

```
1 #! /opt/local/bin/python
2 #!
3 ... /home/dantopa/spackactivity/ubuntu-22.04-dantopa-docker-spack/opt/spack/linux-ubuntu22.04-haswell
4 ... gcc-12.2.0/python-3.10.6-ybcookynohghdr6i72gwalqle6hq27z5/bin/python
5 # Solving Bevington example 6.1 with Python
6 from datetime import date
7 today = date.today( )
8 print( today.strftime("%b-%d-%Y") )
9 import os
10 print(os.path.dirname(os.path.realpath(__file__)))
11
12 print( "importing numpy..." )
13 import numpy as np
14
15 # input data
16 A = np.array([ [1, 1], [1, 2], [1, 3], [1, 4], [1, 5], [1, 6], [1, 7], [1, 8], [1, 9] ])
17 print( "design matrix A\n", np.matrix( A ) )
18 T = np.array([15.6, 17.5, 36.6, 43.8, 58.2, 61.6, 64.2, 70.4, 98.8])
19 print( "data vector T =", np.matrix( T ) )
20
21 # set up normal equations
22 W = np.dot( A.transpose(), A )
23 print( "Gram matrix A*A\n", np.matrix( W ) )
24 b = np.dot( A.transpose(), T )
25
26 # solve normal equations
27 xls = np.linalg.solve( W, b )
28 print( "least squares solution xls =", xls )
29
30 # pseudoinverse solution
31 Winv = np.linalg.inv( W )
32 Ap = np.dot( Winv, A.transpose( ) )
33 xpinv = np.dot( Ap, T.transpose( ) )
34 print( "pseudoinverse xpinv =", xpinv )
35
36 # error propagation
37 residual = np.dot( A, xls ) - T
38 t2 = np.dot( residual, residual )
39 print( "least total squared error =", t2 )
40 [ m, n ] = A.shape
41 print( "A matrix dimensions =", [ m, n ] )
42 diag = np.diag( Winv )
43 sigma = np.sqrt( t2 / ( m - n ) * diag )
44 print( "sigma =", sigma )
45
46 # numerical errors
47 print( "\nnnumerical errors\n" )
48 xlsExact = [ 1733 / 360, 1129 / 120 ]
49 numericErrorXLS = xls - xlsExact
50 print( "numeric errors, fit parameters" )
51 print( numericErrorXLS )
52
53 sigmaExact = np.sqrt( np.array( [ 108297055, 3419907 ] ) / 35 ) / 360
54 numericErrorSigma = sigma - sigmaExact
55 print( "\nnnumeric errors, sigma parameters" )
56 print( numericErrorSigma )
57
58 # machine epsilon
59 machineEpsilon = np.finfo(float).eps
60 print( "\nmachine epsilon =", np.finfo(float).eps )
```

```
60 numericErrorXLseps = numericErrorXLS / machineEpsilon
61 numericErrorXLsigma = numericErrorSigma / machineEpsilon
62 print( "\nnumeric epsilons, fit parameters: ", numericErrorXLseps )
63 print( "\nnumeric epsilons, sigma parameters: ", numericErrorXLsigma )
64
65 # dantopa@Quaxolotl.attlocal.net:least-squares $ ./least-squares.py
66 # Sep-05-2022
67 # /Volumes/T7-Touch/repos/github/jop/python/genesis/least-squares
68
69 # importing numpy...
70 # design matrix A
71 # [[1 1]
72 # [1 2]
73 # [1 3]
74 # [1 4]
75 # [1 5]
76 # [1 6]
77 # [1 7]
78 # [1 8]
79 # [1 9]]
80 # data vector T = [[15.6 17.5 36.6 43.8 58.2 61.6 64.2 70.4 98.8]]
81 # Gram matrix A*A
82 # [[ 9 45]
83 # [45 285]]
84 # least squares solution xls = [4.81388889 9.40833333]
85 # pseudoinverse xpinv = [4.81388889 9.40833333]
86 # least total squared error = 316.6580555555554
87 # A matrix dimensions = [9, 2]
88 # sigma = [4.88620631 0.86830165]
89 #
90 # numerical errors
91 #
92 # numeric errors, fit parameters
93 # [ 9.76996262e-15 -1.77635684e-15]
94 #
95 # numeric errors, sigma parameters
96 # [-8.88178420e-16 -2.22044605e-16]
97 #
98 # machine epsilon = 2.220446049250313e-16
99 #
100 # numeric epsilons, fit parameters: [44. -8.]
101 #
102 # numeric epsilons, sigma parameters: [-4. -1.]
103
```