HUMBOLDT UNIVERSITÄT ZU BERLIN

SEMINAR PAPER

Numerical Methods for solving Eigenvalue-Problems

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NUMERICAL INTRODUCTORY COURSE

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June 30, 2018

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1   Motivation

Abstract

Eigenvalues and eigenvectors are often the solution to multidimensional optimization problems, however computing them by hand for anything but trivial matrices is most of the time infeasible or inpractical. To this extend we would like to deploy an automated procedure which yields the correct eigenvectors and eigenvalues. We demonstrate the relevance of eigenvalues and eigenvectors by revising two applications from statistics, Principal Component Analysis and Fisher's Linear Discriminant Analysis, which we follow up by investigating four algorithms suited for eigenvalue problems. Finally we provide a compound solution that takes advantage of each algorithms strengths.

For many statistical applications eigenvectors provide a formidable solution. Be it dimensionality reduction in terms of a Principal Component Analysis or classification by Fisher's Linear Discriminant Analysis, both come in the guise of optimization problems. But what are eigenvalues and eigenvectors?

If A is an $n \times n$ matrix, v is a non-zero vector and λ is a scalar, such that

$$Av = \lambda v \tag{1}$$

then v is called an *eigenvector* and λ is called an *eigenvalue* of the matrix A. An eigenvalue of A is a root of the characteristic equation,

$$det\,(A - \lambda I) = 0. \tag{2}$$

Geometrically speaking, we require a vector which, when multiplied by matrix A, will not get rotated but only elongated by a factor λ.

When confronted with a high-dimensional data matrix $X \in \mathbb{R}^{n \times m}$ an analyst often wishes to find a lower-dimensional representation, while conserving as much of the structure as possible. One way of achieving this goal is to choose a standardized linear combination of features that aim to maximize the variance of the projection $\delta'X$. We can formalize this as

$$max\ \delta'Var\,(X)\,\delta\ s.t.\ \sum \delta_i^2 = 1. \tag{3}$$

where $X \in \mathbb{R}^{n \times m}; m, n \in \mathbb{N}; \delta \in \mathbb{R}^m$. The Lagrangean that corresponds to the constrained maximization problem in 3 is

$$\mathcal{L}(Var(X), \delta, \lambda) = \delta' Var(X) \delta - \lambda (\delta' \delta - 1),$$

where $\lambda \in \mathbb{R}^m$

Taking derivatives we obtain the first order condition:

$$\frac{\partial \mathcal{L}}{\partial \delta} \overset{!}{=} 0$$

$$2Var(X)\delta - 2\lambda_k \delta \overset{!}{=} 0$$

$$Var(X)\delta = \lambda_k \delta$$

Which is now reduced to a common Eigenvalue problem as posed in (1).

$$Y = \Gamma' (X - \mu) \tag{4}$$

where $Y \in \mathbb{R}^{n \times m}$ is the matrix of rotations, $\Gamma \in \mathbb{R}^{m \times m}$ is the matrix of eigenvectors, $\mu \in \mathbb{R}^m$ is the vector of sample means. [Härdle and Simar, 2015]

In section two we lay out the mathematical foundations for the operations we are about to perform. In particular, we will try to reformulate any complicated eigenvalue problem into a straightforward one by diagonalizing the matrix in question, without altering the eigenvalues we would like to compute. We follow these justifications by proposing two main algorithms for computing eigenvalues, first the Jacobi-Method for symmetric matrices, then the QR-Method for arbitrary square matrices in section 3. Additionally, for the QR-Method we define two extensions which try to increase the initial QR-algorithm's speed. For all algorithms we provide implementations in the `Python`-programming-language [van Rossum, 1995, Hunter, 2007, McKinney, 2010]. In section 4 we will analyse the implemented routines by critically reflecting upon the accuracy of the obtained results as well as their efficiency. In the final section we provide a final algorithm which combines the strengths

of the defined procedures by chosing the algorithm that is most fit for the underlying problem.

2 Similarity Transformations

In general we want to reformulate the eigenvalue problem of a complicated matrix into an eigenvalue problem of a simple matrix, which yields the same eigenvalues. Simple matrices in our case will be diagonal matrices, since with them it is possible to identify their eigenvalues simply as entries on the main diagonal. Such a transformation that conserves the eigenvalues of a matrix is called a *similarity transformation*.

Two $n \times n$ matrices A and B are called *similar* if there exists an invertible matrix P such that

$$A = P^{-1}BP. \tag{5}$$

It is obvious that the similarity relationship is commutative as well as transitive. If A and B are similar, it holds that

$$B - \lambda I = P^{-1}BP - \lambda P^{-1}IP$$
$$= A - \lambda I.$$

Hence A and B have the same eigenvalues. This fact also follows immediately from the transitivity of the similarity relationship and the fact that a matrix is similar to the diagonal matrix formed from its eigenvalues, as stated in the spectral-decomposition. Important types of similarity transformations are based around orthogonal matrices. If Q is orthogonal and

$$A = Q'BQ,$$

A and B are called *orthogonally similar* [Gentle, 1998]. We will use *orthogonal similarity transformations* to diagonalize matrices we wish to know the eigenvalues of.

3   Algorithms

3.1   Jacobi Method

The *Jacobi-Method* for computing the eigenvalues of a symmetric matrix $A \in \mathbb{R}^{n \times n}$ deploys a sequence of orthogonal similarity transformations that eventually results in

$$A = P \Lambda P^{-1} \Leftrightarrow \Lambda = P^{-1} A P,$$

where Λ is diagonal and P consists of a sequence of matrix multiplications $P = \prod_{k=1}^{K} V_{p_k, q_k}(\theta_k)$ and $V_{p_k, q_k}(\theta_k)$ is of the form proposed in (17). More specific the *Jacobi iteration* is

$$A^{(k)} = V'_{p_k, q_k}(\theta_k) A^{(k-1)} V_{p_k, q_k}(\theta_k), \tag{6}$$

where p_k, q_k and θ_k are chosen such that A^k resembles more a diagonal matrix than A^{k-1}. Specifically they will be chosen as to reduce the sum of squares of the off-diagonal elements. As we saw in (17) it is easy to chose an angle θ_k in order to introduce a zero in a single Givens rotation. Here we use the rotations in the context of a similarity transformation, so it is a little more complicated.

