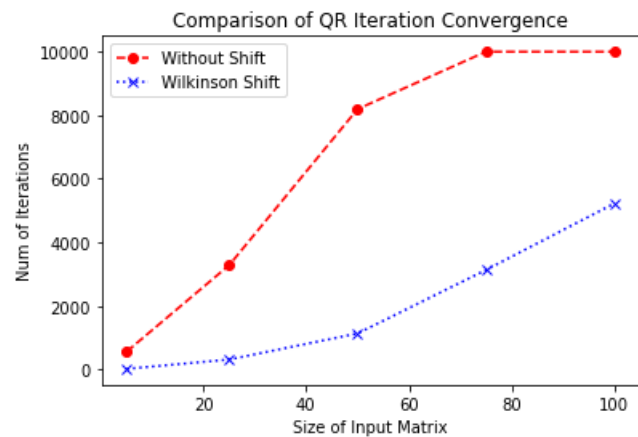
Random Complex >>> Input shape = (100, 100)

QR Iteration without shift:

max_iter=10000 reached, max error=0.013843580120954222 vs tol=1e-06; index of non-convergence=[[21], [22], [37], [38], [39], [40], [41]]

QR Iteration with WILKINSON shift:

Iteration terminates at i=5223 with tol=1e-06 reached



Eigenvectors

Two similar matrices, A and B , with similarity transformation $B = S^{-1}AS$, have the same set of eigenvalues and their eigenvectors are related $v_B = S^{-1}v_A$.

Reference sources:

- Implementing the QR algorithm for efficiently computing matrix eigenvalues and eigenvectors - Section 4.5 (p.51)
https://addi.ehu.es/bitstream/handle/10810/26427/TFG_Erana_Robles_Gorka.pdf?sequence=1 (https://addi.ehu.es/bitstream/handle/10810/26427/TFG_Erana_Robles_Gorka.pdf?sequence=1)
- Find eigenvectors of an upper triangular matrix

(1) <https://math.stackexchange.com/questions/2632460/general-form-of-left-and-right-eigenvectors-of-upper-triangular-matrices> (<https://math.stackexchange.com/questions/2632460/general-form-of-left-and-right-eigenvectors-of-upper-triangular-matrices>)

(2) <https://math.stackexchange.com/questions/3947108/how-to-get-eigenvectors-using-qr-algorithm> (<https://math.stackexchange.com/questions/3947108/how-to-get-eigenvectors-using-qr-algorithm>)

In [18]:

```
1  # Find Eigenvector of an upper triangular matrix given eigenvalues
2
3  def eigenvectors_upperTriangularMatrix(U,eigenvalues):
4
5      """      Compute the eigenvectors of an upper triangular matrix, based on given eigenvalues
6                Source: https://addi.ehu.es/bitstream/handle/10810/26427/TFG_Erana_Robles_Gorka.pdf?sequence=1
7      Input      -----
8                U: 2D np.array in the form of an upper triangular matrix
9                eigenvalues: 1D np.array, real eigenvalues associated with matrix U
10     Return     -----
11                V: 2D np.array with each column represents an eigenvector, in the same order as the associated eigenvalue
12     """
13
14     n = U.shape[0]
15
16     V = np.eye(n, dtype=U.dtype) # in case of complex matrix, enforce dtype
17
18     for i in range(1,n,1):
19         for j in range(i-1,-1,-1):
20             V[j,i] = - np.dot(U[j,:],V[:,i]) / (U[j,j]-eigenvalues[i])
21
22             V[:,i] = V[:,i]/np.linalg.norm(V[:,i]) # vector normalization
23
24     return V
25
26
```



```

In [19]: 1 # Test for eigenvectors
2
3 def test_eigenvectors(eigenvectors, v, verbose=True):
4
5     """    Compare two sets of eigenvectors
6     Input  -----
7           eigenvectors: 2D np.array with real or complex entries, eigenvectors from my function
8           v: 2D np.array, eigenvectors from np.linalg.eig(), basis for comparison
9           verbose: bool, indicating whether to print the two sets of eigenvectors and ratios of eigenvectors/v
10    Return -----
11           None; test results will be printed
12    """
13
14
15    if np.allclose(eigenvectors,v,rtol=RTOL):
16        print('np.linalg.eig and my function return the same eigenvectors? True \n')
17
18    else:
19        print('np.linalg.eig and my function return the same eigenvectors? False \n')
20        d = np.divide(eigenvectors,v, where=(v!=0))
21        if verbose:
22            print('my eigenvectors =\n',eigenvectors,'\nnp.linalg.eig =\n',v, '\nmy eigenvectors / np.linalg.eig =\n', d,'\n')
23        d_ = np.divide(d,d[0], where=(d[0]!=0))
24        print('Eigenvectors all close except sign and/or scaling?', np.allclose(d_,np.ones(d.shape,d.dtype),rtol=RTOL))
25
26        # special case of upper triangular matrix
27        if np.allclose(np.tril(v,-1),np.zeros(d.shape,d.dtype)):
28            print('[Upper Triangular Matrix] Eigenvectors all close except signs?',
29                  np.allclose(np.abs(eigenvectors),np.abs(v),rtol=RTOL),'\n')
30        print('\n\n')
31
32
33    def test_eigenvectors_function(A,eigenvalues,function):
34
35        """    Perform eigenvector testing on selected function; eigenvectors are compared with results from np.linalg.eig()
36        Input  -----
37              A: input matrix, 2D np.array with real or complex entries
38              function: name of the function being tested
39        Return -----
40              None; test results will be printed
41        """
42
43        print("----- Testing for function: {}() -----".format(function.__name__))
44        eigenvectors = function(A, eigenvalues)
45        w,v = np.linalg.eig(A)
46
47        test_eigenvectors(eigenvectors, v)
48
49

```

```

In [20]: 1  ### Testing eigenvectors_upperTriangularMatrix() on Random Real Upper Triangular Matrices
2
3  print('\n\n')
4  print("=====")
5  print('Testing eigenvectors_upperTriangularMatrix() on Random REAL Upper Triangular Matrices')
6  print("=====")
7
8  for A in RANDOM_REAL_MATRICES:
9      U = np.triu(A)
10     print('\nREAL >>> Input shape = {}'.format(U.shape))
11     print('U = \n',U)
12     eigenvalues = np.diag(U)
13     test_eigenvectors_function(U,eigenvalues,eigenvectors_upperTriangularMatrix)
14
15
16  ### Testing eigenvectors_upperTriangularMatrix() on Random COMPLEX Upper Triangular Matrices
17
18  print('\n\n')
19  print("=====")
20  print('Testing eigenvectors_upperTriangularMatrix() on Random COMPLEX Upper Triangular Matrices')
21  print("=====")
22
23  for A in RANDOM_COMPLEX_MATRICES:
24      U = np.triu(A)
25      print('\nCOMPLEX >>> Input shape = {}'.format(U.shape))
26      print('U = \n',U)
27      eigenvalues = np.diag(U)
28      test_eigenvectors_function(U,eigenvalues,eigenvectors_upperTriangularMatrix)
29

```

```

=====
Testing eigenvectors_upperTriangularMatrix() on Random REAL Upper Triangular Matrices
=====

```

```
REAL >>> Input shape = (3, 3)
```

```

U =
[[0.261 0.15  0.741]
 [0.    0.174 0.07 ]
 [0.    0.    0.583]]
----- Testing for function: eigenvectors_upperTriangularMatrix() -----
np.linalg.eig and my function return the same eigenvectors? True

```

```
REAL >>> Input shape = (5, 5)
```

```

U =
[[0.118 0.985 0.164 0.45  0.808]

```

```

[0.    0.35  0.155 0.424 0.595]
[0.    0.    0.497 0.135 0.143]
[0.    0.    0.    0.706 0.689]
[0.    0.    0.    0.    0.418]]
----- Testing for function: eigenvectors_upperTriangularMatrix() -----
np.linalg.eig and my function return the same eigenvectors? True

```

REAL >>> Input shape = (10, 10)

```

U =
[[0.842 0.604 0.581 0.121 0.591 0.322 0.824 0.236 0.569 0.429]
 [0.    0.375 0.832 0.701 0.155 0.575 0.078 0.99  0.485 0.793]
 [0.    0.    0.083 0.414 0.819 0.3    0.075 0.567 0.834 0.001]
 [0.    0.    0.    0.009 0.453 0.353 0.712 0.761 0.973 0.933]
 [0.    0.    0.    0.    0.361 0.201 0.964 0.459 0.884 0.486]
 [0.    0.    0.    0.    0.    0.199 0.453 0.445 0.676 0.858]
 [0.    0.    0.    0.    0.    0.    0.784 0.963 0.477 0.747]
 [0.    0.    0.    0.    0.    0.    0.    0.897 0.068 0.115]
 [0.    0.    0.    0.    0.    0.    0.    0.    0.306 0.268]
 [0.    0.    0.    0.    0.    0.    0.    0.    0.    0.561]]
----- Testing for function: eigenvectors_upperTriangularMatrix() -----
np.linalg.eig and my function return the same eigenvectors? True

```

```

=====
Testing eigenvectors_upperTriangularMatrix() on Random COMPLEX Upper Triangular Matrices
=====

```

COMPLEX >>> Input shape = (3, 3)

```

U =
[[0.9  +0.122j 0.418+0.753j 0.391+0.67j ]
 [0.  +0.j    0.32  +0.669j 0.602+0.798j]
 [0.  +0.j    0.    +0.j    0.763+0.183j]]
----- Testing for function: eigenvectors_upperTriangularMatrix() -----
np.linalg.eig and my function return the same eigenvectors? False

```

```

my eigenvectors =
[[ 1.  +0.j    0.181-0.711j  0.867-0.459j]
 [ 0.  +0.j    0.679+0.j    -0.03  +0.16j ]
 [ 0.  +0.j    0.    +0.j    0.107+0.j   ]]
np.linalg.eig =
[[ 1.  +0.j    0.734+0.j    0.981+0.j   ]
 [ 0.  +0.j    0.168+0.658j -0.102+0.127j]
 [ 0.  +0.j    0.    +0.j    0.095+0.05j ]]
my eigenvectors / np.linalg.eig =
[[1.  +0.j    0.247-0.969j 0.884-0.468j]
 [0.  +0.j    0.247-0.969j 0.884-0.468j]
 [0.  +0.j    0.    +0.j    0.884-0.468j]]

```

```
Eigenvectors all close except sign and/or scaling? False
[Upper Triangular Matrix] Eigenvectors all close except signs? True
```

```
COMPLEX >>> Input shape = (5, 5)
```

```
U =
[[0.893+0.697j 0.926+0.527j 0.219+0.222j 0.412+0.28j 0.684+0.401j]
 [0. +0.j 0. +0.605j 0.197+0.516j 0.827+0.086j 0.448+0.326j]
 [0. +0.j 0. +0.j 0.263+0.364j 0.416+0.594j 0.687+0.376j]
 [0. +0.j 0. +0.j 0. +0.j 0.257+0.995j 0.286+0.426j]
 [0. +0.j 0. +0.j 0. +0.j 0. +0.j 0.157+0.737j]]
----- Testing for function: eigenvectors_upperTriangularMatrix() -----
np.linalg.eig and my function return the same eigenvectors? False

my eigenvectors =
[[ 1. +0.j -0.7 -0.308j 0.17 -0.763j -0.791-0.328j 0.812-0.169j]
 [ 0. +0.j 0.644+0.j -0.193+0.487j 0.36 -0.289j -0.379+0.381j]
 [ 0. +0.j 0. +0.j 0.338+0.j 0.141-0.101j -0.064+0.066j]
 [ 0. +0.j 0. +0.j 0. +0.j 0.151+0.j -0.105+0.024j]
 [ 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0.058+0.j ]]

np.linalg.eig =
[[ 1. +0.j 0.765+0.j 0.782+0.j 0.857+0.j 0.829+0.j ]
 [ 0. +0.j -0.59 +0.259j -0.517-0.083j -0.221+0.405j -0.449+0.295j]
 [ 0. +0.j -0. +0.j 0.074+0.33j -0.092+0.147j -0.076+0.052j]
 [ 0. +0.j -0. +0.j 0. +0.j -0.14 +0.058j -0.108+0.002j]
 [ 0. +0.j -0. +0.j 0. +0.j -0. +0.j 0.057+0.012j]]

my eigenvectors / np.linalg.eig =
[[ 1. +0.j -0.915-0.403j 0.217-0.976j -0.924-0.383j 0.979-0.204j]
 [ 0. +0.j -0.915-0.403j 0.217-0.976j -0.924-0.383j 0.979-0.204j]
 [ 0. +0.j 0. +0.j 0.217-0.976j -0.924-0.383j 0.979-0.204j]
 [ 0. +0.j 0. +0.j 0. +0.j -0.924-0.383j 0.979-0.204j]
 [ 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0.979-0.204j]]
```

```
Eigenvectors all close except sign and/or scaling? False
[Upper Triangular Matrix] Eigenvectors all close except signs? True
```

```
COMPLEX >>> Input shape = (10, 10)
```

```
U =
[[0.685+0.497j 0.168+0.663j 0.181+0.56j 0.225+0.179j 0.347+0.007j 0.236+0.152j 0.646+1.j 0.096+0.474j 0.678+0.406j 0.228+0.469j]
 [0. +0.j 0.253+0.336j 0.681+0.165j 0.438+0.96j 0.717+0.246j 0.117+0.129j 0.889+0.353j 0.402+0.735j 0.205+0.427j 0.34 +0.28j ]
 [0. +0.j 0. +0.j 0.279+0.976j 0.698+0.974j 0.234+0.915j 0.981+0.724j 0.202+0.752j 0.924+0.962j 0.867+0.988j 0.71 +0.413j]
 [0. +0.j 0. +0.j 0. +0.j 0.754+0.469j 0.166+0.42j 0.632+0.601j 0.636+0.471j 0.047+0.719j 0.322+0.934j 0.134+0.476j]
```

```
[0. +0.j 0. +0.j 0. +0.j 0. +0.j 0.011+0.797j 0.927+0.193j 0.572+0.391j 0.149+0.855j 0.352+0.962j 0.794+0.865j]
[0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0.414+0.68j 0.225+0.995j 0.624+0.036j 0.229+0.228j 0.9 +0.424j]
[0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0.038+0.901j 0.533+0.388j 0.101+0.3j 0.032+0.014j]
[0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0.166+0.035j 0.798+0.694j 0.68 +0.182j]
[0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0.788+0.359j 0.03 +0.419j]
[0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0.721+0.572j]]
```

----- Testing for function: eigenvectors_upperTriangularMatrix() -----

np.linalg.eig and my function return the same eigenvectors? False

my eigenvectors =

```
[ [ 1. +0.j -0.472-0.682j -0.109-0.755j -0.994+0.06j 0.145+0.587j 0.506-0.757j 0.598-0.252j 0.597+0.162j 0.048+0.975j -0.211+0.972j]
[ 0. +0.j 0.559+0.j 0.131-0.459j 0.019+0.081j -0.037+0.381j 0.372-0.007j 0.457+0.019j -0.706-0.122j 0.141-0.126j 0.005+0.09j ]
[ 0. +0.j 0. +0.j 0.437+0.j -0.007+0.036j -0.652-0.01j 0.043+0.167j 0.064+0.586j 0.08 +0.177j 0.073-0.042j -0.022+0.035j]
[ 0. +0.j 0. +0.j 0. +0.j 0.021+0.j 0.005-0.121j 0.011-0.044j -0.077+0.015j 0.023-0.128j -0.036-0.045j 0.019+0.006j]
[ 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0.219+0.j 0.021+0.011j -0.057-0.105j -0.161+0.027j -0.006+0.004j -0. +0.002j]
[ 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0.011+0.j 0.004-0.013j 0.033-0.009j -0.002+0.001j 0. +0.001j]
[ 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0.006+0.j -0.041+0.078j -0. +0.002j 0. +0.j ]
[ 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0.117+0.j 0.002+0.001j 0. -0.j ]
[ 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0.002+0.j 0. -0.j ]
[ 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j ]]
```

np.linalg.eig =

```
[ [ 1. +0.j 0.829+0.j 0.762+0.j 0.996+0.j -0.154-0.585j 0.91 +0.j 0.65 +0.j -0.616-0.059j 0.976+0.j 0.995+0.j ]
[ 0. +0.j -0.318+0.46j 0.436+0.195j -0.014-0.082j 0.031-0.382j 0.212+0.306j 0.414+0.196j 0.717+0.j -0.119-0.147j 0.087-0.024j]
[ 0. +0.j -0. +0.j -0.062+0.432j 0.009-0.035j 0.652+0.j -0.115+0.129j -0.169+0.565j -0.109-0.161j -0.038-0.075j 0.039+0.014j]
[ 0. +0.j -0. +0.j -0. +0.j -0.021-0.001j -0.003+0.121j 0.042-0.015j -0.077-0.016j -0.001+0.13j -0.047+0.034j 0.002-0.02j ]
[ 0. +0.j -0. +0.j -0. +0.j 0. -0.j -0.219+0.003j 0.002+0.024j -0.011-0.119j 0.154-0.054j 0.004+0.007j 0.002-0.j ]
[ 0. +0.j -0. +0.j -0. +0.j 0. -0.j -0. +0.j 0.006+0.009j 0.009-0.01j -0.031+0.014j 0.001+0.003j 0.001-0.j ]
[ 0. +0.j -0. +0.j -0. +0.j 0. -0.j -0. +0.j 0. +0.j 0.005+0.002j 0.027-0.084j 0.002+0.j 0. -0.j ]
[ 0. +0.j -0. +0.j -0. +0.j 0. -0.j -0. +0.j 0. +0.j 0. -0.115+0.02j 0.001-0.002j -0. -0.12+0.j ]
[ 0. +0.j -0. +0.j -0. +0.j 0. -0.j -0. +0.j 0. +0.j 0. +0.j -0. +0.j 0. -0.002j -0. -0.j ]
[ 0. +0.j -0. +0.j -0. +0.j 0. -0.j -0. +0.j 0. +0.j 0. +0.j -0. +0.j 0. +0.j -0. -0.j ]]
```

my eigenvectors / np.linalg.eig =

```
[ [ 1. +0.j -0.569-0.822j -0.143-0.99j -0.998+0.06j -1. -0.015j 0.556-0.831j 0.921-0.389j -0.985-0.17j 0.049+0.999j -0.212+0.977j]
[ 0. +0.j -0.569-0.822j -0.143-0.99j -0.998+0.06j -1. -0.015j 0.556-0.831j 0.921-0.389j -0.985-0.17j 0.049+0.999j -0.212+0.977j]
[ 0. +0.j 0. +0.j -0.143-0.99j -0.998+0.06j -1. -0.015j 0.556-0.831j 0.921-0.389j -0.985-0.17j 0.049+0.999j -0.212+0.977j]
[ 0. +0.j 0. +0.j 0. +0.j -0.998+0.06j -1. -0.015j 0.556-0.831j 0.921-0.389j -0.985-0.17j 0.049+0.999j -0.212+0.977j]
[ 0. +0.j 0. +0.j 0. +0.j 0. +0.j -1. -0.015j 0.556-0.831j 0.921-0.389j -0.985-0.17j 0.049+0.999j -0.212+0.977j]
[ 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0.556-0.831j 0.921-0.389j -0.985-0.17j 0.049+0.999j -0.212+0.977j]
[ 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0.921-0.389j -0.985-0.17j 0.049+0.999j -0.212+0.977j]
[ 0. +0.j 0. -0.j 0. +0.j nan+0.j 0. +0.j 0. +0.j 0. +0.j -0.985-0.17j 0.049+0.999j -0.212+0.977j]
[ 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0.049+0.999j -0.212+0.977j]
[ 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j -0.212+0.977j]]
```

Eigenvectors all close except sign and/or scaling? False

[Upper Triangular Matrix] Eigenvectors all close except signs? True

Observations:

