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

Diese Dokumentation enth"alt eine sortierte Liste der wichtigsten LaTeX–Befehle. Die einzelnen Listeneintr"age sind untereinander durch viele Querverweise verkettet, die ein Auffinden inhaltlich zusammengeh"origer Informationen erheblich erleichtern.

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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,

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

2 Similarity Transformations

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

$$A = P^{-1}BP. \tag{3}$$

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

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

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

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

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

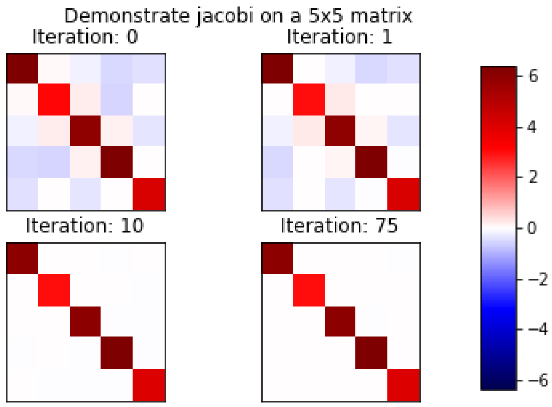
2.2 Givens-Rotations

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.

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

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 $abs(L)$

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

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

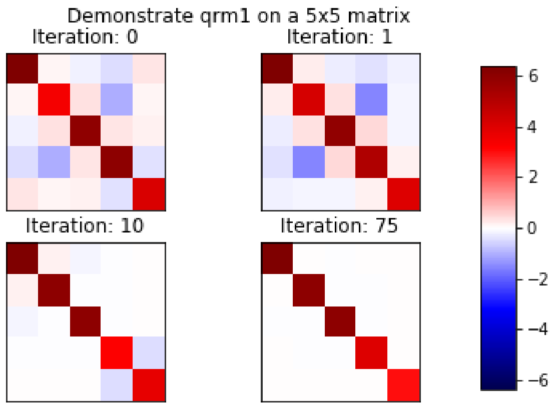
$V \leftarrow I$

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

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

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

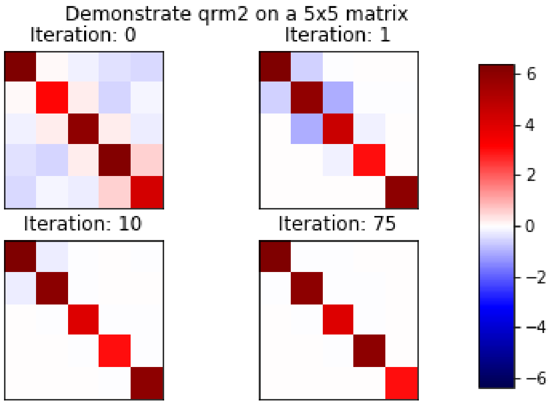
$A \leftarrow RQ$

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

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

continue with: QRM1(A)

