

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 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.

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deserunt mollit anim id est laborum.

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,

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

2 Similarity Transformations

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

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

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

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

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.

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

$$Q = I - 2uu'. (4)$$

$$Qx = c_1 u + c_2 v - 2c_1 u u u' - 2c_2 v u u'$$

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

$$= -c_1 u + c_2 v$$

$$= \tilde{x}$$

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.

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

Figure 1: Progress Jacobi-Method Q

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)

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

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

$$V \leftarrow I$$

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

$$\begin{matrix} A \leftarrow V'AV; \ U \leftarrow UV \\ \mathbf{return} \ diag(A), U \end{matrix}$$

3.2 QR-Method 3 ALGORITHMS

Figure 2: Progress basic QR-Method Demonstrate qrm1 on a 5x5 matrix Iteration: 0 Iteration: 1

Iteration: 10 Iteration: 75

Iteration: 75

3.2 QR-Method

Algorithm 2 QRM1

Require: square matrix A

initialize: $conv \leftarrow False$

while not conv do

 $Q, R \leftarrow \text{QR-Factorization of } A$

 $A \leftarrow RQ$

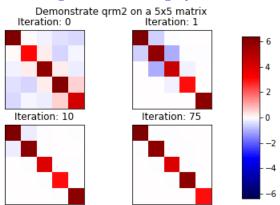
if A is diagonal then

 $conv \gets \mathtt{True}$

 $\mathbf{return}\ diag\left(A\right) ,Q$

3.2 QR-Method 3 ALGORITHMS

Figure 3: Progress Hessenberg-QR-Method Q



3.2.1 Hessenberg Variant

Algorithm 3 QRM2

Require: square matrix A

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

continue with: QRM1(A)

3.2.2 Accelerated Variant

Algorithm 4 QRM3

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

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

while not 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

 $\mathbf{return} \overset{conv}{diag} \overset{-}{(T)}, \overset{True}{Q}$

Demonstrate qrm3 on a 5x5 matrix Iteration: 0 Iteration: 1 Iteration: 10 Iteration: 75

Figure 4: Progress Accelerated QR-Method Q

Analysis

- 4.1 Accuracy
- 4.2 **Efficiency**
- Conclusion **5**

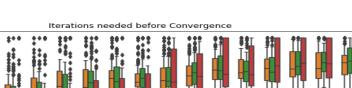
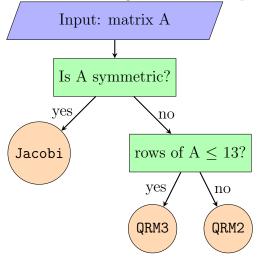


Figure 5: Unit-tests: Iterations Q

Figure 6: Decision process of final eigenvalue routine



6 Appendix

6.1 Eigenvalue Routines

```
import numpy as np
2 import copy
  def hreflect1D(x):
      Calculate Householder reflection: Q = I - 2*uu'.
      Parameters:
          X: numpy array.
10
11
      Returns:
12
          Qx: reflected vector.
13
          Q: Reflector (matrix).
14
      n n n
15
      # Construct v:
16
      v = copy.deepcopy(x)
17
      v[0] += np.linalg.norm(x)
18
19
      # Construct u: normalize v.
20
      vnorm = np.linalg.norm(v)
21
      if vnorm:
22
          u = v / np.linalg.norm(v)
      else:
          u = v
26
```

```
# Construct Q:
27
       Q = np.eye(len(x)) - 2 * np.outer(u, u)
28
       Qx = np.dot(Q, x)
29
30
       return Qx, Q
31
32
33
  def qr_factorize(X, offset=0):
34
       n n n
35
       Compute QR factorization of X s.t. QR = X.
36
37
       Parameters:
38
           - X: square numpy ndarray.
39
           - offset: (int) either 0 or 1. If offset is unity: compute
40
              Hessenberg -
                       matrix.
41
42
       Returns:
43
           {\it Q}: \ {\it square numpy ndarray} , same shape as X. Rotation matrix.
44
           R: square numpy ndarray, same shape as X. Upper triangular
45
              matrix if
               offset is 0, Hessenberg-matrix if offset is 1.
46
       11 11 11
47
       assert offset in [0, 1]
48
       assert type(X) == np.ndarray
49
       assert X.shape[0] == X.shape[1]
50
51
      R = copy.deepcopy(X)
52
       Q = np.eye(X.shape[0])
53
54
```