- Seems to be working except for the signs of eigenvectors

```

In [21]: 1 # General method for obtaining eigenvectors
2
3 def inverse_power_method_with_shift(A, s, max_iter=MAX_ITER, rtol=RTOL):
4
5     """    Apply the inverse power method with shift to compute the eigenvectors associated with an eigenvalue which is close to the shift
6     Input    -----
7             A: input matrix, 2D np.array wiht real or complex entries
8             s: shift to be performed, which is closed to an eigenvalue
9             max_iter: int, maximum number of iterations to be performed
10            rtol: float, relative tolerance between eigenvalues by successive iterations
11     Return    -----
12            x_new: 1D np.array, the eigenvector associated with the eigenvalue which is closed to the given shift
13     """
14
15     n = A.shape[0]
16     A_ = A.astype(s.dtype) - s*np.eye(n,dtype=s.dtype)
17     x_old = np.ones(n, dtype=s.dtype) #initialization as [1,1,1,...]
18
19     for i in range(max_iter):
20         y = np.linalg.solve(A_,x_old) # assuming this can be used? Potentially Singular Matrix Error...
21         x_new = y/np.linalg.norm(y)
22
23         if np.allclose(x_new,x_old,rtol=rtol):
24             print('... num of iterations with inverse power method =',i)
25             break
26         x_old = x_new
27
28     return x_new
29
30
31
32 def eigenvectors_inversePowerMethod(U,eigenvalues):
33
34     """    Compute the eigenvectors of a block triangular matrix, based on given eigenvalues
35     Input    -----
36            U: 2D np.array in the form of a block triangular matrix with complex eigenvalues
37            eigenvalues: 1D np.array, complex eigenvalues associated with matrix U
38     Return    -----
39            V: 2D np.array with each column represents an eigenvector, in the same order as the associated eigenvalues
40     """
41
42     n = U.shape[0]
43     V = np.eye(n, dtype='complex') # only used in case of complex matrix, need to enforce dtype
44
45     for i in range(n):
46         V[:,i] = inverse_power_method_with_shift(U, eigenvalues[i])
47
48     # print('\n ----\n',V.dtype, 'eigenvectors_inversePowerMethod=\n',V,)
49
50     return V
51
52

```

53



In [22]:

```

1  # Testing
2
3  print('\n\n')
4  print("=====")
5  print('Testing eigenvectors_inversePowerMethod() on Random REAL Matrices')
6  print("=====")
7
8  for A in RANDOM_REAL_MATRICES[-1:]:
9      print('\nREAL >>> Input shape = {}'.format(A.shape))
10     w,v = np.linalg.eig(A)
11     eigenvalues = w
12     test_eigenvectors_function(A,eigenvalues,eigenvectors_inversePowerMethod)
13
14
15  print('\n\n')
16  print("=====")
17  print('Testing eigenvectors_inversePowerMethod() on Random COMPLEX Matrices')
18  print("=====")
19
20  for A in RANDOM_COMPLEX_MATRICES[-1:]:
21      print('\nCOMPLEX >>> Input shape = {}'.format(A.shape))
22      w,v = np.linalg.eig(A)
23      eigenvalues = w
24      test_eigenvectors_function(A,eigenvalues,eigenvectors_inversePowerMethod)
25
26
27  print('\n\n')
28  print("=====")
29  print('Testing eigenvectors_inversePowerMethod() on Random COMPLEX Upper *BLOCK* Triangular Matrices')
30  print("=====")
31
32  for A in RANDOM_COMPLEX_MATRICES[-1:]:
33      print('\nCOMPLEX >>> Input shape = {}'.format(A.shape))
34      U = np.triu(A,-1)
35      print('U = \n',U)
36      w,v = np.linalg.eig(U)
37      eigenvalues = w
38      test_eigenvectors_function(U,eigenvalues,eigenvectors_inversePowerMethod)
39

```

```

=====
Testing eigenvectors_inversePowerMethod() on Random REAL Matrices
=====

```

```
REAL >>> Input shape = (10, 10)
```

```

----- Testing for function: eigenvectors_inversePowerMethod() -----
... num of iterations with inverse power method = 1
... num of iterations with inverse power method = 1

```

```
... num of iterations with inverse power method = 1
np.linalg.eig and my function return the same eigenvectors? False
```

```
my eigenvectors =
```

```
[ [ 0.331+0.j    -0.054-0.15j  -0.054+0.15j   0.071+0.129j  0.071-0.129j  -0.311+0.158j  -0.311-0.158j  -0.294+0.j    0.33 +0.j    0.052+0.j ]
 [ 0.348+0.j    0.41 +0.153j  0.41 -0.153j   0.264+0.081j  0.264-0.081j  -0.463-0.138j  -0.463+0.138j  -0.629+0.j    0.176+0.j    0.328+0.j ]
 [ 0.245+0.j   -0.303+0.335j  -0.303-0.335j  -0.341-0.131j  -0.341+0.131j  -0.108-0.036j  -0.108+0.036j  0.131+0.j   -0.443+0.j    0.015+0.j ]
 [ 0.326+0.j    0.13 +0.103j  0.13 -0.103j  -0.222+0.088j  -0.222-0.088j  0.153-0.043j  0.153+0.043j  0.273+0.j   -0.087+0.j   -0.237+0.j ]
 [ 0.332+0.j    0.065-0.392j  0.065+0.392j  -0.393-0.072j  -0.393+0.072j  0.198-0.114j  0.198+0.114j  0.299+0.j   -0.383+0.j    0.196+0.j ]
 [ 0.336+0.j    0.053-0.293j  0.053+0.293j  0.074-0.157j  0.074+0.157j  -0.354-0.077j  -0.354+0.077j  -0.406+0.j    0.706+0.j   -0.795+0.j ]
 [ 0.317+0.j    0.313+0.053j  0.313-0.053j  0.003-0.115j  0.003+0.115j  0.522+0.156j  0.522-0.156j  0.385+0.j   -0.053+0.j   -0.267+0.j ]
 [ 0.35 +0.j   -0.217-0.002j  -0.217+0.002j  0.281+0.038j  0.281-0.038j  0.283-0.008j  0.283+0.008j  -0.116+0.j   -0.096+0.j    0.245+0.j ]
 [ 0.273+0.j   -0.277-0.017j  -0.277+0.017j  0.487+0.037j  0.487-0.037j  -0.194+0.04j  -0.194-0.04j  0.066+0.j   -0.015+0.j   -0.013+0.j ]
 [ 0.286+0.j    0.031+0.282j  0.031-0.282j  -0.435+0.002j  -0.435-0.002j  -0.018-0.083j  -0.018+0.083j  0.079+0.j    0.011+0.j    0.178+0.j ]]
```

```
np.linalg.eig =
```

```
[ [-0.331+0.j    -0.075+0.14j  -0.075-0.14j   0.081+0.123j  0.081-0.123j  0.252-0.241j  0.252+0.241j  -0.294+0.j    0.33 +0.j    0.052+0.j ]
 [-0.348+0.j   -0.161-0.407j  -0.161+0.407j  0.269+0.06j   0.269-0.06j   0.483-0.j    0.483+0.j   -0.629+0.j    0.176+0.j    0.328+0.j ]
 [-0.245+0.j    0.452+0.j    0.452-0.j   -0.35 -0.104j  -0.35 +0.104j  0.114+0.004j  0.114-0.004j  0.131+0.j   -0.443+0.j    0.015+0.j ]
 [-0.326+0.j   -0.011-0.166j  -0.011+0.166j  -0.215+0.105j  -0.215-0.105j  -0.134+0.085j  -0.134-0.085j  0.273+0.j   -0.087+0.j   -0.237+0.j ]
 [-0.332+0.j   -0.334+0.215j  -0.334-0.215j  -0.398-0.042j  -0.398+0.042j  -0.157+0.166j  -0.157-0.166j  0.299+0.j   -0.383+0.j    0.196+0.j ]
 [-0.336+0.j   -0.253+0.157j  -0.253-0.157j  0.062-0.163j  0.062+0.163j  0.361-0.027j  0.361+0.027j  -0.406+0.j    0.706+0.j   -0.795+0.j ]
 [-0.317+0.j   -0.171-0.268j  -0.171+0.268j  -0.006-0.115j  -0.006+0.115j  -0.545+0.j   -0.545-0.j   0.385+0.j   -0.053+0.j   -0.267+0.j ]
 [-0.35 +0.j    0.143+0.162j  0.143-0.162j  0.283+0.017j  0.283-0.017j  -0.269+0.089j  -0.269-0.089j  -0.116+0.j   -0.096+0.j    0.245+0.j ]
 [-0.273+0.j    0.173+0.217j  0.173-0.217j  0.488+0.j    0.488-0.j    0.174-0.093j  0.174+0.093j  0.066+0.j   -0.015+0.j   -0.013+0.j ]
 [-0.286+0.j    0.188-0.212j  0.188+0.212j  -0.433+0.035j  -0.433-0.035j  0.041+0.075j  0.041-0.075j  0.079+0.j    0.011+0.j    0.178+0.j ]]
```

```
my eigenvectors / np.linalg.eig =
```

```
[ [-1.  -0.j    -0.67 +0.742j  -0.67 -0.742j  0.997+0.076j  0.997-0.076j  -0.958-0.286j  -0.958+0.286j  1.  -0.j    1.  +0.j    1.  +0.j ]
 [-1.  -0.j    -0.67 +0.742j  -0.67 -0.742j  0.997+0.076j  0.997-0.076j  -0.958-0.286j  -0.958+0.286j  1.  -0.j    1.  +0.j    1.  +0.j ]
 [-1.  -0.j    -0.67 +0.742j  -0.67 -0.742j  0.997+0.076j  0.997-0.076j  -0.958-0.286j  -0.958+0.286j  1.  +0.j    1.  -0.j    1.  -0.j ]
 [-1.  -0.j    -0.67 +0.742j  -0.67 -0.742j  0.997+0.076j  0.997-0.076j  -0.958-0.286j  -0.958+0.286j  1.  +0.j    1.  -0.j    1.  +0.j ]
 [-1.  -0.j    -0.67 +0.742j  -0.67 -0.742j  0.997+0.076j  0.997-0.076j  -0.958-0.286j  -0.958+0.286j  1.  -0.j    1.  +0.j    1.  -0.j ]
 [-1.  -0.j    -0.67 +0.742j  -0.67 -0.742j  0.997+0.076j  0.997-0.076j  -0.958-0.286j  -0.958+0.286j  1.  +0.j    1.  -0.j    1.  -0.j ]
 [-1.  -0.j    -0.67 +0.742j  -0.67 -0.742j  0.997+0.076j  0.997-0.076j  -0.958-0.286j  -0.958+0.286j  1.  -0.j    1.  -0.j    1.  +0.j ]
 [-1.  -0.j    -0.67 +0.742j  -0.67 -0.742j  0.997+0.076j  0.997-0.076j  -0.958-0.286j  -0.958+0.286j  1.  +0.j    1.  -0.j    1.  -0.j ]
 [-1.  -0.j    -0.67 +0.742j  -0.67 -0.742j  0.997+0.076j  0.997-0.076j  -0.958-0.286j  -0.958+0.286j  1.  +0.j    1.  +0.j    1.  +0.j ]]
```

```
Eigenvectors all close except sign and/or scaling? True
```

```
=====
Testing eigenvectors_inversePowerMethod() on Random COMPLEX Matrices
=====
```

```
COMPLEX >>> Input shape = (10, 10)
```

```
----- Testing for function: eigenvectors_inversePowerMethod() -----
np.linalg.eig and my function return the same eigenvectors? False
```

```

my eigenvectors =
[[ 0.203-0.12j  0.114+0.01j  0.108-0.411j -0.072-0.042j -0.332+0.048j -0.057-0.057j -0.174-0.344j  0.126-0.125j -0.16 +0.196j -0.206-0.021j]
 [ 0.223-0.17j -0.211+0.16j -0.111+0.113j -0.066+0.203j -0.507+0.005j  0.469-0.019j  0.393-0.085j -0.18 -0.117j  0.448+0.133j -0.403+0.513j]
 [ 0.358-0.204j  0.261+0.097j -0.227+0.054j -0.35 -0.063j  0.483-0.119j -0.261-0.197j  0.027-0.229j -0.122+0.156j -0.21 -0.012j  0.171-0.53j ]
 [ 0.248-0.135j  0.035+0.221j  0.113-0.256j -0.026-0.27j -0.102+0.092j  0.201-0.087j  0.21 -0.111j  0.09 +0.555j  0.132-0.358j  0.127+0.075j]
 [ 0.349-0.167j -0.315+0.006j -0.179-0.347j -0.423-0.186j  0.034+0.067j -0.407-0.24j -0.5 +0.076j -0.146-0.479j  0.344+0.181j -0.129+0.155j]
 [ 0.25 -0.202j -0.192-0.267j  0.153-0.049j  0.262+0.389j  0.33 +0.144j -0.332+0.245j -0.115-0.053j  0.067+0.108j -0.217-0.084j  0.19 -0.072j]
 [ 0.201-0.103j -0.157+0.009j  0.085+0.098j  0.253+0.127j -0.068-0.259j -0.086-0.15j -0.117+0.089j  0.206-0.117j -0.083+0.13j  0.066-0.127j]
 [ 0.263-0.176j  0.172-0.174j  0.282+0.402j -0.121+0.017j  0.06 +0.003j  0.132+0.342j -0.177+0.133j  0.224-0.147j -0.108+0.118j -0.064+0.068j]
 [ 0.237-0.225j  0.578-0.255j -0.174+0.081j  0.407-0.128j -0.141-0.167j  0.216+0.101j  0.298+0.369j -0.393+0.018j  0.235-0.074j  0.058+0.126j]
 [ 0.25 -0.206j -0.297+0.098j -0.101+0.422j -0.073-0.175j  0.143+0.292j  0.001-0.063j  0.075+0.09j  0.123+0.048j -0.38 -0.259j  0.14 -0.223j]]

np.linalg.eig =
[[ 0.236-0.004j  0.101+0.055j -0.275-0.325j -0.075+0.036j  0.333-0.045j  0.078+0.021j  0.121+0.366j -0.103-0.145j -0.097+0.234j  0.111+0.175j]
 [ 0.278-0.038j -0.258+0.062j  0.029+0.155j  0.132+0.168j  0.507+0.j -0.395+0.255j -0.401+0.025j -0.144+0.159j  0.468+0.j  0.652+0.j ]
 [ 0.412+0.j  0.2 +0.194j -0.086+0.217j -0.248+0.256j -0.484+0.114j  0.325+0.037j -0.061+0.222j  0.134+0.145j -0.205+0.048j -0.523+0.193j]
 [ 0.282+0.006j -0.057+0.216j -0.145-0.239j -0.239-0.129j  0.103-0.091j -0.129+0.177j -0.224+0.078j  0.562+0.j  0.025-0.381j -0.02 -0.146j]
 [ 0.386-0.028j -0.291-0.121j -0.387-0.053j -0.391+0.246j -0.034-0.067j  0.473+0.j  0.506+0.j -0.497+0.068j  0.381+0.076j  0.201+0.005j]
 [ 0.318-0.052j -0.068-0.322j  0.048-0.154j  0.469+0.j -0.329-0.148j  0.161-0.379j  0.106+0.07j  0.117-0.049j -0.232-0.019j -0.174-0.105j]
 [ 0.225+0.01j -0.148-0.055j  0.129-0.014j  0.247-0.139j  0.066+0.259j  0.15 +0.085j  0.129-0.07j -0.082-0.222j -0.043+0.149j -0.14 +0.027j]
 [ 0.316-0.022j  0.227-0.09j  0.491+0.j -0.054+0.11j -0.06 -0.004j -0.287-0.228j  0.194-0.105j -0.109-0.245j -0.07 +0.144j  0.093+0.008j]
 [ 0.317-0.078j  0.632+0.j -0.033+0.189j  0.121-0.41j  0.139+0.168j -0.237+0.023j -0.24 -0.409j -0.045+0.39j  0.204-0.138j  0.063-0.123j]
 [ 0.319-0.055j -0.311-0.03j  0.288+0.325j -0.186-0.037j -0.14 -0.294j  0.031+0.054j -0.06 -0.1j  0.067-0.114j -0.438-0.14j -0.262+0.027j]]

my eigenvectors / np.linalg.eig =
[[ 0.869-0.495j  0.915-0.404j  0.574+0.819j  0.559+0.829j -1. +0.01j -0.861-0.508j -0.989+0.15j  0.16 +0.987j  0.959+0.284j -0.618+0.786j]
 [ 0.869-0.495j  0.915-0.404j  0.574+0.819j  0.559+0.829j -1. +0.01j -0.861-0.508j -0.989+0.15j  0.16 +0.987j  0.959+0.284j -0.618+0.786j]
 [ 0.869-0.495j  0.915-0.404j  0.574+0.819j  0.559+0.829j -1. +0.01j -0.861-0.508j -0.989+0.15j  0.16 +0.987j  0.959+0.284j -0.618+0.786j]
 [ 0.869-0.495j  0.915-0.404j  0.574+0.819j  0.559+0.829j -1. +0.01j -0.861-0.508j -0.989+0.15j  0.16 +0.987j  0.959+0.284j -0.618+0.786j]
 [ 0.869-0.495j  0.915-0.404j  0.574+0.819j  0.559+0.829j -1. +0.01j -0.861-0.508j -0.989+0.15j  0.16 +0.987j  0.959+0.284j -0.618+0.786j]
 [ 0.869-0.495j  0.915-0.404j  0.574+0.819j  0.559+0.829j -1. +0.01j -0.861-0.508j -0.989+0.15j  0.16 +0.987j  0.959+0.284j -0.618+0.786j]
 [ 0.869-0.495j  0.915-0.404j  0.574+0.819j  0.559+0.829j -1. +0.01j -0.861-0.508j -0.989+0.15j  0.16 +0.987j  0.959+0.284j -0.618+0.786j]
 [ 0.869-0.495j  0.915-0.404j  0.574+0.819j  0.559+0.829j -1. +0.01j -0.861-0.508j -0.989+0.15j  0.16 +0.987j  0.959+0.284j -0.618+0.786j]
 [ 0.869-0.495j  0.915-0.404j  0.574+0.819j  0.559+0.829j -1. +0.01j -0.861-0.508j -0.989+0.15j  0.16 +0.987j  0.959+0.284j -0.618+0.786j]
 [ 0.869-0.495j  0.915-0.404j  0.574+0.819j  0.559+0.829j -1. +0.01j -0.861-0.508j -0.989+0.15j  0.16 +0.987j  0.959+0.284j -0.618+0.786j]]

```

Eigenvectors all close except sign and/or scaling? True

```

=====
Testing eigenvectors_inversePowerMethod() on Random COMPLEX Upper *BLOCK* Triangular Matrices
=====

```

COMPLEX >>> Input shape = (10, 10)

```

U =
[[0.685+0.497j 0.168+0.663j 0.181+0.56j  0.225+0.179j 0.347+0.007j 0.236+0.152j 0.646+1.j  0.096+0.474j 0.678+0.406j 0.228+0.469j]
 [0.508+0.872j 0.253+0.336j 0.681+0.165j 0.438+0.96j  0.717+0.246j 0.117+0.129j 0.889+0.353j 0.402+0.735j 0.205+0.427j 0.34 +0.28j ]
 [0.  +0.j  0.4 +0.483j 0.279+0.976j 0.698+0.974j 0.234+0.915j 0.981+0.724j 0.202+0.752j 0.924+0.962j 0.867+0.988j 0.71 +0.413j]]