We require that $a_{pq}^{(k)} = 0$, this implies

$$a_{pq}^{(k-1)}(\cos^2 \theta - \sin^2 \theta) + \left(a_{pp}^{(k-1)} - a_{qq}^{(k-1)} \right) \cos \theta \sin \theta = 0. \tag{7}$$

Figure 1: Progress Jacobi-Method
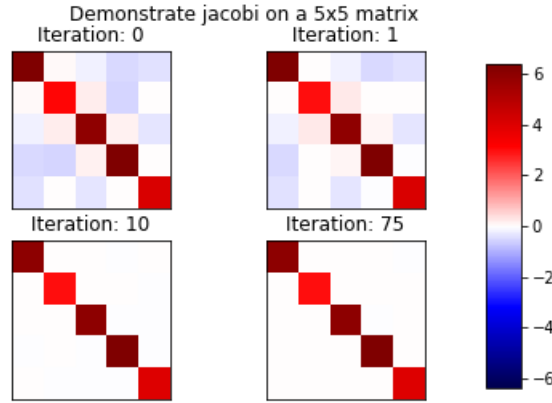
We can use the trigonometric identities

$$\cos(2\theta) = \cos^2 \theta \sin^2 \theta$$

$$\sin(2\theta) = 2 \cos \theta \sin \theta,$$

in (7) we have

$$\tan(2\theta) = \frac{2a_{pq}^{(k-1)}}{a_{pp}^{(k-1)} - a_{qq}^{(k-1)}}.$$

From this we can retrieve the angle and obtain the rotation matrix in each iteration [Gentle, 1998].

The algorithm converges if the off-diagonal elements are sufficiently small. The best index pair at a given iteration is the pair (p, q) that satisfies

$$|a_{pq}^{(k-1)}| = \max_{i<j} |a_{ij}^{(k-1)}|.$$

If this choice is made, the Jacobi Method can be shown to converge [Gentle, 1998].

Figure 1 visualizes the progress of the *Jacobi*-method on a symmetric 5×5 matrix. As we can see, in the first iteration the element $a_4 3$ is eliminated. In the subsequent operations the *Jacobi*-method continues to eliminate any non-zero entries on the off-diagonal until the algorithm convergences after 10 iterations.

Algorithm 1 `jacobi`

Require: symmetric matrix A
Ensure: $0 < precision < 1$

    initialize: $L \leftarrow A; U \leftarrow I; L_{max} \leftarrow 1$
1: **while** $L_{max} > precision$ **do**
2:      Find indices i, j of largest value in lower triangle of $abs(L)$
3:      $L_{max} \leftarrow L_{i,j}$
4:      $\alpha \leftarrow \frac{1}{2} \cdot \arctan(\frac{2A_{i,j}}{A_{i,i}-A_{j,j}})$
5:      $V \leftarrow I$
6:      $V_{i,i}, V_{j,j} \leftarrow \cos\alpha; V_{i,j}, V_{j,i} \leftarrow -\sin\alpha, \sin\alpha$
7:      $A \leftarrow V'AV; U \leftarrow UV$
8: **end while**
9: **return** $diag(A), U$

3.2 QR-Method

The most widely used algorithm to extract eigenvalues is the so called QR-method. The most important advantage of the QR-method over the *Jacobi*-method is that it can be applied to non-symmetric matrices. Note however, that it is simpler for symmetric matrices, since the eigenvalues are real-valued.

The QR-method to extract the eigenvalues of a square matrix $A \in \mathbb{R}^{n \times n}$ is performed by first computing the titular QR decomposition of A.

$$A = QR, \tag{8}$$

where Q is an orthogonal and R is an upper triangular matrix. Then define the QR iteration as

$$A^k = Q'_{k-1}A_{k-1}Q_{k-1} = R_{k-1}Q_{k-1} \tag{9}$$

Note hereby that all matrices in the sequence $\{A_k\}$ share the same eigenvalues, since this procedure is a similarity transformation due to Q's orthogonality. Additionally, in an implementation it is usually preferable to compute the QR-iteration in the way shown at the rightmost part of equation (9) [Börm and Mehl, 2012]. Although, mathematically, each statement is exactly identical there is a practical difference in due to computational imperfections and limited machine precision.

Figure 2: Progress basic QR-Method
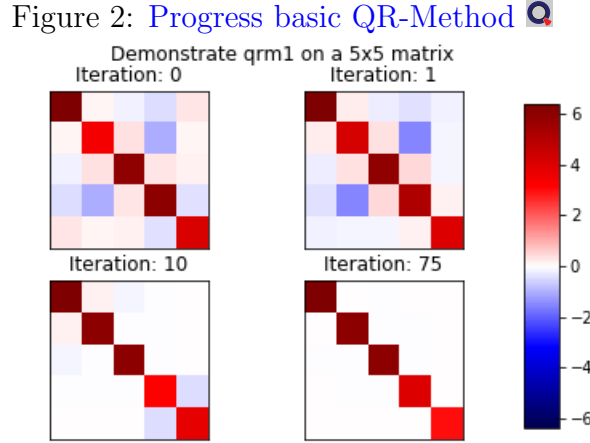
The reason being that the computation of $Q'_{k-1}A_{k-1}Q_{k-1}$ obviously requires two matrix multiplications whereas the result of $R_{k-1}Q_{k-1}$ can be readily obtained by one. When combining multiple steps over a long sequence of QR iterations the additional computations lead to additional rounding errors, which can have an influence on the accuracy of the obtained results. Additionally, less computations lead of course to a faster procedure in general.

