Report on Implementing Symmetric QR Algorithm

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Background

The symmetric QR algorithm is one of the most classical iteration methods for symmetric eigenvalue problem in numerical linear algebra. It consists of tridiagonalization, Wilkinson Shift and implicit iteration, which are important techniques that are supposed to be obtained after learning this course. Moreover, in many situations, problems of symmetric eigenvalues will relatively more frequently occur. Therefore, the topic of implementing symmetric QR algorithm is chosen.

Code Structure

The symmetric QR algorithm is principally composed of preparing functions and the main function.

The preparing functions include the ***upper_hessenber*** function, the ***block_size*** function, and the ***one_step_QR_with_Wilkinson_shift*** function. And the main function is called ***QR_Algorithm_for_symmatric_matrix***. All functions above are stored separately. Thus, it is convenient to exam each of them.

Now we can have a closer and detailed look at the implementation. First, generate a random symmetric real matrix, A. All the elements of A are uniformly distributed between 0 and 1.

Secondly, turn the symmetric matrix A into an upper Hessenberg matrix, T. This process needs to invoke the function ***upper_hessenber***. Since this process can preserve the symmetricity, the matrix T is tridiagonal.

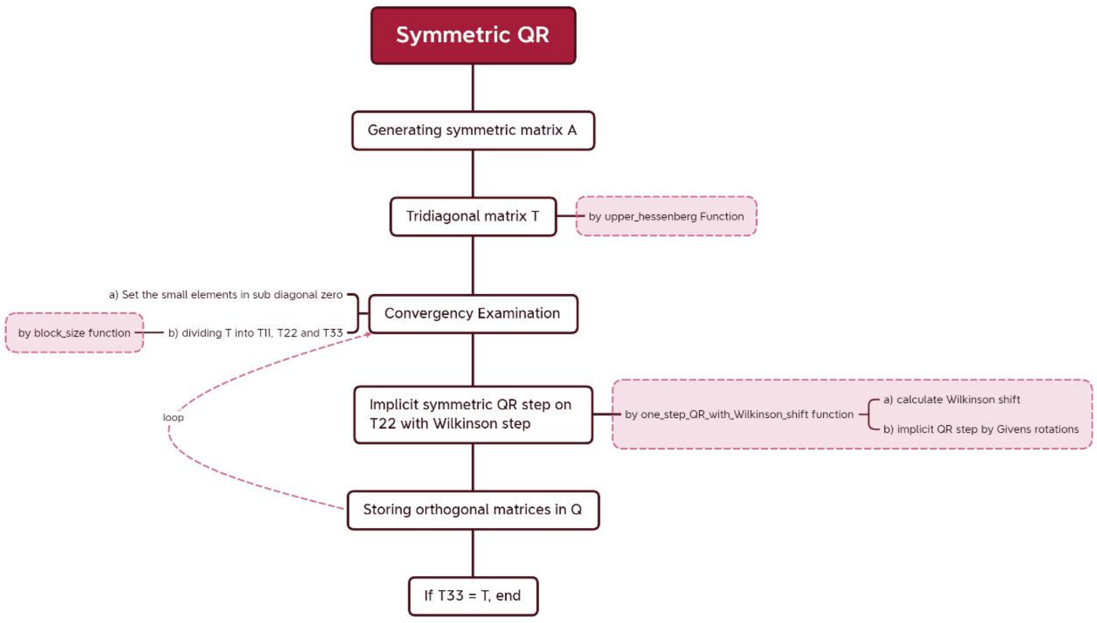
After obtaining T, we have entered the critical part of codes. Before iteration, the matrix T is blocked, which means its convergency is examined. If the elements in the sub diagonal is small enough (the criteria on “small enough” will be omitted here), the algorithm will set them zero. And then, the function ***block_size*** will divide T into three submatrices, namely, T_{11}, T_{22}, T_{33}. T_{33} consists of all the eigenvalues we have obtained and will not be involved in the iteration afterwards. T_{22} is the largest tridiagonal matrix without any zero in its sub diagonal. That is because, when no zero appears in the sub diagonal, the convergency is insured. T_{11} is the remaining part. When T_{33} is n by n, the algorithm will stop since all eigenvalues have been obtained.