```

```
[0.  +0.j  0.  +0.j  0.347+0.289j 0.754+0.469j 0.166+0.42j  0.632+0.601j 0.636+0.471j 0.047+0.719j 0.322+0.934j 0.134+0.476j]
[0.  +0.j  0.  +0.j  0.  +0.j  0.215+0.961j 0.011+0.797j 0.927+0.193j 0.572+0.391j 0.149+0.855j 0.352+0.962j 0.794+0.865j]
[0.  +0.j  0.  +0.j  0.  +0.j  0.  +0.j  0.629+0.281j 0.414+0.68j  0.225+0.995j 0.624+0.036j 0.229+0.228j 0.9  +0.424j]
[0.  +0.j  0.  +0.j  0.  +0.j  0.  +0.j  0.  +0.j  0.527+0.245j 0.038+0.901j 0.533+0.388j 0.101+0.3j  0.032+0.014j]
[0.  +0.j  0.  +0.j  0.  +0.j  0.  +0.j  0.  +0.j  0.  +0.j  0.205+0.451j 0.166+0.035j 0.798+0.694j 0.68  +0.182j]
[0.  +0.j  0.  +0.j  0.  +0.j  0.  +0.j  0.  +0.j  0.  +0.j  0.  +0.j  0.797+0.195j 0.788+0.359j 0.03  +0.419j]
[0.  +0.j  0.  +0.j  0.  +0.j  0.  +0.j  0.  +0.j  0.  +0.j  0.  +0.j  0.062+0.735j 0.721+0.572j]]
----- Testing for function: eigenvectors_inversePowerMethod() -----
```

np.linalg.eig and my function return the same eigenvectors? False

my eigenvectors =

```
[[-0.153-0.476j -0.227-0.105j  0.065+0.077j  0.127+0.002j  0.02  +0.49j   0.422-0.08j   0.146-0.592j -0.453-0.44j  -0.638+0.003j  0.387-0.51j ]
 [-0.294-0.516j  0.564+0.496j -0.677-0.356j -0.288+0.284j -0.205+0.367j -0.615+0.195j  0.398+0.148j  0.192+0.055j -0.612+0.136j  0.213-0.552j]
 [-0.138-0.538j -0.235-0.355j  0.45  +0.303j  0.412+0.199j -0.309-0.364j -0.002-0.3j   -0.25  +0.234j -0.076+0.481j -0.41  +0.088j  0.1  -0.42j ]
 [-0.143-0.191j -0.049+0.202j -0.07  -0.178j -0.018-0.037j -0.148-0.173j  0.252+0.366j -0.059+0.285j  0.4  +0.04j  -0.02  +0.112j -0.147-0.069j]
 [-0.038-0.151j  0.161-0.018j  0.042+0.15j  -0.521-0.172j  0.213-0.38j  -0.267-0.101j -0.055-0.347j -0.107-0.036j  0.033+0.044j -0.105-0.002j]
 [-0.048-0.065j -0.067+0.015j -0.064-0.136j  0.039+0.421j -0.013-0.006j  0.023-0.142j  0.104-0.197j -0.066-0.268j  0.069+0.03j  -0.092+0.043j]
 [-0.021-0.019j  0.123-0.071j  0.023+0.085j  0.017-0.3j   0.141+0.276j  0.061+0.018j  0.054+0.095j  0.064-0.056j  0.045+0.01j  -0.043+0.035j]
 [-0.005-0.004j -0.254-0.076j  0.121-0.012j -0.096-0.136j  0.038+0.079j  0.008+0.027j  0.001+0.11j  -0.001+0.089j  0.009-0.012j  0.02  +0.019j]
 [-0.003+0.j    0.144+0.033j -0.067-0.j    0.018+0.089j  0.01  -0.064j  -0.034-0.038j  0.052-0.14j   0.114+0.003j  0.  -0.017j  0.03  +0.012j]
 [-0.001-0.j    -0.034-0.069j  0.018+0.032j  0.056-0.016j -0.055-0.045j  0.022+0.036j -0.122+0.112j -0.214-0.025j  0.007-0.014j  0.02  +0.027j]]
```

np.linalg.eig =

```
[ [ 0.49  +0.102j -0.24  +0.071j -0.093-0.038j -0.122+0.038j  0.49  +0.j    -0.426-0.051j  0.609+0.j    0.631+0.j    0.638+0.j    0.64  +0.j ]
 [ 0.594+0.j    0.751+0.j    0.764+0.j    0.185-0.36j   0.359+0.22j   0.645+0.j    -0.049+0.422j -0.176+0.094j  0.612-0.133j  0.568-0.165j]
 [ 0.536+0.147j -0.411-0.111j -0.539-0.059j -0.454-0.06j   -0.376+0.294j -0.089+0.287j -0.287-0.187j -0.28  -0.398j  0.41  -0.086j  0.395-0.174j]
 [ 0.237-0.03j   0.096+0.184j  0.145+0.125j  0.029+0.029j -0.179+0.141j -0.129-0.425j -0.291+0.011j -0.314+0.25j  0.021-0.111j -0.034-0.159j]
 [ 0.15  +0.042j  0.109-0.12j  -0.107-0.113j  0.549+0.j    -0.371-0.229j  0.224+0.177j  0.323-0.137j  0.102-0.049j -0.033-0.044j -0.061-0.085j]
 [ 0.08  -0.01j   -0.04  +0.056j  0.12  +0.091j -0.169-0.387j -0.007+0.013j -0.065+0.128j  0.216+0.054j  0.234+0.146j -0.069-0.03j  -0.09  -0.047j]
 [ 0.027-0.008j  0.046-0.134j -0.06  -0.064j  0.078+0.29j   0.282-0.13j  -0.053-0.036j -0.08  +0.075j -0.007+0.085j -0.045-0.01j  -0.054-0.013j]
 [ 0.006-0.003j -0.241+0.111j -0.101+0.066j  0.134+0.099j  0.08  -0.035j  0.  -0.029j -0.106+0.028j -0.061-0.065j -0.01  +0.012j -0.003+0.028j]
 [ 0.001-0.003j  0.13  -0.07j   0.059-0.031j -0.045-0.079j -0.064-0.013j  0.021+0.046j  0.148+0.017j -0.084+0.077j  0.  +0.017j  0.009+0.031j]
 [ 0.001-0.001j -0.071-0.029j -0.031-0.02j  -0.048+0.033j -0.047+0.053j -0.01  -0.041j -0.138-0.092j  0.171-0.132j -0.007+0.014j -0.01  +0.032j]]
```

my eigenvectors / np.linalg.eig =

```
[[-0.495-0.869j  0.751+0.661j -0.885-0.465j -0.949-0.314j  0.041+0.999j -0.953+0.303j  0.239-0.971j -0.717-0.697j -1.  +0.005j  0.605-0.796j]
 [-0.495-0.869j  0.751+0.661j -0.885-0.465j -0.949-0.314j  0.041+0.999j -0.953+0.303j  0.239-0.971j -0.717-0.697j -1.  +0.005j  0.605-0.796j]
 [-0.495-0.869j  0.751+0.661j -0.885-0.465j -0.949-0.314j  0.041+0.999j -0.953+0.303j  0.239-0.971j -0.717-0.697j -1.  +0.005j  0.605-0.796j]
 [-0.495-0.869j  0.751+0.661j -0.885-0.465j -0.949-0.314j  0.041+0.999j -0.953+0.303j  0.239-0.971j -0.717-0.697j -1.  +0.005j  0.605-0.796j]
 [-0.495-0.869j  0.751+0.661j -0.885-0.465j -0.949-0.314j  0.041+0.999j -0.953+0.303j  0.239-0.971j -0.717-0.697j -1.  +0.005j  0.605-0.796j]
 [-0.495-0.869j  0.751+0.661j -0.885-0.465j -0.949-0.314j  0.041+0.999j -0.953+0.303j  0.239-0.971j -0.717-0.697j -1.  +0.005j  0.605-0.796j]
 [-0.495-0.869j  0.751+0.661j -0.885-0.465j -0.949-0.314j  0.041+0.999j -0.953+0.303j  0.239-0.971j -0.717-0.697j -1.  +0.005j  0.605-0.796j]
 [-0.495-0.869j  0.751+0.661j -0.885-0.465j -0.949-0.314j  0.041+0.999j -0.953+0.303j  0.239-0.971j -0.717-0.697j -1.  +0.005j  0.605-0.796j]
 [-0.495-0.869j  0.751+0.661j -0.885-0.465j -0.949-0.314j  0.041+0.999j -0.953+0.303j  0.239-0.971j -0.717-0.697j -1.  +0.005j  0.605-0.796j]]
```

Eigenvectors all close except sign and/or scaling? True

Observations:

- Seems to be working except for the signs and/or scaling of eigenvectors

```

In [28]: 1 # Modified function to take Hessenberg matrix as an input and added optionality to output Q matrix for eigenvector calculation
2
3 def eigen_solver(H, S, max_iter, tol, eigvec, shift, tridiagonal):
4
5     """    Compute the eigenvalues and eigenvectors of a Hessenberg matrix
6     Input    -----
7             H: 2D np.array in the form of a Hessenberg matrix with real or complex entries
8             S: similarity transformation associated with the Hessenberg reduction,  $H = S @ A @ S.T$  where A is the input matrix
9             max_iter: int, maximum number of iterations to be performed
10            tol: float, relative tolerance between eigenvalues by successive iterations
11            eigvec: bool, indicating whether eigenvectors are to be calculated
12            shift: options - None or 'Wilkinson'
13            tridiagonal: bool, indicating whether the input H is a triadiagonal matrix (i.e. original input A is symmetric)
14     Return    -----
15             eigvals_new: 1D np.array, eigenvalues
16             eigenvectors: 2D np.array with each column represents an eigenvector, in the same order as the associated eigenvalues;
17                        if eigvec is False, then this default to a zero matrix
18     """
19
20     n = H.shape[0]
21
22     H_old = H.copy() # H will NOT be updated inplace - this is necessary because we are applying different methods on the same H matrix
23     # H_old = H # for optimizing storage if no need to display comparison of methods
24
25     eigvals_old = diagonal_block(H)
26
27     if eigvec:
28         T = np.eye(n, dtype=eigvals_old.dtype)
29
30     if not shift:
31         print('>>> QR Iteration WITHOUT shift')
32     else:
33         print('>>> QR Iteration with {} shift'.format(shift))
34
35     for i in range(max_iter):
36
37         if shift == 'Wilkinson':
38             datatype, lam = wilkinson_shift(H_old)
39             #print(">>> QR Iteration with Wilkinson's Shift: Lambda = {}, {}".format(lam, datatype))
40
41         if shift:
42             # H_old = H_old - lam * np.eye(n, dtype=datatype) #naive implementation  $O(2n^2)$ 
43             for j in range(n):
44                 H_old[j, j] -= lam #elementwise only  $O(n)$ 
45
46         H_new, G_iter = QR_Givens(H_old, eigvec, True, tridiagonal) # updating H_old in-place # default QR_Givens(H, eigvec=False, inplace=True, tridiagonal)
47
48         if shift:
49             # H_new = H_new + lam * np.eye(n, dtype=datatype) #naive implementation  $O(2n^2)$ 
50             for j in range(n):
51                 H_new[j, j] += lam #elementwise only  $O(n)$ 
52

```

```

53     eigvals_new = diagonal_block(H_new)
54     H_old = H_new # necessary to reset H_old = H_new
55
56
57     # if eigenvectors are required
58     if eigvec:
59         T = G_iter @ T    #  $Q = I.Q1.Q2.Q3...Qk$ ;  $Q1 = G1^*$ ;  $T^* = Q = G1^*...Gk^* \Rightarrow T = Gk...G1.I$ 
60
61     # Test for convergence: relative tol = 1- w / w' for each eigenvalue
62     if np.allclose(eigvals_new, eigvals_old, rtol=tol):
63         print('Iteration terminates at i={} with tol={} reached'.format(i,tol))
64         break
65
66     if i == max_iter-1:
67         err = np.max(abs((eigvals_new - eigvals_old)) / abs(eigvals_old))
68         idx = np.argwhere(np.isclose(eigvals_new, eigvals_old, rtol=tol)==False).tolist()
69         print('max_iter={} reached, max error={} vs tol={}; index of non-convergence={}'.format(max_iter, err, tol, idx))
70
71     eigvals_old = eigvals_new
72
73     # Sort eigenvalues in descending order
74     eigvals_new = sort_(eigvals_new)
75
76     # Compute eigenvectors if required
77     eigenvectors = np.zeros((n,n),dtype=eigvals_new.dtype)
78
79     if eigvec:
80         #print(H_new.dtype, 'H = \n',H_new)
81         if eigvals_new.dtype == 'complex':
82             #print('complex eigenvalues - ',eigvals_new)
83             eig_U = eigenvectors_inversePowerMethod(H_new,eigvals_new)
84         else:
85             #print('real eigenvalues - ',eigvals_new)
86             eig_U = eigenvectors_upperTriangularMatrix(H_new,eigvals_new)
87
88         for i in range(n):
89             eigenvectors[:,i] = S.conjugate().T @ T.conjugate().T @ eig_U[:,i]
90
91     return eigvals_new, eigenvectors
92
93
94
95 def sort_eigen(w, v):
96
97     """    Sort eigenvalues and eigenvectors
98     Input  -----
99           w: 1D np.array containing eigenvalues
100          v: 2D np.array containing eigenvectors in each column
101     Return -----
102           w_sorted: 1D np.array, eigenvalues sorted in descending order
103           v_sorted: 2D np.array, eigenvectors sorted in the same order as its correspondong eigenvalue in w_sorted
104     """

```

```
105
106 w_sorted = np.flip(np.sort(w)) #same as sort_(w) # sort eigenvectors in descending order
107 w_sorted_ix = np.flip(np.argsort(w))
108 # w_sorted_ix = [np.argwhere(w==x).item() for x in w_sorted] # this does not deal with repeating eigenvalues ...
109
110 v_sorted = np.empty_like(v)
111
112 for i,j in enumerate(w_sorted_ix):
113     v_sorted[:,i] = v[:,j]
114
115 return w_sorted, v_sorted
116
117
```



```

In [29]: 1 print('\n\n')
2 print("=====")
3 print('Testing eigen_solver() on Random REAL Matrices')
4 print("=====")
5
6 for A in RANDOM_REAL_MATRICES[1:2]:
7     print('\nREAL >>> Input shape = {}'.format(A.shape))
8
9     w,v = np.linalg.eig(A)
10    w_sorted, v_sorted = sort_eigen(w, v)
11
12    H, S = Hessenberg(A,eigvec=True)
13
14    eigenvalues, eigenvectors = eigen_solver(H, S, max_iter=MAX_ITER, tol=RTOL, eigvec=True, shift=None, tridiagonal=False)
15    test_eigenvalues(eigenvalues,w_sorted)
16    test_eigenvectors(eigenvectors,v_sorted)
17
18
19    eigenvalues, eigenvectors = eigen_solver(H, S, max_iter=MAX_ITER, tol=RTOL, eigvec=True, shift='Wilkinson',tridiagonal=False)
20    test_eigenvalues(eigenvalues,w_sorted)
21    test_eigenvectors(eigenvectors,v_sorted)
22

```

```

=====
Testing eigen_solver() on Random REAL Matrices
=====

```

```
REAL >>> Input shape = (5, 5)
```

```
>>> QR Iteration WITHOUT shift
```

```
Iteration terminates at i=28 with tol=1e-06 reached
```

```
... num of iterations with inverse power method = 1
```

```

my eigenvalues: [ 2.116+0.j      0.207+0.229j  0.207-0.229j  0.073+0.j      -0.515+0.j    ]
np.linalg.eig:  [ 2.116+0.j      0.207+0.229j  0.207-0.229j  0.073+0.j      -0.515+0.j    ]

```

```
np.linalg.eig and my eigenvalues close? True
```

```
np.linalg.eig and my function return the same eigenvectors? False
```

```

my eigenvectors =
[[ 0.496+0.j      -0.055+0.215j -0.055-0.215j -0.116+0.j      -0.549+0.j    ]
 [ 0.409+0.j      -0.117+0.129j -0.117-0.129j -0.222+0.j      0.221+0.j    ]
 [ 0.384+0.j      0.492-0.16j    0.492+0.16j    0.369+0.j      0.398+0.j    ]
 [ 0.576+0.j      -0.537-0.511j -0.537+0.511j -0.681+0.j      -0.576+0.j    ]
 [ 0.328+0.j      0.275+0.167j  0.275-0.167j  0.581+0.j      0.4 +0.j    ]]
np.linalg.eig =

```

```

[[ 0.496+0.j      0.109+0.194j  0.109-0.194j -0.116+0.j      0.549+0.j      ]
 [ 0.409+0.j      0.004+0.174j  0.004-0.174j -0.222+0.j     -0.221+0.j     ]
 [ 0.384+0.j      0.246-0.455j  0.246+0.455j  0.369+0.j     -0.398+0.j     ]
 [ 0.576+0.j     -0.741+0.j     -0.741-0.j     -0.681+0.j     0.576+0.j     ]
 [ 0.328+0.j      0.314-0.068j  0.314+0.068j  0.581+0.j     -0.4  +0.j     ]]
my eigenvectors / np.linalg.eig =
[[ 1.   +0.j      0.725+0.689j  0.725-0.689j  1.   -0.j      -1.   +0.j      ]
 [ 1.   +0.j      0.725+0.689j  0.725-0.689j  1.   -0.j     -1.   -0.j     ]
 [ 1.   +0.j      0.725+0.689j  0.725-0.689j  1.   +0.j     -1.   -0.j     ]
 [ 1.   +0.j      0.725+0.689j  0.725-0.689j  1.   -0.j     -1.   +0.j     ]
 [ 1.   +0.j      0.725+0.689j  0.725-0.689j  1.   +0.j     -1.   -0.j     ]]

```

Eigenvectors all close except sign and/or scaling? True

>>> QR Iteration with Wilkinson shift

C:\ProgramData\Anaconda3\lib\site-packages\ipykernel_launcher.py:32: ComplexWarning: Casting complex values to real discards the imaginary part

```

Iteration terminates at i=14 with tol=1e-06 reached
... num of iterations with inverse power method = 1
... num of iterations with inverse power method = 1

```

```

my eigenvalues: [ 2.116+0.j      0.207+0.229j  0.207-0.229j  0.073+0.j      -0.515+0.j      ]
np.linalg.eig:  [ 2.116+0.j      0.207+0.229j  0.207-0.229j  0.073+0.j      -0.515+0.j      ]

```

np.linalg.eig and my eigenvalues close? True

np.linalg.eig and my function return the same eigenvectors? False

```

my eigenvectors =
[[ 0.496+0.j      -0.213+0.062j -0.213-0.062j -0.116+0.j      0.549+0.j      ]
 [ 0.409+0.j     -0.171-0.035j -0.171+0.035j -0.222+0.j     -0.221+0.j     ]
 [ 0.384+0.j      0.387+0.343j  0.387-0.343j  0.369+0.j     -0.398+0.j     ]
 [ 0.576+0.j      0.169-0.722j  0.169+0.722j -0.681+0.j     0.576+0.j     ]
 [ 0.328+0.j     -0.006+0.321j -0.006-0.321j  0.581+0.j     -0.4  +0.j     ]]
np.linalg.eig =
[[ 0.496+0.j      0.109+0.194j  0.109-0.194j -0.116+0.j      0.549+0.j      ]
 [ 0.409+0.j      0.004+0.174j  0.004-0.174j -0.222+0.j     -0.221+0.j     ]
 [ 0.384+0.j      0.246-0.455j  0.246+0.455j  0.369+0.j     -0.398+0.j     ]
 [ 0.576+0.j     -0.741+0.j     -0.741-0.j     -0.681+0.j     0.576+0.j     ]
 [ 0.328+0.j      0.314-0.068j  0.314+0.068j  0.581+0.j     -0.4  +0.j     ]]
my eigenvectors / np.linalg.eig =
[[ 1.   +0.j      -0.228+0.974j -0.228-0.974j  1.   -0.j      1.   +0.j      ]
 [ 1.   +0.j     -0.228+0.974j -0.228-0.974j  1.   -0.j      1.   -0.j      ]
 [ 1.   +0.j     -0.228+0.974j -0.228-0.974j  1.   +0.j      1.   -0.j      ]
 [ 1.   +0.j     -0.228+0.974j -0.228-0.974j  1.   -0.j      1.   +0.j      ]
 [ 1.   +0.j     -0.228+0.974j -0.228-0.974j  1.   +0.j      1.   -0.j      ]]

