# trial for dominique

## September 20, 2018

## 0.1 trials for Dominique

see if there is a correlation between the different residuals of different species

```
In [123]: import numpy as np
          import pandas as pd
In [124]: datatote = pd.read_csv('parameterfitsFungi/nonlinfit7.txt',header=None)
          datatote
Out [124]:
                   0
                        1
                                       2
                                                      3
                                                                 4
                                                                           5
          0
                   1
                       Ε
                          -14250.087525 -11156.544121
                                                         0.311284
                                                                    0.032444
          1
                   1
                       Η
                                1.018096
                                               0.739876
                                                         0.003008
                                                                    0.000050
          2
                       Q
                   1
                           -9789.440306
                                          -6685.082717
                                                         0.157009
                                                                    0.035848
          3
                   1
                       F
                                                         0.014239
                                                                    0.000071
                                0.761479
                                               0.713766
          4
                   1
                       Y
                           -1684.372161
                                           -908.851026
                                                         0.040757
                                                                    0.038420
          5
                       С
                   1
                                0.895032
                                                         0.008780
                                                                    0.000042
                                               0.821428
          6
                   1
                       N
                           -4140.826663
                                          -2706.734715
                                                         0.095442
                                                                    0.033332
          7
                   1
                       K
                                0.784327
                                               0.687553
                                                         0.011547
                                                                    0.000165
          8
                   1
                       D
                                0.948727
                                              0.697394
                                                         0.004132
                                                                    0.000099
          9
                   2
                       F.
                                                         0.018714
                                0.673710
                                              0.626251
                                                                    0.000086
          10
                   2
                       Η
                                0.989170
                                              0.976107
                                                         0.007740
                                                                    0.000066
                   2
          11
                       Q
                                0.816803
                                               0.767509
                                                         0.012101
                                                                    0.000088
          12
                   2
                       F
                           -3687.720978
                                          -1582.506833
                                                         0.028825
                                                                    0.041911
                   2
                       Y
                                          -2235.826418
          13
                           -2587.001144
                                                         0.012774
                                                                    0.037669
                   2
                       С
          14
                           -3619.955879
                                          -1657.441558
                                                         0.029112
                                                                    0.041324
                   2
          15
                       N
                                0.838011
                                               0.821985
                                                         0.012522
                                                                    0.000583
                   2
                       K
                                               0.605169
                                                         0.010346
                                                                    0.000474
          16
                                0.758210
                   2
                       D
                                                         0.013879
          17
                                0.749415
                                              0.679433
                                                                    0.000553
                   3
                       Ε
                                                         0.000632
                                                                    0.000610
          18
                                0.821380
                                               0.108451
                   3
                       Η
                                          -8094.006009
                                                         0.168378
          19
                         -11589.413849
                                                                    0.048104
                   3
          20
                       Q
                                                         0.002275
                                0.580975
                                               0.006971
                                                                    0.000062
          21
                   3
                       F
                          -11706.062605
                                          -8365.589404
                                                         0.172043
                                                                    0.047108
                   3
                       Y -12928.632809
                                          -9525.001548
          22
                                                         0.227368
                                                                    0.044484
                   3
          23
                         -14402.087881 -10883.053026
                                                         0.214905
                                                                    0.050325
                                                         0.142494
          24
                   3
                       N
                         -12590.830327
                                          -8809.616172
                                                                    0.042703
          25
                   3
                       K
                                0.415288
                                              -0.087842
                                                         0.004799
                                                                    0.000332
          26
                   3
                          -10854.019306 -7339.232054 0.114130
                                                                    0.052524
```

```
27
        4
            Ε
                 -1738.537583 -1140.026394
                                               0.009772
                                                         0.039113
28
        4
            Η
                     0.858932
                                    0.638749
                                               0.006090
                                                          0.000048
        4
             Q
                 -3129.020864
                                -1479.074455
                                               0.052632
                                                          0.038017
29
. . .
                                                     . . .
            . . .
      . . .
4124
      459
            N
                -70721.500960 -70722.002563
                                               0.000382
                                                          0.032644
4125
      459
            K
                     0.756902
                                     0.762496
                                               0.016520
                                                          0.000566
4126
      459
            D
                     0.675254
                                     0.562190
                                               0.015127
                                                          0.000697
                                                          0.046973
4127
      460
            Ε
                 -9906.536888
                                -6936.652662
                                               0.116883
4128
      460
            Η
                     0.741454
                                     0.393203
                                               0.005021
                                                          0.000364
4129
      460
             Q
                -11477.377887
                                -8335.061045
                                               0.133333
                                                          0.066079
4130
      460
             F
                     0.775717
                                     0.602947
                                               0.009124
                                                          0.000302
             Y
                 -1994.476624
                                -1888.340028
                                               0.017021
4131
      460
                                                          0.037689
4132
      460
             С
                     1.131751
                                    0.539917
                                               0.000579
                                                          0.000535
4133
      460
             N
                     0.554127
                                     0.405708
                                               0.017973
                                                          0.002086
4134
      460
             K
                 -2996.703804
                                -2464.957004
                                               0.012048
                                                          0.036406
                                                          0.000457
4135
            D
                     0.927990
                                    0.393748
                                               0.001283
      460
4136
      461
             Ε
                     0.656781
                                     0.378977
                                               0.008698
                                                          0.000745
4137
      461
                 -4417.310371
                                -2372.719802
                                               0.056604
                                                          0.038486
            Η
4138
             Q
                     0.902042
                                     0.824751
                                               0.008444
                                                          0.000183
      461
4139
      461
            F
                -10939.077095
                                -7740.886631
                                               0.136752
                                                          0.048038
4140
      461
             Y
                 -8649.288609
                                -5497.238085
                                               0.122867
                                                          0.038049
4141
            C
                                -4664.165194
      461
                 -7628.836326
                                               0.062992
                                                          0.051539
4142
      461
            N
                 -6368.377297
                                -4153.529721
                                               0.072937
                                                          0.045530
4143
                                    0.430491
                                               0.003677
      461
            K
                     0.810762
                                                          0.000189
4144
      461
            D
                 -5206.456032
                                -3741.356291
                                               0.056818
                                                          0.035351
4145
      462
             Ε
                     0.814121
                                     0.541051
                                               0.005712
                                                          0.000355
4146
      462
                                -1690.633077
                                               0.043682
            Η
                 -3266.399022
                                                          0.037880
4147
      462
             Q
                     0.715664
                                     0.628771
                                               0.014604
                                                          0.000148
      462
            F
4148
                -10000.003514
                                -6615.122663
                                               0.149590
                                                          0.047584
4149
      462
            Y
                 -8795.720937
                                -5880.565076
                                               0.142390
                                                          0.044668
                 -7801.326841
4150
      462
                                -4803.957699
                                               0.066154
            C
                                                          0.040919
4151
      462
            N
                 -6658.170162
                                -4547.657753
                                               0.071813
                                                          0.045060
4152
      462
            K
                     0.903896
                                    0.545003
                                               0.003122
                                                          0.000158
            D
                 -3693.676304 -1974.508790
                                               0.041667
4153
      462
                                                          0.038813
```

[4154 rows x 6 columns]