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

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

```
A - 2x2 numpy array.
21
       Returns:
22
           A - 2x2 diagonal numpy array
23
24
       assert type(A) == np.ndarray
25
       assert A.shape == (2, 2)
26
       assert A[1, 0] == A[0, 1]
27
28
       alpha = 0.5 * np.arctan(2*A[0, 1]/(A[1, 1] - A[0, 0]))
29
       U = np.array([[np.cos(alpha), np.sin(alpha)],
30
                       [-np.sin(alpha), np.cos(alpha)]])
31
       E = np.matmul(U.T, np.matmul(A, U))
32
       return E
33
34
35
  def jacobi(X, precision=1e-6, debug=False):
37
       Compute Eigenvalues and Eigenvectors for symmetric matrices.
38
39
       Parameters:
40
           X - 2D numpy ndarray which represents a symmetric matrix
41
           precision - float in (0, 1). Convergence criterion.
42
43
       Returns:
44
           A - 1D numpy array with eigenvalues sorted by absolute
45
             value
           \it U - 2D numpy array with associated eigenvectors (column).
46
       \boldsymbol{n} \boldsymbol{n} \boldsymbol{n}
47
       assert 0 < precision < 1.
48
       assert type(X) == np.ndarray
49
```

```
n, m = X.shape
50
      assert n == m
51
      assert all(np.isclose(X - X.T, np.zeros(n)).flatten())
52
      A = copy.deepcopy(X)
53
      U = np.eye(A.shape[0])
54
      L = np.array([1])
55
      iterations = 0
56
57
      while L.max() > precision:
58
           L = np.abs(np.tril(A, k=0) - np.diag(A.diagonal()))
59
           i, j = np.unravel_index(L.argmax(), L.shape)
60
           alpha = 0.5 * np.arctan(2*A[i, j] / (A[i, i]-A[j, j]))
61
62
           V = np.eye(A.shape[0])
63
           V[i, i], V[j, j] = np.cos(alpha), np.cos(alpha)
64
           V[i, j], V[j, i] = -np.sin(alpha), np.sin(alpha)
66
           A = np.dot(V.T, A.dot(V))
67
           U = U.dot(V)
68
           iterations += 1
69
70
      # Sort by eigenvalue (descending order) and flatten A
71
      A = np.diag(A)
72
      order = np.abs(A).argsort()[::-1]
73
      if debug:
74
           return iterations
75
76
      return A[order], U[:, order]
77
78
79
```

```
def qrm(X, maxiter=15000, debug=False):
81
       Compute Eigenvalues and Eigenvectors using the QR-Method.
82
83
       Parameters:
84
           - X: square numpy ndarray.
85
       Returns:
86
           - Eigenvalues of A.
87
           - Eigenvectors of A.
88
       n n n
89
       n, m = X.shape
90
       assert n == m
91
92
       \hbox{\it\# First stage: transform to upper Hessenberg-matrix.}
93
       A = copy.deepcopy(X)
94
       conv = False
       k = 0
96
97
       # Second stage: perform QR-transformations.
98
       while (not conv) and (k < maxiter):
99
           k += 1
100
           Q, R = helpers.qr_factorize(A)
101
           A = R.dot(Q)
102
103
           conv = np.alltrue(np.isclose(np.tril(A, k=-1), np.zeros((n
104
              , n))))
105
       if not conv:
106
           warnings.warn("Convergence was not reached. Consider
107
             raising maxiter.")
```

```
if debug:
108
            return k
109
       Evals = A.diagonal()
110
       order = np.abs(Evals).argsort()[::-1]
111
       return Evals[order], Q[order, :]
112
113
114
   def qrm2(X, maxiter=15000, debug=False):
115
        n n n
116
       First compute similar matrix in Hessenberg form, then compute
117
         the
       \label{lem:eigenvalues} \textit{Eigenvectors using the QR-Method}.
118
119
       Parameters:
            - X: square numpy ndarray.
121
        Returns:
122
            - Eigenvalues of A.
123
            - Eigenvectors of A.
124
        n n n
125
       n, m = X.shape
126
        assert n == m
127
128
        # First stage: transform to upper Hessenberg-matrix.
129
       A = lin.hessenberg(X)
130
       conv = False
131
       k = 0
132
133
         \hbox{\it\# Second stage: perform QR-transformations.} \\
134
        while (not conv) and (k < maxiter):
135
            k += 1
136
```

```
Q, R = helpers.qr_factorize(A)
137
           A = R.dot(Q)
138
139
           conv = np.alltrue(np.isclose(np.tril(A, k=-1), np.zeros((n
140
              , n))))
141
       if not conv:
142
           warnings.warn("Convergence was not reached. Consider
143
             raising maxiter.")
       if debug:
144
           return k
145
       Evals = A.diagonal()
146
       order = np.abs(Evals).argsort()[::-1]
147
       return Evals[order], Q[order, :]
148
149
150
  def qrm3(X, maxiter=15000, debug=False):
151
152
       First compute similar matrix in Hessenberg form, then compute
153
       Eigenvalues and Eigenvectors using the QR-Method.
154
155
       Parameters:
156
            - X: square numpy ndarray.
157
       Returns:
158
           - Eigenvalues of A.
159
            - Eigenvectors of A.
160
       H/H/H
161
       n, m = X.shape
162
       assert n == m
163
```

```
164
       # First stage: transform to upper Hessenberg-matrix.
165
       T = lin.hessenberg(X)
166
167
       conv = False
168
169
170
       \# Second stage: perform QR-transformations.
171
       while (not conv) and (k < maxiter):
172
           k += 1
173
           Q, R = helpers.qr_factorize(T - T[n-1, n-1] * np.eye(n))
174
           T = R.dot(Q) + T[n-1, n-1] * np.eye(n)
175
           conv = np.alltrue(np.isclose(np.tril(T, k=-1), np.zeros((n
             , n))))
178
       if not conv:
179
           warnings.warn("Convergence was not reached. Consider
180
             raising maxiter.")
       if debug:
181
           return k
182
       Evals = T.diagonal()
183
       order = np.abs(Evals).argsort()[::-1]
184
       return Evals[order], Q[order, :]
185
```