```

Eigenvectors all close except sign and/or scaling? True

```
C:\ProgramData\Anaconda3\lib\site-packages\ipykernel_launcher.py:44: ComplexWarning: Casting complex values to real discards the imaginary part  
C:\ProgramData\Anaconda3\lib\site-packages\ipykernel_launcher.py:51: ComplexWarning: Casting complex values to real discards the imaginary part
```

```

In [30]: 1 print('\n\n')
2 print("=====")
3 print('Testing eigen_solver() on Random COMPLEX Matrices')
4 print("=====")
5
6 for A in RANDOM_COMPLEX_MATRICES[1:2]:
7     print('\nCOMPLEX >>> Input shape = {}'.format(A.shape))
8
9     w,v = np.linalg.eig(A)
10    w_sorted, v_sorted = sort_eigen(w, v)
11
12    H, S = Hessenberg(A,eigvec=True)
13
14    eigenvalues, eigenvectors = eigen_solver(H, S, max_iter=MAX_ITER, tol=RTOL, eigvec=True, shift=None,tridiagonal=False)
15    test_eigenvalues(eigenvalues,w_sorted)
16    test_eigenvectors(eigenvectors,v_sorted)
17
18
19    eigenvalues, eigenvectors = eigen_solver(H, S, max_iter=MAX_ITER, tol=RTOL, eigvec=True, shift='Wilkinson',tridiagonal=False)
20    test_eigenvalues(eigenvalues,w_sorted)
21    test_eigenvectors(eigenvectors,v_sorted)
22
23

```

```

=====
Testing eigen_solver() on Random COMPLEX Matrices
=====

```

```
COMPLEX >>> Input shape = (5, 5)
```

```
>>> QR Iteration WITHOUT shift
```

```
Iteration terminates at i=935 with tol=1e-06 reached
```

```
my eigenvalues: [ 2.251+2.287j  0.132+0.508j -0.182+0.806j -0.189-0.474j -0.442+0.271j]
np.linalg.eig: [ 2.251+2.287j  0.132+0.508j -0.182+0.806j -0.189-0.474j -0.442+0.271j]
```

```
np.linalg.eig and my eigenvalues close? True
```

```
np.linalg.eig and my function return the same eigenvectors? False
```

```
my eigenvectors =
```

```
[[ 0.51 +0.131j -0.036+0.524j -0.424+0.002j  0.254+0.395j  0.178-0.149j]
 [ 0.325+0.253j -0.415-0.312j  0.325-0.567j  0.15 -0.652j -0.52 +0.098j]
 [ 0.396+0.217j  0.018-0.456j  0.222-0.04j  -0.028+0.334j -0.379-0.102j]
 [ 0.343+0.253j -0.013-0.21j  0.236+0.496j -0.147-0.3j  -0.02 -0.171j]
 [ 0.385+0.138j  0.397+0.209j -0.177+0.096j -0.325+0.042j  0.587+0.371j]]
```

```
np.linalg.eig =
```

```
[[ 0.527+0.j 0.525+0.j -0.213-0.367j -0.327+0.337j  0.071-0.221j]
```

```
[ 0.377+0.164j -0.283+0.436j 0.654+0.j      0.669+0.j      -0.387+0.361j]
[ 0.437+0.111j -0.457+0.014j 0.145+0.173j -0.331+0.048j -0.375+0.117j]
[ 0.396+0.16j  -0.209+0.027j -0.313+0.451j 0.26 -0.211j -0.108-0.134j]
[ 0.407+0.038j 0.181-0.41j  -0.171-0.106j -0.114-0.308j 0.694+0.j  ]]
my eigenvectors / np.linalg.eig =
[[ 0.968+0.249j -0.069+0.998j 0.497-0.868j 0.225-0.974j 0.845+0.535j]
 [ 0.968+0.249j -0.069+0.998j 0.497-0.868j 0.225-0.974j 0.845+0.535j]
 [ 0.968+0.249j -0.069+0.998j 0.497-0.868j 0.225-0.974j 0.845+0.535j]
 [ 0.968+0.249j -0.069+0.998j 0.497-0.868j 0.225-0.974j 0.845+0.535j]
 [ 0.968+0.249j -0.069+0.998j 0.497-0.868j 0.225-0.974j 0.845+0.535j]]
```

Eigenvectors all close except sign and/or scaling? True

```
>>> QR Iteration with Wilkinson shift
Iteration terminates at i=12 with tol=1e-06 reached
```

```
my eigenvalues: [ 2.251+2.287j 0.132+0.508j -0.182+0.806j -0.189-0.474j -0.442+0.271j]
np.linalg.eig: [ 2.251+2.287j 0.132+0.508j -0.182+0.806j -0.189-0.474j -0.442+0.271j]
```

np.linalg.eig and my eigenvalues close? True

np.linalg.eig and my function return the same eigenvectors? False

```
my eigenvectors =
[[ 0.356+0.389j 0.507+0.137j 0.362+0.221j -0.029+0.469j -0.233+0.001j]
 [ 0.134+0.389j -0.386+0.347j -0.575+0.312j 0.508-0.436j 0.463+0.257j]
 [ 0.213+0.397j -0.444-0.106j -0.209-0.083j -0.22 +0.252j 0.227+0.32j ]
 [ 0.149+0.4j   -0.209-0.028j 0.06 -0.546j 0.06 -0.329j -0.094+0.144j]
 [ 0.247+0.326j 0.282-0.349j 0.201+0.012j -0.287-0.159j -0.214-0.66j ]]
np.linalg.eig =
[[ 0.527+0.j      0.525+0.j      -0.213-0.367j -0.327+0.337j 0.071-0.221j]
 [ 0.377+0.164j -0.283+0.436j 0.654+0.j      0.669+0.j      -0.387+0.361j]
 [ 0.437+0.111j -0.457+0.014j 0.145+0.173j -0.331+0.048j -0.375+0.117j]
 [ 0.396+0.16j  -0.209+0.027j -0.313+0.451j 0.26 -0.211j -0.108-0.134j]
 [ 0.407+0.038j 0.181-0.41j  -0.171-0.106j -0.114-0.308j 0.694+0.j  ]]
my eigenvectors / np.linalg.eig =
[[ 0.676+0.737j 0.966+0.26j -0.879+0.477j 0.759-0.652j -0.309-0.951j]
 [ 0.676+0.737j 0.966+0.26j -0.879+0.477j 0.759-0.652j -0.309-0.951j]
 [ 0.676+0.737j 0.966+0.26j -0.879+0.477j 0.759-0.652j -0.309-0.951j]
 [ 0.676+0.737j 0.966+0.26j -0.879+0.477j 0.759-0.652j -0.309-0.951j]
 [ 0.676+0.737j 0.966+0.26j -0.879+0.477j 0.759-0.652j -0.309-0.951j]]
```

Eigenvectors all close except sign and/or scaling? True

Observations

- Seems to be working for real and complex matrices

In []: 1

References for Francis Double-Shift QR Algorithm

- <https://www.cs.cornell.edu/~bindel/class/cs6210-f12/notes/lec28.pdf> (<https://www.cs.cornell.edu/~bindel/class/cs6210-f12/notes/lec28.pdf>)
- <https://people.inf.ethz.ch/arbenz/ewp/Lnotes/chapter4.pdf> (<https://people.inf.ethz.ch/arbenz/ewp/Lnotes/chapter4.pdf>)
- <https://people.eecs.berkeley.edu/~wkahan/Math128/Parlett.pdf> (<https://people.eecs.berkeley.edu/~wkahan/Math128/Parlett.pdf>)
- <https://www.math.usm.edu/lambers/mat610/class0331.pdf> (<https://www.math.usm.edu/lambers/mat610/class0331.pdf>)
- http://math.ntnu.edu.tw/~min/matrix_computation/QR_alg_ch2_1.pdf (http://math.ntnu.edu.tw/~min/matrix_computation/QR_alg_ch2_1.pdf)
- <https://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.215.3553&rep=rep1&type=pdf> (<https://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.215.3553&rep=rep1&type=pdf>)
- https://www.youtube.com/watch?v=RSm_Mqi0aSA (https://www.youtube.com/watch?v=RSm_Mqi0aSA)

Background

Implicit double shifts

Apply 1st shift s_1 on H_0 :

- $H_0 - s_1 I = Q_1 R_1 \dots (1)$
- $H_1 = R_1 Q_1 + s_1 I \dots (2)$

Apply 2nd shift s_2 on H_1 :

- $H_1 - s_2 I = Q_2 R_2 \dots (3)$
- $H_2 = R_2 Q_2 + s_2 I \dots (4)$

Now combining the two shifts (without explicitly forming H_1), from (2) and (3):

- $R_1 Q_1 + s_1 I = Q_2 R_2 + s_2 I$

Apply Q_1 from left and R_1 from right on both sides and expand terms:

- $Q_1(R_1 Q_1)R_1 + Q_1(s_1 I)R_1 = Q_1(Q_2 R_2)R_1 + Q_1(s_2 I)R_1$

Substitute $Q_1 R_1$ from (1) and re-arrange:

- $(Q_1 Q_2)(R_2 R_1) = (H_0 - s_1 I)^2 + (H_0 - s_1 I)(s_1 - s_2) = (H_0 - s_1 I)(H_0 - s_2 I)$

This is effectively the QR decomposition of matrix $M = (H_0 - s_1 I)(H_0 - s_2 I)$, i.e. performing two shifts on H_0 to obtain H_2 :

- $H_2 = (Q_1 Q_2)^* H_0 (Q_1 Q_2)$

When s_1 and s_2 are a conjugate pair of a complex eigenvalue λ , matrix M is real, thus avoiding QR decomposition in complex arithmetics

- $M = H_0^2 - 2\text{Re}(\lambda)H + |\lambda|^2 I$

A few observations:

- Naive implementation involves forming M explicitly by matrix multiplication, which is computationally expensive $\sim O(n^3)$
- Note also the matrix M is *not* in Hessenberg form; it has two lower sub-diagonals due to the multiplication of two Hessenberg matrices.
- Implicit Q-Theorem ...
- Need to restore M to Hessenberg by Givens rotation

Implicit Q theorem

- "The gist of the implicit Q theorem is that if $Q^T A Q = H$ and $Z^T A Z = G$ are both unreduced Hessenberg matrices and Q and Z have the same first column, the G and H are "essentially equal" in the sense that $G = D H D$ with $D = \text{diag}(\pm 1, \dots, \pm 1)$." -- Golub and van Loan [5, p.347]

Bulge chasing not implemented

- Instead of forming M in its entirety, we only form its first column, which being a second degree polynomial of a Hessenberg matrix, has only three nonzero entries.
- Compute a Householder reflection P_0 that makes $M e_1$ a multiple of e_1 .
- Then, we compute $P_0^T H P_0$, which is no longer Hessenberg, because P_0 operates on the first three rows and columns of H .
- Finally, we apply a series of Householder reflections P_1, P_2, \dots, P_{n-2} that restore Hessenberg form
- Because the reflections P_1, P_2, \dots, P_{n-2} do not affect the first row (when applied on the left) or column (when applied on the right),
- it follows that if we define $Z = P_0 P_1 P_2 \cdots P_{n-2}$, then Z and Z^* have the same first column
- Since both matrices implement similarity transformations that preserve the Hessenberg form of H , it follows from the Implicit Q Theorem that
- Z and Z^* are essentially equal, and that they essentially produce the same updated matrix H_2
- This variation of a Hessenberg QR step is called a Francis QR Step.
- (Source: <https://www.math.usm.edu/lambers/mat610/class0331.pdf> (<https://www.math.usm.edu/lambers/mat610/class0331.pdf>))

```

In [ ]: 1 #####
2  ### IGNORE ###
3  #####
4
5  # Naive implementation of Francis Double-shift QR Algorithm
6
7  def construct_M_full(H,lam_re,lam_im):
8
9      """      Naive implementation of the full matrix  $M = (H-s1.I)(H-s2.I)$  where  $s1$  and  $s2$  are complex conjugate pair
10
11      Input      -----
12                  H: 2D np.array in the form of a Hessenberg matrix with real entries
13                  lam_re: real part of a complex eigenvalue
14                  lam_im: imaginary part of a complex eigenvalue
15      Return      -----
16                  M: 2D np.array with only real entries
17      """
18
19      I = np.eye(H.shape[0])
20
21      M = H@H - 2*lam_re*H + (lam_re**2+lam_im**2)*I #Note: H@H complexity =  $O(n^3)$  expensive!
22      # RuntimeError: overflow encountered in matmul
23      # RuntimeError: invalid value encountered in matmul
24      #print(M)
25
26      return M
27
28
29
30 # for eigenvalues only
31
32 def QR_Iteration_DoubleShift(A, max_iter, tol):
33
34     """      Perform QR iteration with double shift to obtain eigenvalues
35     Input      -----
36                  A: 2D np.array with real or complex entries
37                  max_iter: int, maximum number of iterations to be performed
38                  tol: float, relative tolerance between eigenvalues by successive iterations
39     Return      -----
40                  eigvals_new: 1D np.array with real or complex entries
41     """
42
43     n = A.shape[0]
44
45     # step 1: tranform A to Hessenberg
46     H, _ = Hessenberg(A)
47
48     # step 2: QR iteration
49     H_old = H.copy()
50     eigvals_old = diagonal_block(H)
51
52     for i in range(max_iter):

```



```

53
54     # calculate Wilkinson shift
55     datatype, lam = wilkinson_shift(H_old)
56     # print(">>> Wilkinson_shift = {},{}".format(lam,datatype))
57
58     if datatype == 'complex':
59         M = construct_M_full(H_old, lam.real, lam.imag)
60         H_old, _ = Hessenberg(M) # Hessenberg(A, eigvec=False, inplace=True)
61         H_new, _ = QR_Givens(H_old) # updating H_old in-place ## default QR_Givens(H, eigvec=False, inplace=True, tridiagonal=False)
62
63     else:
64         H_old = H_old - lam * np.eye(n)
65         H_new, _ = QR_Givens(H_old) + lam * np.eye(n) # updating H_old in-place
66
67     eigvals_new = diagonal_block(H_new)
68
69     H_old = H_new
70
71     # Test for convergence: relative tol = 1- w / w' for each eigenvalue
72     if np.allclose(eigvals_new, eigvals_old, rtol=tol):
73         print('Iteration terminates at i={} with tol={} reached'.format(i, tol))
74         break
75
76     if i == max_iter-1:
77         err = np.max(abs((eigvals_new - eigvals_old)) / abs(eigvals_old))
78         idx = np.argwhere(np.isclose(eigvals_new, eigvals_old, rtol=tol)==False).tolist()
79         print('max_iter={} reached, max error={} vs tol={}; index of non-convergence={}'.format(max_iter, err, tol, idx))
80
81     eigvals_old = eigvals_new
82
83     return eigvals_new
84
85

```

```

In [ ]: 1 print('\n\n')
2 print("=====")
3 print('Testing QR_Iteration_DoubleShift on Random REAL Matrices')
4 print("=====")
5
6 for A in RANDOM_REAL_MATRICES[1:-1]:
7     print('\nREAL >>> Input shape = {}'.format(A.shape))
8
9     test_eigenvalues_function(A, QR_Iteration_Eigenvalues)
10    test_eigenvalues_function(A, QR_Iteration_WilkinsonShift)
11    test_eigenvalues_function(A, QR_Iteration_DoubleShift)

```

Observations:

- Double-shift does not work **#TODO**

- Overflow issues with repeated matrix multiplication $H@H$ in order to get M in the iteration
- Need implement element-wise Bulge-chasing (based on implicit Q)

```
In [ ]: 1 #####
2  ### IGNORE ###
3  #####
4
5  def eigen_solver_real(H, S, max_iter, tol, eigvec):
6
7      """    Compute the eigenvalues and eigenvectors of a Hessenberg matrix with real entries
8              with Wilkinson' shift (if real) or double shift (if complex)
9      Input  -----
10             H: 2D np.array in the form of a Hessenberg matrix with real entries
11             S: similarity transformation associated with the Hessenberg reduction,  $H = S @ A @ S.T$  where A is the input real matrix
12             max_iter: int, maximum number of iterations to be performed
13             tol: float, relative tolerance between eigenvalues by successive iterations
14             eigvec: bool, indicating whether eigenvectors are to be calculated
15      Return -----
16             eigvals_new: 1D np.array, eigenvalues
17             eigenvectors: 2D np.array with each column represents an eigenvector, in the same order as the associated eigenvalues;
18                           if eigvec is False, then this default to a zero matrix
19      """
20
21      datatype, lam = Wilkinson_shift(H_old)
22
23      if datatype == 'complex':
24          shift = 'Double-'
25      else:
26          shift = "Wilkinson's "
27      print(">>> QR Iteration with Real Shift: lambda = {}, {} -> Applying {}Shift".format(lam, datatype, shift))
28
29      pass # TODO
30
31
32  def eigen_solver_realsymmetric(H, S, max_iter, tol, eigvec):
33      pass # TODO
34
35
```

```
In [ ]: 1
```

Visualization

```

In [31]: 1 # Visualization
2
3 def plot_eigenvalues_real(w_sorted,eigenvalues):
4
5     '''Plotting line chart for two sets of REAL eigenvalues in comparison
6     Input -----
7         w_sorted: eigenvalues from np.linalg.eig(), sorted in descending order by magnitude
8         eigenvalues: eigenvalues from my function, sorted in descending order by magnitude
9     Return -----
10        None; chart on display
11    '''
12    plt.plot(w_sorted, color='red', marker='o', linestyle='dashed', label = 'np.linalg.eig()')
13    plt.plot(eigenvalues, color='green', marker='x', linestyle='dotted', label='my eigenvalues')
14    plt.title('Real Eigenvalues')
15    plt.legend()
16    plt.show()
17
18
19 def plot_eigenvalues_complex(w_sorted,eigenvalues):
20
21     '''Plotting line chart for two sets of COMPLEX eigenvalues in comparison
22     Input -----
23         w_sorted: eigenvalues from np.linalg.eig(), sorted in descending order by magnitude
24         eigenvalues: eigenvalues from my function, sorted in descending order by magnitude
25     Return -----
26        None; two charts on display, one for real parts and the other for imaginary parts
27    '''
28    f, ax = plt.subplots(1,2,figsize=(10,5))
29    ax[0].plot(w_sorted.real, color='red', marker='o', linestyle='dashed', label = 'np.linalg.eig()')
30    ax[0].plot(eigenvalues.real, color='green', marker='x', linestyle='dotted', label='my eigenvalues')
31    ax[0].set_title('Complex Eigenvalues - Real')
32    ax[0].legend()
33
34
35    x = np.arange(len(eigenvalues)) # the Label Locations
36    width = 0.02 # the width of the bars
37    ax[1].bar(x - width/2, w_sorted.imag, width, color='red',label = 'np.linalg.eig()')
38    ax[1].bar(x + width/2, eigenvalues.imag, width,color='green', label='my eigenvalues')
39    ax[1].set_title('Complex Eigenvalues - Imaginary')
40    ax[1].legend()
41
42    plt.show()
43