## 0.1.1 we remove uninsteresting data

```
In [125]: data = datatot.drop([1,4,5], axis=1)
In [126]: data
Out[126]:
                                  2
                                                 3
                   0
          0
                     -14250.087525 -11156.544121
          1
                   1
                          1.018096
                                         0.739876
          2
                      -9789.440306
                                     -6685.082717
          3
                          0.761479
                                         0.713766
```

```
4
           -1684.372161
                            -908.851026
        1
5
        1
                0.895032
                               0.821428
6
        1
           -4140.826663
                          -2706.734715
7
        1
                0.784327
                               0.687553
        1
8
                0.948727
                               0.697394
9
        2
                0.673710
                               0.626251
        2
10
                0.989170
                               0.976107
11
        2
                0.816803
                               0.767509
12
        2
           -3687.720978
                          -1582.506833
13
        2
           -2587.001144
                          -2235.826418
14
        2
                          -1657.441558
           -3619.955879
15
        2
                0.838011
                               0.821985
        2
16
                0.758210
                               0.605169
        2
17
                0.749415
                               0.679433
18
        3
                0.821380
                               0.108451
19
        3 -11589.413849
                          -8094.006009
20
        3
                0.580975
                               0.006971
21
        3 -11706.062605
                          -8365.589404
22
        3 -12928.632809
                          -9525.001548
23
        3 -14402.087881 -10883.053026
        3 -12590.830327
24
                          -8809.616172
25
        3
                0.415288
                             -0.087842
26
        3 -10854.019306
                          -7339.232054
27
           -1738.537583
                          -1140.026394
28
        4
                0.858932
                               0.638749
                          -1479.074455
29
           -3129.020864
. . .
4124
      459 -70721.500960 -70722.002563
4125
      459
                0.756902
                               0.762496
4126
      459
                0.675254
                               0.562190
4127
      460
           -9906.536888
                          -6936.652662
4128
      460
                0.741454
                               0.393203
4129
      460 -11477.377887
                          -8335.061045
4130
      460
                0.775717
                               0.602947
4131
      460
           -1994.476624
                          -1888.340028
4132
      460
                1.131751
                               0.539917
4133
      460
                0.554127
                               0.405708
4134
      460
           -2996.703804
                          -2464.957004
4135
      460
                0.927990
                               0.393748
4136
      461
                0.656781
                               0.378977
4137
      461
           -4417.310371
                          -2372.719802
4138
      461
                0.902042
                               0.824751
4139
      461 -10939.077095
                          -7740.886631
4140
      461
           -8649.288609
                          -5497.238085
4141
      461
           -7628.836326
                          -4664.165194
4142
      461
           -6368.377297
                          -4153.529721
4143
      461
                0.810762
                               0.430491
4144
      461
           -5206.456032
                          -3741.356291
```

```
4145 462
                        0.814121
                                      0.541051
         4146 462 -3266.399022 -1690.633077
         4147
               462
                        0.715664
                                      0.628771
         4148 462 -10000.003514 -6615.122663
         4149
               462 -8795.720937 -5880.565076
         4150
              462 -7801.326841 -4803.957699
         4151 462 -6658.170162 -4547.657753
         4152
              462
                        0.903896
                                      0.545003
         4153 462 -3693.676304 -1974.508790
         [4154 rows x 3 columns]
In [127]: len(data)/data[0][len(data)-1]
Out[127]: 8
In [128]: arr = np.zeros((data[0][len(data)-1],9))
         data = np.array(data)
```

0.1.2 we put everything in a corresponding array organized by species and averaging the two regressors.