After blocking the matrix T, only the T_{22} will be iterated, which invokes the function ***one_step_QR_with_Wilkinson_shift***. It first calculates the famous Wilkinson shift and apply the implicit iteration symmetric QR step to T_{22}. Every step of the implicit iteration is a simply Givens rotation doing the bubble-chasing job, but all the Givens rotations add up to a virtually QR step which tries to bring the eigenvalues of T_{22} out. Now we get back to the convergency examining step to see whether any new eigenvalue is found.

During all the steps above, all the orthogonal matrices are stored in ***Q***, which will show the corresponding eigenvectors if the user need them.

The last step visualizes the convergency history as well as the average iteration steps for an eigenvalue, and then calculate the error by 2-norm of (Q*T*Q'-A), where T is now a diagonal matrix with all the eigenvalues.

For clarity, I draw a picture to show the algorithm. Every block with red background is separately stored in a MATLAB file.


Symmetric QR
Generating symmetric matrix A
Tridiagonal matrix T
by upper_hessenberg Function
a) Set the small elements in sub diagonal zero
b) dividing T into T11, T22 and T33
by block_size function
Convergency Examination
loop
Implicit symmetric QR step on T22 with Wilkinson step
by one_step_QR_with_Wilkinson_shift function
a) calculate Wilkinson shift
b) implicit QR step by Givens rotations
Storing orthogonal matrices in Q
If T33 = T, end

Picture 1: the big picture of my symmetric QR algorithm

Detailed algorithm

First, the *upper_Hessenberg* function is as follows.

```
%% the function "upper_hessenberg" using householder orthogonalization to
make matrix A an upper Hessenberg matrix
% 最后返回 A，U，满足：H=U'AU，其中 H 是上海森伯格阵
function [A,U] = upper_hessenberg(A)
n = size(A);
n = n(1,1);
U = eye(n);
for i = 1:n-2
    u = A(i+1:n,i);
    u(1,1) = u(1,1) + sign(u(1,1)) * norm(u);
    if norm(u)==0
        continue
    end
    w = [zeros(i,1);u];
    Q = eye(n)-(2/(w'*w))*(w*w');  %generate the Householder orthogonalizer
    A = Q*A*Q';
    U = U*Q';
end
end
```

Secondly, the *block_size* function is as follow.

```
function [l,m] = block_size(T)
n = size(T);
n = n(1,1);
% 分块【分块部分有 bug】
    % 首先确定 m
    flg = 0;
    for i = n-1:-1:1
        if T(i+1,i) ~= 0
            flg = i; %flg 所指的是 T22 的最右侧元素
            break
        end
    end
    if flg ~=0
        m = n-flg-1;
        %only for test
    else
        m = n;
        %only for test
        % 注意：此时已经变成对角阵，应当结束循环，跳出循环输出有关信息
    end

    % 确定 l【这一步有 bug？】
    flg = 0;
    for j = n-m-1:-1:1
        % 这一步是在确定 m 后且没有结束循环的情况下进行的，也就是仍有一个三对角阵
T22
        % 此时 n-m 所指向的就是三对角阵最右侧的位置
        if T(j+1,j) == 0
            flg  = j; % 此时 j 所指的是 T11 最右侧的位置
            break;
        end
    end
    if flg == 0
        % 此时从 1 到 i+1 都是三对角阵的范围
        l = 0;
    else
        % 此时从 1 到 j 都是 T11 的部分
        l = flg;
    end
end
```