```

Attampt at Object-Oriented Programming

```

In [32]: 1 # Object-Oriented Programming: implement algorithm 1.4.14 in a way, that H is either Hessenberg or tridiagonal, either real or complex, but encapsulat
2
3 class Matrix:
4
5     # General matrix class for both complex and real matrices
6
7     def __init__(self, A, calc_eigvec=False):
8         self.calc_eigvec = calc_eigvec
9         self.A = A
10        self.n = A.shape[0]
11        self.dtype = A.dtype
12
13        self.is_symmetric = False
14        if np.allclose(A,A.T) or np.allclose(A, A.conjugate().T):
15            self.is_symmetric = True
16
17        self.is_hessenberg = False
18        zeros = np.zeros([self.n,self.n],dtype=self.dtype)
19        if np.allclose(np.tril(self.A, -2),zeros):
20            self.is_hessenberg = True
21            self.H = self.A
22            self.S = None
23        else:
24            self.H,self.S = Hessenberg(self.A, self.calc_eigvec)
25
26        self.is_tridiagonal = False
27        tridiag = self.A - np.tril(self.A,-2) - np.triu(self.A,2)
28        if self.is_hessenberg and np.allclose(np.triu(self.A,2),zeros) and not np.allclose(tridiag,zeros):
29            self.is_tridiagonal = True
30
31    def __eq__(self, other):
32        return np.allclose(self.A,other.A)
33
34    def __repr__(self):
35        return self.A
36
37    def __str__(self):
38        return 'Matrix dtype={}, shape={}x{}, is_symmetric={}, is_hessenberg={}, is_tridiagonal={} \n{}'.format(self.dtype,self.n,self.n,self.is_symme
39
40
41    # Wilkson's shift in complex arithmetics
42    def eigen_solver(self, shift=None):
43        # shift = None or 'Wilkinson'
44        tridiagonal = self.is_symmetric
45        # tridiagonal = False
46        print('activiating tridigonal:', tridiagonal)
47
48        if self.calc_eigvec:
49            print('\n ----- Processing both eigenvalues and eigenvectors ----- ')
50            self.eigenvalues, self.eigenvectors = eigen_solver(self.H, self.S, MAX_ITER, RTOL, self.calc_eigvec,shift,tridiagonal)
51            #eigen_solver(H, S, max_iter, tol, eigvec, shift, tridiagonal)
52        else:

```

```
53     print('\n ----- Processing eigenvalues only ----- ')
54     self.eigenvalues, _ = eigen_solver(self.H, self.S, MAX_ITER, RTOL, self.calc_eigvec, shift, tridiagonal)
55
56 def eigen_test(self, verbose):
57     w, v = np.linalg.eig(self.A)
58     w_sorted, v_sorted = sort_eigen(w, v)
59
60     print('\n ----- Checking Eigenvalues -----')
61     test_eigenvalues(self.eigenvalues, w_sorted, verbose)
62     if self.calc_eigvec:
63         print('\n ----- Checking Eigenvectors -----')
64         test_eigenvectors(self.eigenvectors, v_sorted, verbose)
65     if verbose:
66         print(self.eigenvalues.dtype)
67
68     if self.eigenvalues.dtype == 'complex128':
69         plot_eigenvalues_complex(w_sorted, self.eigenvalues)
70     else:
71         plot_eigenvalues_real(w_sorted, self.eigenvalues)
72
73
74
```

```

In [ ]: 1 #####
2  ### IGNORE ###
3  #####
4
5
6  class RealMatrix(Matrix):
7
8      def __init__(self, A, calc_eigvec=False):
9          super().__init__(A, calc_eigvec)
10
11
12      # double-shifts for complex eigenvalues
13      def eigen_solver(self):
14
15          if self.calc_eigvec:
16              print('\n ----- Processing both eigenvalues and eigenvectors ----- ')
17              self.eigenvalues, self.eigenvectors = eigen_solver_real(self.H, self.S, max_iter=MAX_ITER, tol=RTOL, eigvec=self.calc_eigvec)
18
19          else:
20              print('\n ----- Processing eigenvalues only ----- ')
21              self.eigenvalues, _ = eigen_solver_real(self.H, self.S, max_iter=MAX_ITER, tol=RTOL, eigvec=self.calc_eigvec)
22
23
24  class SymmetricRealMatrix(RealMatrix):
25
26      def __init__(self, A, calc_eigvec=False):
27          super().__init__(A, calc_eigvec)
28
29
30      # transformation to tridiagonal form with optimized storage
31      def eigen_solver(self):
32
33          if self.calc_eigvec:
34              print('\n ----- Processing both eigenvalues and eigenvectors ----- ')
35              self.eigenvalues, self.eigenvectors = eigen_solver_realsymmetric(self.H, self.S, max_iter=MAX_ITER, tol=RTOL, eigvec=self.calc_eigvec)
36
37          else:
38              print('\n ----- Processing eigenvalues only ----- ')
39              self.eigenvalues, _ = eigen_solver_realsymmetric(self.H, self.S, max_iter=MAX_ITER, tol=RTOL, eigvec=self.calc_eigvec)
40

```

```

In [ ]: 1

```

Matric Market

from scipy.io import mmread

- BCSSTK01 (real symmetric positive definite, 48 by 48, 224 entries), Small test problem; source: <https://math.nist.gov/MatrixMarket/data/Harwell-Boeing/bcsstruc1/bcsstruc1.html> (<https://math.nist.gov/MatrixMarket/data/Harwell-Boeing/bcsstruc1/bcsstruc1.html>)
- CK104 (real unsymmetric, 104 by 104, 992 entries) The matrices have several multiple eigenvalues and clustered eigenvalues. source: <https://math.nist.gov/MatrixMarket/data/NEP/chuck/ck104.html> (<https://math.nist.gov/MatrixMarket/data/NEP/chuck/ck104.html>)
- QC324 (complex symmetric indefinite, 324 x 324, 26730 entries) H2PLUS: Model of H2+ in an Electromagnetic Field source: <https://math.nist.gov/MatrixMarket/data/NEP/h2plus/h2plus.html> (<https://math.nist.gov/MatrixMarket/data/NEP/h2plus/h2plus.html>)
- MHD1280 (complex unsymmetric, 1280 by 1280, 47906 entries) MHD: Alfven Spectra in Magnetohydrodynamicssource: <https://math.nist.gov/MatrixMarket/data/NEP/mhd/mhd.html> (<https://math.nist.gov/MatrixMarket/data/NEP/mhd/mhd.html>)
- RBS480A (real unsymmetric, 480 by 480, 17088 entries) The computational task is to compute the real eigenvalues and the corresponding eigenvectors (most of the eigenvalues are complex). source: <https://math.nist.gov/MatrixMarket/data/NEP/robotics/robotics.html> (<https://math.nist.gov/MatrixMarket/data/NEP/robotics/robotics.html>)
- QH1484 (real unsymmetric, 1484 by 1484, 6110 entries) This set of matrices if from the application of the Hydro-Quebec power systems' small-signal model. In the application, one wants to compute all eigenvalues $a + bi$ in a box of the complex plane. <https://math.nist.gov/MatrixMarket/data/NEP/quebec/quebec.html> (<https://math.nist.gov/MatrixMarket/data/NEP/quebec/quebec.html>)
- ORANI678 (real unsymmetric, 2529 by 2529, 90158 entries) Australian Economic Models Economic model of Australia, 1968-69 data source: <https://math.nist.gov/MatrixMarket/data/Harwell-Boeing/econaus/orani678.html> (<https://math.nist.gov/MatrixMarket/data/Harwell-Boeing/econaus/orani678.html>)

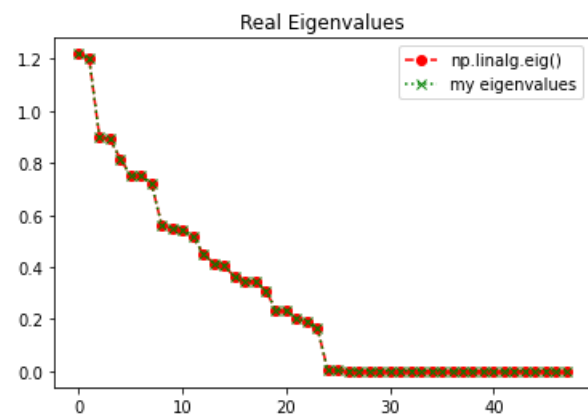
```

In [33]: 1 def normalize(A):
2         """ normalize a matrix to between [-1,1]
3         """
4         scaler = max(abs(A.max()),abs(A.min()))
5         return A/scaler, scaler
6
7
8 def runtest_matrixmarket(source, matrix_class,shift):
9     """
10    Testing on matrix from matrix market
11    Input -----
12        source: str, filename in the form of 'xxxn.mtx.gz'
13        matrix_class: options = [Matrix,RealMatrix, SymmetricRealMatrix]; currently only Matrix option is available
14        shift: None or 'Wilkinson'
15    Return -----
16        None; print test results
17    """
18
19    # read data from matrix market format
20    A = mmread(source)
21    print("From Matrix Market: \nmatrix source={}, matrix type={}, shape={}, data type={}, max={}, min={} "
22          .format(source, type(A), A.shape,A.dtype, A.max(),A.min()))
23
24    # convert to np.array
25    A = np.asarray(A.todense())
26
27    # normalization
28    A, s = normalize(A)
29
30    # wrap into a matrix class object
31    a = matrix_class(A, calc_eigvec=False)
32    print('is_symmetric={}', a.is_symmetric)
33
34    # run test on eigen_solver()
35    a.eigen_solver(shift)
36    a.eigen_test(verbose=True)
37
38

```



```
In [34]: 1 # real symmetric 48x48
2
3 source = 'matricmarket/bcsstk01.mtx.gz'
4 matrix_class = Matrix
5
6 runtest_matricmarket(source, matrix_class, shift=None)
7
```



```
In [38]: 1 # real symmetric 48x48
2
3 source = 'matricmarket/bcsstk01.mtx.gz'
4 matrix_class = Matrix
5
6 runtest_matrixmarket(source, matrix_class, shift='Wilkinson')
7
```

Observation

- General QR iteration without shift seems to be working for small real symmetric matrix
- QR iteration with Wilkinson shift seems to be working for small real symmetric matrix
- Similar convergence rate...

```
In [35]: 1 MAX_ITER = 10000 # increased max iteration
2
3 # real unsymmetric matrix 104x104 - WIHTOUT SHIFT
4
5 source = 'matricmarket/ck104.mtx.gz'
6 matrix_class = Matrix
7
8 runtest_matrixmarket(source, matrix_class, shift=None)
9
```

From Matrix Market:

matrix source=matricmarket/ck104.mtx.gz, matrix type=<class 'scipy.sparse.coo.coo_matrix'>, shape=(104, 104), data type=float64, max=4.7481454523109, min=-2.6168329561089

is_symmetric={} False

activating tridigonal: False

----- Processing eigenvalues only -----

>>> QR Iteration WITHOUT shift

C:\ProgramData\Anaconda3\lib\site-packages\ipykernel_launcher.py:32: ComplexWarning: Casting complex values to real discards the imaginary part

Iteration terminates at i=2982 with tol=1e-06 reached

----- Checking Eigenvalues -----

```
my eigenvalues: [1.159+0.j  1.159-0.j  0.336+0.j  0.336-0.j  0.299+0.j  0.299-0.j  0.297+0.j  0.297-0.j  0.252+0.j  0.252-0.j  0.2
4 +0.j  0.24 -0.j  0.24 +0.j  0.24 -0.j  0.228+0.j  0.228-0.j  0.216+0.j  0.216-0.j  0.211+0.j  0.211-0.j  0.211+0.j  0.211-0.j
0.204+0.j
0.204+0.j  0.198+0.j  0.198+0.j  0.194+0.j  0.194-0.j  0.194+0.j  0.194-0.j  0.189+0.j  0.189+0.j  0.175+0.j  0.175-0.j  0.172+
0.j  0.172+0.j  0.172+0.j  0.172+0.j  0.167+0.j  0.167+0.j  0.148+0.j  0.148+0.j  0.145+0.j  0.145+0.j  0.145+0.j  0.145+0.j
0.142+0.j  0.142-0.j  0.119+0.j  0.119+0.j  0.117+0.j  0.117+0.j  0.117+0.j  0.117+0.j  0.116+0.j  0.116+0.j  0.116+0.j  0.089+0.j  0.089+
0.j  0.089+0.j  0.089+0.j  0.089+0.j  0.089-0.j  0.089+0.j  0.089-0.j  0.063+0.j  0.063+0.j  0.063+0.j  0.063+0.j  0.062+0.001j
0.062-0.001j 0.062+0.001j 0.062-0.001j 0.04 +0.j  0.04 +0.j  0.039+0.j  0.039+0.j  0.039+0.j  0.039+0.j  0.039-0.j  0.039+0.j  0.021+
0.j  0.021+0.j  0.021+0.j  0.021-0.j  0.02 +0.j  0.02 +0.j  0.02 +0.j  0.02 +0.j  0.008+0.j  0.008+0.j  0.008+0.j  0.008+0.j
0.008+0.j  0.008+0.j  0.007+0.j  0.007+0.j  0.001+0.j  0.001+0.j  0.001+0.j  0.001+0.j  0.001+0.j  0.001+0.j  0.001+0.j  0.001+
0.j ]
np.linalg.eig: [1.159+0.j  1.159+0.j  0.336+0.j  0.336+0.j  0.299+0.j  0.299+0.j  0.297+0.j  0.297+0.j  0.252+0.j  0.252+0.j  0.2
4 +0.j  0.24 -0.j  0.24 +0.j  0.24 -0.j  0.228+0.j  0.228+0.j  0.216+0.j  0.216+0.j  0.211+0.j  0.211-0.j  0.211+0.j  0.211-0.j
0.204+0.j
0.204+0.j  0.198+0.j  0.198+0.j  0.194+0.j  0.194-0.j  0.194+0.j  0.194-0.j  0.189+0.j  0.189+0.j  0.175+0.j  0.175-0.j  0.172+
0.j  0.172+0.j  0.172+0.j  0.172+0.j  0.167+0.j  0.167+0.j  0.148+0.j  0.148-0.j  0.145+0.j  0.145+0.j  0.145+0.j  0.145+0.j
0.142+0.j  0.142+0.j  0.119+0.j  0.119+0.j  0.117+0.j  0.117+0.j  0.117+0.j  0.117+0.j  0.116+0.j  0.116+0.j  0.116+0.j  0.089+0.j  0.089+
0.j  0.089+0.j  0.089+0.j  0.089+0.j  0.089-0.j  0.089+0.j  0.089-0.j  0.063+0.j  0.063+0.j  0.063+0.j  0.063+0.j  0.062+0.001j
0.062-0.001j 0.062+0.001j 0.062-0.001j 0.04 +0.j  0.04 +0.j  0.039+0.j  0.039+0.j  0.039+0.j  0.039+0.j  0.039-0.j  0.039+0.j  0.021+
0.j  0.021+0.j  0.021+0.j  0.021+0.j  0.02 +0.j  0.02 +0.j  0.02 -0.j  0.02 +0.j  0.02 +0.j  0.008+0.j  0.008+0.j  0.008+0.j  0.008+0.j
0.008+0.j  0.008+0.j  0.007+0.j  0.007+0.j  0.001+0.j  0.001+0.j  0.001+0.j  0.001+0.j  0.001+0.j  0.001+0.j  0.001+0.j  0.001+
0.j ]
```

np.linalg.eig and my eigenvalues close? False

my eigenvalues - np.linalg.eig =

```
[-0.+0.j  0.-0.j  -0.+0.j  -0.+0.j  0.+0.j  -0.+0.j  -0.+0.j  -0.+0.j  0.+0.j  -0.+0.j  -0.-0.j  -0.+0.j  -0.-0.j  -0.+
```

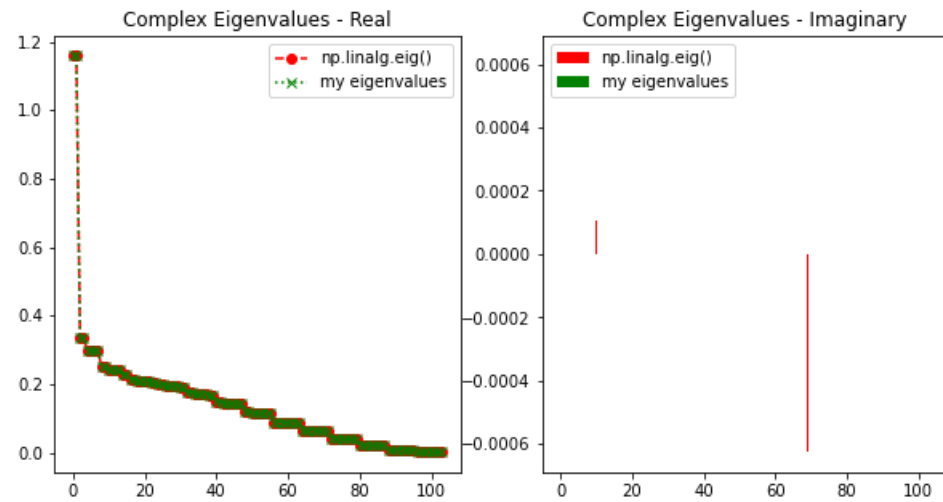
```

0.j      -0.+0.j      -0.-0.j      -0.+0.j      -0.+0.j      -0.+0.j      -0.-0.j      -0.+0.j      -0.-0.j      -0.+0.j      -0.+0.j      -0.+0.j      -0.+0.j      -0.+0.j
-0.-0.j   -0.+0.j      -0.-0.j      -0.+0.j      -0.+0.j      0.+0.j      0.-0.j      0.+0.j      -0.+0.j      0.+0.j      -0.+0.j      -0.+0.j      0.+0.j      -0.-0.
j      -0.+0.j      0.+0.j      -0.+0.j      0.+0.j      -0.+0.j      -0.+0.j      -0.-0.j      0.+0.j      -0.+0.j      0.+0.j      0.+0.j      -0.+0.j      -0.+0.j
0.+0.j      0.+0.j      0.+0.j      -0.+0.j      0.+0.j      0.+0.j      0.-0.j      0.+0.j      -0.+0.j      -0.-0.j      -0.+0.j      -0.+0.j      0.+0.j      -0.+0.
j      0.+0.j      0.-0.j      -0.-0.j      -0.+0.j      -0.+0.j      -0.+0.j      0.+0.j      -0.+0.j      0.-0.j      0.+0.001j  0.-0.001j  -0.+0.j      0.+0.j
-0.+0.j   -0.+0.j      -0.-0.j      0.-0.j      -0.+0.j      0.+0.j      0.+0.j      0.+0.j      -0.+0.j      -0.+0.j      -0.+0.j      0.+0.j      -0.+0.j      -0.+0.
j      0.+0.j      -0.+0.j      0.+0.j      -0.+0.j      -0.+0.j      0.+0.j      0.+0.j      -0.+0.j      0.+0.j      ]

```

max abs diff = 0.0007594189357278833

complex128



```
In [36]: 1 # real unsymmetric matrix 104x104 - WILKINSON SHIFT
2
3 source = 'matricmarket/ck104.mtx.gz'
4 matrix_class = Matrix
5
6 runtest_matrixmarket(source, matrix_class, shift='Wilkinson')
7
```

From Matrix Market:

```
matrix source=matricmarket/ck104.mtx.gz, matrix type=<class 'scipy.sparse.coo.coo_matrix'>, shape=(104, 104), data type=float64, max=4.7481454523109, min=-2.6168329561089
```

```
is_symmetric={} False
```

activating tridigonal: False

```
----- Processing eigenvalues only -----
>>> QR Iteration with Wilkinson shift
```

```
C:\ProgramData\Anaconda3\lib\site-packages\ipykernel_launcher.py:32: ComplexWarning: Casting complex values to real discards the imaginary part
```

```
max_iter=10000 reached, max error=0.0029218219274107005 vs tol=1e-06; index of non-convergence=[[67], [69]]
```

```
----- Checking Eigenvalues -----
```

[illegible]

np.linalg.eig and my eigenvalues close? False

```
my_eigenvalues = np.linalg.eig(
    [-0.  +0.j  0.   -0.j -0.  +0.j -0.  +0.j -0.  +0.j  0.   +0.j -0.  +0.j -0.  +0.j  0.   -0.j  0.   +0.j  0.
     -0.j -0.  +0.j -0.  -0.j -0.  +0.j -0.  +0.j  0.   -0.j  0.   +0.j  0.   +0.j  0.   -0.j  0.   +0.j -0.  -0.j
     -0.  +0.j -0.  -0.j -0.  +0.j  0.   +0.j -0.  +0.j -0.  -0.j -0.  +0.j -0.  +0.j  0.   +0.j -0.  +0.j  0.]
)
```