6.2 Analysis: Figures

```
import os
import copy
```

```
3 import pandas as pd
4 import numpy as np
5 import seaborn as sns
6 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)
13
  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")
21 plt.savefig(os.path.join(outpath, "iterations_boxplot.png"))
  plt.show()
  plt.close()
23
24
25 # Boxplot elapsed time:
fig = plt.figure(figsize=(10, 5))
27 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()
33
34
  # Visualize Algorithm-Progress:
35
np.random.seed(42)
  size = 5
37
  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))
41
42
  def plot_factory(func):
43
      def plotter(savepath, **fig_kw):
44
           def algorithm_generator(*args, **kwargs):
               return func(*args, **kwargs)
47
          fig, ax = plt.subplots(nrows=2, ncols=2, **fig_kw)
48
          algorithm_iterator = algorithm_generator()
49
           j = -1
50
51
          for i, A in enumerate(algorithm_iterator):
52
               if i in (0, 1, 10, 75):
53
                   j += 1
54
55
                   hm = ax[j // 2, j \% 2].imshow(A,
56
                                                    cmap=plt.get_cmap('
57
                                                      seismic'),
                                                    vmin=-X.max(),
58
                                                    vmax=X.max())
59
                   ax[j // 2, j % 2].set_yticks([])
60
```

```
ax[j // 2, j % 2].set_xticks([])
61
                    ax[j // 2, j % 2].set_title("Iteration: " + str(i)
62
                      )
63
                    if i > 75:
64
                         break
65
66
           fig.subplots_adjust(right=0.8)
67
           cbar_ax = fig.add_axes([0.85, 0.15, 0.05, 0.7])
68
           fig.colorbar(hm, cax=cbar_ax)
69
70
           sup_title = "Demonstrate {} on a {}x{} matrix".format(
71
               func.__name__,
72
               *X.shape)
73
74
           fig.suptitle(sup_title)
75
           fig.savefig(savepath)
76
77
           return fig, ax
78
79
       return plotter
80
81
82
  @plot_factory
83
  def jacobi():
84
       n n n
85
       Compute Eigenvalues and Eigenvectors for symmetric matrices
86
        using the
       jacobi method.
87
88
```

```
Yields:
89
            * A - 2D numpy array of current iteration step.
90
       11 11 11
91
       A = copy.deepcopy(X)
92
       U = np.eye(A.shape[0])
93
       L = np.array([1])
94
       iterations = 0
95
96
       while iterations < 5000:
97
           L = np.abs(np.tril(A, k=0) - np.diag(A.diagonal()))
98
           i, j = np.unravel_index(L.argmax(), L.shape)
99
            alpha = 0.5 * np.arctan(2*A[i, j] / (A[i, i]-A[j, j]))
100
101
           V = np.eye(A.shape[0])
102
           V[i, i], V[j, j] = np.cos(alpha), np.cos(alpha)
103
           V[i, j], V[j, i] = -np.sin(alpha), np.sin(alpha)
104
105
           A = np.dot(V.T, A.dot(V))
106
           U = U.dot(V)
107
            iterations += 1
108
           yield A
109
110
111
  @plot_factory
112
  def qrm1():
113
       n n n
114
       Create generator for transformed matrices after applying the
115
         QR-Method.
116
       Yields:
117
```

```