3.2.2 Accelerated Variant

Algorithm 4 `QRM3`

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

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

while not $conv$ **do**

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

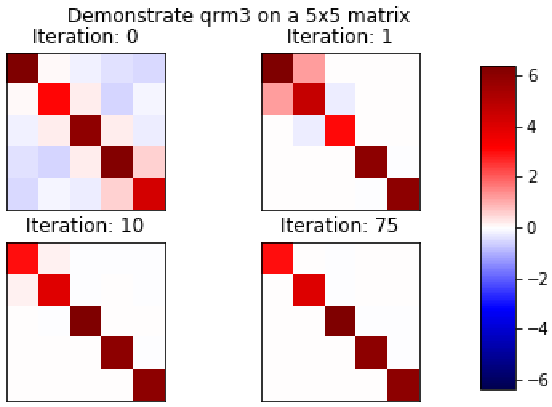
$T \leftarrow RQ + t_{p-1,p-1}I$

if T is diagonal **then**

$conv \leftarrow True$

return $diag(T), Q$

Figure 4: Progress Accelerated QR-Method



4 Analysis

4.1 Accuracy

4.2 Efficiency

5 Conclusion

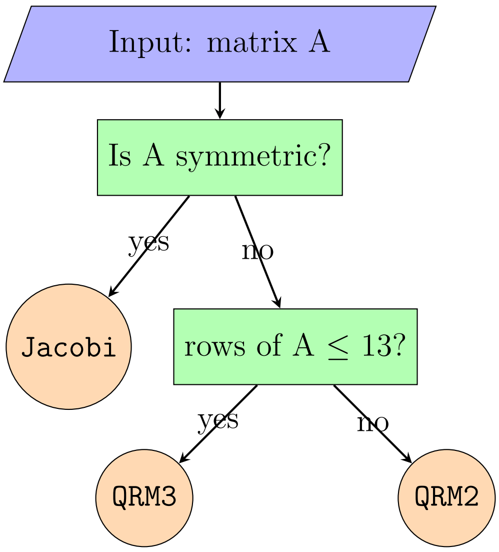
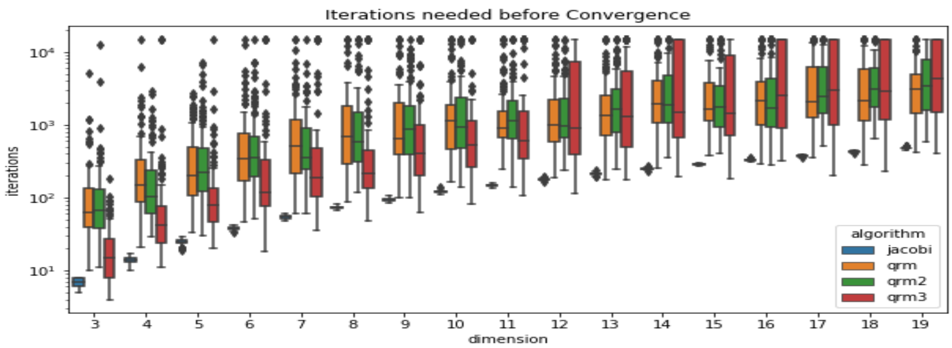


Figure 5: Unit-tests: Iterations



6 Appendix

6.1 Eigenvalue Routines

```
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)
    v[0] += np.linalg.norm(x)

    # Construct u: normalize v.
    vnorm = np.linalg.norm(v)
    if vnorm:
        u = v / np.linalg.norm(v)
    else:
        u = v

    # Construct Q:
    Q = np.eye(len(x)) - 2 * np.outer(u, u)
    Qx = np.dot(Q, x)

    return Qx, Q


def qr_factorize(X, offset=0):
    """
    Compute QR factorization of X s.t. QR = X.

    Parameters:
        - X: square numpy ndarray.
        - offset: (int) either 0 or 1. If offset is unity: compute Hessenberg-
                   matrix.

    Returns:
        Q: square numpy ndarray, same shape as X. Rotation matrix.
```

```
        R: square numpy ndarray, same shape as X. Upper triangular matrix if
           offset is 0, Hessenberg-matrix if offset is 1.
    """
    assert offset in [0, 1]
    assert type(X) == np.ndarray
    assert X.shape[0] == X.shape[1]

    R = copy.deepcopy(X)
    Q = np.eye(X.shape[0])

    for i in range(X.shape[0]-offset):
        Pi = np.eye(R.shape[0])
        _, Qi = hreflect1D(R[i+offset:, i])
        Pi[i+offset:, i+offset:] = Qi

        Q = Pi.dot(Q)
        R = Pi.dot(R)

    return Q.T, R
```

```
"""
Algorithms for solving eigenvalue problems.

1. Compute diagonalization of 2x2 matrices via jacobi iteration.
2. Generalize Jacobi iteration for symmetric matrices.
"""
import numpy as np
import copy
import warnings
```

```python
from scipy import linalg as lin
from algorithms import helpers


def jacobi2x2(A):
    """
    Diagonalize a 2x2 matrix through jacobi step.

    Solve: U' A U = E s.t. E is a diagonal matrix.

    Parameters:
        A - 2x2 numpy array.
    Returns:
        A - 2x2 diagonal numpy array
    """
    assert type(A) == np.ndarray
    assert A.shape == (2, 2)
    assert A[1, 0] == A[0, 1]

    alpha = 0.5 * np.arctan(2*A[0, 1]/(A[1, 1] - A[0, 0]))
    U = np.array([[np.cos(alpha), np.sin(alpha)],
                  [-np.sin(alpha), np.cos(alpha)]])
    E = np.matmul(U.T, np.matmul(A, U))
    return E


def jacobi(X, precision=1e-6, debug=False):
    """
    Compute Eigenvalues and Eigenvectors for symmetric matrices.