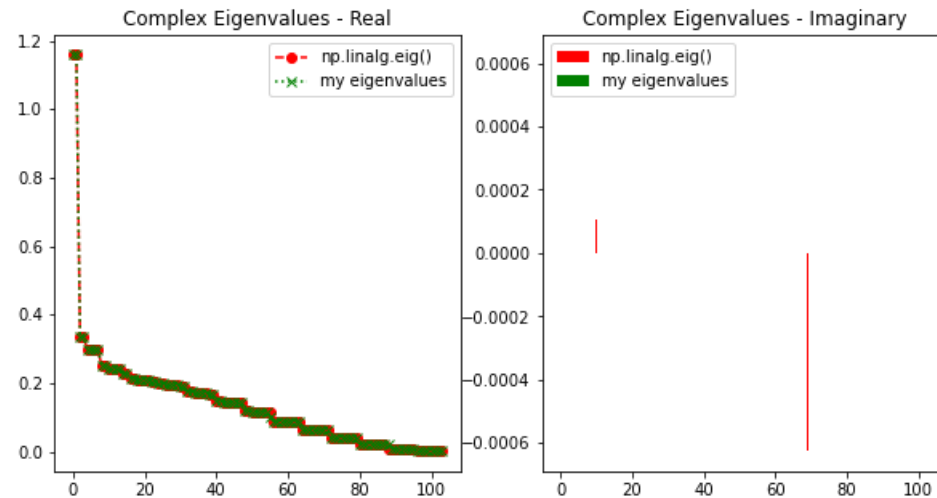
```

-0.j 0. +0.j 0. +0.j 0. +0.j -0. +0.j -0. +0.j 0. +0.j 0. +0.j -0. +0.j -0. +0.j -0. +0.j -0.001+0.j
0. +0.j -0.014+0.j -0. +0.j 0. +0.j -0. +0.j -0. +0.j -0. -0.j -0. +0.j -0. -0.j -0. +0.j -0. +0.j -0.
+0.j -0. +0.j -0. -0.j -0. +0.j -0. -0.j -0. +0.j 0. +0.j -0. +0.j -0. +0.j 0. +0.j 0. -0.j 0. +0.j 0. -0.j 0.002+0.j
0. +0.j 0. +0.j 0. +0.j 0. -0.j -0. +0.j 0. +0.j 0. +0.j 0.012+0.j -0. +0.j 0. +0.j 0. +0.j 0. +0.j -0. +0.j -0.
+0.j 0. +0.j 0. +0.j 0. +0.j -0. +0.j -0. +0.j 0. +0.j 0. +0.j 0. +0.j 0. +0.j]

```

max abs diff = 0.014099740514612172

complex128



Observation

- General QR iteration without shift seems to be working for real unsymmetric matrix
- However, applying Wilkinson's shift seems to converge slower than without shift... **WHY??**


```
In [37]: 1 MAX_ITER = 10000
2
3 # complex symmetric matrix - WIHTOUT SHIFT
4
5 source = 'matricmarket/qc324.mtx.gz'
6 matrix_class = Matrix
7
8 runtest_matrixmarket(source, matrix_class, shift=None)
9
```

From Matrix Market:

matrix source=matricmarket/qc324.mtx.gz, matrix type=<class 'scipy.sparse.coo.coo_matrix'>, shape=(324, 324), data type=complex128, max=(1.4957127687965-0.087585823232133j), min=(-0.40837438550439-0.017204228197979j)

is_symmetric={} True

activating tridigonal: True

----- Processing eigenvalues only -----

>>> QR Iteration WITHOUT shift

max_iter=10000 reached, max error=0.034575504317016725 vs tol=1e-06; index of non-convergence=[[52], [54], [142], [144], [178], [180], [268], [270], [271]]

----- Checking Eigenvalues -----

my eigenvalues: [1.014-0.063j 0.859-0.064j 0.786-0.072j 0.741-0.07j 0.632-0.069j 0.628-0.06j 0.548-0.058j 0.519-0.048j 0.48 -0.056j 0.41 -0.042j 0.401-0.048j 0.354-0.054j 0.324-0.039j 0.312-0.042j 0.305-0.041j 0.275-0.039j 0.248-0.034j 0.235-0.039j 0.218-0.038j 0.203-0.033j 0.2 -0.038j 0.193-0.039j 0.189-0.036j 0.184-0.026j 0.182-0.028j 0.17 -0.027j 0.168-0.03j 0.167-0.031j 0.164-0.028j 0.155-0.027j 0.152-0.023j 0.148-0.032j 0.144-0.03j 0.141-0.031j 0.141-0.03j 0.137-0.032j 0.133-0.028j 0.131-0.033j 0.124-0.037j 0.115-0.033j 0.112-0.037j 0.112-0.03j 0.111-0.043j 0.108-0.027j 0.101-0.025j 0.095-0.017j 0.094-0.023j 0.092-0.021j 0.091-0.017j 0.091-0.025j 0.088-0.031j 0.085-0.032j 0.079-0.042j 0.066-0.042j 0.064-0.048j 0.056-0.043j 0.056-0.049j 0.051-0.04j 0.046-0.045j 0.04 -0.04j 0.039-0.036j 0.036-0.036j 0.033-0.042j 0.032-0.03j 0.031-0.036j 0.031-0.037j 0.031-0.038j 0.028-0.03j 0.027-0.031j 0.027-0.034j 0.026-0.023j 0.025-0.036j 0.024-0.025j 0.022-0.024j 0.021-0.032j 0.021-0.022j 0.021-0.018j 0.02 -0.024j 0.018-0.019j 0.017-0.016j 0.016-0.019j 0.016-0.032j 0.015-0.022j 0.015-0.019j 0.015-0.015j 0.015-0.02j 0.014-0.017j 0.014-0.015j 0.014-0.018j 0.013-0.016j 0.013-0.021j 0.012-0.01j 0.012-0.017j 0.012-0.019j 0.011-0.019j 0.011-0.02j 0.01 -0.008j 0.009-0.015j 0.009-0.014j 0.008-0.007j 0.008-0.014j 0.008-0.027j 0.007-0.013j 0.006-0.01j 0.005-0.006j 0.003-0.003j 0.002-0.009j 0.002-0.008j 0.002-0.011j 0.002-0.008j 0.001-0.014j 0. -0.016j -0. -0.004j -0. -0.01j -0. -0.006j -0.001-0.013j -0.001-0.002j -0.002-0.002j -0.002-0.004j -0.002-0.005j -0.003-0.003j -0.004-0.009j -0.005-0.006j -0.005-0.007j -0.006-0.006j -0.006-0.001j -0.007-0.007j -0.007-0.004j -0.008-0.006j -0.009-0.007j -0.009-0.008j -0.012-0.008j -0.013-0.012j -0.015-0.007j -0.015-0.007j -0.015-0.016j -0.016-0.008j -0.017-0.01j -0.017-0.01j -0.018-0.01j -0.018-0.008j -0.018-0.014j -0.019-0.01j -0.02 -0.01j -0.02 -0.01j -0.021-0.013j -0.021-0.016j -0.021-0.014j -0.027-0.014j -0.029-0.012j -0.03 -0.015j -0.031-0.012j -0.032-0.011j -0.035-0.013j -0.036-0.012j -0.036-0.015j -0.037-0.01j -0.038-0.01j -0.038-0.013j -0.041-0.016j -0.044-0.009j -0.044-0.008j -0.046-0.014j -0.046-0.017j -0.047-0.011j -0.049-0.01j -0.051-0.013j -0.052-0.016j -0.053-0.017j -0.055-0.011j -0.056-0.022j -0.058-0.017j -0.059-0.012j -0.06 -0.022j -0.063-0.007j -0.064-0.013j -0.064-0.016j -0.067-0.017j -0.069-0.012j -0.071-0.018j -0.072-0.024j -0.074-0.011j -0.077-0.018j -0.08 -0.017j -0.082-0.019j -0.083-0.013j -0.089-0.021j -0.089-0.017j -0.094-0.02j -0.094-0.021j -0.095-0.018j -0.097-0.018j -0.098-0.013j -0.099-0.019j -0.107-0.026j -0.109-0.011j -0.111-0.024j -0.112-0.017j -0.114-0.009j -0.114-0.009j -0.115-0.015j -0.117-0.016j -0.119-0.022j -0.124-0.019j -0.126-0.006j -0.128-0.013j -0.128-0.021j -0.131-0.02j -0.141-0.015j -0.141-0.013j -0.144-0.013j -0.148-0.012j -0.148-0.016j -0.149-0.012j -0.149-0.009j -0.153-0.02j -0.156-0.007j -0.157-0.01j -0.16 -0.019j -0.164-0.014j -0.167-0.013j -0.168-0.015j -0.169-0.005j -0.171-0.001j -0.172-0.013j -0.178-0.012j -0.18 -0.013j -0.181-0.008j -0.182-0.012j -0.183-0.023j -0.186-0.012j -0.186-0.02j -0.187-0.011j -0.189-0.017j -0.192-0.009j -0.193-0.009j -0.196-0.016j -0.196-0.015j -0.201-0.016j -0.204-0.013j -0.205-0.013j -0.207-0.004j -0.208-0.009j -0.209-0.012j -0.21 -0.014j -0.211-0.013j -0.211-0.012j -0.212-0.007j -0.217-0.009j -0.218-0.016j -0.22 -0.018j -0.22 -0.015j -0.222-0.014j -0.222-0.014j -0.227-0.013j -0.227-0.01j -0.229-0.005j -0.23 -0.008j -0.234-0.012j -0.235-0.014j -0.235-0.01j -0.237-0.009j -0.239-0.006j -0.239-0.004j -0.24 -0.012j -0.243-0.013j -0.244-0.009j -0.245-0.014j -0.246-0.006j -0.246-0.012j -0.249-0.008j -0.25 -0.012j -0.251-0.015j -0.253-0.016j -0.254-0.008j -0.256-0.013j -0.256-0.012j -0.259-0.013j -0.26 -0.011j -0.261-0.014j -0.267-0.011j -0.267-0.015j -0.268-0.01j -0.269-0.009

```

j -0.272-0.014j -0.272-0.006j -0.274-0.008j -0.275-0.007j -0.278-0.011j -0.284-0.003j -0.285-0.013j -0.287-0.014j -0.288-0.008j -0.288-0.011j
-0.289-0.009j -0.292+0.006j -0.295-0.004j -0.297-0.004j -0.299-0.004j -0.302-0.005j -0.302+0.002j -0.302-0.002j -0.306+0.007j -0.308-0.004j -0.309-0.006
j -0.315-0.003j -0.316-0.013j -0.317-0.001j -0.318+0.006j -0.319-0.005j -0.323-0.005j -0.323-0.009j -0.325+0.004j -0.332-0.004j -0.333+0.004j
-0.335+0.005j -0.336-0.002j -0.337+0.007j -0.338+0.004j -0.34 +0.009j -0.341-0.002j -0.341+0.008j -0.342+0.017j -0.343+0.003j]
np.linalg.eig: [ 1.014-0.064j 0.859-0.063j 0.785-0.064j 0.739-0.064j 0.637-0.064j 0.631-0.063j 0.549-0.063j 0.511-0.064j 0.474-0.062j 0.41 -0.0
6j 0.408-0.064j 0.355-0.058j 0.32 -0.063j 0.307-0.055j 0.301-0.045j 0.267-0.053j 0.245-0.062j 0.232-0.05j 0.208-0.038j 0.202-0.048j 0.201-0.
032j
0.193-0.03j 0.184-0.029j 0.181-0.06j 0.177-0.028j 0.176-0.046j 0.17 -0.027j 0.164-0.026j 0.159-0.035j 0.158-0.025j 0.154-0.044j 0.152-0.024
j 0.146-0.023j 0.14 -0.022j 0.136-0.042j 0.135-0.022j 0.13 -0.021j 0.127-0.031j 0.126-0.058j 0.125-0.021j 0.12 -0.04j 0.12 -0.02j
0.115-0.019j 0.111-0.019j 0.108-0.038j 0.106-0.019j 0.103-0.02j 0.1 -0.018j 0.098-0.037j 0.096-0.017j 0.092-0.017j 0.092-0.035j 0.088-0.016
j 0.087-0.034j 0.085-0.015j 0.082-0.033j 0.081-0.015j 0.079-0.055j 0.078-0.014j 0.077-0.033j 0.074-0.014j 0.073-0.045j 0.072-0.032j
0.071-0.013j 0.068-0.013j 0.067-0.031j 0.064-0.012j 0.062-0.03j 0.061-0.012j 0.058-0.011j 0.057-0.03j 0.055-0.011j 0.053-0.029j 0.052-0.01j
0.049-0.01j 0.048-0.028j 0.046-0.009j 0.044-0.009j 0.043-0.027j 0.041-0.008j 0.039-0.027j 0.038-0.008j 0.038-0.053j 0.036-0.007j
0.034-0.026j 0.033-0.007j 0.031-0.006j 0.03 -0.025j 0.028-0.006j 0.026-0.006j 0.025-0.024j 0.024-0.005j 0.021-0.005j 0.021-0.024j 0.019-0.004
j 0.017-0.004j 0.016-0.023j 0.015-0.004j 0.014-0.003j 0.012-0.022j 0.012-0.003j 0.01 -0.003j 0.008-0.002j 0.008-0.022j 0.007-0.002j
0.006-0.002j 0.004-0.001j 0.004-0.021j 0.003-0.05j 0.003-0.001j 0.002-0.001j 0.001-0.j 0. -0.j -0. -0.02j -0. -0.j -0.001-0.j
-0.002-0.j -0.004-0.j -0.004-0.02j -0.006-0.j -0.008-0.j -0.008-0.019j -0.011-0.j -0.012-0.018j -0.014-0.j -0.016-0.018j
-0.017-0.j -0.02 -0.017j -0.021-0.j -0.021-0.038j -0.024-0.017j -0.025-0.j -0.027-0.048j -0.027-0.016j -0.027-0.032j -0.03 -0.j -0.031-0.015
j -0.034-0.015j -0.035-0.j -0.036-0.03j -0.038-0.014j -0.04 -0.j -0.041-0.014j -0.044-0.029j -0.045-0.013j -0.046-0.j -0.048-0.013j
-0.051-0.012j -0.051-0.028j -0.052-0.j -0.052-0.046j -0.054-0.011j -0.058-0.011j -0.058-0.j -0.058-0.027j -0.061-0.01j -0.064-0.01j -0.065-0.026
j -0.065-0.j -0.066-0.009j -0.069-0.009j -0.07 -0.035j -0.071-0.025j -0.072-0.008j -0.074-0.044j -0.075-0.008j -0.077-0.024j -0.078-0.008j
-0.08 -0.007j -0.083-0.007j -0.083-0.023j -0.085-0.006j -0.087-0.006j -0.088-0.022j -0.09 -0.005j -0.092-0.005j -0.093-0.042j -0.094-0.022j -0.094-0.004
j -0.096-0.004j -0.098-0.004j -0.099-0.021j -0.1 -0.003j -0.102-0.031j -0.102-0.003j -0.104-0.003j -0.104-0.021j -0.105-0.002j -0.107-0.002j
-0.108-0.04j -0.109-0.002j -0.109-0.02j -0.11 -0.001j -0.111-0.001j -0.112-0.001j -0.113-0.j -0.114-0.019j -0.118-0.019j -0.121-0.038j -0.122-0.019
j -0.125-0.02j -0.129-0.018j -0.13 -0.037j -0.133-0.017j -0.137-0.017j -0.137-0.035j -0.14 -0.016j -0.142-0.034j -0.144-0.015j -0.147-0.033j
-0.147-0.015j -0.151-0.014j -0.152-0.033j -0.154-0.014j -0.157-0.032j -0.158-0.013j -0.161-0.013j -0.162-0.031j -0.164-0.012j -0.166-0.03j -0.167-0.012
j -0.171-0.011j -0.171-0.03j -0.174-0.011j -0.176-0.029j -0.177-0.01j -0.179-0.01j -0.181-0.028j -0.182-0.009j -0.185-0.009j -0.185-0.027j
-0.188-0.008j -0.19 -0.027j -0.191-0.008j -0.193-0.007j -0.195-0.026j -0.196-0.007j -0.198-0.006j -0.199-0.025j -0.2 -0.006j -0.203-0.006j -0.203-0.024
j -0.205-0.005j -0.207-0.005j -0.208-0.024j -0.209-0.004j -0.211-0.004j -0.212-0.023j -0.213-0.004j -0.215-0.003j -0.216-0.022j -0.217-0.003j
-0.219-0.003j -0.22 -0.002j -0.221-0.022j -0.222-0.002j -0.223-0.002j -0.224-0.001j -0.225-0.021j -0.226-0.001j -0.227-0.001j -0.228-0.j -0.228-0.j
-0.229-0.02j -0.229-0.j -0.23 -0.j -0.231-0.j -0.233-0.j -0.233-0.02j -0.234-0.j -0.237-0.j -0.237-0.019j -0.239-0.j
-0.241-0.018j -0.242-0.j -0.245-0.018j -0.246-0.j -0.248-0.017j -0.25 -0.j -0.252-0.017j -0.254-0.j -0.256-0.016j -0.258-0.j -0.259-0.015
j -0.263-0.015j -0.263-0.j -0.266-0.014j -0.269-0.j -0.27 -0.014j -0.273-0.013j -0.274-0.j -0.277-0.013j -0.28 -0.012j -0.28 -0.j
-0.283-0.011j -0.286-0.011j -0.287-0.j -0.289-0.01j -0.292-0.01j -0.294-0.j -0.295-0.009j -0.298-0.009j -0.301-0.008j -0.304-0.008j -0.306-0.008
j -0.309-0.007j -0.311-0.007j -0.314-0.006j -0.316-0.006j -0.318-0.005j -0.321-0.005j -0.323-0.004j -0.325-0.004j -0.327-0.004j -0.329-0.003j
-0.331-0.003j -0.332-0.003j -0.334-0.002j -0.336-0.002j -0.337-0.002j -0.339-0.001j -0.34 -0.001j -0.341-0.001j -0.342-0.j ]

```

np.linalg.eig and my eigenvalues close? False

```

my eigenvalues - np.linalg.eig =
[-0. +0.001j -0.001-0.002j 0.001-0.008j 0.002-0.006j -0.005-0.005j -0.003+0.003j -0.001+0.005j 0.008+0.016j 0.005+0.006j 0. +0.018j -0.007+0.01
6j -0.001+0.004j 0.003+0.024j 0.005+0.013j 0.004+0.003j 0.008+0.014j 0.003+0.028j 0.003+0.011j 0.011+0.j 0.002+0.015j -0.001-0.006j
0.001-0.008j 0.004-0.007j 0.003+0.033j 0.005-0.001j -0.006+0.019j -0.003-0.004j 0.003-0.005j 0.006+0.007j -0.003-0.002j -0.003+0.02j -0.004-0.008
j -0.002-0.007j 0.001-0.009j 0.005+0.012j 0.002-0.01j 0.003-0.007j 0.004-0.002j -0.002+0.021j -0.01 -0.013j -0.008+0.003j -0.008-0.01j
-0.004-0.024j -0.003-0.007j -0.007+0.013j -0.011+0.002j -0.009-0.003j -0.008-0.003j -0.007+0.02j -0.005-0.008j -0.004-0.014j -0.007+0.003j -0.01 -0.026
j -0.021-0.008j -0.021-0.032j -0.026-0.01j -0.026-0.034j -0.028+0.016j -0.031-0.031j -0.037-0.008j -0.036-0.022j -0.036+0.008j -0.039-0.01j
-0.039-0.016j -0.036-0.023j -0.036-0.006j -0.034-0.026j -0.034+0.001j -0.034-0.02j -0.031-0.023j -0.031+0.007j -0.03 -0.025j -0.029+0.004j -0.03 -0.014
j -0.028-0.023j -0.027+0.006j -0.026-0.009j -0.024-0.016j -0.026+0.009j -0.023-0.007j -0.022+0.007j -0.022-0.024j -0.023+0.031j -0.02 -0.012j
-0.019+0.011j -0.018-0.013j -0.016-0.011j -0.016+0.01j -0.015-0.012j -0.013-0.011j -0.013+0.004j -0.011-0.005j -0.01 -0.012j -0.009+0.005j -0.008-0.015
j -0.006-0.016j -0.006+0.015j -0.006-0.012j -0.005-0.011j -0.004+0.015j -0.004-0.012j -0.002-0.024j -0.002-0.011j -0.002+0.011j -0.002-0.004j
-0.002-0.002j -0.002-0.007j -0.002+0.013j -0.001+0.039j -0.001-0.007j -0.001-0.013j -0.001-0.016j -0. -0.004j -0. +0.01j 0. -0.006j 0. -0.013
j 0.001-0.002j 0.002-0.002j 0.002+0.016j 0.003-0.005j 0.005-0.003j 0.004+0.01j 0.006-0.006j 0.007+0.011j 0.008-0.006j 0.01 +0.017j