Figure 3.2 visualizes the progress of the basic QR-method on the same 5×5 matrix as in Figure 1. Compared to the *Jacobi*-method it does not explicitly pick a single element that will be eliminated per iteration. Instead, the QR-method extracts the eigenvalues by a process that is called "chasing". By that we mean that alternating steps are being performed, which create non-zero eintries in positions $(i + 2, i)$, $(i + 3, i)$ and $(i + 3, i + 1)$ and restore them to zero, as the nonzero entries are moved farther down the matrix [Gentle, 1998]. We can also see that compared to the *Jacobi*-Method, so far, the QR-algorithm lacks in speed. Where the *Jacobi*-method was almost done diagonalizing the matrix in iteration 10, the basic QR-algorithm still had multiple non-zero entries left. Thus we would like to make minor improvements on the algorithm's efficiency.

Algorithm 2 `QRM1`

Require: square matrix A

    initialize: $conv \leftarrow False$

 1: **while** not $conv$ **do**

 2:     $Q, R \leftarrow$ QR-Factorization of A

 3:     $A \leftarrow RQ$

 4:     **if** A is diagonal **then**

 5:         $conv \leftarrow$ `True`

 6:     **end if**

 7: **end while**

 8: **return** $diag\left(A\right), Q$

3.2.1 Hessenberg Variant

In order to speed up the QR-method it is advisable to transform the matrix to its upper *Hessenberg* form. A matrix A is of upper *Hessenberg* form if it is upper triangular except for the first subdiagonal, which may be non-zero. In particular $a_{ij} = 0 \; \forall i > j + 1$:

$$\begin{bmatrix} X & X & X & \ldots & X & X \\ X & X & X & \ldots & X & X \\ 0 & X & X & \ldots & X & X \\ 0 & 0 & X & \ldots & X & X \\ \vdots & \vdots & & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & X & X \end{bmatrix}$$

A matrix can be reduced to *Hessenberg* form in a finite number of similarity transformations using Householder transformations or Givens rotations. For symmetric matrices the transformation into a *Hessenberg*-form results in a tridiagonal matrix. But even for non-symmetric matrices, the *Hessenberg*-form allows a large saving in subsequent computations. After the transformation we can deploy the previously defined QR-method [Gentle, 1998].
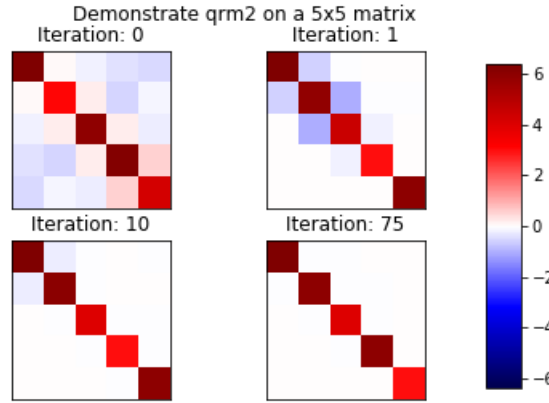
Figure 3: Progress Hessenberg-QR-Method 🔍

Figure 3 visualizes the progress of the *Hessenberg* variant of the *QR*-method. In order to make it comparable to the previous algorithms the same 5×5-dimensional matrix is being evaluated. We can readily see, that the transformation to *Hessenberg*-form results in a tridiagonal matrix. This facilitates computations and explains the vastly improved resulting matrix after 10 iterations compared to the basic *QR*-method. However, it still does not match the progress of the *Jacobi*-method after the same number of iterations.

Algorithm 3 `QRM2`

Require: square matrix A

  1: $A \leftarrow$ `hessenberg`(A)

  2: continue with: $\mathrm{QRM1(A)}$

3.2.2 Accelerated Variant

We could already improve the *QR*-method and cut down on computational cost. However, we still cannot match the results of the *Jacobi* method. To this effect we present the final adjustment on the *QR*-method to improve convergence speed. The general idea is, that we deliberately create an additional zero entry on the main diagonal by subtracting a scalar on each element, perform the *QR*-iteration and finally undo the subtraction. In particular, we define

$$T^m = \begin{bmatrix} \alpha_1^m & \beta_1^m & 0 & 0 & \dots & & 0 \\ \beta_1^m & \alpha_2^m & \beta_2^m & & & & \\ 0 & \beta_2^m & \alpha_3^m & \beta_3^m & & & \vdots \\ & & \ddots & \ddots & \ddots & & \\ & & & & \beta_{n-2}^m & \alpha_{n-1}^m & \beta_{n-1}^m \\ 0 & & & & & \beta_{n-1}^m & \alpha_n^m \end{bmatrix} \tag{10}$$

$$T^m = T - t_{n,n}I$$

$$T^m = QR$$

$$T^{m+1} = T^m + t_{n,n}I$$

After this we can define the accelerated iteration step as

$$R_m = Q_m' \left(T_m - \alpha_n^m I \right) \tag{11}$$

$$T_{m+1} = Q_m' \left(T_m - \alpha_n^m I \right) Q_m + \alpha_n^m I \tag{12}$$

$$= Q_m' T_m Q_m \tag{13}$$

Again T_{m+1} is similar to T_m.