Thirdly, the *one_step_QR_with_Wilkinson_shift* function is as follows.

```
%% 带 Wilkinson 位移的隐式 QR 迭代
function [A,G_accumulated] = one_step_QR_with_Wilkinson_shift(A)
% 返回 A 与 G_accumulated，满足关系：A(output) = G_accumulated' * A(input) *
G_accumulated
n = size(A);
n = n(1,1);
sigma = (A(n-1,n-1)-A(n,n))/2;
Wilkinson_shift = A(n,n) - (A(n,n-1)^2) / (sigma + sign(sigma) *
sqrt(sigma^2 + A(n,n-1)^2));
x = A(1,1)-Wilkinson_shift;
% x = A(1,1)-A(n,n);
y = A(2,1);
G_accumulated = eye(n);
for k = 1:n-1
    %生成 Givens 旋转中的角度
    %[c,s] = givens(x,y);
    if y == 0
        c = 1; s = 0;
    else
        if abs(y)>abs(x)
            tao = x/y; s = 1/sqrt(1+tao^2); c = s*tao;
        else
            tao = y/x; c=1/sqrt(1+tao^2); s=c*tao;
        end
    end
    %生成 Givens 旋转矩阵
    G = eye(n); G(k,k) = c; G(k+1,k+1) = c; G(k,k+1) = -s; G(k+1,k) = s;
    %驱赶"气泡"
    A = (G'*A)*G;
    G_accumulated = G_accumulated * G;
    %为下一次迭代的 Givens 矩阵所需参数做准备
    if k<n-1
    x = A(k+1,k);
    y = A(k+2,k);
    end
end
```

```
end
```

Most importantly, the main function called *QR_Algorithm_for_symmatric_matrix*, is as follows.

```
%% QR_Algorithm_for_symmatric_matrix

%% 准备工作：生成对称矩阵 A
n = 20; %n 为矩阵阶数
A = zeros(n);
for i = 1:n
    for j = 1:i
        A(j,i)=-2+4*rand();
        A(i,j) = A(j,i);
    end
end

% M 用于记录 T33 阶数的变化（即已经算出的特征值的个数）
M=zeros(n,1);

%% 准备工作：三对角化（调用自己写的函数）
    % T 与 U 满足：T=U'AU
[T,U] = upper_hessenberg(A); %对 A 进行上海森伯格化，由于 A 是对称的，故实际上为
三对角化

%% QR 算法的主体部分
tol = 1e-14;
Q = eye(n); %用于储存所有的 Givens 旋转阵
max = 1000; %迭代次数保护
m=0; % m 是 T33 阶数，即已经算出的特征值的个数
for count = 1:max
    % 一、收敛性判定
    % 把足够小的次对角元变成 0
    for i = 1:n-m-1
        if abs(T(i+1,i))<=(abs(T(i,i))+abs(T(i+1,i+1)))*tol
            T(i+1,i) = 0;
            T(i,i+1) = 0;
        end
    end

    % 二、对 T 进行分块（调用自己写的函数）
        % 从左上角到右下角分别记作 T11，T22，T33，其中 T33 是对角阵，T22 是最大的
不可约三对角阵
        % 分块的目的以及细节可参见北大教材《数值线性代数》对称 QR 算法有关章节
    [l,m] = block_size(T); %l 是 T11 阶数, m 是 T33 阶数
    M(count,1) = m; %记录已经得到的特征值的个数
    if m==n  % 此时已经是对角阵，得到全部特征值
        break;
    end

    % 三、对 T22 进行一次 Wilkinson 位移隐式 QR 迭代（调用自己写的函数）
    [T(l+1:n-m,l+1:n-m),G] = one_step_QR_with_Wilkinson_shift(T(l+1:n-
m,l+1:n-m));

    % 四、储存旋转阵
    Q = Q*blkdiag(eye(l),G,eye(m)); %Q 用于存储 Givens 旋转阵

end %最外层循环结束（有迭代次数保护的那个）

Q = U*Q; %把三对角化时的 U 也包含进来，此处的 Q 满足 A=QDQ',其中 D=T 为对角阵，元素
为特征值，得到 A 的谱分解

%% 对称 QR 算法成果展示
plot([1:count],M,"-o"); %迭代次数和 T33（已经算出的特征值）大小的关系
xlabel("rounds of iteration")
ylabel("the number of obtained eigenvalue")
title({['QR algorithm for symmatric matrix'];['matrix size:',num2str(n),'
by ',num2str(n)];['tol = ',num2str(tol)]});

disp(["Average iter for an eigenvalue:",count/n])

disp(["Depature:",norm(Q*T*Q'-A)])
```

