

leggi_pdb

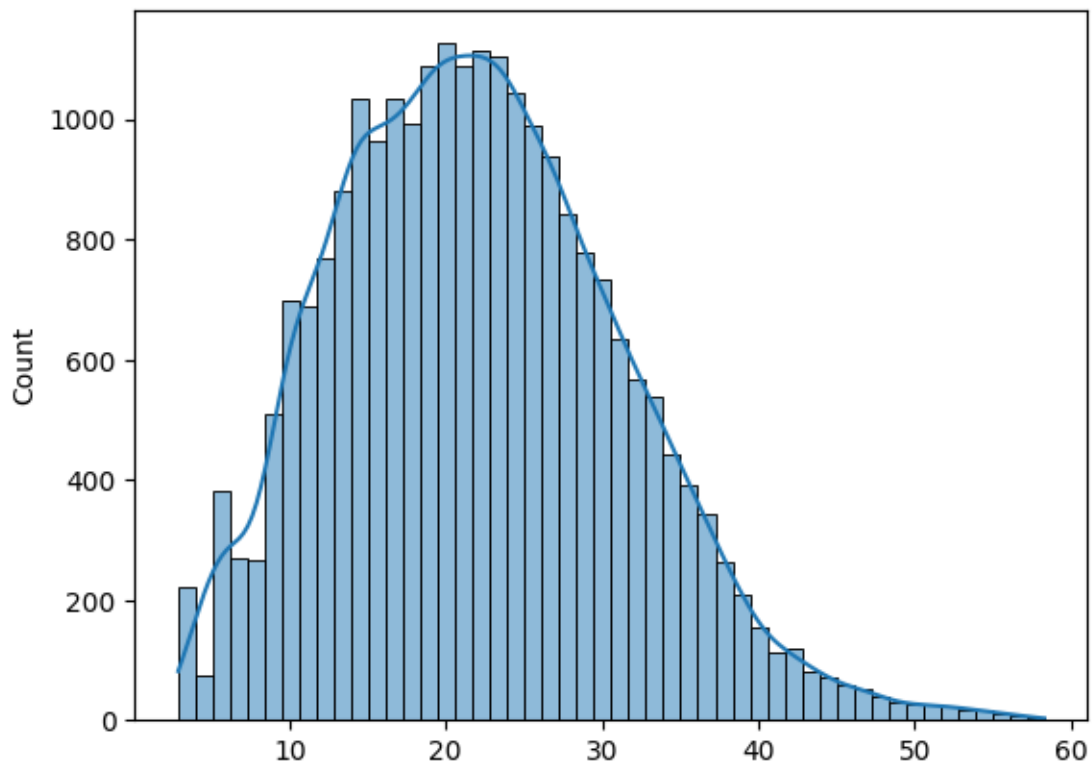
April 15, 2023

```
[117]: import scipy as sp
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
```

```
[118]: data = sp.io.loadmat('coord1PHP.mat')
protlist = data['protlist'][:,0]
A = data['A']
coord = data['coord']
Nnode = A.shape[0]

sns.histplot(protlist, kde=True, bins=50)
```

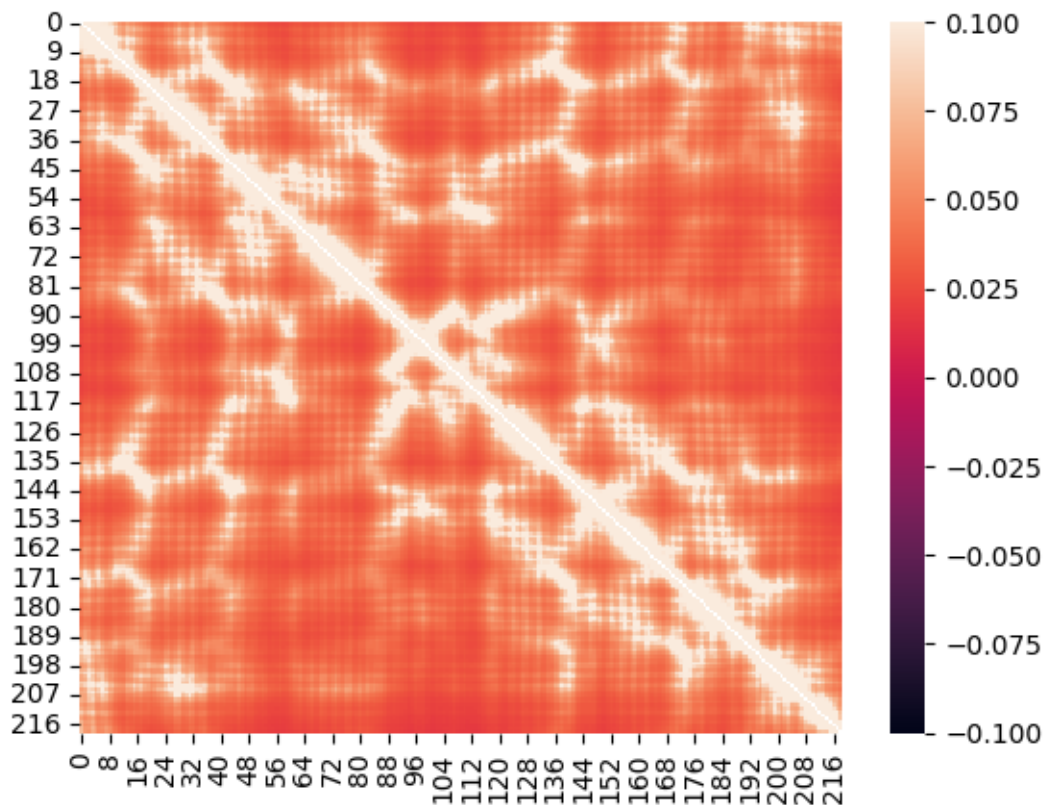
```
[118]: <Axes: ylabel='Count'>
```



```
[119]: D = sp.spatial.distance.squareform(protdist)
sns.heatmap(1./D)
```