we can see that the values vary a lot, from 9 to -10,000 with a lot of very low numbers. this creates quite high variances. However, High number for one AA often means the same for another.

```
1.33168360e+06, 3.33227600e+06, 5.87558032e+06, 4.59123591e+06,
3.03355034e+06, 2.45890719e+06, 2.55713215e+06, 2.86463372e+06,
1.63368004e+06, 3.85745337e+06, 2.34380078e+06, 1.94293020e+06,
5.92445632e+06, 3.97194954e+06, 1.23150844e+07, 4.37447250e+06,
1.09796225e+07, 5.89096574e+06, 1.39090088e+07, 3.97052243e+06,
1.00380710e+07, 1.79882205e+07, 5.41169803e+06, 6.55981651e+06,
4.88902117e+06, 4.94541570e+06, 5.48681438e+06, 3.85717731e+06,
2.86394650e+06, 3.84317066e+06, 2.83628470e+06, 3.74389095e+06,
3.26953862e+05, 5.78246176e+06, 1.49316012e+07, 1.30144580e+07,
4.37046332e+07, 2.46755944e+07, 4.48815885e+06, 2.98772807e+07,
6.87974192e+06, 3.86565664e+07, 2.36927258e+07, 1.95623164e+07,
1.99481461e+07, 6.32308803e+06, 4.78252731e+08, 6.22502400e+06,
3.64617707e+06, 5.22190817e+06, 1.17093701e+07, 5.27698951e+06,
3.38054897e+06, 1.76455182e+07, 7.51754389e+06, 1.59776475e+07,
2.21454442e+06, 7.18669846e+06, 3.51090303e+06, 3.17123798e+06,
1.20604726e+07, 3.69905139e+06, 5.04433414e+06, 1.26668732e+06,
1.06905913e+06, 1.53474280e+07, 1.69079859e+07, 2.07075905e+07,
2.42201599e+07, 1.34099967e+07, 1.26650020e+07, 2.37231941e+07,
1.43004093e+07, 1.49120454e+07, 1.83995894e+07, 2.14378793e+07,
2.01599243e+07, 1.01046063e+07, 1.28098163e+07, 6.38373755e+06,
1.97839810e+07, 2.32459961e+07, 2.29265291e+07, 5.53194271e+06,
1.63919467e+06, 1.62717734e+06, 2.35072835e+06, 1.83852730e+06,
1.58536422e+06, 4.21419641e+06, 3.07130736e+07, 8.68655203e+06,
3.37935250e+06, 6.55805306e+06, 5.90843689e+06, 9.17023805e+06,
2.91149217e+07, 1.14810482e+07, 3.99649447e+07, 1.70703681e+07,
1.63093448e+07, 4.63117522e+07, 6.53035783e+06, 2.77565551e+07,
1.16463941e+07, 6.31852637e+07, 6.90915583e+05, 3.18942283e+06,
1.22394205e+06, 6.39633024e+06, 9.90753087e+05, 5.06260549e-02,
6.03045849e-01, 2.61134652e+06, 1.74098171e+07, 1.16715220e+06,
1.46259650e+06, 6.67530784e+06, 5.67530042e+07, 1.61486981e+07,
1.60781642e+07, 1.95150996e+06, 4.40356468e+06, 9.59475968e+05,
4.26347682e+06, 4.16116123e+06, 6.53982775e+06, 6.58502212e+06,
5.15489567e+06, 5.24978724e+06, 2.10989060e+06, 5.27896028e+06,
2.32195793e+07, 7.23585676e+06, 4.78554234e+06, 3.19049531e+06,
6.01784591e+06, 6.19861757e+06, 4.68382382e+06, 2.99302999e+06,
5.04097425e+06, 4.08687606e+06, 2.24222816e+06, 4.58821310e+06,
4.94997979e+06, 6.95500986e+06, 3.56843375e+06, 2.80198597e+07,
6.86389391e+05, 9.17994391e+06, 1.21316992e+07, 2.37831377e+06,
8.95224692e+06, 9.23015861e+06, 4.13769908e+06, 2.29496299e+07,
7.87008825e+05, 2.73050118e+07, 1.85128758e+07, 6.36773204e+07,
1.35541657e+08, 1.44615748e+06, 5.55521107e+06, 1.02479985e+07,
1.58164750e+06, 4.00406855e+06, 4.31400365e+06, 2.88568664e+07,
2.60832179e+06, 3.22386503e+07, 1.52216684e+06, 3.48264500e+07,
9.68331583e+06, 1.82697615e+07, 1.54121893e+07, 6.77521100e+06,
8.25528638e+05, 1.08542815e+06, 1.52890700e+06, 7.78605148e+06,
1.33796491e+07, 1.97745032e+07, 9.18654343e+06, 1.96972466e+07,
1.11054751e+06, 1.38791053e+06, 2.05460727e+06, 8.67058856e+06,
4.84675118e+06, 3.13369186e+06, 4.16571060e+06, 9.94191912e+06,
```

```
2.01582541e+07, 1.52861652e+06, 1.04830068e+07, 1.33461266e+07,
1.95876975e+07, 1.83932232e+07, 2.56055688e+07, 2.67689960e+06,
1.05542167e+07, 8.20731198e+06, 1.13753191e+07, 5.64520923e+06,
1.26836441e+07, 7.68381979e+06, 6.34826399e+06, 6.62274641e+06,
5.85627481e+06, 5.14294820e+06, 4.97408874e+06, 8.47531462e+06,
1.69730729e+06, 1.17912395e+07, 2.99436970e+07, 3.64545266e+06,
3.51211819e+06, 1.44956046e+06, 6.69134135e+06, 8.28803800e+07,
4.14704909e+07, 2.05873585e+06, 4.72873840e+05, 5.66083084e+06,
1.17229216e+07, 1.03304139e+07, 1.22865948e+07, 2.83782261e+07,
5.73942758e+06, 1.17907880e+07, 1.80165735e+07, 3.57793555e+07,
3.01143016e+06, 5.78403869e+06, 4.98246436e+07, 4.20907550e+06,
1.50520799e+07, 5.29772231e+06, 7.81432761e+06, 9.90867594e+06,
1.24057228e+08, 3.43579933e+07, 1.66956835e+08, 7.62859255e+06,
8.43518843e+06, 1.80551265e+06, 3.30203405e+07, 1.65763081e+07,
2.68283846e+07, 1.72915325e+01, 4.12590574e+07, 1.24848910e+05,
2.51873890e+05, 9.77528832e+06, 8.13973144e+06, 2.64148194e+06,
1.60038996e+06, 4.61519779e+06, 2.99009070e+06, 2.41859317e+06,
2.10296963e+06, 3.58443889e+06, 3.02089820e+06, 4.82079126e+06,
4.51896794e+06, 4.02154173e+06, 3.46358527e+06, 3.07673421e+06,
2.80870096e+06, 7.53179410e+06, 4.42138338e+06, 9.08593367e+06,
3.00691183e+06, 8.34010112e+06, 7.44651706e+06, 1.93017175e+06,
7.79572110e+06, 1.04239342e+07, 4.75729187e+06, 5.90087987e+06,
1.39370897e+07, 3.45942074e+05, 7.90278670e+05, 1.10088455e+06,
5.60566049e+06, 7.19917831e+06, 3.79348414e+07, 2.22384380e+07,
1.40133676e+08, 1.21543800e+06, 8.25017708e+06, 7.75083985e+06,
3.76622051e+06, 5.23813155e+06, 3.85506830e+06, 4.56368349e+06,
5.23379822e+06, 5.43756400e+06, 6.64785660e+06, 3.95081556e+06,
2.94733229e+06, 4.95199416e+06, 4.69818107e+06, 4.86564973e+06,
4.64040329e+06, 3.94305960e+06, 4.61178414e+06, 4.07642036e+06,
5.26336553e+06, 3.52848173e+06, 6.32809768e+06, 5.01382507e+06,
5.03483287e+06, 5.10822495e+06, 4.02557358e+07, 2.00945209e+07,
3.36501980e+06, 4.34892369e+06, 3.93617828e+06, 2.96558121e+06,
1.40604209e+07, 2.12266298e+07, 4.36724776e+06, 6.54385218e+06,
5.55194958e+06, 3.87626707e+06, 3.29377475e+06, 1.51826439e+06,
9.37999925e+05, 3.36073430e+07, 9.07656549e+05, 1.89510601e+07,
1.94816494e+08, 4.75831280e+07, 1.06583672e+08, 1.24617752e+07,
2.44581184e+07, 4.75834899e+08, 6.82491663e+06, 6.06789436e+06,
8.12656041e+06, 1.06683344e+07, 5.72758183e+06, 1.49120622e+07,
4.21211354e+06, 9.76848926e+06, 8.87133956e+06, 2.03235643e+07,
2.36784670e+06, 1.27205110e+07, 4.14394006e+06, 1.56190824e+07,
1.73631546e+07, 7.08569844e+05, 3.51081851e+06, 3.52644062e+06,
4.21911748e+05, 7.36412785e+05, 6.83779729e+05, 9.34570508e+06,
2.97913232e+06, 3.79177370e+06, 1.24840065e+07, 1.04519897e+08,
9.48024335e+05, 2.34031965e+06, 9.92277753e+05, 6.08757611e+07,
3.57570321e+07, 1.62612437e+07, 4.01948923e+07, 4.05616728e+07,
4.14063150e+07, 7.92694106e+07, 1.50006633e+07, 1.45089031e+07,
5.80395868e+06, 1.18598491e+07, 3.24824187e+06, 2.99964244e+06,
6.62106846e+05, 1.00557573e+06, 2.14978966e+06, 1.27117776e+06,
```

```
4.23182053e+05, 7.60094000e+05, 3.96055906e+07, 2.20187261e+07, 3.51621868e+07, 1.85421409e+07, 1.80177020e+07, 2.05574460e+07, 2.17109974e+07, 1.21648256e+07, 2.03800012e+07, 2.05764445e+07, 7.90366115e+06, 6.03541385e+07, 1.41614217e+06, 3.06125797e+06, 2.24503067e+07, 3.22979463e+07, 5.77298334e+06, 7.27681976e+06, 5.72277348e+06, 4.90141674e+06, 1.92305063e+07, 5.67383354e+06, 3.77912724e+06, 3.92947762e+06, 2.46157269e+06, 3.07665615e+06, 2.48992135e+06, 3.31623450e+06, 3.63110727e+06, 2.77053443e+07, 5.76350053e+06, 2.15446710e+06, 2.87738003e+06, 1.11224560e+06, 2.07609476e+07, 7.92735489e+06, 9.89938257e+06, 1.33606368e+07, 2.12840266e+07, 1.54804038e+06, 3.77961794e+06, 1.84245907e+07, 2.12522405e+07, 2.35397018e+07, 1.22732600e+05, 4.83443472e+06, 6.37423034e+06, 4.32173712e+07, 5.16333749e+08, 6.89368180e+06, 2.22570555e+06, 2.04592591e+07, 4.82631052e+08, 1.35023802e+07, 1.03059546e+07, 9.79626493e+06])
```

In [132]: arr.var()

Out[132]: 22724635.591483254

variance accross measures/ mean variance accross species

```
In [133]: arr.mean(0).var()
Out[133]: 1388583.6554276315
```

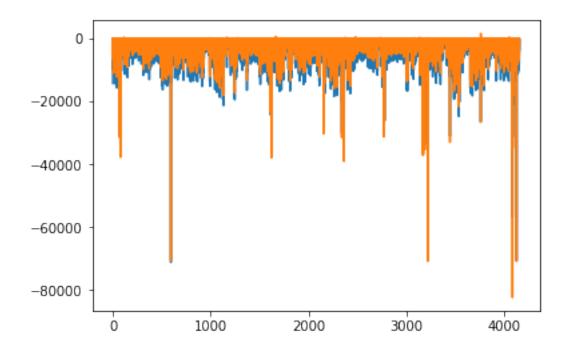
#### 0.1.3 we can see that the mean is still pretty high.