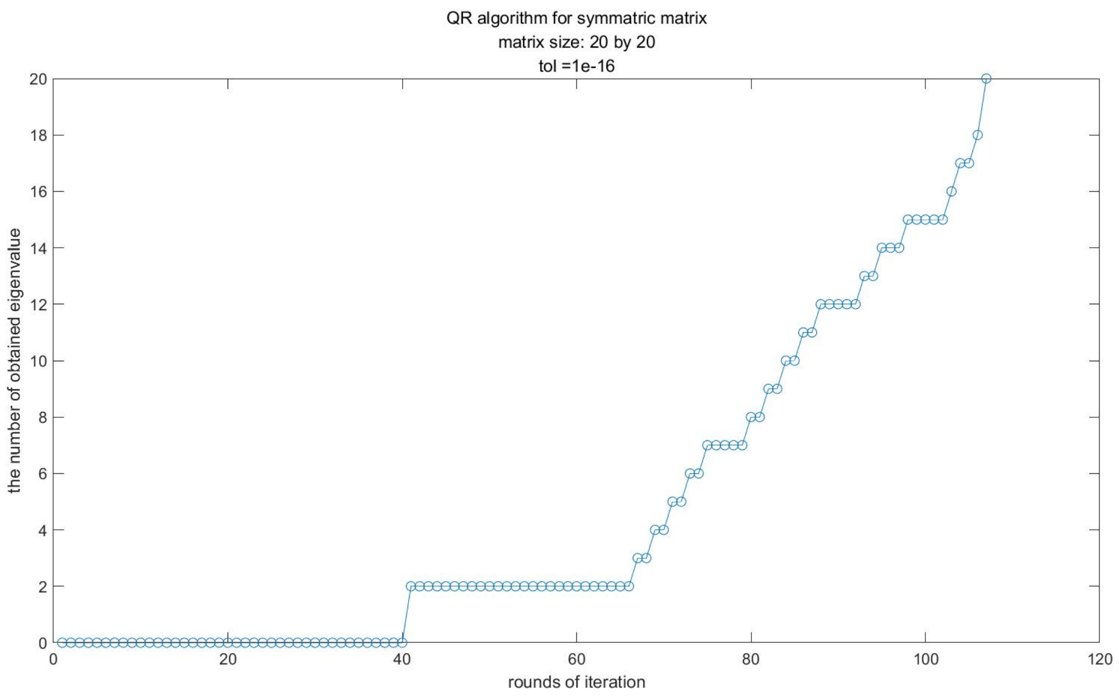
The details of functions above can be found in the MATLAB files of the same package where this report belongs!

Numerical experiments

Set the size of A 20 by 20.

Firstly, set the **tol = 1e-16**. It is a strict tolerance, considering that only when **abs(T(i+1,i))<=(abs(T(i,i))+abs(T(i+1,i+1)))*tol** can the elements in sub diagonal be set zero.

Now run the algorithm and we get the following result.



Picture 2: the typical convergence history when the size of A is 20 by 20 and tol = 1e-16