```

```
    Parameters:
        X - 2D numpy ndarray which represents a symmetric matrix
        precision - float in (0, 1). Convergence criterion.

    Returns:
        A - 1D numpy array with eigenvalues sorted by absolute
          value
        U - 2D numpy array with associated eigenvectors (column).
    """
    assert 0 < precision < 1.
    assert type(X) == np.ndarray
    n, m = X.shape
    assert n == m
    assert all(np.isclose(X - X.T, np.zeros(n)).flatten())
    A = copy.deepcopy(X)
    U = np.eye(A.shape[0])
    L = np.array([1])
    iterations = 0

    while L.max() > precision:
        L = np.abs(np.tril(A, k=0) - np.diag(A.diagonal()))
        i, j = np.unravel_index(L.argmax(), L.shape)
        alpha = 0.5 * np.arctan(2*A[i, j] / (A[i, i]-A[j, j]))

        V = np.eye(A.shape[0])
        V[i, i], V[j, j] = np.cos(alpha), np.cos(alpha)
        V[i, j], V[j, i] = -np.sin(alpha), np.sin(alpha)

        A = np.dot(V.T, A.dot(V))
        U = U.dot(V)
```

```
            iterations += 1

    # Sort by eigenvalue (descending order) and flatten A
    A = np.diag(A)
    order = np.abs(A).argsort()[::-1]
    if debug:
        return iterations

    return A[order], U[:, order]


def qrm(X, maxiter=15000, debug=False):
    """
    Compute Eigenvalues and Eigenvectors using the QR-Method.

    Parameters:
        - X: square numpy ndarray.
    Returns:
        - Eigenvalues of A.
        - Eigenvectors of A.
    """
    n, m = X.shape
    assert n == m

    # First stage: transform to upper Hessenberg-matrix.
    A = copy.deepcopy(X)
    conv = False
    k = 0

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

```
    while (not conv) and (k < maxiter):
        k += 1
        Q, R = helpers.qr_factorize(A)
        A = R.dot(Q)

        conv = np.alltrue(np.isclose(np.tril(A, k=-1), np.zeros((n
          , n))))

    if not conv:
        warnings.warn("Convergence was not reached. Consider
          raising maxiter.")
    if debug:
        return k
    Evals = A.diagonal()
    order = np.abs(Evals).argsort()[::-1]
    return Evals[order], Q[order, :]


def qrm2(X, maxiter=15000, debug=False):
    """
    First compute similar matrix in Hessenberg form, then compute
      the
    Eigenvalues and Eigenvectors using the QR-Method.

    Parameters:
        - X: square numpy ndarray.
    Returns:
        - Eigenvalues of A.
        - Eigenvectors of A.
    """
```

```
    n, m = X.shape
    assert n == m

    # First stage: transform to upper Hessenberg-matrix.
    A = lin.hessenberg(X)
    conv = False
    k = 0

    # Second stage: perform QR-transformations.
    while (not conv) and (k < maxiter):
        k += 1
        Q, R = helpers.qr_factorize(A)
        A = R.dot(Q)

        conv = np.alltrue(np.isclose(np.tril(A, k=-1), np.zeros((n
          , n))))

    if not conv:
        warnings.warn("Convergence was not reached. Consider
          raising maxiter.")
    if debug:
        return k
    Evals = A.diagonal()
    order = np.abs(Evals).argsort()[::-1]
    return Evals[order], Q[order, :]


def qrm3(X, maxiter=15000, debug=False):
    """
    First compute similar matrix in Hessenberg form, then compute
```

```
        the
    Eigenvalues and Eigenvectors using the QR-Method.