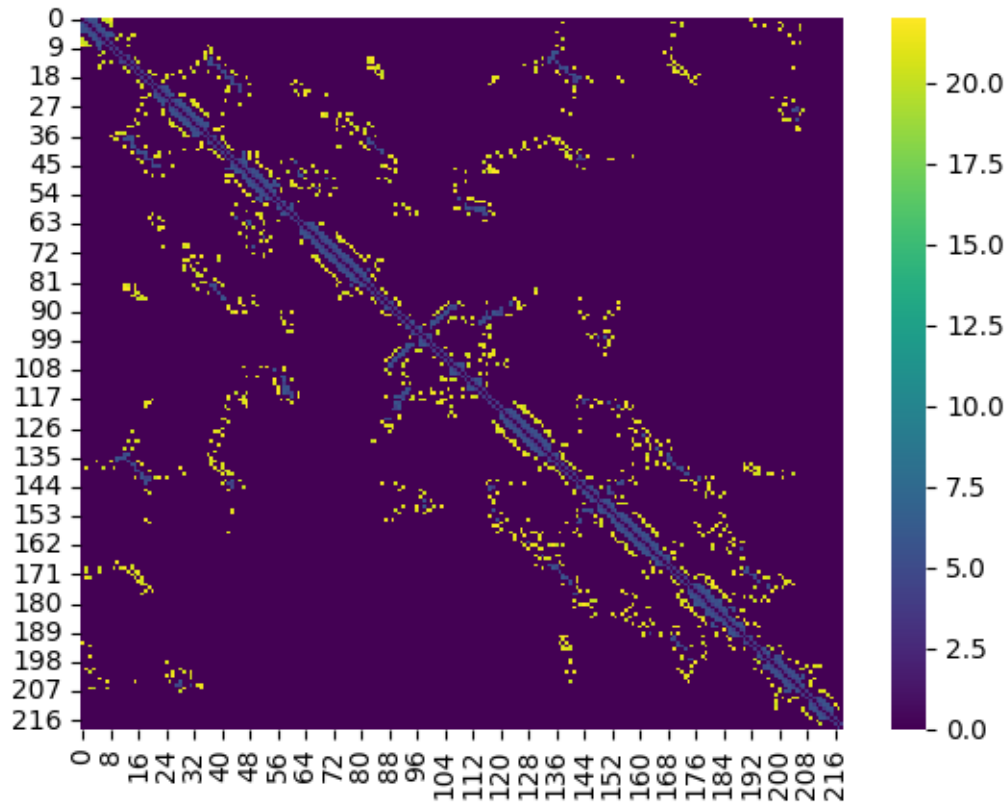
```
/tmp/ipykernel_833/2899854611.py:2: RuntimeWarning: divide by zero encountered
in divide
  sns.heatmap(1./D)
```

[119]: <Axes: >



```
[120]: Net6 = (D < 6) * D
Net10 = (D > 10) * (D < 11) * D
N1 = (D < 11) * D
sns.heatmap(Net6 + 2*Net10, cmap='viridis')
```

[120]: <Axes: >

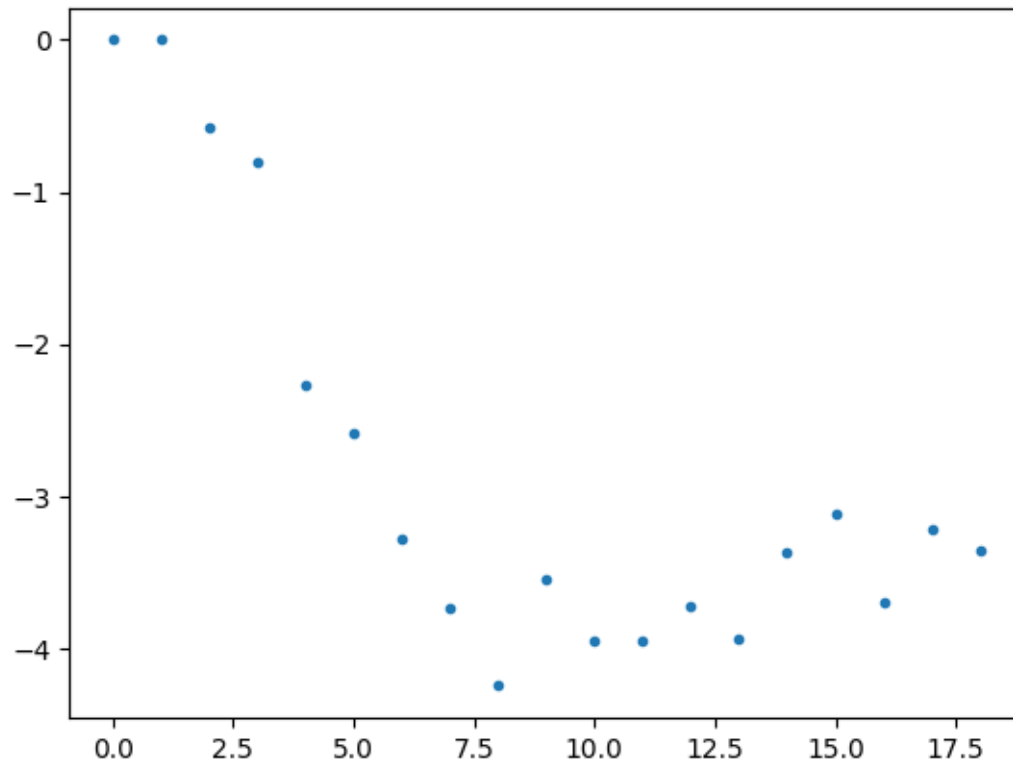


```
[121]: Kdiag = []

for index in range(Nnode):
    Kdiag.append(np.sum(np.diag(A, index))/(Nnode - index))

plt.plot(np.log(Kdiag[1:20]), '.')
```