however, mixing AA between different species, shows that a random association is finding much worse variance than the one we have (on average a difference of 2,832,176)

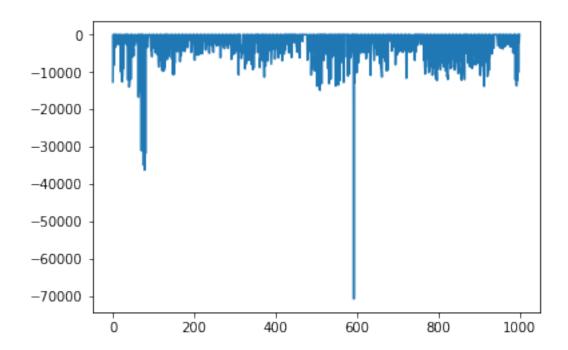
```
Out[137]: array([[ 4.15145500e-01, -6.20570878e+03, 6.97707000e-01, ...,
                  -1.49103579e+03, 1.06608050e+00, 8.41851000e-01],
                 [-5.15551749e+03, -3.06515524e+03, 6.26267500e-01, ...,
                 -1.03056625e+04, 4.93779000e-01, -3.08304566e+03],
                 [3.32430000e-01, -1.86764586e+03, 3.92859000e-01, ...,
                  -2.51911140e+03, 7.77000000e-01, -3.12708306e+03],
                 [-1.56705559e+04, -3.47117630e+03, 5.81732000e-01, ...,
                 -4.28548748e+03, -8.39942050e+03, -1.02534611e+04],
                 [-1.24855159e+03, -6.34379273e+03, 7.27223000e-01, ...,
                 -3.62731461e+03, 5.13653500e-01, -5.19541578e+03],
                 [ 5.54347000e-01, -2.13428459e+03, -2.30404766e+03, ...,
                  -9.43247771e+03, 5.71346000e-01, -2.95652433e+03]])
In [138]: randarr.mean(0)
Out[138]: array([-2219.06645714, -2919.84412463, -2015.18948926, -4288.21485415,
                 -4477.73292545, -4078.47555626, -4687.57869146, -1166.91552409,
                 -2855.27048881])
In [147]: randarr.mean(0).var()-arr.mean(0).var()
Out[147]: 2.3283064365386963e-10
In [153]: randarr = np.zeros(arr.shape)
          X = 2000
          a=0
          for _ in range(X):
             for i in range(arr.shape[1]):
                  ind = np.arange(len(arr))
                 np.random.shuffle(ind)
                  randarr[:,i] = arr[ind,i]
              a += randarr.var(1).mean()-arr.var(1).mean()
          print a/X
2832176.8380952715
In [150]: randarr.var(1).mean()-arr.var(1).mean()
Out[150]: 2653785.4159249514
In [70]: arr.var(0)
Out[70]: array([41333202.63856429, 10727555.04310829, 19414596.46349642,
                12230304.06525019, 22099342.25172593, 19543347.84000982,
                28742207.88900693, 21790682.06159877, 16143229.1717399 ])
```

## 0.2 we can explore how the data looks like

we see here that even if there is some correlation, the variation is too high to be able to cluster it

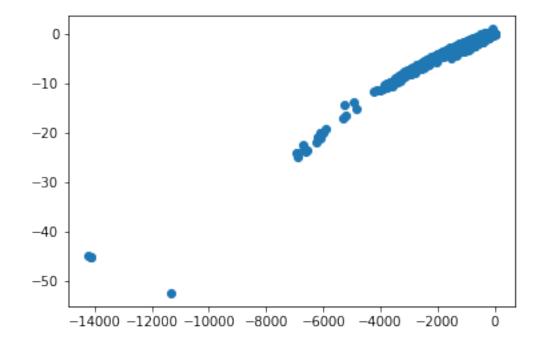


```
In [73]: plot(data[:1000,1:].mean(1))
Out[73]: [<matplotlib.lines.Line2D at 0x103c5a650>]
```



In [75]: scatter(data[:,1]/data[:,1].max(),data[:,2]/data[:,2].max())

Out[75]: <matplotlib.collections.PathCollection at 0x10a510690>



## 0.3 Given the repartition of the data (outliers) it will be almost impossible to cluster

we should better use direct exploration

0.3.1 We can see that it is confirmed here, even if it does not cluster, we can see some correlation

this view allows us to zoom in the data

```
In [77]: X = -1
         species = [1,2,3,4,5,6,7,8,9,10]
         col = ['#f39c12', "#1abc9c", "#3498db", "#2ecc71", "#9b59b6", '#34495e', '#492000', '*
         '#043927', '#8F9779', '#f1c40f', '#e67e22', '#e74c3c', '#7f8c8d']
         source = ColumnDataSource(data=dict(x = data[:X,1]/data[:,1].min(),
                                             y = data[:X,2]/data[:,2].min(),
                                             names = np.array(datatot[0])[:X],
                                             colors= [col[0] if i-30 not in species else\
                                                      col[i-30] for i in np.array(datatot[0])[::
         output_notebook()
         hover = HoverTool(tooltips=[("species: ", "@names")])
         p = figure(title="Plot of the regressors",
                    tools=[hover, WheelZoomTool(), PanTool(), SaveTool(), ResetTool()],
                    plot_width=800, plot_height=600)
         p.circle(x='x', y='y', source=source, size=10,color='colors')
         show(p)
```

0.3.2 we can further test it by running classifier to see if they are able to cluster the data according to our labels

the results are very low....