    Parameters:
        - X: square numpy ndarray.
    Returns:
        - Eigenvalues of A.
        - Eigenvectors of A.
    """
    n, m = X.shape
    assert n == m

    # First stage: transform to upper Hessenberg-matrix.
    T = lin.hessenberg(X)

    conv = False
    k = 0

    # Second stage: perform QR-transformations.
    while (not conv) and (k < maxiter):
        k += 1
        Q, R = helpers.qr_factorize(T - T[n-1, n-1] * np.eye(n))
        T = R.dot(Q) + T[n-1, n-1] * np.eye(n)

        conv = np.alltrue(np.isclose(np.tril(T, k=-1), np.zeros((n
          , n))))

    if not conv:
        warnings.warn("Convergence was not reached. Consider
          raising maxiter.")
```

```
    if debug:
        return k
    Evals = T.diagonal()
    order = np.abs(Evals).argsort()[::-1]
    return Evals[order], Q[order, :]
```

6.2 Analysis: Figures

```
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()

# Visualize Algorithm-Progress:
np.random.seed(42)
size = 5
Lambda = np.diag(np.random.randint(low=0, high=10, size=size))
G = ortho_group.rvs(dim=size)
X = np.dot(G, Lambda.dot(G.T))


def plot_factory(func):
    def plotter(savepath, **fig_kw):
        def algorithm_generator(*args, **kwargs):
            return func(*args, **kwargs)

        fig, ax = plt.subplots(nrows=2, ncols=2, **fig_kw)
        algorithm_iterator = algorithm_generator()
        j = -1
```

```

        for i, A in enumerate(algorithm_iterator):
            if i in (0, 1, 10, 75):
                j += 1

                hm = ax[j // 2, j % 2].imshow(A,
                                              cmap=plt.get_cmap('seismic'),
                                              vmin=-X.max(),
                                              vmax=X.max())
                ax[j // 2, j % 2].set_yticks([])
                ax[j // 2, j % 2].set_xticks([])
                ax[j // 2, j % 2].set_title("Iteration: " + str(i))

                if i > 75:
                    break

        fig.subplots_adjust(right=0.8)
        cbar_ax = fig.add_axes([0.85, 0.15, 0.05, 0.7])
        fig.colorbar(hm, cax=cbar_ax)

        sup_title = "Demonstrate {} on a {}x{} matrix".format(
            func.__name__,
            *X.shape)

        fig.suptitle(sup_title)
        fig.savefig(savepath)

        return fig, ax
```

```python

    return plotter


@plot_factory
def jacobi():
    """
    Compute Eigenvalues and Eigenvectors for symmetric matrices
      using the
    jacobi method.

    Yields:
        * A - 2D numpy array of current iteration step.
    """
    A = copy.deepcopy(X)
    U = np.eye(A.shape[0])
    L = np.array([1])
    iterations = 0

    while iterations < 5000:
        L = np.abs(np.tril(A, k=0) - np.diag(A.diagonal()))
        i, j = np.unravel_index(L.argmax(), L.shape)
        alpha = 0.5 * np.arctan(2*A[i, j] / (A[i, i]-A[j, j]))

        V = np.eye(A.shape[0])
        V[i, i], V[j, j] = np.cos(alpha), np.cos(alpha)
        V[i, j], V[j, i] = -np.sin(alpha), np.sin(alpha)

        A = np.dot(V.T, A.dot(V))
        U = U.dot(V)
```

```
            iterations += 1
            yield A


@plot_factory
def qrm1():
    """
    Create generator for transformed matrices after applying the
      QR-Method.

    Yields:
        - T: 2D-numpy array. Similar matrix to X.
    """
    # First stage: transform to upper Hessenberg-matrix.
    T = copy.deepcopy(X)

    k = 0
    # Second stage: perform QR-transformations.
    while k < 5000:
        k += 1
        Q, R = np.linalg.qr(T)
        T = R.dot(Q)
        yield T


@plot_factory
def qrm2():
    """
    Create generator for transformed matrices after applying the
      QR-Method.
```

```

    Yields:
        - T: 2D-numpy array. Similar matrix to X.
    """
    # First stage: transform to upper Hessenberg-matrix.
    T = lin.hessenberg(X)

    k = 0
    # Second stage: perform QR-transformations.
    while k < 5000:
        if k == 0:
            yield X
        k += 1
        Q, R = np.linalg.qr(T)
        T = R.dot(Q)
        yield T


@plot_factory
def qrm3():
    """
    First compute similar matrix in Hessenberg form, then compute the
    Eigenvalues and Eigenvectors using the accelerated QR-Method.

