



HUMBOLDT UNIVERSITÄT ZU BERLIN

SEMINAR PAPER

# Numerical Methods for solving Eigenvalue-Problems

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NUMERICAL INTRODUCTORY COURSE

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# 1 Motivation

---

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 impractical. 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.

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deserunt mollit anim id est laborum.

[3] [2] [1] If  $A$  is an  $n \times n$  matrix,  $v$  is a non-zero vector and  $\lambda$  is a scalar, such that

$$Av = \lambda v \quad (1)$$

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

$$\det(A - \lambda I) = 0 \quad (2)$$

## 2 Similarity Transformations

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

$$A = P^{-1}BP. \quad (3)$$

This transformation defined in 3 is also called a *similarity transformation*. It is obvious that the similarity relationship is commutative as well as transitive. If  $A$  and  $B$  are similar, it holds that

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

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*.

## 2.1 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

$$x = c_1u + c_2v$$

for some scalars  $c_1$  and  $c_2$ . The vector

$$\tilde{x} = -c_1u + c_2v$$

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

$$Q = I - 2uu'. \tag{4}$$

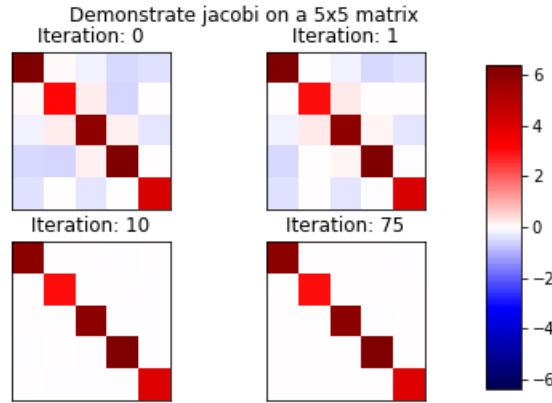
$$\begin{aligned}
Qx &= c_1u + c_2v - 2c_1uuu' - 2c_2vuu' \\
&= c_1u + c_2v - 2c_1u'uu - 2c_2u'vu \\
&= -c_1u + c_2v \\
&= \tilde{x}
\end{aligned}$$

## 2.2 Givens-Rotations

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.

$$V_{pq}(\theta) = \begin{bmatrix} 1 & & & & & & \\ & \ddots & & & & & \\ & & 1 & & & & \\ & & & \cos \theta & \sin \theta & & \\ & & & & \ddots & & \\ & & & -\sin \theta & \cos \theta & & \\ & & & & & 1 & \\ & & & & & & \ddots \\ & & & & & & & 1 \end{bmatrix} \quad (5)$$

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

Figure 1: Progress Jacobi-Method 

### 3 Algorithms

#### 3.1 Jacobi Method

---

**Algorithm 1** jacobi

---

**Require:** symmetric matrix  $A$

**Ensure:**  $0 < precision < 1$

**initialize:**  $L \leftarrow A; U \leftarrow I; L_{max} \leftarrow 1$

**while**  $L_{max} > precision$  **do**

    Find indices  $i, j$  of largest value in lower triangle of  $abs(L)$

$L_{max} \leftarrow L_{i,j}$

$\alpha \leftarrow \frac{1}{2} \cdot \arctan\left(\frac{2A_{i,j}}{A_{i,i} - A_{j,j}}\right)$

$V \leftarrow I$

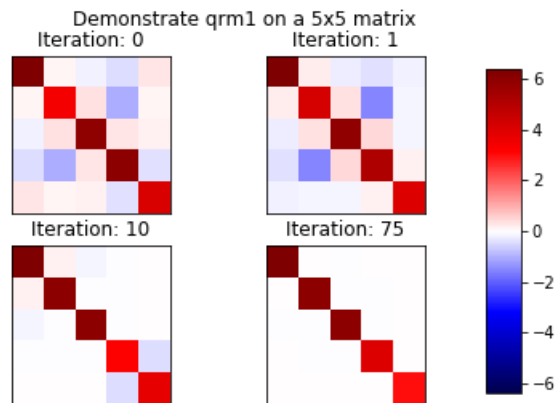
$V_{i,i}, V_{j,j} \leftarrow \cos \alpha; V_{i,j}, V_{j,i} \leftarrow -\sin \alpha, \sin \alpha$