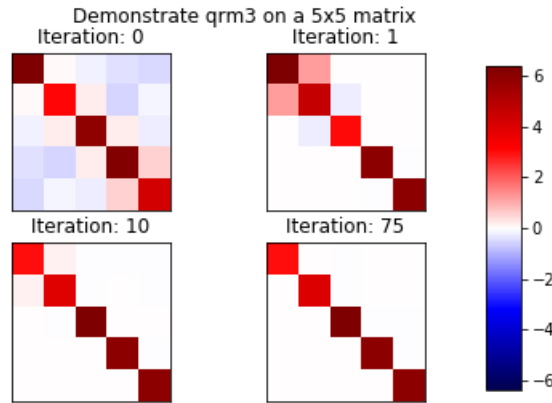Figure 4: Progress Accelerated QR-Method

Demonstrate qrm3 on a 5x5 matrix

Table 1: Unit tests accross matrix-sizes

awesome	sauce
nothing	to
see	here

Figure 4 visualizes the progress of the accelerated QR-method. For comparability, the matrix used is the same 5×5 matrix as before. Most notably is, that the accelerated method still performs worse than the *Jacobi* method. So far results seem similar compared to the *Hessenberg* variant of the QR-method. The case can be made that the accelerated method performs considerably better than the basic QR-method and slightly better than the *Hessenberg* variant after 10 iterations than the. Howbeit, this claim warrants further analysis.

Algorithm 4 `QRM3`

Require: square matrix $A \in \mathbb{R}^{p \times p}$
1: $T \leftarrow \texttt{hessenberg}(A)$, $conv \leftarrow False$
2: **while** not $conv$ **do**
3:     $Q, R \leftarrow$ QR-Factorization of $T - t_{p-1,p-1}I$
4:     $T \leftarrow RQ + t_{p-1,p-1}I$
5:     **if** T is diagonal **then**
6:         $conv \leftarrow True$
7:     **end if**
8: **end while**
9: **return** $diag\left(T\right)$, Q

---

4   Analysis

4.1   Accuracy

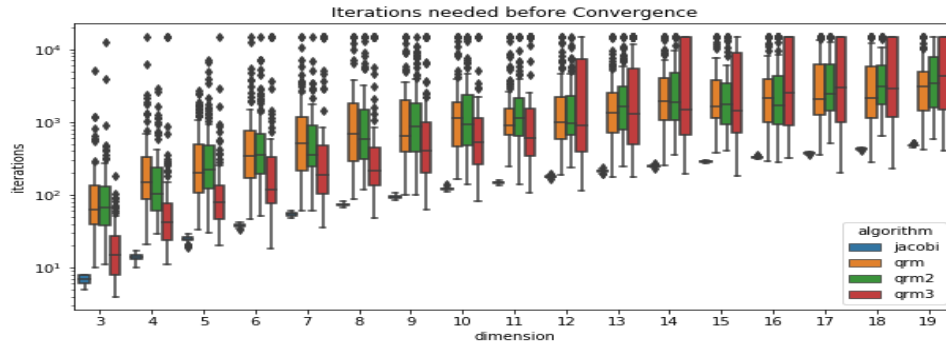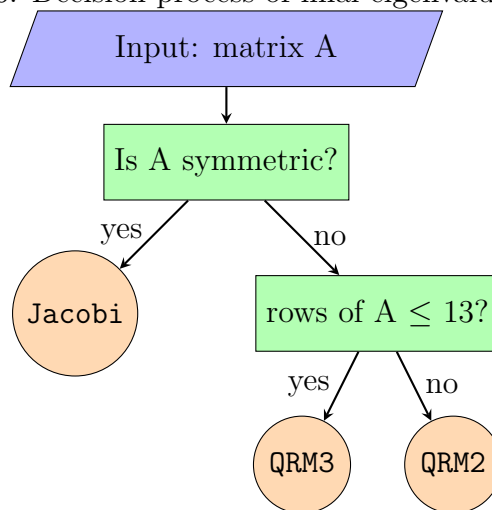## 4.2   Efficiency

5   Conclusion

Figure 5: Unit-tests: Iterations

Figure 6: Decision process of final eigenvalue routine

6 Appendix

6.1 Householder-Reflections

Our goal is still to diagonalize a matrix in order to programmatically extract it's eigenvalues. So far we have seen that there exist such transformations that conserve the eigenvalues of a given matrix. However, we require transformations that, additionally, eliminate non-zero entries on the off-diagonal elements of said matrix. A greedy technique, that eliminates all but the first elements of a vector is proposed in the form of Householder-Reflections.

Let u and v be orthonormal vectors and let x be a vector in the space spanned by u and v, such that

$$x = c_1 u + c_2 + v$$

for some scalars c_1 and c_2. The vector

$$\tilde{x} = -c_1 u + c_2 v$$

is a *reflection* of x through the line difined by the vector u. Now consider the matrix

$$P = I - 2uu'. \tag{14}$$

Note that

$$Px = c_1 u + c_2 v - 2c_1 uuu' - 2c_2 vuu'$$

$$= c_1 u + c_2 v - 2c_1 u'uu - 2c_2 u'vu$$

$$= -c_1 u + c_2 v$$

$$= \hat{x}.$$

The matrix P is called a reflector. The usefulness of Householder-Reflections stems from the fact that it is easy to transform a vector of the form

$$x = (x_1, x_2, \ldots, x_n)$$

into a vector

$$\hat{x} = (\hat{x}_1, 0, \ldots, 0).$$

If $Qx = \hat{x}$, then $||x||_2 = ||\hat{x}||_2$ and thus $\hat{x}_1 = \pm||x||_2$, since it is the only non-zero entry. To construct the reflector let

$$v = (x_1 + sign(x_1)||x||_2, x2, \ldots, x_n) \tag{15}$$

and $u = \frac{v}{||v||_2}$ [Gentle, 1998]. We use the *sign*-function, which simply returns the sign of its argument in order to avoid the numerical problem known as *catastrophic cancellation*. It can occur when adding two very close, but different, floating point numbers of differing signs. In some unfortunate cases both of these numbers get represented by the same computer number and, because of their opposing signs cancel each other out. In our case this would mean, that we reflect the vector onto the origin. Fortunately, by making use of the *sign* function we can make sure that both summands will share the same sign, thus mitigating any concerns about catastrophic cancellation.