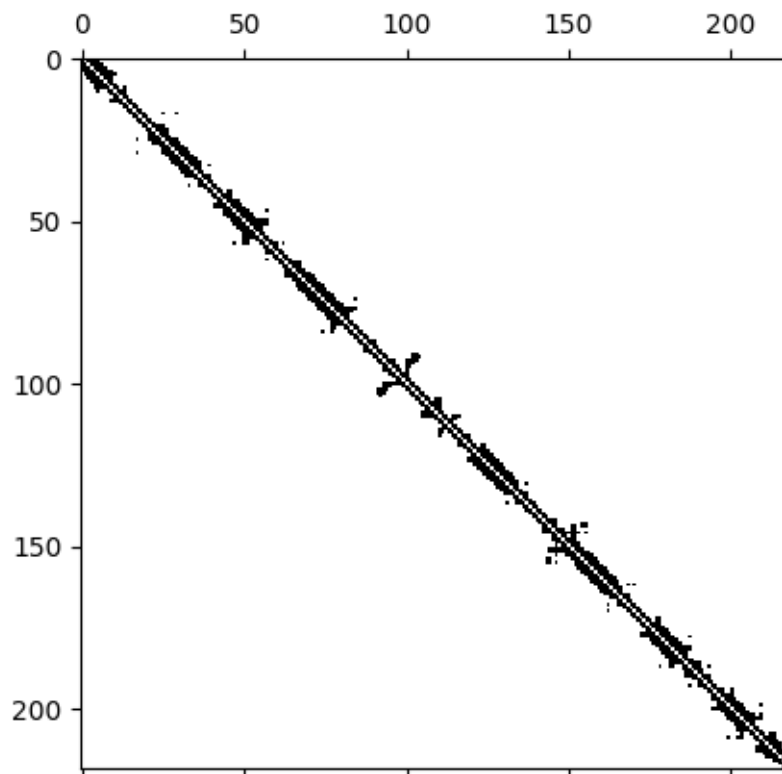
```
[121]: [<matplotlib.lines.Line2D at 0x7f64fe7fa980>]
```



```
[122]: Nkd = 12
Ad = np.zeros((Nnode, Nnode))

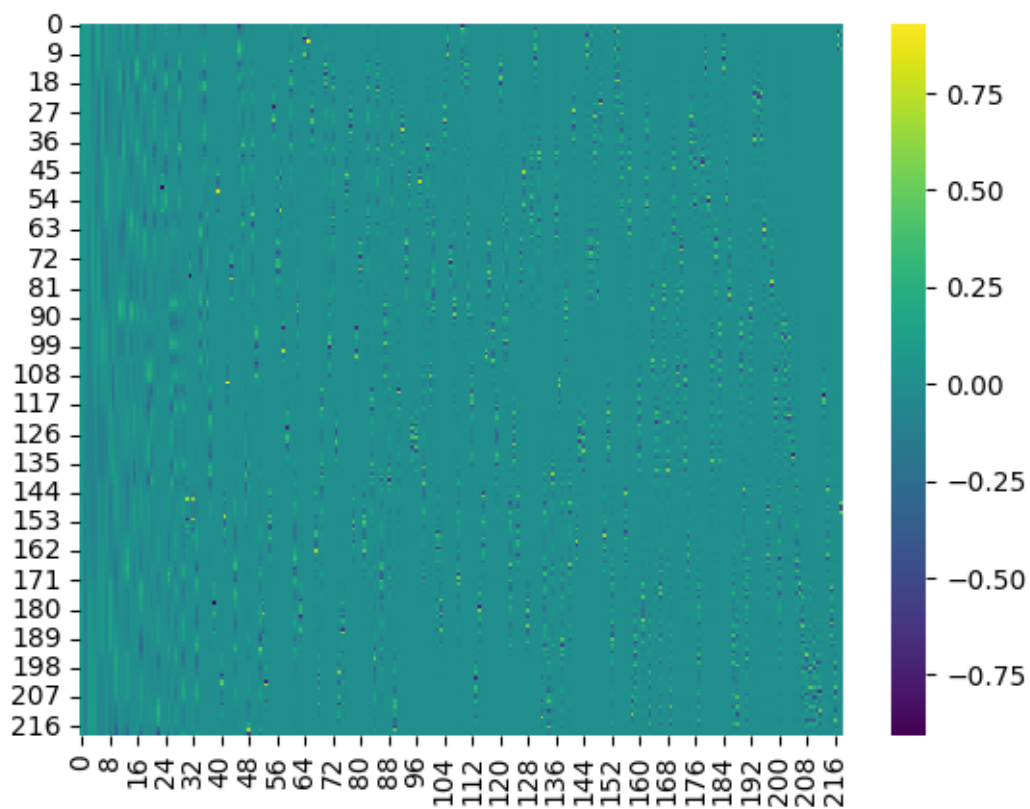
for ind in range(-Nkd, Nkd):
    Ad += np.diagflat(A.diagonal(ind), ind)
Ad = Ad + Ad.T
plt.spy(Ad)
```

```
[122]: <matplotlib.image.AxesImage at 0x7f64fe675510>
```



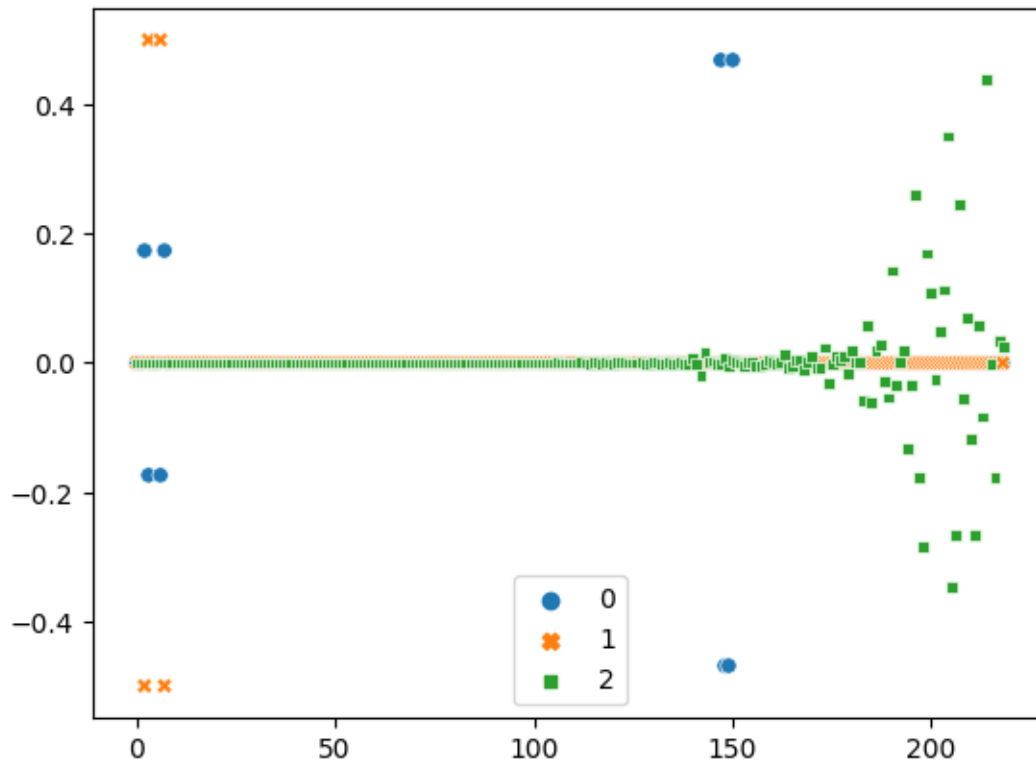
```
[123]: ValAd, VecAd = np.linalg.eig(sp.sparse.csgraph.laplacian(Ad))  
sns.heatmap(VecAd, cmap='viridis')
```

```
[123]: <Axes: >
```



```
[124]: i1 = Nnode - 1
        i2 = Nnode - 2
        i3 = Nnode - 3
        sns.scatterplot(VecAd[:, [i1, i2, i3]])
```