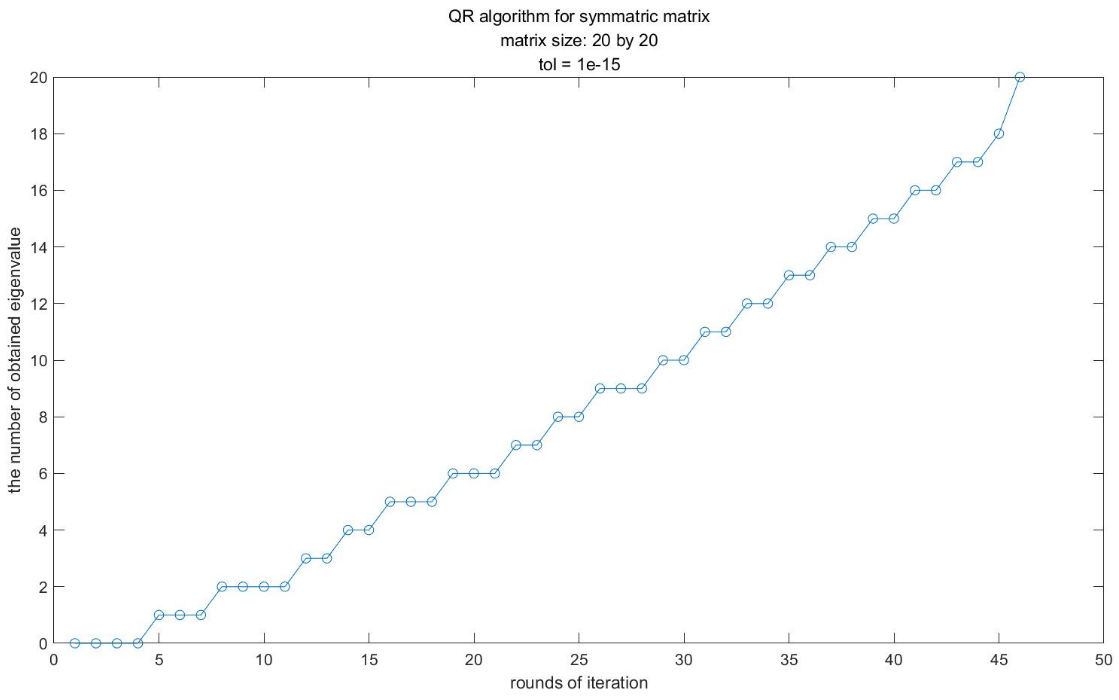
The **average iteration** for an eigenvalue is **5.35**(it costs too much). And the **error**, i.e., 2-norm of (Q*T*Q'-A), is **8.7322e-14**.

The matrix A in this experiment can be observed in the file "A of size 20 by 20 in experiment 1".

After many experiments with tol = 1e-16, it is certain that the convergence history is the **typical case**. Therefore, more results will not be presented here.

Now set **tol = 1e-15** and here are the **different** results.

A **good** case with tol = 1e-15 looks like this:

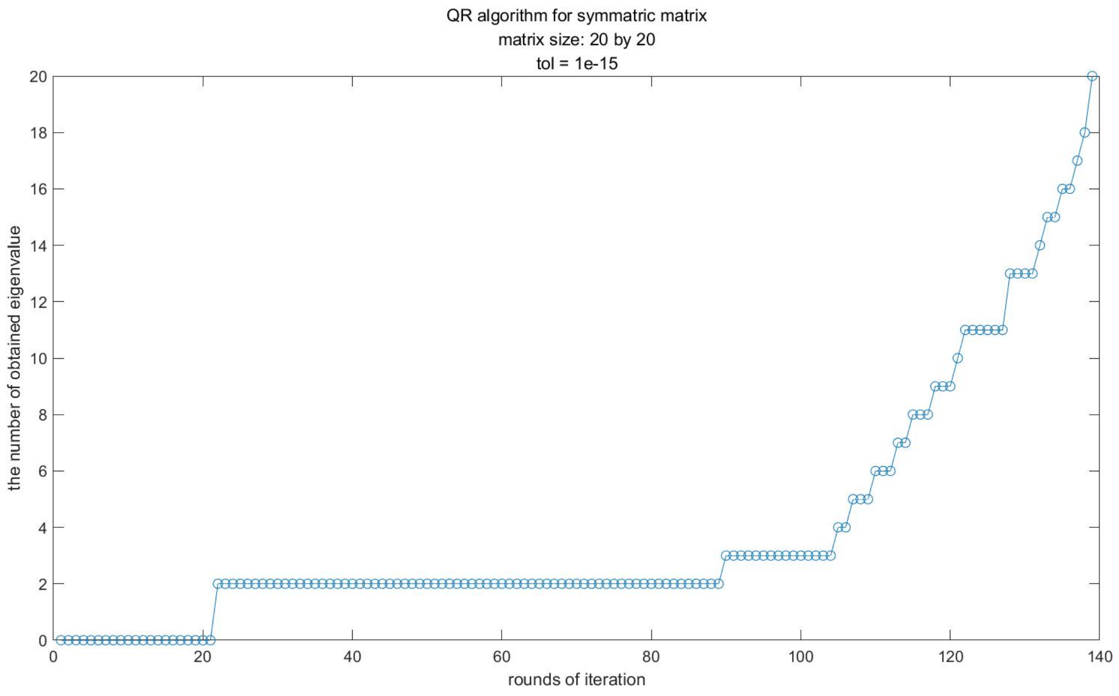


Picture 3: the good convergence history when the size of A is 20 by 20 and tol = 1e-15

The **average iteration** for an eigenvalue is **2.3** (much cheaper). And the **error**, i.e., 2-norm of (Q*T*Q'-A), is **4.1854e-14** (still as good as the last experiment).

The matrix A in this experiment can be observed in the file “A of size 20 by 20 in experiment 2”.

Nevertheless, here comes a **bad case** with tol = 1e-15:

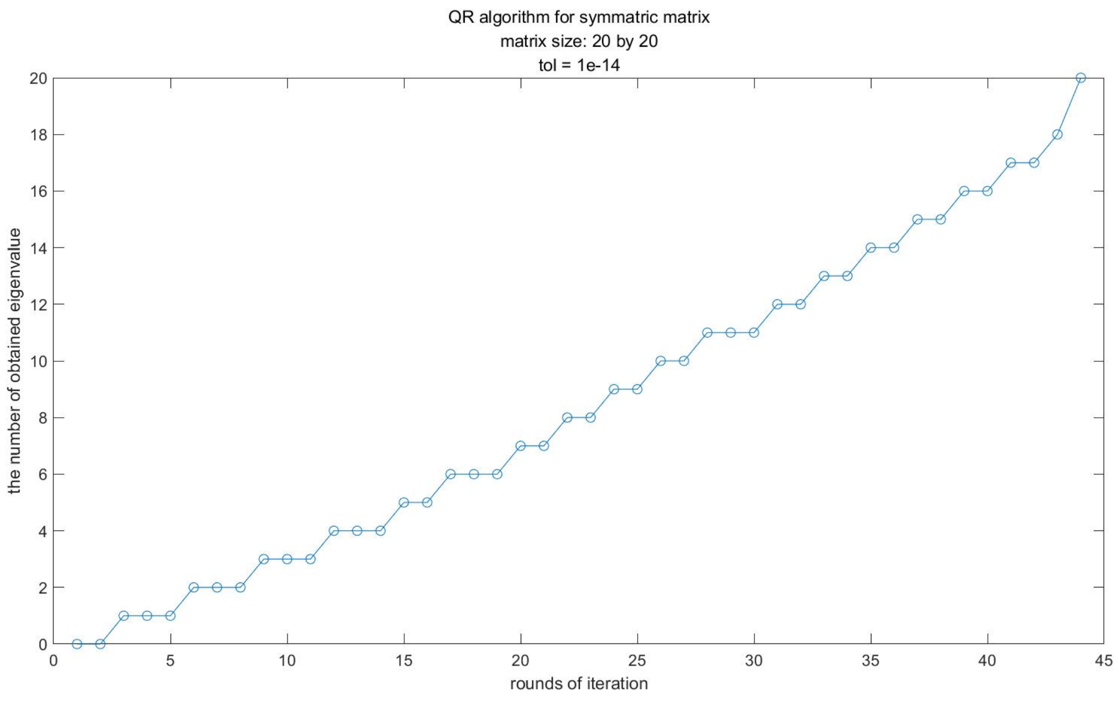


Picture 4: the bad convergence history when the size of A is 20 by 20 and tol = 1e-15

The **average iteration** for an eigenvalue is **6.95** (unbearable). And the **error**, i.e., 2-norm of (Q*T*Q'-A), is **2.1044e-13** (not that good).

The matrix A in this experiment can be observed in the file “A of size 20 by 20 in experiment 3”.