We use reflectors to compute the so called QR factorization of an aribitrary square matrix $A \in \mathbb{R}^{n \times n}$.

$$A = QR \tag{16}$$

where Q is orthogonal and R is upper triangular. We use Householder transformations to reflect the ith column and produce zeros below the (i, i) element. The QR-factorization of a matrix $A \in \mathbb{R}^5$ would therefore consist of five Householder-reflections with $Q = P_5 P_4 P_3 P_2 P_1$. The number of computations for the QR factorization in this fashion is $2n^3/3$ multiplications and $2n^3/3$ additions [Gentle, 1998].

6.2   Givens-Rotations

Another way of forming the QR-factorization is by using orthogonal transformations which rotate a vector in a way such that a specific element becomes 0 and only one other element in the vector being changed. These transformations are called *Givens transformations, Givens Rotations* or *Jacobi transformations*

Figure 7: Rotation of x

A Givens rotation in $\mathbb{R}^2$.

Using orthogonal transformations we can also rotate a vector in such a way that a specified element becomes 0 and only one other element in the vector is changed. The basic idea can be seen in a two-dimensional space. We wish to rotate the vector $x = (x_1, x_2)$ to $\tilde{x} = (\tilde{x_1}, 0)$ as with a reflector.

It is easy to see that the orthogonal matrix

$$Q = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix}$$

performs the desired rotation, if $\cos\theta = \frac{x_1}{||x||_2}$ and $\sin\theta = \frac{x_2}{||x||_2}$

In general, we can construct an orthogonal $matrix V_{pq}$, that will transform the vector

$$x = (x_1, \ldots, x_p, \ldots x_q, \ldots, x_n)$$

to

$$\tilde{x} = (x_1, \ldots, \tilde{x}_p, \ldots 0, \ldots, x_n)$$
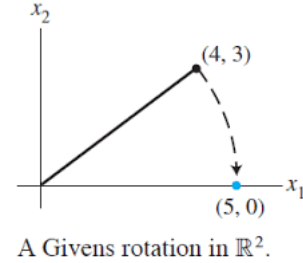
. The matrix that does this is

$$V_{pq}(\theta) = \begin{bmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & \cos\theta & & \sin\theta & & \\ & & & \ddots & & & \\ & & -\sin\theta & & \cos\theta & & \\ & & & & & \ddots & \\ & & & & & & 1 \end{bmatrix} \tag{17}$$

where $\cos\theta = \frac{x_p}{||x||}$ and $\sin\theta = \frac{x_q}{||x||}$.

A rotation matrix is therefore the same as an identitiy matrix, in which we change four elements [Börm and Mehl, 2012]. We will use Givens rotations primarily in the Jacobi-Method.