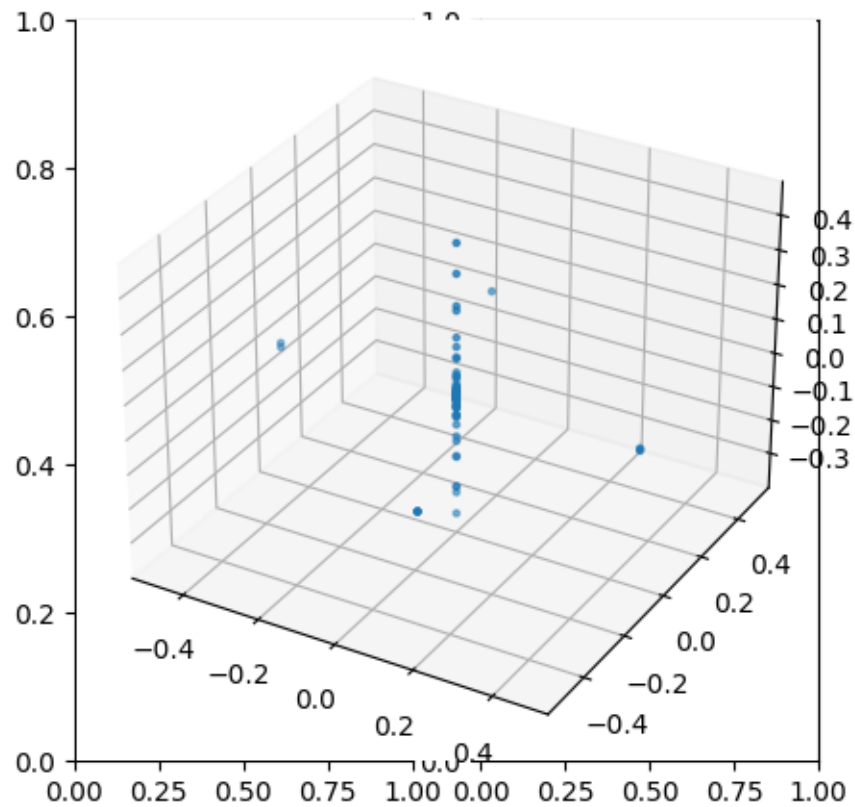
```
[124]: <Axes: >
```



```
[142]: fig, ax = plt.subplots(ncols=2 , figsize=(5, 5))
ax = fig.add_subplot(projection='3d')

ax.scatter(VecAd[:, i1], VecAd[:, i2], VecAd[:, i3], marker='.'.)
```

```
[142]: <mpl_toolkits.mplot3d.art3d.Path3DCollection at 0x7f64fdb419c0>
```

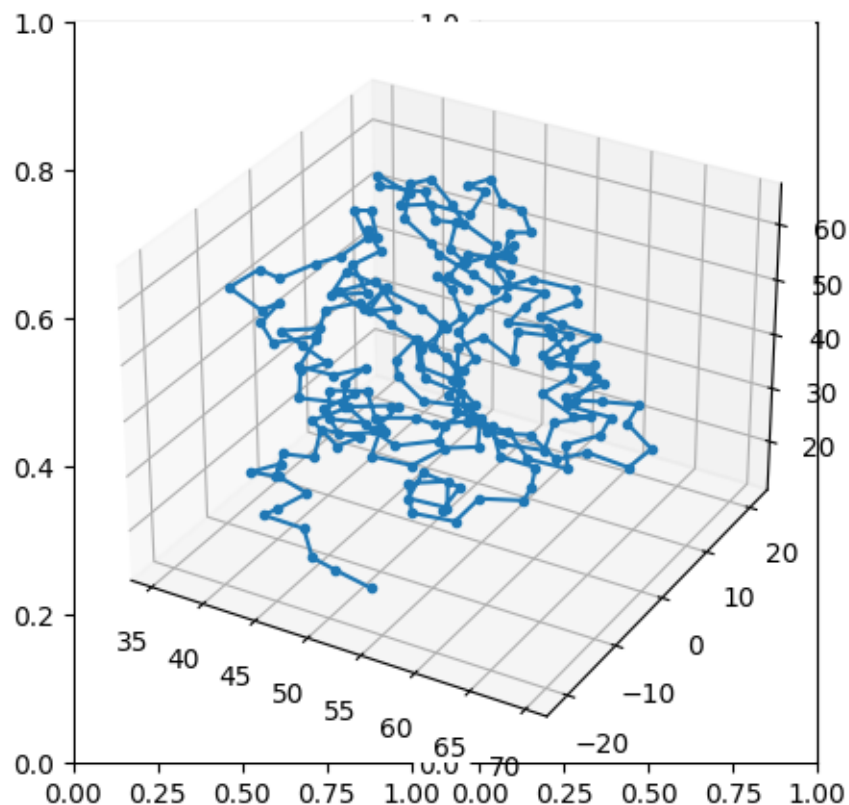


```
[143]: fig, ax = plt.subplots(ncols=2 , figsize=(5, 5))
ax = fig.add_subplot(projection='3d')

ax.plot(coord[:,0], coord[:,1], coord[:,2], marker='.')

```

```
[143]: [<mpl_toolkits.mplot3d.art3d.Line3D at 0x7f64fda7b970>]
```

```
[127]: import networkx as nx

D, P = sp.sparse.csgraph.dijkstra(Ad, directed=False, return_predecessors=True)
Cl = 1 / np.mean(D)
K = np.sum(A, axis=0)
BC = nx.betweenness centrality(nx.from_numpy_array(A))

print(Cl)
print(K)
print(BC)
```

0.029674209219849382

```
[ 4  6  8  7  9  9  9  6  6  9  8  8 11 14 14 12 13 14 14 13  9 11 10  6
  6  9  8  9 11 11 10 11 11 12  7  8 12 11 12 14 12 12 16 17 16 15 12 11
16 11 12 11 11  6  6  8 10 14 11  9 11 10 10  9  6  5 10 12  8  7 11 10
 8 10  9  8  9 12  9  7  8  7 12  9  9  8  8 12  9 13 16 14 14 13 10  8
 7  6  8  5  9  7  8  7  9 11  9 10  6  7 14  8  8  7 13 15 14 14 15 16
14  9  8 12 12  8  8 10 11  8  8 13 10  8 13 11 14 14 11 11 12 14 14 14
15 11 13  6  9  8  8 14 13 10 14 12 11 10 11 10  9 11 12 10  6  9  5  7
13  9 12 13 13 17 14  8  8 12 13  8 12 12  9  7  7  7 12  9  6  7 13  8
 8 10 11  6  8 10  8  8 12 11 12 11 12 12  7  7  7  9  6  6  7  8  6  6]
```