$A \leftarrow V'AV; U \leftarrow UV$

**return**  $diag(A), U$

---



Figure 2: Progress basic QR-Method 

## 3.2 QR-Method

---

### Algorithm 2 QRM1

---

**Require:** square matrix  $A$

---

**initialize:**  $conv \leftarrow False$

**while** not  $conv$  **do**

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

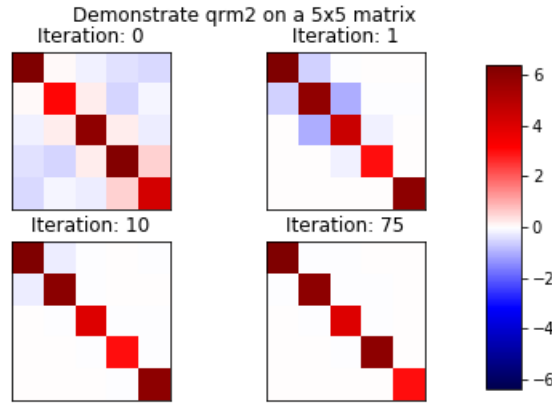
$A \leftarrow RQ$

**if**  $A$  is diagonal **then**

$conv \leftarrow True$

**return**  $diag(A), Q$

---

Figure 3: Progress Hessenberg-QR-Method 

### 3.2.1 Hessenberg Variant

---

#### Algorithm 3 QRM2

---

**Require:** square matrix  $A$

---

$A \leftarrow \text{hessenberg}(A)$

continue with: QRM1(A)

---

### 3.2.2 Accelerated Variant

---

#### Algorithm 4 QRM3

---

**Require:** square matrix  $A \in \mathbb{R}^{p \times p}$

---

$T \leftarrow \text{hessenberg}(A)$ ,  $\text{conv} \leftarrow \text{False}$

**while** not  $\text{conv}$  **do**

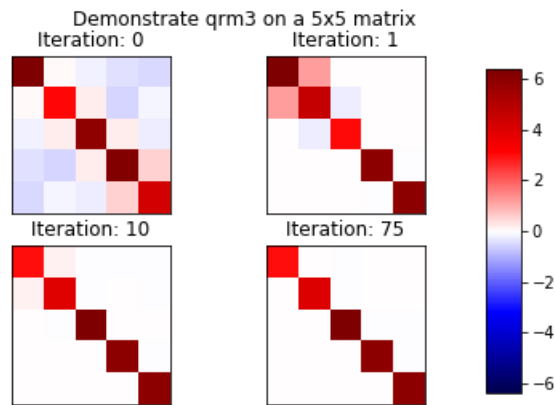
$Q, R \leftarrow \text{QR-Factorization of } T - t_{p-1,p-1}I$