```

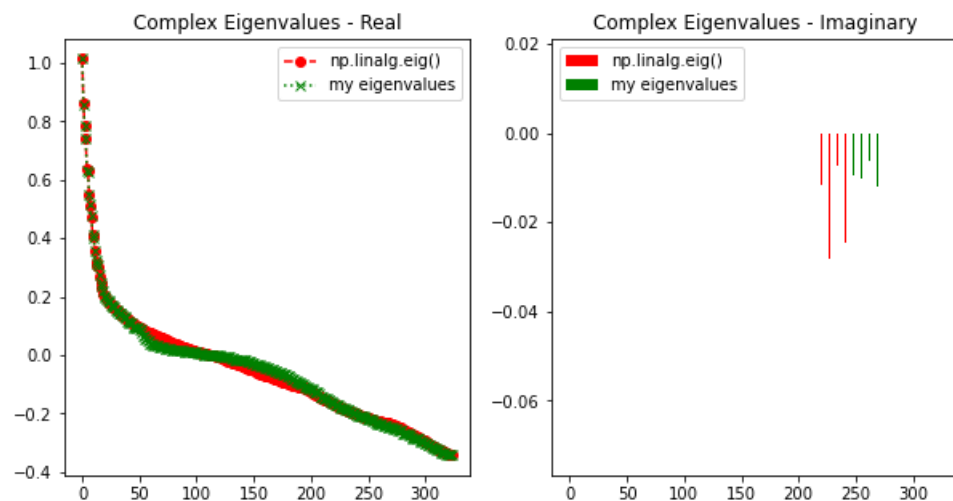
```

0.01 -0.007j 0.012+0.013j 0.013-0.006j 0.013+0.031j 0.014+0.009j 0.013-0.008j 0.014+0.036j 0.013+0.009j 0.012+0.025j 0.014-0.016j 0.014+0.007
j 0.018+0.005j 0.017-0.01j 0.018+0.021j 0.02 +0.006j 0.022-0.014j 0.022+0.004j 0.025+0.019j 0.025+0.003j 0.024-0.013j 0.027-0.003j
0.03 -0.002j 0.025+0.014j 0.023-0.012j 0.022+0.031j 0.023-0.001j 0.025-0.j 0.023-0.013j 0.023+0.015j 0.025-0.004j 0.027-0.001j 0.027+0.016
j 0.027-0.013j 0.025-0.006j 0.026+0.j 0.026+0.027j 0.025+0.01j 0.026-0.008j 0.027+0.032j 0.026-0.002j 0.026+0.011j 0.026-0.009j
0.027-0.01j 0.028-0.004j 0.027+0.001j 0.027-0.011j 0.028-0.006j 0.028+0.001j 0.027-0.002j 0.028-0.008j 0.029+0.025j 0.026+0.005j 0.025-0.008
j 0.026-0.014j 0.026-0.021j 0.024+0.01j 0.024-0.014j 0.022+0.014j 0.02 -0.016j 0.021-0.01j 0.015+0.j 0.016-0.015j 0.013-0.018j
0.014+0.019j 0.014-0.016j 0.012+0.002j 0.012-0.011j 0.012-0.018j 0.005-0.026j 0.005-0.01j 0.003-0.005j 0.006+0.003j 0.006+0.029j 0.008+0.01j
0.01 +0.005j 0.012+0.003j 0.012+0.015j 0.008-0.002j 0.011+0.01j 0.009+0.021j 0.012-0.005j 0.01 +0.014j 0.003+0.001j 0.005+0.02j
0.004+0.002j 0.003+0.002j 0.004+0.017j 0.005+0.002j 0.007+0.023j 0.005-0.007j 0.005+0.006j 0.005+0.021j 0.005-0.007j 0.002+0.016j 0. -0.001
j 0.002-0.004j 0.003+0.024j 0.002+0.009j 0.004+0.015j -0.001-0.002j -0. -0.003j -0.001+0.02j 0.001-0.003j 0.002-0.015j -0. +0.015j
0.002-0.012j 0.003+0.015j 0.002-0.01j 0.001-0.002j 0.002+0.017j -0. -0.009j 0.002-0.008j -0.002+0.009j -0.004-0.007j -0.002-0.007j -0.004+0.02j
-0.003-0.004j -0.002-0.007j -0.003+0.01j -0.002-0.008j 0. -0.008j 0. +0.016j -0.004-0.006j -0.003-0.013j -0.003+0.004j -0.003-0.012j
-0.003-0.012j -0.002-0.012j -0.006+0.009j -0.005-0.008j -0.006-0.003j -0.006-0.007j -0.01 +0.009j -0.009-0.013j -0.008-0.01j -0.009-0.009j -0.011-0.006
j -0.011+0.017j -0.011-0.012j -0.013-0.013j -0.013-0.009j -0.013-0.014j -0.013+0.014j -0.012-0.012j -0.012-0.008j -0.013+0.007j -0.012-0.015j
-0.012+0.003j -0.012-0.008j -0.011+0.005j -0.01 -0.012j -0.011+0.004j -0.011-0.011j -0.009+0.003j -0.013-0.011j -0.011+0.001j -0.01 -0.01j -0.013-0.011j
j -0.009+0.j -0.008-0.006j -0.007+0.006j -0.006-0.007j -0.009+0.003j -0.011+0.01j -0.011-0.013j -0.01 -0.002j -0.008+0.004j -0.007-0.011j
-0.006+0.002j -0.006+0.017j -0.008-0.004j -0.008+0.007j -0.006+0.006j -0.008-0.005j -0.006+0.011j -0.004+0.007j -0.006+0.016j -0.005+0.004j -0.002+0.001
j -0.006+0.004j -0.004-0.006j -0.003+0.005j -0.002+0.012j -0. +0.j -0.002-0.j -0. -0.004j 0. +0.008j -0.005-0.j -0.004+0.007j
-0.004+0.008j -0.004+0.j -0.002+0.009j -0.003+0.006j -0.003+0.011j -0.002-0.001j -0.001+0.009j -0.001+0.017j -0.001+0.004j]

```

max abs diff = 0.04387580291749045

complex128



Observation

- General QR iteration without shift seems to be working for complex symmetric matrix

```
In [39]: 1 MAX_ITER = 10000
2
3 # complex symmetric matrix - WILKINSON SHIFT
4
5 source = 'matricmarket/qc324.mtx.gz'
6 matrix_class = Matrix
7 runtest_matrixmarket(source, matrix_class, shift='Wilkinson')
8
```

From Matrix Market:

matrix source=matricmarket/qc324.mtx.gz, matrix type=<class 'scipy.sparse.coo.coo_matrix'>, shape=(324, 324), data type=complex128, max=(1.4957127687965-0.087585823232133j), min=(-0.40837438550439-0.017204228197979j)

is_symmetric={} True

activiating tridigonal: True

----- Processing eigenvalues only -----

>>> QR Iteration with Wilkinson shift

Iteration terminates at i=9047 with tol=1e-06 reached

----- Checking Eigenvalues -----

```
my eigenvalues: [ 1.013-0.063j  0.859-0.064j  0.788-0.067j  0.741-0.071j  0.635-0.061j  0.634-0.072j  0.547-0.058j  0.517-0.061j  0.471-0.053j  0.414-0.0
47j  0.402-0.046j  0.357-0.035j  0.317-0.036j  0.309-0.038j  0.304-0.044j  0.265-0.04j   0.243-0.042j  0.241-0.037j  0.213-0.034j  0.206-0.031j  0.202-0.
033j
  0.196-0.037j  0.191-0.036j  0.188-0.03j   0.184-0.039j  0.178-0.04j   0.171-0.031j  0.168-0.028j  0.164-0.031j  0.158-0.036j  0.156-0.024j  0.152-0.026
j  0.147-0.03j   0.142-0.022j  0.141-0.031j  0.14 -0.027j  0.137-0.018j  0.134-0.021j  0.13 -0.025j  0.125-0.035j  0.122-0.038j  0.12 -0.026j
  0.118-0.028j  0.114-0.027j  0.112-0.029j  0.11 -0.028j  0.107-0.031j  0.104-0.031j  0.102-0.032j  0.098-0.037j  0.098-0.02j   0.097-0.019j  0.096-0.016
j  0.094-0.02j   0.091-0.02j   0.088-0.024j  0.088-0.013j  0.085-0.017j  0.082-0.021j  0.077-0.021j  0.076-0.025j  0.076-0.023j  0.07 -0.028j
  0.067-0.035j  0.065-0.036j  0.062-0.044j  0.061-0.039j  0.059-0.035j  0.055-0.046j  0.054-0.037j  0.052-0.045j  0.049-0.047j  0.049-0.035j  0.046-0.03j
  0.046-0.03j   0.045-0.05j   0.043-0.023j  0.043-0.033j  0.042-0.035j  0.042-0.014j  0.037-0.025j  0.037-0.007j  0.034-0.024j  0.03 -0.026j
  0.029-0.024j  0.029-0.019j  0.028-0.017j  0.026-0.022j  0.025-0.024j  0.021-0.026j  0.021-0.026j  0.017-0.023j  0.016-0.023j  0.015-0.028j  0.015-0.017
j  0.011-0.022j  0.01 -0.021j  0.009-0.025j  0.008-0.027j  0.006-0.023j  0.003-0.008j  0.002-0.001j  0. -0.029j  0. -0.017j  0. -0.006j
  -0.002-0.012j  -0.003-0.041j  -0.004-0.016j  -0.005-0.045j  -0.005-0.011j  -0.007-0.017j  -0.009-0.007j  -0.011-0.021j  -0.013-0.009j  -0.013-0.011j  -0.015-0.015
j  -0.021-0.011j  -0.022-0.017j  -0.022-0.017j  -0.023-0.015j  -0.023-0.011j  -0.025-0.012j  -0.031-0.01j   -0.031-0.012j  -0.036-0.008j  -0.037-0.008j
  -0.038-0.012j  -0.038-0.014j  -0.039-0.011j  -0.04 -0.007j  -0.041-0.009j  -0.043-0.008j  -0.043-0.01j   -0.043-0.006j  -0.044-0.005j  -0.047-0.008j  -0.047-0.013
j  -0.047-0.007j  -0.052-0.016j  -0.053-0.014j  -0.054-0.01j   -0.055-0.007j  -0.056-0.011j  -0.058-0.007j  -0.061-0.013j  -0.063-0.005j  -0.065-0.007j
  -0.065-0.004j  -0.065-0.005j  -0.065-0.005j  -0.067-0.007j  -0.067-0.005j  -0.067-0.004j  -0.068-0.005j  -0.068-0.004j  -0.068-0.009j  -0.068-0.005j  -0.068-0.004
j  -0.068-0.005j  -0.068-0.004j  -0.068-0.004j  -0.068-0.003j  -0.068-0.005j  -0.068-0.007j  -0.068-0.006j  -0.068-0.004j  -0.069-0.009j  -0.069-0.003j
  -0.069-0.004j  -0.07 -0.006j  -0.07 -0.07 -0.07 -0.011j  -0.071-0.007j  -0.072-0.012j  -0.072-0.007j  -0.073-0.008j  -0.076-0.011j  -0.078-0.014j  -0.079-0.012
j  -0.083-0.013j  -0.084-0.018j  -0.084-0.011j  -0.084-0.009j  -0.085-0.008j  -0.088-0.011j  -0.088-0.017j  -0.088-0.009j  -0.089-0.013j  -0.09 -0.011j
  -0.091-0.018j  -0.092-0.016j  -0.092-0.013j  -0.097-0.011j  -0.098-0.018j  -0.098-0.015j  -0.098-0.017j  -0.1 -0.017j  -0.105-0.018j  -0.106-0.011j  -0.106-0.02j
  -0.107-0.014j  -0.109-0.011j  -0.113-0.013j  -0.115-0.019j  -0.116-0.021j  -0.119-0.016j  -0.121-0.025j  -0.126-0.021j  -0.133-0.011j  -0.133-0.008j
  -0.137-0.01j   -0.137-0.017j  -0.142-0.005j  -0.143-0.013j  -0.143-0.004j  -0.145-0.007j  -0.146-0.017j  -0.149-0.006j  -0.15 -0.004j  -0.155-0.006j  -0.155-0.008
j  -0.156-0.011j  -0.162-0.011j  -0.165-0.016j  -0.166-0.019j  -0.173-0.018j  -0.173-0.008j  -0.173-0.011j  -0.173-0.006j  -0.174-0.016j  -0.181-0.007j
  -0.181-0.019j  -0.183-0.018j  -0.186-0.014j  -0.188-0.011j  -0.189-0.016j  -0.19 -0.017j  -0.19 -0.01j   -0.193-0.015j  -0.196-0.025j  -0.2 -0.005j  -0.201-0.016
j  -0.202-0.023j  -0.202-0.021j  -0.203-0.014j  -0.204-0.022j  -0.207-0.01j   -0.208-0.019j  -0.209-0.018j  -0.21 -0.022j  -0.212-0.023j  -0.215-0.02j
  -0.217-0.011j  -0.22 -0.017j  -0.221-0.01j   -0.222-0.014j  -0.223-0.019j  -0.227-0.015j  -0.227-0.017j  -0.228-0.018j  -0.232-0.016j  -0.232-0.015j  -0.234-0.013
j  -0.236-0.017j  -0.236-0.02j   -0.237-0.016j  -0.239-0.011j  -0.241-0.019j  -0.243-0.018j  -0.244-0.017j  -0.244-0.017j  -0.245-0.009j  -0.246-0.011j
  -0.249-0.01j   -0.25 -0.017j  -0.253-0.007j  -0.254-0.013j  -0.254-0.018j  -0.256-0.014j  -0.258-0.007j  -0.261-0.011j  -0.263-0.011j  -0.263-0.015j  -0.267-0.015
j  -0.269-0.012j  -0.271-0.008j  -0.272-0.019j  -0.274-0.012j  -0.275-0.014j  -0.277-0.011j  -0.279-0.009j  -0.28 -0.008j  -0.284-0.01j   -0.285-0.003j
  -0.288-0.005j  -0.289+0.003j  -0.291-0.005j  -0.292+0.001j  -0.293-0.005j  -0.295+0.003j  -0.298-0.008j  -0.301-0.001j  -0.301-0.004j  -0.302-0.004j  -0.305-0.006
j  -0.308+0.002j  -0.312-0.007j  -0.315-0.009j  -0.316-0.002j  -0.317-0.003j  -0.321-0.004j  -0.323+0.004j  -0.323+0.003j  -0.329+0.002j  -0.331+0.002j
```

```

-0.332+0.004j -0.336+0.005j -0.337+0.004j -0.337+0.003j -0.338+0.007j -0.338+0.011j -0.34 +0.009j -0.341+0.007j -0.343+0.02j ]
np.linalg.eig: [ 1.014-0.064j 0.859-0.063j 0.785-0.064j 0.739-0.064j 0.637-0.064j 0.631-0.063j 0.549-0.063j 0.511-0.064j 0.474-0.062j 0.41 -0.0
6j 0.408-0.064j 0.355-0.058j 0.32 -0.063j 0.307-0.055j 0.301-0.045j 0.267-0.053j 0.245-0.062j 0.232-0.05j 0.208-0.038j 0.202-0.048j 0.201-0.
032j
0.193-0.03j 0.184-0.029j 0.181-0.06j 0.177-0.028j 0.176-0.046j 0.17 -0.027j 0.164-0.026j 0.159-0.035j 0.158-0.025j 0.154-0.044j 0.152-0.024
j 0.146-0.023j 0.14 -0.022j 0.136-0.042j 0.135-0.022j 0.13 -0.021j 0.127-0.031j 0.126-0.058j 0.125-0.021j 0.12 -0.04j 0.12 -0.02j
0.115-0.019j 0.111-0.019j 0.108-0.038j 0.106-0.019j 0.103-0.02j 0.1 -0.018j 0.098-0.037j 0.096-0.017j 0.092-0.017j 0.092-0.035j 0.088-0.016
j 0.087-0.034j 0.085-0.015j 0.082-0.033j 0.081-0.015j 0.079-0.055j 0.078-0.014j 0.077-0.033j 0.074-0.014j 0.073-0.045j 0.072-0.032j
0.071-0.013j 0.068-0.013j 0.067-0.031j 0.064-0.012j 0.062-0.03j 0.061-0.012j 0.058-0.011j 0.057-0.03j 0.055-0.011j 0.053-0.029j 0.052-0.01j
0.049-0.01j 0.048-0.028j 0.046-0.009j 0.044-0.009j 0.043-0.027j 0.041-0.008j 0.039-0.027j 0.038-0.008j 0.038-0.053j 0.036-0.007j
0.034-0.026j 0.033-0.007j 0.031-0.006j 0.03 -0.025j 0.028-0.006j 0.026-0.006j 0.025-0.024j 0.024-0.005j 0.021-0.005j 0.021-0.024j 0.019-0.004
j 0.017-0.004j 0.016-0.023j 0.015-0.004j 0.014-0.003j 0.012-0.022j 0.012-0.003j 0.01 -0.003j 0.008-0.002j 0.008-0.022j 0.007-0.002j
0.006-0.002j 0.004-0.001j 0.004-0.021j 0.003-0.05j 0.003-0.001j 0.002-0.001j 0.001-0.j 0. -0.j -0. -0.02j -0. -0.j -0.001-0.j
-0.002-0.j -0.004-0.j -0.004-0.02j -0.006-0.j -0.008-0.j -0.008-0.019j -0.011-0.j -0.012-0.018j -0.014-0.j -0.016-0.018j
-0.017-0.j -0.02 -0.017j -0.021-0.j -0.021-0.038j -0.024-0.017j -0.025-0.j -0.027-0.048j -0.027-0.016j -0.027-0.032j -0.03 -0.j -0.031-0.015
j -0.034-0.015j -0.035-0.j -0.036-0.03j -0.038-0.014j -0.04 -0.j -0.041-0.014j -0.044-0.029j -0.045-0.013j -0.046-0.j -0.048-0.013j
-0.051-0.012j -0.051-0.028j -0.052-0.j -0.052-0.046j -0.054-0.011j -0.058-0.011j -0.058-0.j -0.058-0.027j -0.061-0.01j -0.064-0.01j -0.065-0.026
j -0.065-0.j -0.066-0.009j -0.069-0.009j -0.07 -0.035j -0.071-0.025j -0.072-0.008j -0.074-0.044j -0.075-0.008j -0.077-0.024j -0.078-0.008j
-0.08 -0.007j -0.083-0.007j -0.083-0.023j -0.085-0.006j -0.087-0.006j -0.088-0.022j -0.09 -0.005j -0.092-0.005j -0.093-0.042j -0.094-0.022j -0.094-0.004
j -0.096-0.004j -0.098-0.004j -0.099-0.021j -0.1 -0.003j -0.102-0.031j -0.102-0.003j -0.104-0.003j -0.104-0.021j -0.105-0.002j -0.107-0.002j
-0.108-0.04j -0.109-0.002j -0.109-0.02j -0.11 -0.001j -0.111-0.001j -0.112-0.001j -0.113-0.j -0.114-0.019j -0.118-0.019j -0.121-0.038j -0.122-0.019
j -0.125-0.02j -0.129-0.018j -0.13 -0.037j -0.133-0.017j -0.137-0.017j -0.137-0.035j -0.14 -0.016j -0.142-0.034j -0.144-0.015j -0.147-0.033j
-0.147-0.015j -0.151-0.014j -0.152-0.033j -0.154-0.014j -0.157-0.032j -0.158-0.013j -0.161-0.013j -0.162-0.031j -0.164-0.012j -0.166-0.03j -0.167-0.012
j -0.171-0.011j -0.171-0.03j -0.174-0.011j -0.176-0.029j -0.177-0.01j -0.179-0.01j -0.181-0.028j -0.182-0.009j -0.185-0.009j -0.185-0.027j
-0.188-0.008j -0.19 -0.027j -0.191-0.008j -0.193-0.007j -0.195-0.026j -0.196-0.007j -0.198-0.006j -0.199-0.025j -0.2 -0.006j -0.203-0.006j -0.203-0.024
j -0.205-0.005j -0.207-0.005j -0.208-0.024j -0.209-0.004j -0.211-0.004j -0.212-0.023j -0.213-0.004j -0.215-0.003j -0.216-0.022j -0.217-0.003j
-0.219-0.003j -0.22 -0.002j -0.221-0.022j -0.222-0.002j -0.223-0.002j -0.224-0.001j -0.225-0.021j -0.226-0.001j -0.227-0.001j -0.228-0.j -0.228-0.j
-0.229-0.02j -0.229-0.j -0.23 -0.j -0.231-0.j -0.233-0.j -0.233-0.02j -0.234-0.j -0.237-0.j -0.237-0.019j -0.239-0.j
-0.241-0.018j -0.242-0.j -0.245-0.018j -0.246-0.j -0.248-0.017j -0.25 -0.j -0.252-0.017j -0.254-0.j -0.256-0.016j -0.258-0.j -0.259-0.015
j -0.263-0.015j -0.263-0.j -0.266-0.014j -0.269-0.j -0.27 -0.014j -0.273-0.013j -0.274-0.j -0.277-0.013j -0.28 -0.012j -0.28 -0.j
-0.283-0.011j -0.286-0.011j -0.287-0.j -0.289-0.01j -0.292-0.01j -0.294-0.j -0.295-0.009j -0.298-0.009j -0.301-0.008j -0.304-0.008j -0.306-0.008
j -0.309-0.007j -0.311-0.007j -0.314-0.006j -0.316-0.006j -0.318-0.005j -0.321-0.005j -0.323-0.004j -0.325-0.004j -0.327-0.004j -0.329-0.003j
-0.331-0.003j -0.332-0.003j -0.334-0.002j -0.336-0.002j -0.337-0.002j -0.339-0.001j -0.34 -0.001j -0.341-0.001j -0.342-0.j ]