5 3 2]

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PCM_permute

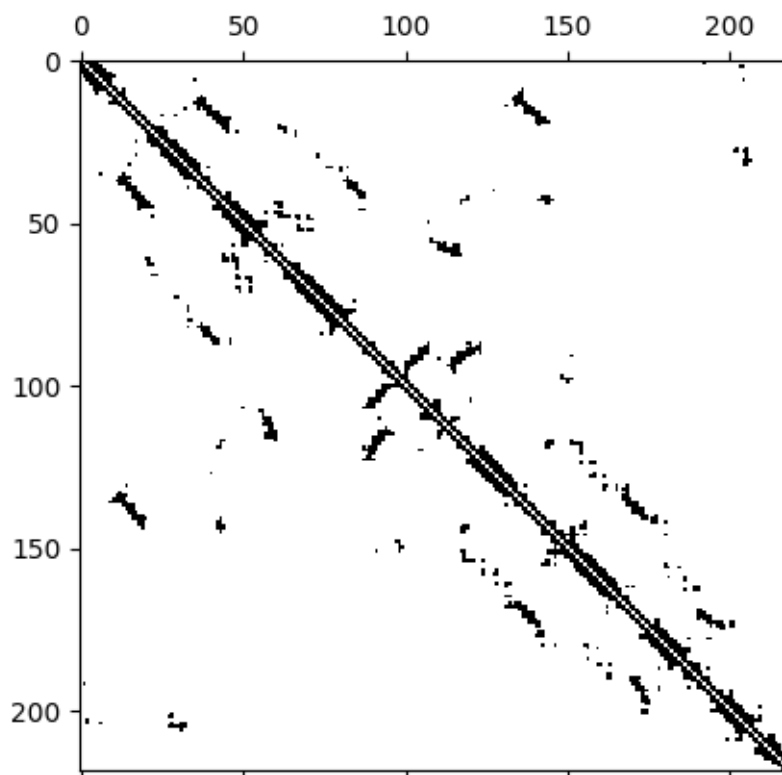
April 15, 2023

1 Permutation effects

```
[20]: import scipy as sp  
import numpy as np  
from matplotlib import pyplot as plt
```

```
[29]: data = sp.io.loadmat('coord1PHP.mat')  
A = data['A']  
coord = data['coord']  
Nnode = A.shape[0]  
plt.spy(A)
```

```
[29]: <matplotlib.image.AxesImage at 0x7fc8e8b04790>
```



```
[22]: Index = np.arange(Nnode)
      PermIndex = np.random.permutation(Nnode)
      PermMat = np.zeros((Nnode,Nnode))
```

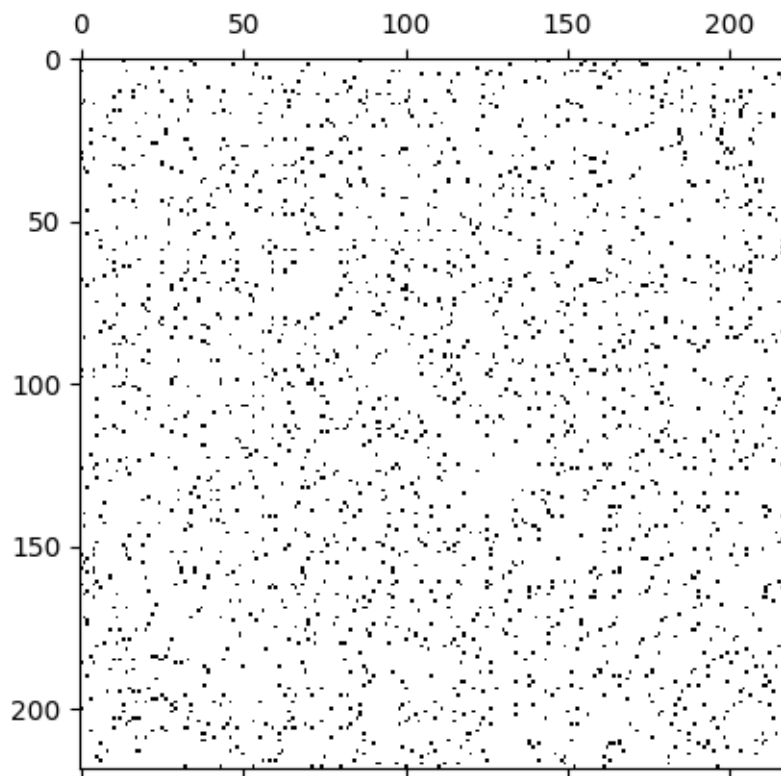
```
[23]: for ind in Index:
      PermMat[Index[ind], PermIndex[ind]] = 1
```

A faster method could be

```
[24]: PermMat = sp.sparse.coo_matrix((np.ones(Nnode), (Index, PermIndex)),
      ↪shape=(Nnode, Nnode)).toarray()
```

```
[25]: A2 = PermMat.dot(A).dot(PermMat.T)
      plt.spy(A2)
```

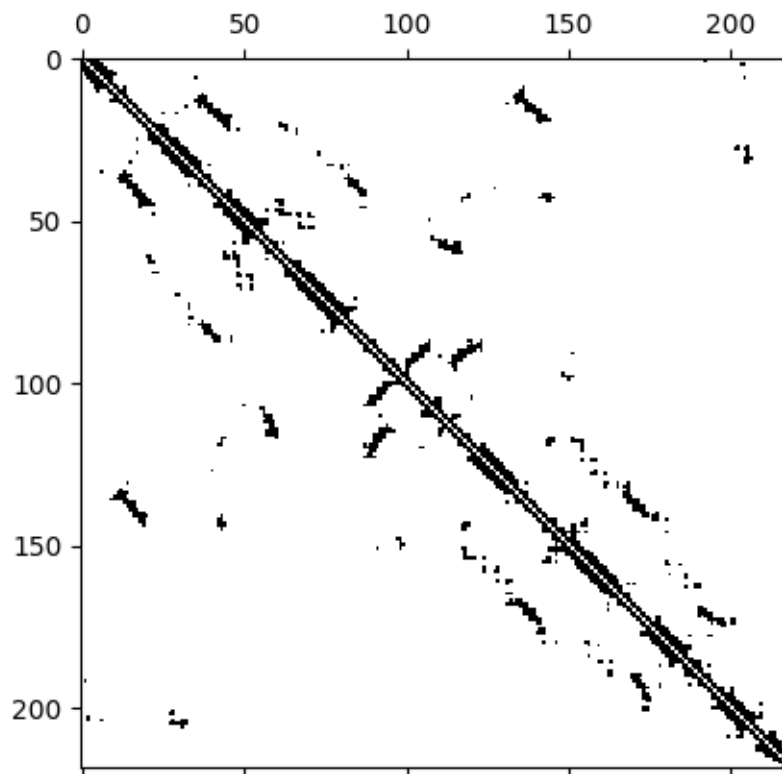
```
[25]: <matplotlib.image.AxesImage at 0x7fc8e8d9c190>
```