6.3 Eigenvalue Routines

```python
import numpy as np
import copy


def hreflect1D(x):
    """
    Calculate Householder reflection: Q = I - 2*uu'.

    Parameters:
        X: numpy array.

    Returns:
        Qx: reflected vector.
        Q: Reflector (matrix).
    """
    # Construct v:
    v = copy.deepcopy(x)
```

```python
18      v[0] += np.linalg.norm(x)
19
20      # Construct u: normalize v.
21      vnorm = np.linalg.norm(v)
22      if vnorm:
23          u = v / np.linalg.norm(v)
24      else:
25          u = v
26
27      # Construct Q:
28      Q = np.eye(len(x)) - 2 * np.outer(u, u)
29      Qx = np.dot(Q, x)
30
31      return Qx, Q
32
33
34  def qr_factorize(X, offset=0):
35      """
36      Compute QR factorization of X s.t. QR = X.
37
38      Parameters:
39          - X: square numpy ndarray.
40          - offset: (int) either 0 or 1. If offset is unity: compute
             Hessenberg-
41                    matrix.
42
43      Returns:
44          Q: square numpy ndarray, same shape as X. Rotation matrix.
45          R: square numpy ndarray, same shape as X. Upper triangular
             matrix if
46              offset is 0, Hessenberg-matrix if offset is 1.
47      """
48      assert offset in [0, 1]
49      assert type(X) == np.ndarray
50      assert X.shape[0] == X.shape[1]
```

```
51
52      R = copy.deepcopy(X)
53      Q = np.eye(X.shape[0])
54
55      for i in range(X.shape[0]-offset):
56          Pi = np.eye(R.shape[0])
57          _, Qi = hreflect1D(R[i+offset:, i])
58          Pi[i+offset:, i+offset:] = Qi
59
60          Q = Pi.dot(Q)
61          R = Pi.dot(R)
62
63      return Q.T, R
```

```
1   """
2   Algorithms for solving eigenvalue problems.
3
4   1. Compute diagonalization of 2x2 matrices via jacobi iteration.
5   2. Generalize Jacobi iteration for symmetric matrices.
6   """
7   import numpy as np
8   import copy
9   import warnings
10  from scipy import linalg as lin
11  from algorithms import helpers
12
13
14  def jacobi2x2(A):
15      """
16      Diagonalize a 2x2 matrix through jacobi step.
17
18      Solve: U' A U = E s.t. E is a diagonal matrix.
19
20      Parameters:
21          A - 2x2 numpy array.
22      Returns:
```

```python
23          A - 2x2 diagonal numpy array
24      """
25      assert type(A) == np.ndarray
26      assert A.shape == (2, 2)
27      assert A[1, 0] == A[0, 1]
28
29      alpha = 0.5 * np.arctan(2*A[0, 1]/(A[1, 1] - A[0, 0]))
30      U = np.array([[np.cos(alpha), np.sin(alpha)],
31                    [-np.sin(alpha), np.cos(alpha)]])
32      E = np.matmul(U.T, np.matmul(A, U))
33      return E
34
35
36  def jacobi(X, precision=1e-6, debug=False):
37      """
38      Compute Eigenvalues and Eigenvectors for symmetric matrices.
39
40      Parameters:
41          X - 2D numpy ndarray which represents a symmetric matrix
42          precision - float in (0, 1). Convergence criterion.
43
44      Returns:
45          A - 1D numpy array with eigenvalues sorted by absolute
               value
46          U - 2D numpy array with associated eigenvectors (column).
47      """
48      assert 0 < precision < 1.
49      assert type(X) == np.ndarray
50      n, m = X.shape
51      assert n == m
52      assert all(np.isclose(X - X.T, np.zeros(n)).flatten())
53      A = copy.deepcopy(X)
54      U = np.eye(A.shape[0])
55      L = np.array([1])
56      iterations = 0
```

```python
57
58     while L.max() > precision:
59         L = np.abs(np.tril(A, k=0) - np.diag(A.diagonal()))
60         i, j = np.unravel_index(L.argmax(), L.shape)
61         alpha = 0.5 * np.arctan(2*A[i, j] / (A[i, i]-A[j, j]))
62
63         V = np.eye(A.shape[0])
64         V[i, i], V[j, j] = np.cos(alpha), np.cos(alpha)
65         V[i, j], V[j, i] = -np.sin(alpha), np.sin(alpha)
66
67         A = np.dot(V.T, A.dot(V))
68         U = U.dot(V)
69         iterations += 1
70
71     # Sort by eigenvalue (descending order) and flatten A
72     A = np.diag(A)
73     order = np.abs(A).argsort()[::-1]
74     if debug:
75         return iterations
76
77     return A[order], U[:, order]
78
79
80 def qrm(X, maxiter=15000, debug=False):
81     """
82     Compute Eigenvalues and Eigenvectors using the QR-Method.
83
84     Parameters:
85         - X: square numpy ndarray.
86     Returns:
87         - Eigenvalues of A.
88         - Eigenvectors of A.
89     """
90     n, m = X.shape
91     assert n == m
```

```python
92
93      # First stage: transform to upper Hessenberg-matrix.
94      A = copy.deepcopy(X)
95      conv = False
96      k = 0
97
98      # Second stage: perform QR-transformations.
99      while (not conv) and (k < maxiter):
100         k += 1
101         Q, R = helpers.qr_factorize(A)
102         A = R.dot(Q)
103
104         conv = np.alltrue(np.isclose(np.tril(A, k=-1), np.zeros((n
            , n))))
105
106     if not conv:
107         warnings.warn("Convergence was not reached. Consider
            raising maxiter.")
108     if debug:
109         return k
110     Evals = A.diagonal()
111     order = np.abs(Evals).argsort()[::-1]
112     return Evals[order], Q[order, :]
113
114
115 def qrm2(X, maxiter=15000, debug=False):
116     """
117     First compute similar matrix in Hessenberg form, then compute
            the
118     Eigenvalues and Eigenvectors using the QR-Method.
119
120     Parameters:
121         - X: square numpy ndarray.
122     Returns:
123         - Eigenvalues of A.
```

```python
124            - Eigenvectors of A.
125        """
126     n, m = X.shape
127     assert n == m
128
129     # First stage: transform to upper Hessenberg-matrix.
130     A = lin.hessenberg(X)
131     conv = False
132     k = 0
133
134     # Second stage: perform QR-transformations.
135     while (not conv) and (k < maxiter):
136         k += 1
137         Q, R = helpers.qr_factorize(A)
138         A = R.dot(Q)
139
140         conv = np.alltrue(np.isclose(np.tril(A, k=-1), np.zeros((n
             , n))))
141
142     if not conv:
143         warnings.warn("Convergence was not reached. Consider
             raising maxiter.")
144     if debug:
145         return k
146     Evals = A.diagonal()
147     order = np.abs(Evals).argsort()[::-1]
148     return Evals[order], Q[order, :]
149
150
151 def qrm3(X, maxiter=15000, debug=False):
152     """
153     First compute similar matrix in Hessenberg form, then compute
             the
154     Eigenvalues and Eigenvectors using the QR-Method.
155
```

```python
156        Parameters:
157            - X: square numpy ndarray.
158        Returns:
159            - Eigenvalues of A.
160            - Eigenvectors of A.
161        """
162        n, m = X.shape
163        assert n == m
164
165        # First stage: transform to upper Hessenberg-matrix.
166        T = lin.hessenberg(X)
167
168        conv = False
169        k = 0
170
171        # Second stage: perform QR-transformations.
172        while (not conv) and (k < maxiter):
173            k += 1
174            Q, R = helpers.qr_factorize(T - T[n-1, n-1] * np.eye(n))
175            T = R.dot(Q) + T[n-1, n-1] * np.eye(n)
176
177            conv = np.alltrue(np.isclose(np.tril(T, k=-1), np.zeros((n
                , n))))
178
179        if not conv:
180            warnings.warn("Convergence was not reached. Consider
                raising maxiter.")
181        if debug:
182            return k
183        Evals = T.diagonal()
184        order = np.abs(Evals).argsort()[::-1]
185        return Evals[order], Q[order, :]
```