$T \leftarrow RQ + t_{p-1,p-1}I$

**if**  $T$  is diagonal **then**

$\text{conv} \leftarrow \text{True}$   
**return**  $\text{diag}(T), Q$

---

Figure 4: Progress Accelerated QR-Method 

## 4 Analysis

### 4.1 Accuracy

### 4.2 Efficiency

## 5 Conclusion

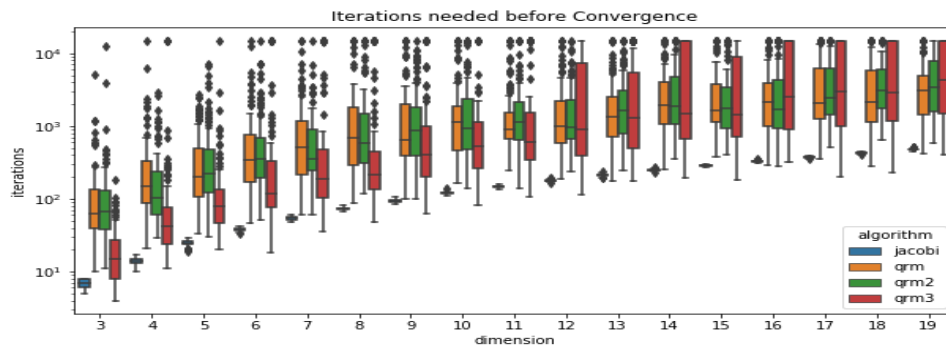
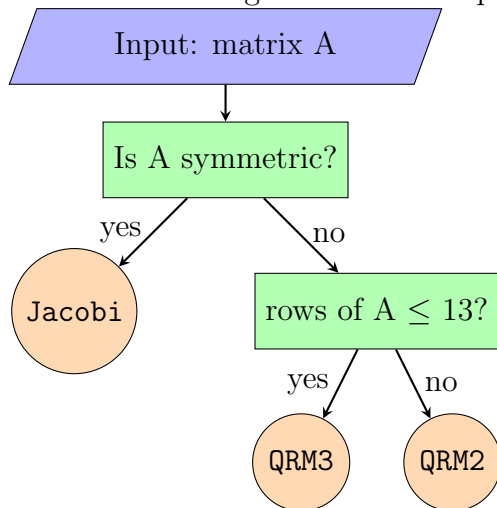
Figure 5: Unit-tests: Iterations 

Figure 6: Decision process of final eigenvalue routine



## 6 Appendix

### 6.1 Eigenvalue Routines

```
1 import numpy as np
2 import copy
3
4
5 def hreflect1D(x):
6     """
7     Calculate Householder reflection:  $Q = I - 2*uu'$ .
8
9     Parameters:
10        X: numpy array.
11
12     Returns:
13        Qx: reflected vector.
14        Q: Reflector (matrix).
15     """
16     # Construct v:
17     v = copy.deepcopy(x)
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
41             Hessenberg-
42             matrix.
43
44     Returns:
45         Q: square numpy ndarray, same shape as X. Rotation matrix.
46         R: square numpy ndarray, same shape as X. Upper triangular
47             matrix if
48             offset is 0, Hessenberg-matrix if offset is 1.
49     """
50     assert offset in [0, 1]
51     assert type(X) == np.ndarray
52     assert X.shape[0] == X.shape[1]
53
54     R = copy.deepcopy(X)
55     Q = np.eye(X.shape[0])

```

```

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:  $U^T A U = E$  s.t.  $E$  is a diagonal matrix.
19
20     Parameters:

```

```

21     A - 2x2 numpy array.
22     Returns:
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
46     value
47     U - 2D numpy array with associated eigenvectors (column).
48     """
49     assert 0 < precision < 1.
50     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
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
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
105             , n))))
106
107     if not conv:
108         warnings.warn("Convergence was not reached. Consider
109             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
118     the
119
120     Eigenvalues and Eigenvectors using the QR-Method.
121
122     Parameters:
123         - X: square numpy ndarray.
124
125     Returns:
126         - Eigenvalues of A.
127         - Eigenvectors of A.
128     """
129     n, m = X.shape
130     assert n == m
131
132     # First stage: transform to upper Hessenberg-matrix.
133     A = lin.hessenberg(X)
134     conv = False
135     k = 0
136
137     # Second stage: perform QR-transformations.
138     while (not conv) and (k < maxiter):
139         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
141         , n))))
142
143     if not conv:
144         warnings.warn("Convergence was not reached. Consider
145             raising maxiter.")
146     if debug:
147         return k
148     Evals = A.diagonal()
149     order = np.abs(Evals).argsort()[::-1]
150     return Evals[order], Q[order, :]
151
152 def qrm3(X, maxiter=15000, debug=False):
153     """
154     First compute similar matrix in Hessenberg form, then compute
155     the
156     Eigenvalues and Eigenvectors using the QR-Method.
157
158     Parameters:
159         - X: square numpy ndarray.
160
161     Returns:
162         - Eigenvalues of A.
163         - Eigenvectors of A.
164     """
165     n, m = X.shape
166     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
178             , n))))
179
180     if not conv:
181         warnings.warn("Convergence was not reached. Consider
182             raising maxiter.")
183
184     if debug:
185         return k
186
187     Evals = T.diagonal()
188     order = np.abs(Evals).argsort()[::-1]
189     return Evals[order], Q[order, :]