We can invert the permutation effect

```
[26]: A3 = (PermMat.T).dot(A2).dot(PermMat)
      plt.spy(A3)
```

[26]: <matplotlib.image.AxesImage at 0x7fc8e8c082b0>



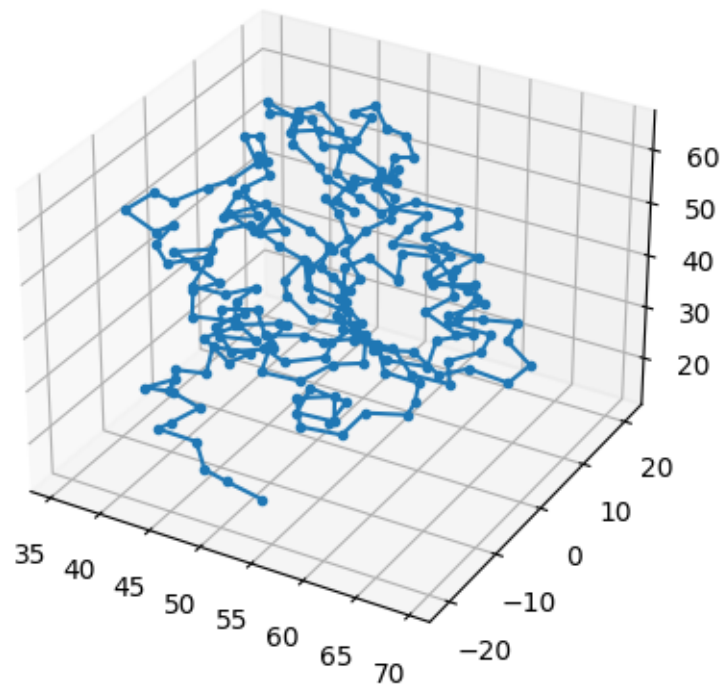
Let's try to visualize the 3d structure of the protein

```
[38]: fig = plt.figure()
      ax = fig.add_subplot(projection='3d')

      ax.plot(coord[:,0], coord[:,1], coord[:,2], marker='.')

```

[38]: [<mpl_toolkits.mplot3d.art3d.Line3D at 0x7fc8e19db5b0>]



ER_networks

April 15, 2023

1 Code from ER class

```
[57]: import scipy as sp
import numpy as np
import sys
import seaborn as sns
import matplotlib.pyplot as plt
import networkx as nx

def rand_canonical_f(Nnode, Plink):
    A = np.triu(np.random.rand(Nnode, Nnode), k=1)
    A = A > 1 - (2*Plink)
    A = A + A.T
    return A
```

Let's compare the memory usage between a sparse and a normal matrix. Moreover, we assume a microcanonical ensemble, fixing the number of nodes and links.

```
[58]: Nnode = int(1e3)
Nlink = int(3e4)
Net1 = sp.sparse.lil_matrix((Nnode,Nnode))
Net2 = np.zeros((Nnode,Nnode))

print(sys.getsizeof(Net1))
print(sys.getsizeof(Net2))
```

48
8000128

1.1 Microcanonical ensemble

Now, let's try to generate a random graph without using Networkx functions.

```
[59]: for index in range(100):
    # generate a random link
    ii = np.random.randint(Nnode, size=(Nlink, 2))
    # create a sparse matrix using these links
```



```

NetM = sp.sparse.coo_matrix((np.ones(Nlink), (ii[:,0], ii[:,1])),
↪shape=(Nnode, Nnode))
#remove loops
NetM.setdiag(0)
# symmetrize
NetM = NetM + NetM.T
print(NetM)

```

```

(0, 16)      1.0
(0, 17)      1.0
(0, 25)      1.0
(0, 51)      1.0
(0, 59)      1.0
(0, 92)      1.0
(0, 99)      1.0
(0, 103)     1.0
(0, 140)     1.0
(0, 168)     1.0
(0, 174)     1.0
(0, 175)     1.0
(0, 196)     1.0
(0, 221)     3.0
(0, 235)     1.0
(0, 271)     1.0
(0, 272)     1.0
(0, 299)     1.0
(0, 304)     1.0
(0, 320)     1.0
(0, 324)     1.0
(0, 333)     1.0
(0, 352)     1.0
(0, 356)     1.0
(0, 359)     1.0
:           :
(999, 675)   1.0
(999, 688)   1.0
(999, 695)   1.0
(999, 713)   1.0
(999, 716)   1.0
(999, 719)   1.0
(999, 723)   1.0
(999, 733)   1.0
(999, 742)   1.0
(999, 770)   1.0
(999, 788)   1.0
(999, 790)   1.0
(999, 807)   1.0

```

(999, 817)	1.0
(999, 821)	1.0
(999, 842)	1.0
(999, 849)	1.0
(999, 855)	1.0
(999, 868)	1.0
(999, 889)	1.0
(999, 891)	1.0
(999, 903)	2.0
(999, 911)	1.0
(999, 960)	1.0
(999, 961)	1.0

NOTE that reciprocal links and repeated links randomly created reduce symmetric links with a probability that scales as $\frac{1}{N_{node}^2}$

Let's count the number of links in the matrix.

```
[60]: Nl = int(NetM.count_nonzero()/2)
print('Randomly generated links: {:d}'.format(Nl))
print('Missing links for microcanonical ensemble: {:d}'.format(Nlink-Nl))
```

Randomly generated links: 29035

Missing links for microcanonical ensemble: 965

We notice that we miss some links, then we add one by one missing links until microcanonical constraint fulfilled.

```
[61]: while Nl < Nlink:
    i1 = np.random.randint(Nnode)
    i2 = np.random.randint(Nnode)
    if i1 != i2 and NetM[i1,i2] == 0:
        NetM[i1,i2] = 1
        NetM[i2,i1] = 1 # symmetric link
        Nl += 1
```