6.4   Analysis: Figures

```python
import os
import copy
import pandas as pd
import numpy as np
import seaborn as sns
from scipy import linalg as lin
from scipy.stats import ortho_group
from matplotlib import pyplot as plt

datadir = os.path.join("analysis", "benchmarks.csv")
outpath = os.path.join("media", "plots")
trials = pd.read_csv(datadir, index_col=0)

trials.groupby(["algorithm", "dimension"]).iterations.describe()

# Boxplot iteration:
fig = plt.figure(figsize=(10, 5))
sns.boxplot(x="dimension", y="iterations", hue="algorithm", data=
    trials)
plt.yscale("log")
plt.title("Iterations needed before Convergence")
plt.savefig(os.path.join(outpath, "iterations_boxplot.png"))
plt.show()
plt.close()

# Boxplot elapsed time:
fig = plt.figure(figsize=(10, 5))
sns.boxplot(x="dimension", y="time", hue="algorithm", data=trials)
plt.title("Time needed before Convergence")
plt.ylabel("time (sec)")
plt.yscale('log')
plt.savefig(os.path.join(outpath, "time_boxplot.png"))
plt.show()
plt.close()
```

```python
34
35  # Visualize Algorithm-Progress:
36  np.random.seed(42)
37  size = 5
38  Lambda = np.diag(np.random.randint(low=0, high=10, size=size))
39  G = ortho_group.rvs(dim=size)
40  X = np.dot(G, Lambda.dot(G.T))
41
42
43  def plot_factory(func):
44      def plotter(savepath, **fig_kw):
45          def algorithm_generator(*args, **kwargs):
46              return func(*args, **kwargs)
47
48          fig, ax = plt.subplots(nrows=2, ncols=2, **fig_kw)
49          algorithm_iterator = algorithm_generator()
50          j = -1
51
52          for i, A in enumerate(algorithm_iterator):
53              if i in (0, 1, 10, 75):
54                  j += 1
55
56                  hm = ax[j // 2, j % 2].imshow(A,
57                                                cmap=plt.get_cmap('
                                                  seismic'),
58                                                vmin=-X.max(),
59                                                vmax=X.max())
60                  ax[j // 2, j % 2].set_yticks([])
61                  ax[j // 2, j % 2].set_xticks([])
62                  ax[j // 2, j % 2].set_title("Iteration: " + str(i)
                    )
63
64                  if i > 75:
65                      break
66
```

27

```python
67          fig.subplots_adjust(right=0.8)

68          cbar_ax = fig.add_axes([0.85, 0.15, 0.05, 0.7])

69          fig.colorbar(hm, cax=cbar_ax)


71          sup_title = "Demonstrate {} on a {}x{} matrix".format(

72              func.__name__,

73              *X.shape)


75          fig.suptitle(sup_title)

76          fig.savefig(savepath)


78          return fig, ax


80      return plotter



83  @plot_factory

84  def jacobi():

85      """

86      Compute Eigenvalues and Eigenvectors for symmetric matrices
          using the

87      jacobi method.


89      Yields:

90          * A - 2D numpy array of current iteration step.

91      """

92      A = copy.deepcopy(X)

93      U = np.eye(A.shape[0])

94      L = np.array([1])

95      iterations = 0


97      while iterations < 5000:

98          L = np.abs(np.tril(A, k=0) - np.diag(A.diagonal()))

99          i, j = np.unravel_index(L.argmax(), L.shape)

100         alpha = 0.5 * np.arctan(2*A[i, j] / (A[i, i]-A[j, j]))
```

```python
101
102          V = np.eye(A.shape[0])
103          V[i, i], V[j, j] = np.cos(alpha), np.cos(alpha)
104          V[i, j], V[j, i] = -np.sin(alpha), np.sin(alpha)
105
106          A = np.dot(V.T, A.dot(V))
107          U = U.dot(V)
108          iterations += 1
109          yield A
110
111
112 @plot_factory
113 def qrm1():
114     """
115     Create generator for transformed matrices after applying the
          QR-Method.
116
117     Yields:
118         - T: 2D-numpy array. Similar matrix to X.
119     """
120     # First stage: transform to upper Hessenberg-matrix.
121     T = copy.deepcopy(X)
122
123     k = 0
124     # Second stage: perform QR-transformations.
125     while k < 5000:
126         k += 1
127         Q, R = np.linalg.qr(T)
128         T = R.dot(Q)
129         yield T
130
131
132 @plot_factory
133 def qrm2():
134     """
```

```
135         Create generator for transformed matrices after applying the
             QR-Method.
136
137         Yields:
138             - T: 2D-numpy array. Similar matrix to X.
139         """
140         # First stage: transform to upper Hessenberg-matrix.
141         T = lin.hessenberg(X)
142
143         k = 0
144         # Second stage: perform QR-transformations.
145         while k < 5000:
146             if k == 0:
147                 yield X
148             k += 1
149             Q, R = np.linalg.qr(T)
150             T = R.dot(Q)
151             yield T
152
153
154 @plot_factory
155 def qrm3():
156         """
157         First compute similar matrix in Hessenberg form, then compute
             the
158         Eigenvalues and Eigenvectors using the accelerated QR-Method.
159
160         Yields:
161             * T - 2D numpy array of current iteration step.
162         """
163         # First stage: transform to upper Hessenberg-matrix.
164         T = lin.hessenberg(X)
165         k = 0
166         n, _ = X.shape
167
```

```python
168        # Second stage: perform QR-transformations.

169        while k < 5000:

170            if k == 0:

171                yield X

172            k += 1

173            Q, R = np.linalg.qr(T - T[n-1, n-1] * np.eye(n))

174            T = R.dot(Q) + T[n-1, n-1] * np.eye(n)


176            yield T



179  jacobi(os.path.join(outpath, "jacobi.png"))

180  qrm1(os.path.join(outpath, "qrm1.png"))

181  qrm2(os.path.join(outpath, "qrm2.png"))

182  qrm3(os.path.join(outpath, "qrm3.png"))


184  plt.show()

185  plt.close()
```