Out[156]: 0.5642753972075109

## 0.4 Same for bacterias

	aabab	00					
Out[120]:		0	1	2	3	4	5
	0	1	E	-14250.087525	-11156.544121	0.311284	0.032444
	1	1	Н	1.018096	0.739876	0.003008	0.000050
	2	1	Q	-9789.440306	-6685.082717	0.157009	0.035848
	3	1	F	0.761479	0.713766	0.014239	0.000071
	4	1	Y	-1684.372161	-908.851026	0.040757	0.038420
	5	1	С	0.895032	0.821428	0.008780	0.000042
	6	1	N	-4140.826663	-2706.734715	0.095442	0.033332
	7	1	K	0.784327	0.687553	0.011547	0.000165
	8	1	D	0.948727	0.697394	0.004132	0.000099
	9	2	E	0.673710	0.626251	0.018714	0.000086
	10	2	Η	0.989170	0.976107	0.007740	0.000066
	11	2	Q	0.816803	0.767509	0.012101	0.000088
	12	2	F		-1582.506833	0.028825	0.041911
	13	2	Y	-2587.001144	-2235.826418	0.012774	0.037669
	14	2	С	-3619.955879	-1657.441558	0.029112	0.041324
	15	2	N	0.838011	0.821985	0.012522	0.000583
	16	2	K	0.758210	0.605169	0.010346	0.000474
	17	2	D	0.749415	0.679433	0.013879	0.000553
	18	3	E	0.821380	0.108451	0.000632	0.000610
	19	3	Н		-8094.006009	0.168378	0.048104
	20	3	Q	0.580975	0.006971	0.002275	0.000062
	21	3	F	-11706.062605	-8365.589404	0.172043	0.047108
	22	3	Y	-12928.632809	-9525.001548	0.227368	0.044484
	23	3	С		-10883.053026	0.214905	0.050325
	24	3	N	-12590.830327	-8809.616172	0.142494	0.042703
	25	3	K	0.415288	-0.087842	0.004799	0.000332
	26	3	D	-10854.019306		0.114130	0.052524
	27	4	E	-1738.537583	-1140.026394	0.009772	0.039113
	28	4	Η	0.858932	0.638749	0.006090	0.000048
	29	4	Q	-3129.020864	-1479.074455	0.052632	0.038017
			• • •				
	4124	459	N		-70722.002563	0.000382	0.032644
	4125	459	K	0.756902	0.762496	0.016520	0.000566
	4126	459	D	0.675254	0.562190	0.015127	0.000697
	4127	460	E	-9906.536888	-6936.652662	0.116883	0.046973
	4128	460	H	0.741454	0.393203	0.005021	0.000364
	4129	460	Q	-11477.377887	-8335.061045	0.133333	0.066079
	4130	460	F	0.775717	0.602947	0.009124	0.000302
	4131	460	Y	-1994.476624	-1888.340028	0.017021	0.037689
	4132	460	C	1.131751	0.539917	0.000579	0.000535
	4133	460	N	0.554127	0.405708	0.017973	0.002086
	4134	460	K	-2996.703804	-2464.957004	0.012048	0.036406
	4135	460	D	0.927990	0.393748	0.001283	0.000457

```
4136
      461
            Ε
                                              0.008698
                                                         0.000745
                     0.656781
                                    0.378977
4137
      461
            Η
                 -4417.310371
                               -2372.719802
                                              0.056604
                                                         0.038486
4138
      461
            Q
                                               0.008444
                                                         0.000183
                     0.902042
                                    0.824751
4139
            F
               -10939.077095
                                -7740.886631
      461
                                               0.136752
                                                         0.048038
            Y
4140
      461
                 -8649.288609
                                -5497.238085
                                               0.122867
                                                         0.038049
4141
            C
                                -4664.165194
                                               0.062992
      461
                 -7628.836326
                                                         0.051539
4142
      461
            N
                 -6368.377297
                                -4153.529721
                                               0.072937
                                                         0.045530
                                                         0.000189
4143
      461
            K
                     0.810762
                                    0.430491
                                              0.003677
4144
            D
      461
                 -5206.456032
                               -3741.356291
                                               0.056818
                                                         0.035351
4145
      462
            Ε
                     0.814121
                                    0.541051
                                               0.005712
                                                         0.000355
4146
                 -3266.399022
      462
            Η
                               -1690.633077
                                               0.043682
                                                         0.037880
4147
            Q
      462
                     0.715664
                                    0.628771
                                               0.014604
                                                         0.000148
4148
      462
            F
               -10000.003514
                               -6615.122663
                                               0.149590
                                                         0.047584
            Y
4149
      462
                -8795.720937
                                -5880.565076
                                               0.142390
                                                         0.044668
4150
      462
            C
                 -7801.326841
                                -4803.957699
                                               0.066154
                                                         0.040919
4151
      462
                 -6658.170162
                               -4547.657753
            N
                                               0.071813
                                                         0.045060
4152
      462
            K
                     0.903896
                                    0.545003
                                               0.003122
                                                         0.000158
4153
      462
            D
                 -3693.676304 -1974.508790
                                              0.041667
                                                         0.038813
```

[4154 rows x 6 columns]

```
In [103]: data = datatot.drop([1,4,5], axis=1)
```

In [104]: data

```
Out[104]:
                   0
                                   2
                                                  3
           0
                      -14250.087525 -11156.544121
           1
                   1
                           1.018096
                                           0.739876
           2
                   1
                       -9789.440306
                                      -6685.082717
           3
                   1
                           0.761479
                                           0.713766
           4
                   1
                       -1684.372161
                                       -908.851026
           5
                   1
                           0.895032
                                           0.821428
           6
                   1
                       -4140.826663
                                      -2706.734715
           7
                   1
                           0.784327
                                           0.687553
           8
                   1
                           0.948727
                                           0.697394
                   2
           9
                           0.673710
                                           0.626251
           10
                   2
                           0.989170
                                           0.976107
           11
                   2
                           0.816803
                                           0.767509
           12
                   2
                       -3687.720978
                                      -1582.506833
           13
                   2
                       -2587.001144
                                      -2235.826418
                   2
           14
                       -3619.955879
                                      -1657.441558
                   2
           15
                           0.838011
                                           0.821985
                   2
           16
                           0.758210
                                           0.605169
                   2
           17
                           0.749415
                                           0.679433
           18
                   3
                           0.821380
                                           0.108451
           19
                   3
                     -11589.413849
                                      -8094.006009
           20
                   3
                           0.580975
                                           0.006971
           21
                   3 -11706.062605
                                      -8365.589404
```

```
25
                          0.415288
                                        -0.087842
          26
                   3 -10854.019306
                                     -7339.232054
          27
                      -1738.537583
                                     -1140.026394
          28
                          0.858932
                                         0.638749
          29
                      -3129.020864
                                     -1479.074455
           . . .
          4124
                 459 -70721.500960 -70722.002563
          4125
                 459
                          0.756902
                                         0.762496
          4126
                 459
                          0.675254
                                         0.562190
          4127
                 460
                      -9906.536888
                                     -6936.652662
          4128
                 460
                          0.741454
                                         0.393203
          4129
                 460 -11477.377887
                                     -8335.061045
          4130
                 460
                          0.775717
                                         0.602947
          4131
                 460
                      -1994.476624
                                     -1888.340028
          4132
                 460
                          1.131751
                                         0.539917
          4133
                 460
                          0.554127
                                         0.405708
          4134
                 460
                      -2996.703804
                                     -2464.957004
          4135
                 460
                          0.927990
                                         0.393748
          4136
                 461
                          0.656781
                                         0.378977
          4137
                 461
                      -4417.310371
                                     -2372.719802
          4138
                          0.902042
                                         0.824751
                 461
          4139
                 461 -10939.077095
                                     -7740.886631
          4140
                      -8649.288609
                 461
                                     -5497.238085
          4141
                 461
                      -7628.836326
                                     -4664.165194
          4142
                 461
                      -6368.377297
                                     -4153.529721
          4143
                 461
                          0.810762
                                         0.430491
          4144
                 461
                      -5206.456032
                                     -3741.356291
          4145
                 462
                          0.814121
                                         0.541051
          4146
                 462
                      -3266.399022
                                     -1690.633077
          4147
                 462
                          0.715664
                                         0.628771
          4148
                 462 -10000.003514
                                     -6615.122663
          4149
                      -8795.720937
                 462
                                     -5880.565076
          4150
                 462
                      -7801.326841
                                     -4803.957699
          4151
                 462
                      -6658.170162
                                     -4547.657753
          4152
                 462
                          0.903896
                                         0.545003
          4153
                 462
                      -3693.676304
                                     -1974.508790
          [4154 rows x 3 columns]
In [105]: len(data)/data[0][len(data)-1]
Out[105]: 8
In [106]: arr = np.zeros((data[0][len(data)-1],9))
          data = np.array(data)
```

3 -12928.632809 -9525.001548

3 -14402.087881 -10883.053026

-8809.616172

3 -12590.830327

22

23

24

At first I thought that as the distance inter cluster is higher than the overhall distance, there is correlation. However by shuffling, one can see that even a randomize set produce the exact same variance.