```

## 6.2 Analysis: Figures

```

1 import os
2 import copy

```

```
3 import pandas as pd
4 import numpy as np
5 import seaborn as sns
6 from scipy import linalg as lin
7 from scipy.stats import ortho_group
8 from matplotlib import pyplot as plt
9
10 datadir = os.path.join("analysis", "benchmarks.csv")
11 outpath = os.path.join("media", "plots")
12 trials = pd.read_csv(datadir, index_col=0)
13
14 trials.groupby(["algorithm", "dimension"]).iterations.describe()
15
16 # Boxplot iteration:
17 fig = plt.figure(figsize=(10, 5))
18 sns.boxplot(x="dimension", y="iterations", hue="algorithm", data=
    trials)
19 plt.yscale("log")
20 plt.title("Iterations needed before Convergence")
21 plt.savefig(os.path.join(outpath, "iterations_boxplot.png"))
22 plt.show()
23 plt.close()
24
25 # Boxplot elapsed time:
26 fig = plt.figure(figsize=(10, 5))
27 sns.boxplot(x="dimension", y="time", hue="algorithm", data=trials)
28 plt.title("Time needed before Convergence")
29 plt.ylabel("time (sec)")
30 plt.yscale('log')
31 plt.savefig(os.path.join(outpath, "time_boxplot.png"))
```

```

32 plt.show()
33 plt.close()
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('
58                                                         seismic'),
59                                                         vmin=-X.max(),
60                                                         vmax=X.max())
61
62                 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
65         if i > 75:
66             break
67
68         fig.subplots_adjust(right=0.8)
69         cbar_ax = fig.add_axes([0.85, 0.15, 0.05, 0.7])
70         fig.colorbar(hm, cax=cbar_ax)
71
72         sup_title = "Demonstrate {} on a {}x{} matrix".format(
73             func.__name__,
74             *X.shape)
75
76         fig.suptitle(sup_title)
77         fig.savefig(savepath)
78
79         return fig, ax
80
81     return plotter
82
83 @plot_factory
84 def jacobi():
85     """
86     Compute Eigenvalues and Eigenvectors for symmetric matrices
87     using the
88     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
96
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]))
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
116     QR-Method.
117
118     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
136     QR-Method.
137
138     Yields:
139         - T: 2D-numpy array. Similar matrix to X.
140         """
141         # First stage: transform to upper Hessenberg-matrix.
142         T = lin.hessenberg(X)
143
144         k = 0
145         # Second stage: perform QR-transformations.
146         while k < 5000:
147             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
158     the
159     Eigenvalues and Eigenvectors using the accelerated QR-Method.
160
161     Yields:
162     * T - 2D numpy array of current iteration step.
163     """
164     # First stage: transform to upper Hessenberg-matrix.
165     T = lin.hessenberg(X)
166     k = 0
167     n, _ = X.shape
168
169     # Second stage: perform QR-transformations.
170     while k < 5000:
171         if k == 0:
172             yield X
173             k += 1
174             Q, R = np.linalg.qr(T - T[n-1, n-1] * np.eye(n))
175             T = R.dot(Q) + T[n-1, n-1] * np.eye(n)