Now set **tol = 1e-14**. This “tol” is too tolerant, or maybe too “benevolent” to my computer. The result is as follows.



Picture 5: the typical convergence history when the size of A is 20 by 20 and tol = 1e-14

The **average iteration** for an eigenvalue is **2.2**(good). And the **error**, i.e., 2-norm of (Q*T*Q'-A), is **2.8603e-14** (God, still as good).

The matrix A in this experiment can be observed in the file "A of size 20 by 20 in experiment 4".

When tol = 1e-14, the convergence history above is typical and thus I shall not present more results here. I have observed that when tol = 1e-14, the average iteration is usually cheap (a little more than 2) and the error (i.e., 2-norm of (Q*T*Q'-A)), is as good as the error when tol = 1e-16.

Discussion

The discussion will focus on tol that determines whether the elements in the sub diagonal is zero and that strongly influence the convergence history.

According to James W. Demmel's famous textbook[①], the number of average iterations, namely, the QR steps for an eigenvalue, is usually **2**. Nonetheless, according to Golub and Van Loan's famous work[②], the structure of my algorithm is similar to the pseudocodes in their book except that I separately write important functions like ***upper_hessenberg*** as a black box, mainly for clarity. The only tricky part is that the tol is left for me to devise.

When tol = 1e-16 or 1e-15, it seems too strict to my computer, since the errors (i.e., 2-norm of (Q*T*Q'-A)) are no better than the result when tol = 1e = 14 and it costs too many QR step averagely. Correspondingly, in the picture 2 and picture 4 are some "plat stages"

[①] （美）德梅尔:《应用数值线性代数》，王国荣译，北京：人民邮电出版社，2007.6，第 179 页

[②] Gene H. Golub and Charles F. Van Loan: *Matrix Computation*, 4th edition, the Johns Hopkins University Press, 2013, P463 where no eigenvalue could be found.

We can have a closer observation now. Considering the critical codes below that strongly influence the convergency examination:

```
% 一、收敛性判定
    % 把足够小的次对角元变成0
    for i = 1:n-m-1
        if abs(T(i+1,i))<=(abs(T(i,i))+abs(T(i+1,i+1)))*tol
            T(i+1,i) = 0;
            T(i,i+1) = 0;
        end
    end

……

% 三、对T22进行一次Wilkinson位移隐式QR迭代（调用自己写的函数）
[T(l+1:n-m,l+1:n-m),G] =
one_step_QR_with_Wilkinson_shift(T(l+1:n-m,l+1:n-m));
```

When tol is too strict (i.e., 1e-15 or less), even T_{22} has converged after 2 QR steps, the machine error makes the elements in the sub diagonal of T_{22} still too large such that they cannot be set zero. That means there would be many useless “plat stages”. In other word, within the “plat stages”, the algorithm cannot make those elements in the sub diagonal smaller when they are $O(\varepsilon_{\text{machine}})$, even if T22 has virtually converged. When we are more “tolerant”, or probably “benevolent”, setting tol = 1e-14, the algorithm can **set the elements small enough in the sub diagonal zero in time without losing accuracy**, compared with the case when tol = 1e-16. As far as I am concerned, a reasonable assumption is that unfortunately the machine error of my computer is only around 1e-14.

Another reason (however, far less possible) is that the QR step might makes those elements in the top left or in the middle but not in the bottom right, converge toward zero. Since only T33 (on the tail) is responsible for storing all the eigenvalues obtained, and since the T_{22} is the largest tridiagonal sub matrix of T, the algorithm can help nothing but iterate once again. In this case, even some eigenvalues not in the bottom right corner of T_{22} has been found, the size of T_{33} doesn't change and we will see the “plat stages” in the convergence history picture.

Reference

[1]（美）德梅尔：《应用数值线性代数》，王国荣译，北京：人民邮电出版社，2007.6

[2] Golub G H, Van Loan C F. ***Matrix Computation***. 4th edition. Baltimore: The Johns Hopkins University Press, 2013

[3] 徐树方，高立，张平文：《数值线性代数》，第二版，北京：北京大学出版社，2013.1