Lastly, let's compute the degree vector, finding minimum and maximum.

```
[62]: K = sum(NetM)
print('Average degree: {:.2f}'.format(np.mean(K)))
print('Minimum degree: {:d}'.format(int(np.min(K))))
print('Maximum degree: {:d}'.format(int(np.max(K))))
```

Average degree: 61.87

Minimum degree: 39

Maximum degree: 87

1.2 Canonical ensemble

Let's now try to build a canonical ensemble.

```
[63]: Nnode = int(1e2)
      Plink = 0.3
      Nexp = int(1e4)
```

```
[64]: LinkS = np.zeros((Nexp, 1))
      for index in range(Nexp):
          NetC = sp.sparse.triu(sp.sparse.rand(Nnode, Nnode, density=Plink,
          ↪format='csr'), k=1)
          NetC = NetC + NetC.T
          LinkS[index] = NetC.count_nonzero()/2
```

Let's see some stats

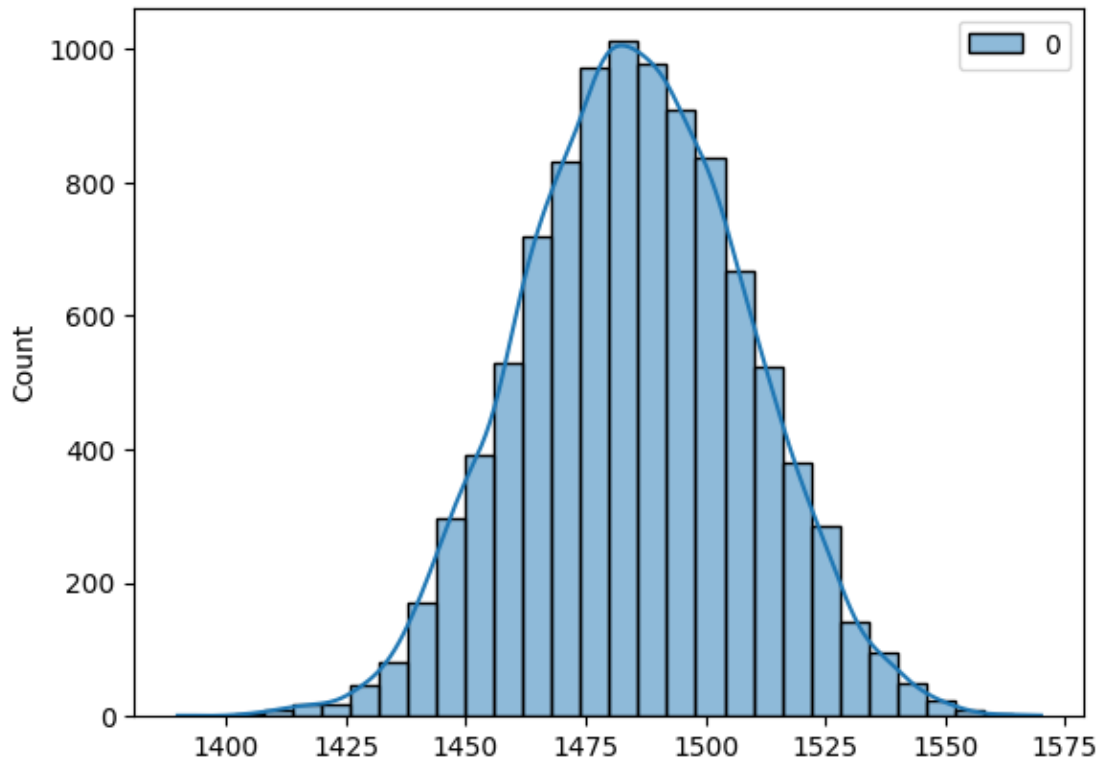
```
[65]: print('Average number of links: {:.2f}'.format(np.mean(LinkS)))
      print('Standard deviation: {:.2f}'.format(np.std(LinkS)))

      print('Expected number of links: {:.2f}'.format(Plink*Nnode*(Nnode-1)/2))
      print('Expected standard deviation: {:.2f}'.format(np.
      ↪sqrt(Plink*(1-Plink)*Nnode*(Nnode-1)/2)))

      sns.histplot(data=LinkS, bins=30, kde=True)
```

```
Average number of links: 1485.08
Standard deviation: 23.30
Expected number of links: 1485.00
Expected standard deviation: 32.24
```

```
[65]: <Axes: ylabel='Count'>
```



The degree distribution for increasing size - CV decreases. Tends to the delta function - regular graph.

```
[66]: Pow = 4.21 # max network size
      Pl = 0.1
      Cnt = 0

      M = []
      S = []
      CV = []
      Nnodes = []

[67]: for index in np.arange(2, Pow, step=0.3):
      Nnodes.append(int(10**index))
      NetC = sp.sparse.triu(sp.sparse.rand(Nnodes[Cnt], Nnodes[Cnt], density=Pl,
      ↪format='csr'), k=1)
      NetC = NetC + NetC.T
      K = sum(NetC).todense()
      M.append(np.mean(K))
      S.append(np.std(K))
      CV.append(np.std(K)/np.mean(K))
```

```

    # sns.histplot(data=K, bins=30, kde=True, label='N={:d}'.
↪format(Nnodes[Cnt]))
    print('N={:d} - Average degree: {:.2f}'.format(Nnodes[Cnt], M[Cnt]))
    print('N={:d} - Standard deviation: {:.2f}'.format(Nnodes[Cnt], S[Cnt]))
    print('N={:d} - CV: {:.2f}'.format(Nnodes[Cnt], CV[Cnt]))
    Cnt += 1