mean variance across measures / total variance in dataset

```
In [109]: arr.var(1)
Out[109]: array([1.88320167e+07, 1.46298823e+06, 2.57848672e+07, 1.23875859e+06,
                 3.38089684e+07, 5.81636619e+06, 9.85721808e+05, 1.15497369e+08,
                 2.11076435e+08, 1.48011996e+06, 4.29659097e+06, 3.06602532e+06,
                 1.13877470e+07, 1.56978859e+07, 1.58120395e+07, 3.36395088e+06,
                 1.67513007e+07, 3.04943265e+06, 6.56091388e+06, 2.96761685e+06,
                 1.33168360e+06, 3.33227600e+06, 5.87558032e+06, 4.59123591e+06,
                 3.03355034e+06, 2.45890719e+06, 2.55713215e+06, 2.86463372e+06,
                 1.63368004e+06, 3.85745337e+06, 2.34380078e+06, 1.94293020e+06,
                 5.92445632e+06, 3.97194954e+06, 1.23150844e+07, 4.37447250e+06,
                 1.09796225e+07, 5.89096574e+06, 1.39090088e+07, 3.97052243e+06,
                 1.00380710e+07, 1.79882205e+07, 5.41169803e+06, 6.55981651e+06,
                 4.88902117e+06, 4.94541570e+06, 5.48681438e+06, 3.85717731e+06,
                 2.86394650e+06, 3.84317066e+06, 2.83628470e+06, 3.74389095e+06,
                 3.26953862e+05, 5.78246176e+06, 1.49316012e+07, 1.30144580e+07,
                 4.37046332e+07, 2.46755944e+07, 4.48815885e+06, 2.98772807e+07,
                 6.87974192e+06, 3.86565664e+07, 2.36927258e+07, 1.95623164e+07,
                 1.99481461e+07, 6.32308803e+06, 4.78252731e+08, 6.22502400e+06,
                 3.64617707e+06, 5.22190817e+06, 1.17093701e+07, 5.27698951e+06,
                 3.38054897e+06, 1.76455182e+07, 7.51754389e+06, 1.59776475e+07,
                 2.21454442e+06, 7.18669846e+06, 3.51090303e+06, 3.17123798e+06,
                 1.20604726e+07, 3.69905139e+06, 5.04433414e+06, 1.26668732e+06,
                 1.06905913e+06, 1.53474280e+07, 1.69079859e+07, 2.07075905e+07,
                 2.42201599e+07, 1.34099967e+07, 1.26650020e+07, 2.37231941e+07,
                 1.43004093e+07, 1.49120454e+07, 1.83995894e+07, 2.14378793e+07,
                 2.01599243e+07, 1.01046063e+07, 1.28098163e+07, 6.38373755e+06,
                 1.97839810e+07, 2.32459961e+07, 2.29265291e+07, 5.53194271e+06,
```

```
1.63919467e+06, 1.62717734e+06, 2.35072835e+06, 1.83852730e+06,
1.58536422e+06, 4.21419641e+06, 3.07130736e+07, 8.68655203e+06,
3.37935250e+06, 6.55805306e+06, 5.90843689e+06, 9.17023805e+06,
2.91149217e+07, 1.14810482e+07, 3.99649447e+07, 1.70703681e+07,
1.63093448e+07, 4.63117522e+07, 6.53035783e+06, 2.77565551e+07,
1.16463941e+07, 6.31852637e+07, 6.90915583e+05, 3.18942283e+06,
1.22394205e+06, 6.39633024e+06, 9.90753087e+05, 5.06260549e-02,
6.03045849e-01, 2.61134652e+06, 1.74098171e+07, 1.16715220e+06,
1.46259650e+06, 6.67530784e+06, 5.67530042e+07, 1.61486981e+07,
1.60781642e+07, 1.95150996e+06, 4.40356468e+06, 9.59475968e+05,
4.26347682e+06, 4.16116123e+06, 6.53982775e+06, 6.58502212e+06,
5.15489567e+06, 5.24978724e+06, 2.10989060e+06, 5.27896028e+06,
2.32195793e+07, 7.23585676e+06, 4.78554234e+06, 3.19049531e+06,
6.01784591e+06, 6.19861757e+06, 4.68382382e+06, 2.99302999e+06,
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4.94997979e+06, 6.95500986e+06, 3.56843375e+06, 2.80198597e+07,
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8.95224692e+06, 9.23015861e+06, 4.13769908e+06, 2.29496299e+07,
7.87008825e+05, 2.73050118e+07, 1.85128758e+07, 6.36773204e+07,
1.35541657e+08, 1.44615748e+06, 5.55521107e+06, 1.02479985e+07,
1.58164750e+06, 4.00406855e+06, 4.31400365e+06, 2.88568664e+07,
2.60832179e+06, 3.22386503e+07, 1.52216684e+06, 3.48264500e+07,
9.68331583e+06, 1.82697615e+07, 1.54121893e+07, 6.77521100e+06,
8.25528638e+05, 1.08542815e+06, 1.52890700e+06, 7.78605148e+06,
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1.11054751e+06, 1.38791053e+06, 2.05460727e+06, 8.67058856e+06,
4.84675118e+06, 3.13369186e+06, 4.16571060e+06, 9.94191912e+06,
2.01582541e+07, 1.52861652e+06, 1.04830068e+07, 1.33461266e+07,
1.95876975e+07, 1.83932232e+07, 2.56055688e+07, 2.67689960e+06,
1.05542167e+07, 8.20731198e+06, 1.13753191e+07, 5.64520923e+06,
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5.85627481e+06, 5.14294820e+06, 4.97408874e+06, 8.47531462e+06,
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3.51211819e+06, 1.44956046e+06, 6.69134135e+06, 8.28803800e+07,
4.14704909e+07, 2.05873585e+06, 4.72873840e+05, 5.66083084e+06,
1.17229216e+07, 1.03304139e+07, 1.22865948e+07, 2.83782261e+07,
5.73942758e+06, 1.17907880e+07, 1.80165735e+07, 3.57793555e+07,
3.01143016e+06, 5.78403869e+06, 4.98246436e+07, 4.20907550e+06,
1.50520799e+07, 5.29772231e+06, 7.81432761e+06, 9.90867594e+06,
1.24057228e+08, 3.43579933e+07, 1.66956835e+08, 7.62859255e+06,
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4.51896794e+06, 4.02154173e+06, 3.46358527e+06, 3.07673421e+06,
2.80870096e+06, 7.53179410e+06, 4.42138338e+06, 9.08593367e+06,
3.00691183e+06, 8.34010112e+06, 7.44651706e+06, 1.93017175e+06,
```

```
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1.39370897e+07, 3.45942074e+05, 7.90278670e+05, 1.10088455e+06,
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1.40133676e+08, 1.21543800e+06, 8.25017708e+06, 7.75083985e+06,
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5.55194958e+06, 3.87626707e+06, 3.29377475e+06, 1.51826439e+06,
9.37999925e+05, 3.36073430e+07, 9.07656549e+05, 1.89510601e+07,
1.94816494e+08, 4.75831280e+07, 1.06583672e+08, 1.24617752e+07,
2.44581184e+07, 4.75834899e+08, 6.82491663e+06, 6.06789436e+06,
8.12656041e+06, 1.06683344e+07, 5.72758183e+06, 1.49120622e+07,
4.21211354e+06, 9.76848926e+06, 8.87133956e+06, 2.03235643e+07,
2.36784670e+06, 1.27205110e+07, 4.14394006e+06, 1.56190824e+07,
1.73631546e+07, 7.08569844e+05, 3.51081851e+06, 3.52644062e+06,
4.21911748e+05, 7.36412785e+05, 6.83779729e+05, 9.34570508e+06,
2.97913232e+06, 3.79177370e+06, 1.24840065e+07, 1.04519897e+08,
9.48024335e+05, 2.34031965e+06, 9.92277753e+05, 6.08757611e+07,
3.57570321e+07, 1.62612437e+07, 4.01948923e+07, 4.05616728e+07,
4.14063150e+07, 7.92694106e+07, 1.50006633e+07, 1.45089031e+07,
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6.62106846e+05, 1.00557573e+06, 2.14978966e+06, 1.27117776e+06,
4.23182053e+05, 7.60094000e+05, 3.96055906e+07, 2.20187261e+07,
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2.17109974e+07, 1.21648256e+07, 2.03800012e+07, 2.05764445e+07,
7.90366115e+06, 6.03541385e+07, 1.41614217e+06, 3.06125797e+06,
2.24503067e+07, 3.22979463e+07, 5.77298334e+06, 7.27681976e+06,
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3.77912724e+06, 3.92947762e+06, 2.46157269e+06, 3.07665615e+06,
2.48992135e+06, 3.31623450e+06, 3.63110727e+06, 2.77053443e+07,
5.76350053e+06, 2.15446710e+06, 2.87738003e+06, 1.11224560e+06,
2.07609476e+07, 7.92735489e+06, 9.89938257e+06, 1.33606368e+07,
2.12840266e+07, 1.54804038e+06, 3.77961794e+06, 1.84245907e+07,
2.12522405e+07, 2.35397018e+07, 1.22732600e+05, 4.83443472e+06,
6.37423034e+06, 4.32173712e+07, 5.16333749e+08, 6.89368180e+06,
2.22570555e+06, 2.04592591e+07, 4.82631052e+08, 1.35023802e+07,
1.03059546e+07, 9.79626493e+06])
```