6.5   Analysis: Unit tests

```python
"""
Automated tests for different algorithms.
"""
import os
import sys
import numpy as np
from threading import Thread
import pandas as pd
from algorithms import eigen
from scipy.stats import ortho_group
from tqdm import tqdm
from functools import wraps


data_out = os.path.join("data", "accuracy_tests.csv")


class AlgoTest(object):
    tests = {"algorithm": [],
             "dimension": [],
             "maxiter": [],
             "failed": []}

    def __init__(self, algo, dim, filepath, n_tests=1000, jobs=1,
                 *args, **kwargs):
        assert n_tests % jobs == 0
        self.algorithm = self.__get_test_algorithm(algo, *args, **
          kwargs)
        self.dim = dim
        self.n = n_tests // jobs
        self.failed = []
        self.jobs = jobs
        self.result = None
        self.path = filepath
```

```python
34         self.maxiter = kwargs.get("maxiter", None)

35

36         if not os.path.exists(self.path):
37             self.save(header=["algorithm", "dimension", "maxiter",
                   "failed"])

38

39     def __get_test_algorithm(self, algorithm, *args, **kwargs):
40         @wraps(algorithm)
41         def algo(X):
42             return algorithm(X, *args, **kwargs)
43         return algo

44

45     def __get_test_matrix(self):
46         """Return matrix with assosiated Eigenvalues."""
47         eigenvalues = np.random.uniform(size=self.dim)
48         eigenvectors = ortho_group.rvs(dim=self.dim)
49         Lambda = np.diag(eigenvalues)

50

51         matrix = np.dot(eigenvectors, Lambda).dot(eigenvectors.T)

52

53         order = np.abs(eigenvalues).argsort()[::-1]
54         return matrix, eigenvalues[order]

55

56     def __run_test(self):
57         """Run singular test."""
58         mat, true_eig = self.__get_test_matrix()
59         test_eig, _ = self.algorithm(mat)
60         test_res = np.alltrue(np.isclose(true_eig, test_eig))
61         self.failed.append(not test_res)

62

63     def __run_tests(self):
64         """Run multiple tests."""
65         for _ in range(self.n):
66             try:
67                 self.__run_test()
```

```python
68              except (KeyboardInterrupt, SystemExit):
69                  self.__save()
70                  sys.exit(0)

72      def run(self):
73          """Distribute tests accross threads."""

75          threadlist = [None] * self.jobs

77          for i in range(self.jobs):
78              threadlist[i] = Thread(target=self.__run_tests, daemon
                    =True)
79              threadlist[i].start()

81          for thread in threadlist:
82              thread.join()

84          self.result = sum(self.failed)
85          self.tests["algorithm"].append(self.algorithm.__name__)
86          self.tests["dimension"].append(self.dim)
87          self.tests["failed"].append(self.result)
88          if self.algorithm.__name__ == "jacobi":
89              self.tests["maxiter"].append(None)
90          else:
91              self.tests["maxiter"].append(self.maxiter)

93      def save(self, header=False):
94          if os.path.exists(self.path):
95                  print("Saving results.")
96          df = pd.DataFrame(self.tests)
97          with open(self.path, 'a') as f:
98              df.to_csv(f, header=header, index=False,
99                      columns=["algorithm", "dimension", "maxiter"
                          , "failed"])
100
```

```python
101
102  # Unit tests
103  if __name__ == "__main__":
104      # Define Flags.
105      JOBS = 20
106      MAXITER = (10, 100, 1000, 10000, 100000)
107      DIMS = range(3, 8)
108      ALGOS = {'jacobi': eigen.jacobi,
109               'qrm': eigen.qrm,
110               'qrm2': eigen.qrm2,
111               'qrm3': eigen.qrm3}
112
113      # Define parameters of all runs.
114      parameters = []
115      for algo in ALGOS.values():
116          for maxiter in MAXITER:
117              for dim in range(3, 8):
118                  param = (algo,
119                           maxiter if algo.__name__ != "jacobi" else
                                None,
120                           dim)
121                  parameters.append(param)
122
123      # Check progress of previous runs.
124      if os.path.exists(data_out):
125          print("Check progress:")
126          required = [(algo.__name__, m, dim) for (algo, m, dim) in
                parameters]
127          required = set(required)
128
129          progress = pd.read_csv(data_out)
130
131          done = []
132          for (a, d, m, _) in progress.values:
133              if np.isnan(m):
```

35

```python
134                   param = (a, None, d)
135               else:
136                   param = (a, int(m), d)
137               done.append(param)
138           done = set(done)
139           print(len(done))
140
141           to_do = required.difference(done)
142           parameters = [(ALGOS[a], m, d) for a, m, d in to_do]
143           print("Perform tests on:")
144           print(to_do)
145           print(len(to_do))
146
147       for algo, maxiter, dim in tqdm(parameters):
148           if algo is eigen.jacobi:
149               algo_test = AlgoTest(filepath=data_out,
150                                    algo=algo,
151                                    dim=dim,
152                                    jobs=JOBS)
153           else:
154               algo_test = AlgoTest(filepath=data_out,
155                                    algo=algo,
156                                    dim=dim,
157                                    maxiter=maxiter,
158                                    jobs=JOBS)
159           algo_test.run()
160
161       algo_test.save()
```

7   References

[Börm and Mehl, 2012] Börm, S. and Mehl, C. (2012). *Numerical Methods for Eigenvalue Problems.* Walter de Gruyter GmbH & Co.KG, Berlin/Boston.

[Gentle, 1998] Gentle, J. E. (1998). *Numerical Linear Algebra for Applications in Statistics.* Springer Science and Business Media, New York.

[Härdle and Simar, 2015] Härdle, W. K. and Simar, L. (2015). *Applied Multivariate Statistical Analysis.* Springer-Verlag Gmbh, Berlin, Heidelberg.

[Hunter, 2007] Hunter, J. D. (2007). Matplotlib: A 2d graphics environment. *Computing In Science & Engineering*, 9(3):90–95.

[McKinney, 2010] McKinney, W. (2010). Data structures for statistical computing in python. In van der Walt, S. and Millman, J., editors, *Proceedings of the 9th Python in Science Conference*, pages 51 – 56.

[van Rossum, 1995] van Rossum, G. (1995). Python tutorial. Technical Report CS-R9526, Centrum voor Wiskunde en Informatica (CWI), Amsterdam.