```

```
176         yield T
177
178
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"))
183
184     plt.show()
185     plt.close()
```

### 6.3 Analysis: Unit tests

```
1  """
2  Automated tests for different algorithms.
3  """
4  import os
5  import numpy as np
6  import threading
7  import pandas as pd
8  from algorithms import eigen
9  from scipy.stats import ortho_group
10 from tqdm import trange, tqdm
11
12 data_out = os.path.join("data", "accuracy_tests.csv")
13
14
15 def get_test_matrix(dim):
16     """Return matrix with associated Eigenvalues."""
```

```
17     eigenvalues = np.random.uniform(size=dim)
18     eigenvectors = ortho_group.rvs(dim=dim)
19     Lambda = np.diag(eigenvalues)
20
21     matrix = np.dot(eigenvectors, Lambda).dot(eigenvectors.T)
22
23     order = np.abs(eigenvalues).argsort()[::-1]
24     return matrix, eigenvalues[order]
25
26
27 def test_algo(algo, Ntests=1000, dim=3, *args, **kwargs):
28     """
29     Test routine that allows for threading. Note that the
30     variables:
31     failed, critical and problematic need to be defined in the
32     enveloping or
33     global scope beforehand.
34
35     Parameters:
36
37     - algo: algorithm to be tested
38     - Ntests: number of tests to compute
39     - dim: dimensions of matrix
40     - *args, **kwargs: additional arguments to be passed to
41       algo.
42
43     Returns:
44
45     - None, but will update the variables failed, critical and
46       problematic.
47     + failed: number of failed tests
48     + critical: number of ZeroDivisionErrors
```

```
43         + problematic: list of numpy arrays which led to wrong
          eigenvalues.
44
45     """
46     global failed
47     global critical
48     global problematic
49
50     for _ in range(Ntests):
51         try:
52             A, true_eig = get_test_matrix(dim=dim)
53             my_eig, _ = algo(A, *args, **kwargs)
54             assert np.alltrue(np.isclose(my_eig, true_eig))
55
56         except AssertionError:
57             failed += 1
58             problematic.append(A)
59
60         except ZeroDivisionError:
61             critical += 1
62
63 def threaded_tests(algo, N, nWorkers=10, verbose=True, *args, **
64     kwargs):
65     global failed
66     global critical
67     global problematic
68
69     assert N % nWorkers == 0
70
71     n = N // nWorkers
```

```
71     threadlist = [None] * nWorkers
72
73     for i in range(nWorkers):
74         threadlist[i] = threading.Thread(target=test_algo,
75                                         args=(algo, n, *args))
76         threadlist[i].start()
77
78     for i in range(nWorkers):
79         threadlist[i].join()
80
81     logstr = """
82     {} out of {} tests failed.
83     {} tests failed critically.
84     """.format(failed, N, critical)
85
86     if verbose:
87         print(logstr)
88
89
90 # Tests
91 results = {
92     "algorithm": [],
93     "dimension": [],
94     "maxiter": [],
95     "failed": []}
96
97 for algo in tqdm([eigen.jacobi, eigen.qrm, eigen.qrm2, eigen.qrm3
98 ]):
99     for dim in trange(3, 15):
100         for maxiter in 1000, 10000, 100000:
```

```
100         if algo.__name__ == eigen.jacobi:
101             maxiter = 1e-6
102             failed = 0
103             critical = 0
104             problematic = []
105             threaded_tests(algo, 1000, 20, False, dim, maxiter)
106             results["algorithm"].append(algo.__name__)
107             results["dimension"].append(dim)
108             results["maxiter"].append(maxiter)
109             results["failed"].append(failed)
110
111 test_data = pd.DataFrame(results)
112 test_data.to_csv(data_out)
```

## References

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- [3] Wolfgang K. Härdle and Léopold Simar. *Applied Multivariate Statistical Analysis*. Springer-Verlag GmbH, Berlin, Heidelberg, 2015.