In [110]: arr.var()

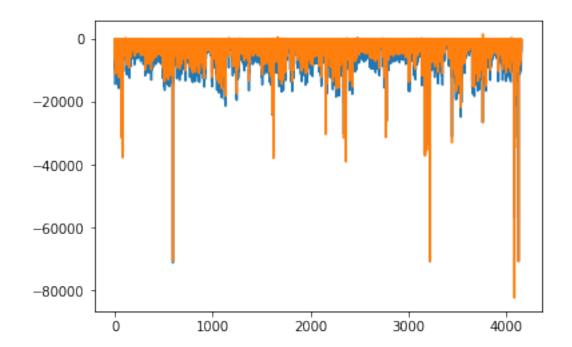
Out[110]: 22724635.591483254

variance accross measures/ mean variance accross species

```
In [111]: arr.mean(0).var()
Out[111]: 1388583.6554276315
In [112]: arr.mean(0)
Out[112]: array([-2219.06645714, -2919.84412463, -2015.18948926, -4288.21485415,
                 -4477.73292545, -4078.47555626, -4687.57869146, -1166.91552409,
                 -2855.27048881])
In [113]: arr.shape
Out[113]: (462, 9)
In [114]: randarr = np.zeros(arr.shape)
          for i in range(arr.shape[1]):
              ind = np.arange(len(arr))
             np.random.shuffle(ind)
             randarr[:,i] = arr[ind,i]
In [115]: randarr
Out[115]: array([[ 4.80310500e-01, -8.20665403e+03, 8.27506000e-01, ...,
                   5.09000000e-01, 8.14207000e-01, 6.83017500e-01],
                 [ 1.81295400e+00, -5.50839054e+03, -7.39452358e+03, ...,
                   3.26664000e-01, 5.96259000e-01, 6.67008500e-01],
                 [ 5.86694000e-01, -2.05983162e+03, 7.60942000e-01, ...,
                  -7.16414784e+03, -1.12670978e+03, 1.31595050e+00],
                 [-8.42159477e+03, 7.28880000e-01, -6.37472343e+03, ...,
                   7.98908000e-01, 5.62661000e-01, -3.39828738e+03],
                 [ 6.15312500e-01, 8.96209500e-01, 6.26267500e-01, ...,
                 -3.29407793e+03, 8.95917000e-01, 8.86115000e-01],
                 [-3.56788777e+03, -2.26486971e+03, 6.17829500e-01, ...,
                   5.02751500e-01, 1.02734500e+00, -2.88560159e+03]])
In [116]: randarr.mean(0).var()-arr.mean(0).var()
Out[116]: 4.656612873077393e-10
In [117]: randarr.var(1).mean()-arr.var(1).mean()
Out[117]: 2882412.743031189
In [97]: arr.var(0)
Out [97]: array([41333202.63856429, 10727555.04310829, 19414596.46349642,
                12230304.06525019, 22099342.25172593, 19543347.84000982,
                28742207.88900693, 21790682.06159877, 16143229.1717399 ])
```

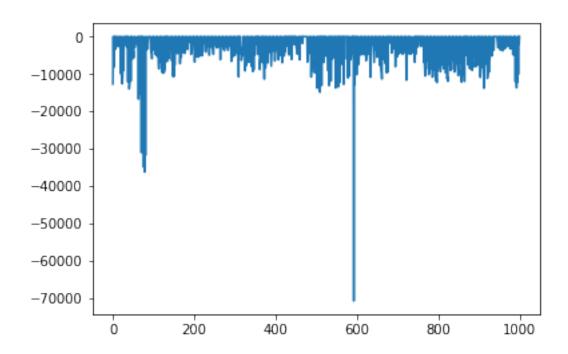
```
In [31]: from matplotlib.pyplot import *
```

In [118]: plot(data[:,1:])



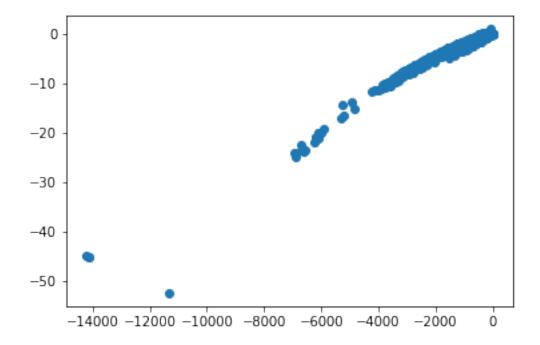
In [119]: plot(data[:1000,1:].mean(1))

Out[119]: [<matplotlib.lines.Line2D at 0x109c419d0>]



In [75]: scatter(data[:,1]/data[:,1].max(),data[:,2]/data[:,2].max())

Out[75]: <matplotlib.collections.PathCollection at 0x10a510690>



Given the repartition of the data (outliers) it will be almost impossible to cluster we should better use direct exploration

We can see that it is confirmed here, even if it does not cluster, it is more a relation of variance and

```
In [77]: X = -1
         species = [1,2,3,4,5,6,7,8,9,10]
         col = ['#f39c12', "#1abc9c", "#3498db", "#2ecc71", "#9b59b6", '#34495e', '#492000', '*
         '#043927', '#8F9779', '#f1c40f', '#e67e22', '#e74c3c', '#7f8c8d']
         source = ColumnDataSource(data=dict(x = data[:X,1]/data[:,1].min(),
                                             y = data[:X,2]/data[:,2].min(),
                                             names = np.array(datatot[0])[:X],
                                             colors= [col[0] if i-30 not in species else\
                                                     col[i-30] for i in np.array(datatot[0])[::
         output_notebook()
         hover = HoverTool(tooltips=[("species: ", "@names")])
         p = figure(title="Plot of the regressors",
                    tools=[hover, WheelZoomTool(), PanTool(), SaveTool(), ResetTool()],
                    plot_width=800, plot_height=600)
         p.circle(x='x', y='y', source=source, size=10,color='colors')
         show(p)
In [47]: from sklearn.neighbors import KNeighborsClassifier
         from sklearn.gaussian_process import GaussianProcessClassifier
         from sklearn.svm import SVC
         svc = SVC(C=1.0, kernel='rbf', degree=40, gamma='auto', coef0=0.0, shrinking=True, pre
                tol=0.001, cache_size=200, class_weight=None, verbose=False,
                max_iter=-1, random_state=None).fit(data[:,1:], data[:,0].astype(int))
         neigh = KNeighborsClassifier(n_neighbors=462).fit(data[:,1:], data[:,0].astype(int))
In [48]: neigh.score(data[:,1:], data[:,0].astype(int))
Out [48]: 0.010582010582010581
In [49]: svc.score(data[:,1:], data[:,0].astype(int))
Out [49]: 0.02356902356902357
```