```

np.linalg.eig and my eigenvalues close? False

```

my eigenvalues - np.linalg.eig =
[-0.001+0.001j -0.001-0.001j 0.002-0.003j 0.002-0.006j -0.001+0.003j 0.003-0.009j -0.002+0.006j 0.007+0.004j -0.003+0.009j 0.005+0.013j -0.006+0.01
8j 0.003+0.022j -0.003+0.027j 0.001+0.018j 0.003+0.001j -0.002+0.012j -0.002+0.02j 0.009+0.013j 0.006+0.004j 0.005+0.017j 0.001-0.002j
0.003-0.007j 0.007-0.008j 0.007+0.029j 0.007-0.011j 0.002+0.006j 0.001-0.004j 0.004-0.002j 0.005+0.004j 0.001-0.011j 0.002+0.019j 0.001-0.002
j 0.002-0.007j 0.001+0.001j 0.006+0.011j 0.005-0.005j 0.007+0.003j 0.007+0.01j 0.004+0.032j -0. -0.014j 0.002+0.002j 0. -0.006j
0.003-0.009j 0.003-0.008j 0.004+0.009j 0.004-0.008j 0.003-0.011j 0.004-0.012j 0.004+0.004j 0.002-0.02j 0.006-0.004j 0.005+0.016j 0.007+0.j
0.007+0.014j 0.006-0.004j 0.006+0.009j 0.007+0.002j 0.006+0.038j 0.004-0.007j 0. +0.012j 0.002-0.011j 0.003+0.021j -0.002+0.004j
-0.004-0.022j -0.002-0.024j -0.005-0.013j -0.004-0.027j -0.003-0.004j -0.006-0.034j -0.005-0.026j -0.005-0.016j -0.006-0.037j -0.004-0.006j -0.006-0.02j
-0.004-0.021j -0.003-0.022j -0.004-0.014j -0.001-0.024j -0.001-0.007j 0.001-0.006j -0.001+0.002j -0.001+0.001j -0.004+0.029j -0.006-0.019j
-0.005+0.002j -0.004-0.013j -0.002-0.011j -0.004+0.004j -0.003-0.018j -0.005-0.021j -0.004-0.001j -0.007-0.018j -0.006-0.018j -0.006-0.004j -0.004-0.013
j -0.006-0.019j -0.006+0.002j -0.006-0.021j -0.006-0.024j -0.006-0.j -0.009-0.005j -0.008+0.001j -0.008-0.027j -0.008+0.004j -0.007-0.004j
-0.007-0.011j -0.008-0.04j -0.008+0.005j -0.008+0.005j -0.008-0.01j -0.009-0.016j -0.01 -0.007j -0.011-0.02j -0.013+0.011j -0.013-0.011j -0.014-0.015
j -0.018-0.011j -0.018-0.017j -0.018+0.003j -0.017-0.015j -0.015-0.011j -0.016+0.008j -0.02 -0.01j -0.019+0.007j -0.022-0.008j -0.021+0.01j
-0.02 -0.012j -0.018+0.004j -0.018-0.011j -0.019+0.031j -0.018+0.007j -0.018-0.008j -0.016+0.038j -0.016+0.01j -0.017+0.027j -0.017-0.008j -0.016+0.003
j -0.013+0.008j -0.017-0.016j -0.017+0.016j -0.016+0.005j -0.015-0.007j -0.015+0.003j -0.014+0.022j -0.016+0.j -0.017-0.005j -0.017+0.005j
-0.014+0.008j -0.014+0.022j -0.014-0.005j -0.014+0.039j -0.013+0.006j -0.01 +0.007j -0.009-0.005j -0.009+0.023j -0.007+0.001j -0.004+0.005j -0.003+0.022

```

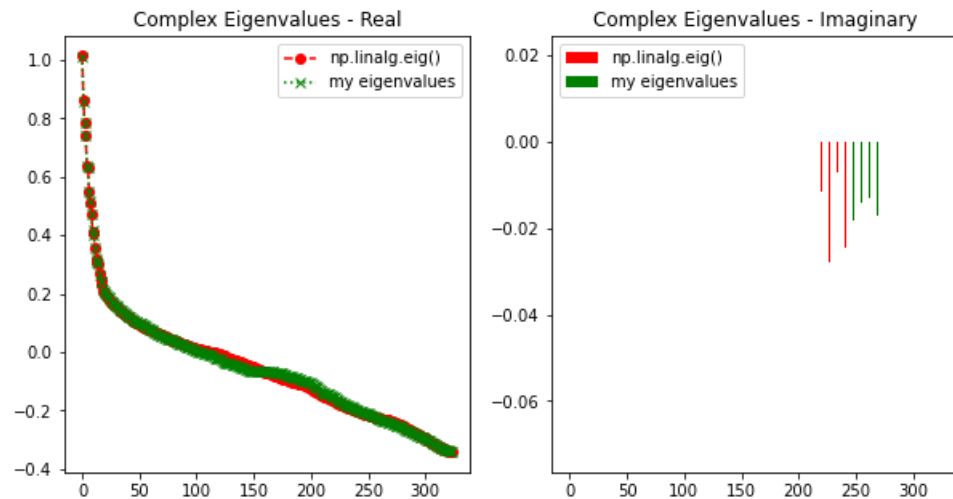
```

j -0.003-0.005j -0.001+0.005j 0.001+0.005j 0.002+0.032j 0.003+0.02j 0.004+0.001j 0.006+0.038j 0.006+0.004j 0.008+0.015j 0.009+0.004j
0.011+0.003j 0.013+0.001j 0.013+0.023j 0.015-0.005j 0.016-0.002j 0.016+0.011j 0.018-0.002j 0.019-0.003j 0.017+0.03j 0.016+0.008j 0.016-0.007
j 0.013-0.009j 0.014-0.014j 0.015+0.01j 0.016-0.005j 0.017+0.023j 0.014-0.008j 0.016-0.014j 0.016+0.012j 0.016-0.011j 0.018-0.01j
0.017+0.022j 0.017-0.014j 0.017+0.007j 0.013-0.01j 0.013-0.017j 0.015-0.014j 0.015-0.016j 0.013+0.003j 0.013+0.001j 0.015+0.028j 0.016-0.001
j 0.018+0.006j 0.02 +0.007j 0.018+0.024j 0.017-0.001j 0.02 -0.004j 0.018+0.019j 0.019-0.009j 0.016+0.013j 0.011+0.004j 0.013+0.025j
0.011+0.005j 0.014-0.002j 0.009+0.027j 0.012+0.001j 0.014+0.028j 0.013+0.006j 0.015-0.004j 0.013+0.025j 0.014+0.008j 0.012+0.024j 0.012+0.003
j 0.015-0.j 0.009+0.018j 0.008-0.006j 0.01 +0.01j 0.004-0.007j 0.007+0.002j 0.008+0.017j 0.009+0.003j 0.011-0.008j 0.005+0.02j
0.007-0.01j 0.007+0.009j 0.005-0.006j 0.005-0.004j 0.006+0.01j 0.006-0.01j 0.008-0.004j 0.006+0.01j 0.004-0.019j 0.002+0.001j 0.003+0.008
j 0.003-0.018j 0.005-0.016j 0.005+0.009j 0.005-0.018j 0.004-0.006j 0.004+0.004j 0.004-0.015j 0.005-0.019j 0.005-0.j 0.002-0.017j
0.001-0.008j -0. -0.015j -0.001+0.012j -0. -0.012j 0.001-0.017j -0.002-0.013j -0.002+0.004j -0.003-0.017j -0.005-0.015j -0.005-0.015j -0.006-0.013
j -0.007+0.003j -0.007-0.02j -0.007-0.016j -0.008-0.011j -0.008-0.019j -0.01 +0.002j -0.009-0.017j -0.007-0.017j -0.009+0.01j -0.007-0.011j
-0.008+0.008j -0.008-0.017j -0.008+0.011j -0.008-0.013j -0.006-0.001j -0.006-0.014j -0.006+0.009j -0.007-0.011j -0.007+0.005j -0.004-0.015j -0.008+0.j
-0.006+0.002j -0.007-0.008j -0.005-0.005j -0.005-0.012j -0.005-0.j -0.004+0.002j -0.005-0.009j -0.004+0.005j -0.005+0.002j -0.004-0.003j
-0.005+0.007j -0.003+0.014j -0.004-0.005j -0.002+0.011j -0.001+0.005j -0.001+0.003j -0.003+0.002j -0.003+0.008j -0. +0.004j 0.002+0.004j 0.002+0.002
j 0.001+0.009j -0.001+0.j -0.001-0.002j 0.001+0.004j 0.002+0.002j -0. +0.001j 0. +0.008j 0.002+0.007j -0.002+0.005j -0.002+0.005j
-0.002+0.007j -0.004+0.007j -0.003+0.006j -0.001+0.005j -0.001+0.009j 0. +0.012j -0. +0.01j 0. +0.008j -0.001+0.02j ]

```

max abs diff = 0.04126956850298427

complex128



Observation

- QR iteration with Wilkinson's shift seems to be working for complex symmetric matrix
- Slightly better convergence than the general method without shift
- Max iteration increased to 1e4


```
In [40]: 1 MAX_ITER = 100000
2
3 # Complex unsymmetric
4 source = 'matricmarket/mhd1280a.mtx.gz'
5 matrix_class = Matrix
6 runtest_matrixmarket(source, matrix_class, shift=None)
7
```

From Matrix Market:

matrix source=matricmarket/mhd1280a.mtx.gz, matrix type=<class 'scipy.sparse.coo.coo_matrix'>, shape=(1280, 1280), data type=complex128, max=(74619.3808+3.84011238e-11j), min=(-15906.7974-2.73633283e-07j)

is_symmetric={} False

activiating tridigonal: False

```
----- Processing eigenvalues only -----
>>> QR Iteration WITHOUT shift
Iteration terminates at i=33607 with tol=1e-06 reached
```

```
----- Checking Eigenvalues -----
```

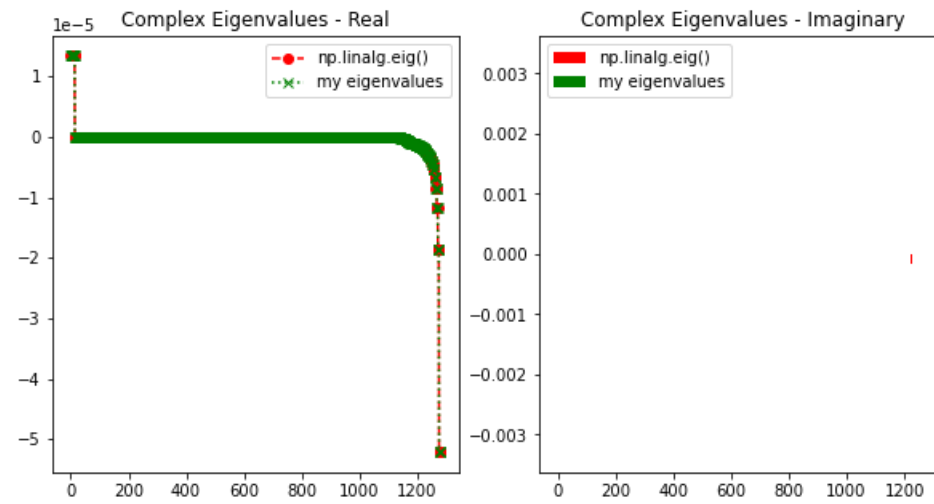
```
my eigenvalues: [ 0.-0.j      0.-0.j      0.-0.j      ... -0.-0.003j -0.-0.003j -0.+0.003j]
np.linalg.eig:  [ 0.+0.j      0.+0.j      0.+0.j      ... -0.-0.003j -0.-0.003j -0.+0.003j]
```

np.linalg.eig and my eigenvalues close? False

```
my eigenvalues - np.linalg.eig =
[0.-0.j 0.-0.j 0.-0.j ... 0.+0.j 0.+0.j 0.-0.j]
```

max abs diff = 0.00017325703855534271

complex128



```
In [41]: 1 MAX_ITER = 100000
2
3 # Complex unsymmetric
4 source = 'matricmarket/mhd1280a.mtx.gz'
5 matrix_class = Matrix
6 runtest_matrixmarket(source, matrix_class, shift='Wilkinson')
7
```

From Matrix Market:

```
matrix source=matricmarket/mhd1280a.mtx.gz, matrix type=<class 'scipy.sparse.coo.coo_matrix'>, shape=(1280, 1280), data type=complex128, max=(74619.3808+3.84011238e-11j), min=(-15906.7974-2.73633283e-07j)
```

```
is_symmetric={} False
```

```
activiating tridigonal: False
```

```
----- Processing eigenvalues only -----
```

```
>>> QR Iteration with Wilkinson shift
```

```
Iteration terminates at i=13234 with tol=1e-06 reached
```

```
----- Checking Eigenvalues -----
```

```
my eigenvalues: [ 0.-0.j      0.-0.j      0.+0.j      ... -0.-0.003j -0.-0.003j -0.+0.003j]
```

```
np.linalg.eig: [ 0.+0.j      0.+0.j      0.+0.j      ... -0.-0.003j -0.-0.003j -0.+0.003j]
```

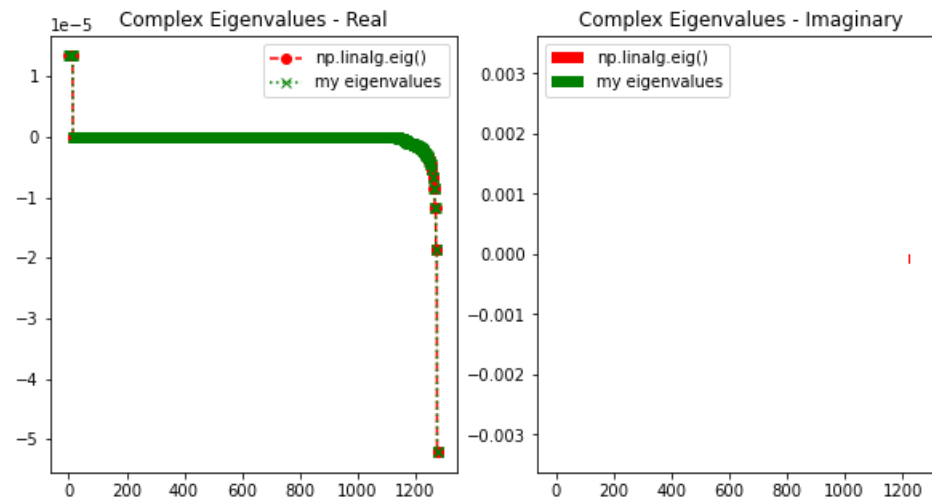
```
np.linalg.eig and my eigenvalues close? False
```

```
my eigenvalues - np.linalg.eig =
```

```
[ 0.-0.j  0.-0.j  0.+0.j ...  0.+0.j -0.+0.j -0.-0.j]
```

```
max abs diff = 0.00015237568085155927
```

```
complex128
```



Observation

- Increased max iteration number to $1e5$
- General QR iteration without shift seems to be working for complex unsymmetric matrix
- This demonstrates that QR iteration with Wilkinson shift indeed converges faster

In []:

1

Checklist / To-Dos:

Option 1

General complex matrices with transformation to Hessenberg form

- Hessenberg form via Householder Transformation ***[Done]***
- QR Iteration with Givens Rotation ***[Done]***
- Test for convergence ***[Done]***
- Modify Householder to accommodate for complex matrices ***[Done]***
- Modify Givens to accommodate for complex matrices ***[Done]***
- Diagonal blocks for real matrix with complex conjugate eigenvalues ***[Done]***
- Use Wilkinson shifts to accelerate convergence ***[Done]***
- Investigate convergence - comparison visualization ***[Done]***

- Compute not only eigenvalues but also eigenvectors ***[Done]***
 - Apply your program to several suitable matrices from the Matrix Market. Use suitable library functions for reading the matrices. ***[Done]***
 - Object-oriented programming: is it possible to implement algorithm 1.4.14 in a way, that H is either Hessenberg or tridiagonal, either real or complex, but encapsulate the differences inside the QR-decompositions applied in every step _ element-wise application (special case of tridiagonal) ***[Done]***
-

Option 2

General real matrices with transformation to Hessenberg form and double shifts for complex eigenvalues

- Use double shifts to avoid complex arithmetic _ Matrix multiplication ***[Done]***
- "Bulge-chasing" for element-wise computation **#NOT IMPLEMENTED**

Option 3

Symmetric real matrices with transformation to tridiagonal form with optimized storage

- Use deflation when the subdiagonal element in the last row is sufficiently small (implementation may be hard if not option 3)
- Use deflation**, if any other subdiagonal element is small (seems very hard)
- Add SVD capability to option 3

Additional Considerations

- Well-chosen tests for correctness
 - Investigation into convergence
 - Write very well structured code
 - Well-prepared jupyter notebooks with code, accompanying text, and results
-

In []:

1