    Yields:
        * T - 2D numpy array of current iteration step.
    """
    # First stage: transform to upper Hessenberg-matrix.
    T = lin.hessenberg(X)
```

```
    k = 0
    n, _ = X.shape

    # Second stage: perform QR-transformations.
    while k < 5000:
        if k == 0:
            yield X
        k += 1
        Q, R = np.linalg.qr(T - T[n-1, n-1] * np.eye(n))
        T = R.dot(Q) + T[n-1, n-1] * np.eye(n)

        yield T


jacobi(os.path.join(outpath, "jacobi.png"))
qrm1(os.path.join(outpath, "qrm1.png"))
qrm2(os.path.join(outpath, "qrm2.png"))
qrm3(os.path.join(outpath, "qrm3.png"))

plt.show()
plt.close()
```

6.3 Analysis: Unit tests

```
"""
Automated tests for different algorithms.
"""
import os
import numpy as np
```

```python
import threading
import pandas as pd
from algorithms import eigen
from scipy.stats import ortho_group
from tqdm import trange, tqdm

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


def get_test_matrix(dim):
    """Return matrix with assosiated Eigenvalues."""
    eigenvalues = np.random.uniform(size=dim)
    eigenvectors = ortho_group.rvs(dim=dim)
    Lambda = np.diag(eigenvalues)

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

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


def test_algo(algo, Ntests=1000, dim=3, *args, **kwargs):
    """
    Test routine that allows for threading. Note that the variables:
    failed, critical and problematic need to be defined in the enveloping or
    global scope beforehand.

    Parameters:
```

```
        - algo: algorithm to be tested
        - Ntests: number of tests to compute
        - dim: dimensions of matrix
        - *args, **kwargs: additional arguments to be passed to algo.

    Returns:
        - None, but will update the variables failed, critical and problematic.
            + failed: number of failed tests
            + critical: number of ZeroDivisionErrors
            + problematic: list of numpy arrays which led to wrong eigenvalues.
    """
    global failed
    global critical
    global problematic

    for _ in range(Ntests):
        try:
            A, true_eig = get_test_matrix(dim=dim)
            my_eig, _ = algo(A, *args, **kwargs)
            assert np.alltrue(np.isclose(my_eig, true_eig))

        except AssertionError:
            failed += 1
            problematic.append(A)

        except ZeroDivisionError:
            critical += 1
```

```python


def threaded_tests(algo, N, nWorkers=10, verbose=True, *args, **
    kwargs):
    global failed
    global critical
    global problematic

    assert N % nWorkers == 0

    n = N // nWorkers
    threadlist = [None] * nWorkers

    for i in range(nWorkers):
        threadlist[i] = threading.Thread(target=test_algo,
                                         args=(algo, n, *args))
        threadlist[i].start()

    for i in range(nWorkers):
        threadlist[i].join()

    logstr = """
    {} out of {} tests failed.
    {} tests failed critically.
    """.format(failed, N, critical)

    if verbose:
        print(logstr)


```

```
# Tests
results = {
    "algorithm": [],
    "dimension": [],
    "maxiter": [],
    "failed": []}

for algo in tqdm([eigen.jacobi, eigen.qrm, eigen.qrm2, eigen.qrm3
 ]):
    for dim in trange(3, 15):
        for maxiter in 1000, 10000, 100000:
            if algo.__name__ == eigen.jacobi:
                maxiter = 1e-6
            failed = 0
            critical = 0
            problematic = []
            threaded_tests(algo, 1000, 20, False, dim, maxiter)
            results["algorithm"].append(algo.__name__)
            results["dimension"].append(dim)
            results["maxiter"].append(maxiter)
            results["failed"].append(failed)

test_data = pd.DataFrame(results)
test_data.to_csv(data_out)
```

References

[1] Seffen Börm and Christian Mehl. *Numerical Methods for Eigenvalue Problems.* Walter de Gruyter GmbH & Co.KG, Berlin/Boston, 2012.

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

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