- T: 2D-numpy array. Similar matrix to X.
118
       n n n
119
       # First stage: transform to upper Hessenberg-matrix.
120
       T = copy.deepcopy(X)
121
122
       k = 0
123
        \hbox{\it\# Second stage: perform QR-transformations.} \\
124
       while k < 5000:
125
           k += 1
126
            Q, R = np.linalg.qr(T)
127
            T = R.dot(Q)
128
            yield T
129
130
0plot_factory
   def qrm2():
134
       Create generator for transformed matrices after applying the
135
         QR-Method.
136
       Yields:
137
            - T: 2D-numpy array. Similar matrix to X.
138
       n n n
139
       # First stage: transform to upper Hessenberg-matrix.
140
       T = lin.hessenberg(X)
141
142
       k = 0
143
       \# Second stage: perform QR-transformations.
144
       while k < 5000:
145
           if k == 0:
146
```

```
yield X
147
            k += 1
148
            Q, R = np.linalg.qr(T)
149
            T = R.dot(Q)
150
            yield T
151
152
153
   @plot_factory
154
   def qrm3():
155
        n n n
156
       First compute similar matrix in Hessenberg form, then compute
157
       Eigenvalues \ \ and \ \ Eigenvectors \ \ using \ \ the \ \ accelerated \ \ QR-Method.
158
159
        Yields:
160
            * T - 2D numpy array of current iteration step.
        n/n/n
162
        # First stage: transform to upper Hessenberg-matrix.
163
       T = lin.hessenberg(X)
164
       k = 0
165
       n, _= X.shape
166
167
        \# Second stage: perform QR-transformations.
168
        while k < 5000:
169
            if k == 0:
170
                 yield X
171
            k += 1
172
            Q, R = np.linalg.qr(T - T[n-1, n-1] * np.eye(n))
173
            T = R.dot(Q) + T[n-1, n-1] * np.eye(n)
174
175
```

```
yield T
176
177
178
  jacobi(os.path.join(outpath, "jacobi.png"))
179
  qrm1(os.path.join(outpath, "qrm1.png"))
180
  qrm2(os.path.join(outpath, "qrm2.png"))
181
  qrm3(os.path.join(outpath, "qrm3.png"))
182
183
  plt.show()
184
  plt.close()
```

6.3 Analysis: Unit tests

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

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

```
+ problematic: list of numpy arrays which led to wrong
43
                   eigenvalues.
       11 11 11
44
       global failed
45
       global critical
46
       global problematic
47
48
      for _ in range(Ntests):
49
           try:
50
               A, true_eig = get_test_matrix(dim=dim)
51
               my_eig, _ = algo(A, *args, **kwargs)
52
               assert np.alltrue(np.isclose(my_eig, true_eig))
53
54
           except AssertionError:
55
               failed += 1
               problematic.append(A)
57
58
           except ZeroDivisionError:
59
               critical += 1
60
61
62
  def threaded_tests(algo, N, nWorkers=10, verbose=True, *args, **
63
    kwargs):
       global failed
64
       global critical
65
       global problematic
66
67
       assert N % nWorkers == 0
68
69
      n = N // nWorkers
70
```

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

REFERENCES REFERENCES

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

References

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