### 0.5 we are now looking at the full dataset

```
In [6]: datatot = pd.DataFrame({'': []})
        for i in range (5,15):
            datatot = pd.concat([datatot, pd.read_csv('parameterFitsBacteria/nonlinfit'+str(i)
        datatot
Out[6]:
                  0
                       1
                                      2
                                                    3
                                                                         5
        0
                1.0
                      Ε
                         -62792.363178 -41171.105942
                                                       0.387295
                                                                 0.053507 NaN
        1
                1.0
                              0.884914
                                             0.625735
                                                       0.025491
                                                                  0.000321 NaN
                      Η
        2
                1.0
                      Q
                         -34078.001362 -14052.539028
                                                       0.223853
                                                                 0.072042 NaN
        3
                                                                 0.073091 NaN
                1.0
                      F
                          -7417.175624
                                        -7323.722600
                                                       0.052349
        4
                1.0
                      Y
                                                                 0.073580 NaN
                         -11366.590431
                                         -8018.684126
                                                       0.055767
        5
                1.0
                      C
                                                       0.028707
                                                                 0.000434 NaN
                              0.968817
                                             0.864984
        6
                1.0
                      Ν
                         -14509.094395
                                         -5446.502499
                                                       0.083904
                                                                 0.075813 NaN
        7
                1.0
                      K
                               1.851802
                                             1.645036
                                                       0.003847
                                                                 0.001664 NaN
        8
                                                       0.024459 0.000370 NaN
                1.0
                      D
                              0.907276
                                             0.647303
        9
                2.0
                      Ε
                                             0.975947
                                                       0.021372 0.000522 NaN
                               1.094369
        10
                2.0
                                                       0.028694 0.077360 NaN
                      Η
                         -19868.512605 -19868.590216
        11
                2.0
                      Q
                                                       0.036053 0.000334 NaN
                              0.879460
                                             0.826876
        12
                2.0
                      F
                         -17245.573218 -10324.527574 0.076132 0.071973 NaN
        13
                2.0
                      Y
                          -3340.967483
                                          -825.185441
                                                       0.041597
                                                                  0.078089 NaN
        14
                2.0
                      С
                         -13539.463661
                                        -2431.330570
                                                       0.082519
                                                                 0.080565 NaN
        15
                2.0
                      N
                          -4876.630557
                                         -4453.878513
                                                       0.024482 0.078637 NaN
        16
                2.0
                      K
                              0.953721
                                             0.839989
                                                       0.028875
                                                                 0.000569 NaN
        17
                2.0
                      D
                                                       0.032383
                                                                 0.000105 NaN
                              0.955444
                                             0.927154
        18
                3.0
                      Ε
                              0.648022
                                            -0.061252
                                                       0.012024
                                                                 0.000051 NaN
                3.0
                                                       0.287958 0.059913 NaN
        19
                      Η
                         -48419.842753 -29259.971830
        20
                3.0
                      Q
                               0.718656
                                            -0.090369
                                                       0.008074
                                                                 0.000410 NaN
        21
                3.0
                      F
                         -49899.734542 -29418.743313
                                                       0.234177
                                                                 0.109418 NaN
        22
                3.0
                         -61797.377808 -40902.629785
                                                      0.354978 0.057879 NaN
                      Y
        23
                3.0
                      C
                         -56755.199293 -35080.077306
                                                       0.358516 0.056577 NaN
        24
                3.0
                         -43746.892027 -22584.086268
                                                       0.251196
                                                                 0.069826 NaN
                      N
        25
                3.0
                      K
                              0.801362
                                            -0.063157
                                                       0.006064 0.000021 NaN
        26
                3.0
                         -41138.321246 -23718.158629
                                                       D
                4.0
        27
                      Ε
                           -102.507859
                                          6077.565657
                                                       0.048571
                                                                  0.085363 NaN
        28
                4.0
                      Η
                              0.856398
                                             0.638767
                                                       0.028769
                                                                 0.000050 NaN
        29
                4.0
                      Q
                          -9391.532128
                                         -5847.378522
                                                       0.063551
                                                                  0.074700 NaN
                                                                       . . .
        . . .
                . . .
                                                             . . .
        4128
              459.0
                              0.839945
                                             0.699710
                                                       0.000050
                                                                 0.000131 NaN
                      N
        4129
              459.0
                      K
                                             0.442044
                                                       0.004320
                                                                 0.000214 NaN
                              0.436508
        4130
              459.0
                      D
                              0.667253
                                             0.528199
                                                       0.000174
                                                                 0.000182 NaN
              460.0
                      Ε
                                                       0.021962
                                                                 0.000381 NaN
        4131
                              0.406190
                                             0.634501
        4132
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                      Η
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                                                       0.00001
                                                                  0.000645 NaN
                              0.985126
              460.0
                                                                  0.000436 NaN
        4133
                      Q
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                                             0.726891
                                                       0.021257
        4134
              460.0
                      F
                                             0.694422
                                                       0.000074 0.000418 NaN
                              0.816020
        4135
              460.0
                      Y
                              0.930689
                                             0.838514
                                                       0.000041
                                                                  0.000352 NaN
        4136
              460.0
                      С
                                             0.611306
                                                       0.000000 0.000733 NaN
                              1.021081
              460.0
                              0.677209
                                             0.490812 0.000091 0.000128 NaN
        4137
                      Ν
```

4138	460.0	K	0.869084	0.978546	0.000364	0.000636 NaN	
4139	460.0	D	0.781626	0.442542	0.000005	0.000741 NaN	
4140	461.0	E	0.757875	0.587377	0.000063	0.000267 NaN	
4141	461.0	Н	0.571183	0.688012	0.003767	0.000529 NaN	
4142	461.0	Q	0.815468	0.722794	0.000099	0.000167 NaN	
4143	461.0	F	0.536594	0.908253	0.016678	0.000051 NaN	
4144	461.0	Y	0.417824	0.662918	0.021889	0.000208 NaN	
4145	461.0	C	0.577827	0.928626	0.011756	0.001116 NaN	
4146	461.0	N	0.480479	0.637362	0.009399	0.000121 NaN	
4147	461.0	K	0.564361	0.378703	0.000202	0.000135 NaN	
4148	461.0	D	0.681498	0.810177	0.001866	0.000187 NaN	
4149	462.0	E	0.658475	0.512497	0.000175	0.000150 NaN	
4150	462.0	Н	0.557306	0.676898	0.004250	0.000283 NaN	
4151	462.0	Q	0.702023	0.639770	0.000324	0.000139 NaN	
4152	462.0	F	1.490475	2.449030	0.000149	0.003616 NaN	
4153	462.0	Y	0.503267	0.801784	0.015582	0.000323 NaN	
4154	462.0	C	0.480082	0.733640	0.015162	0.000319 NaN	
4155	462.0	N	0.560325	0.737822	0.005977	0.000271 NaN	
4156	462.0	K	0.696857	0.477855	0.000052	0.000184 NaN	
4157	462.0	D	0.755843	0.842702	0.000732	0.000813 NaN	

[41550 rows x 7 columns]