```

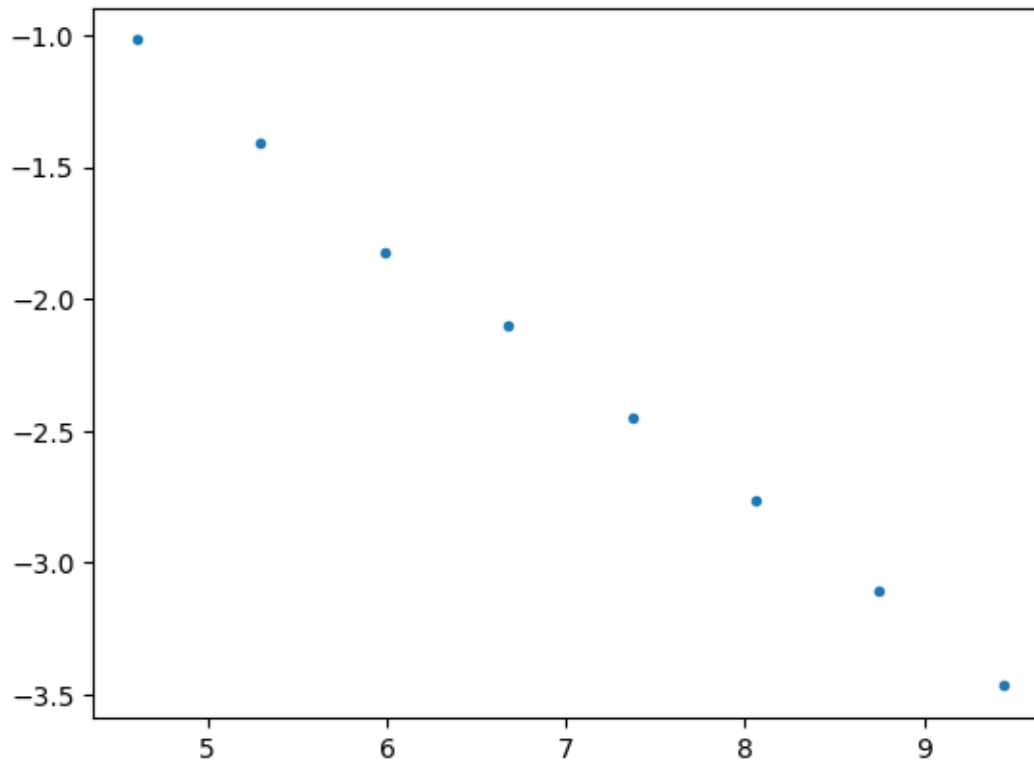
```

N=100 - Average degree: 4.50
N=100 - Standard deviation: 1.62
N=100 - CV: 0.36
N=199 - Average degree: 9.76
N=199 - Standard deviation: 2.39
N=199 - CV: 0.25
N=398 - Average degree: 19.72
N=398 - Standard deviation: 3.19
N=398 - CV: 0.16
N=794 - Average degree: 39.65
N=794 - Standard deviation: 4.83
N=794 - CV: 0.12
N=1584 - Average degree: 79.53
N=1584 - Standard deviation: 6.86
N=1584 - CV: 0.09
N=3162 - Average degree: 158.26
N=3162 - Standard deviation: 9.98
N=3162 - CV: 0.06
N=6309 - Average degree: 314.95
N=6309 - Standard deviation: 14.07
N=6309 - CV: 0.04
N=12589 - Average degree: 629.21
N=12589 - Standard deviation: 19.65
N=12589 - CV: 0.03

```

```
[68]: plt.plot(np.log(Nnodes), np.log(CV), '.')
```

```
[68]: [<matplotlib.lines.Line2D at 0x7fafb89a6860>]
```



1.3 Giant component transition

```
[69]: Nnode = int(1e2)

rr = np.triu(np.random.rand(Nnode, Nnode), k=1)
rr = rr + rr.T
```

```
[70]: Pmin = 1 / (20 * Nnode)
Pmax = 6 / Nnode
xP = np.arange(Pmin, Pmax, step=0.00002)
```

NOTE that $\lambda = xP * Nnode$

```
[71]: Rc = np.zeros(len(xP))
Rm = np.zeros(len(xP))
Cnt = 0

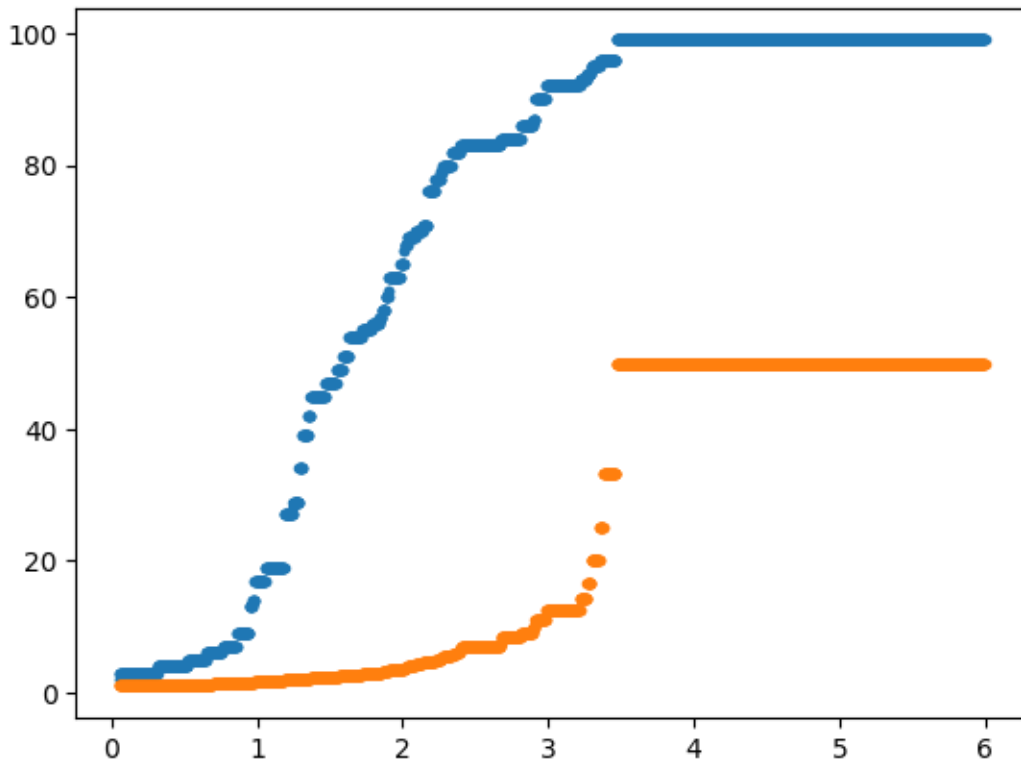
for index in xP:
    Net = nx.from_numpy_array(rr > 1 - index)
    CompList = nx.connected_components(Net)
    Comps = [len(x) for x in CompList]
    Rc[Cnt] = max(Comps)
```

```
Rm[Cnt] = np.mean(Comps)
Cnt += 1
```

```
[72]: plt.plot(xP*Nnode, Rc, '.')
```

```
plt.plot(xP*Nnode, Rm, '.')
```

```
[72]: [<matplotlib.lines.Line2D at 0x7fafb882d990>]
```



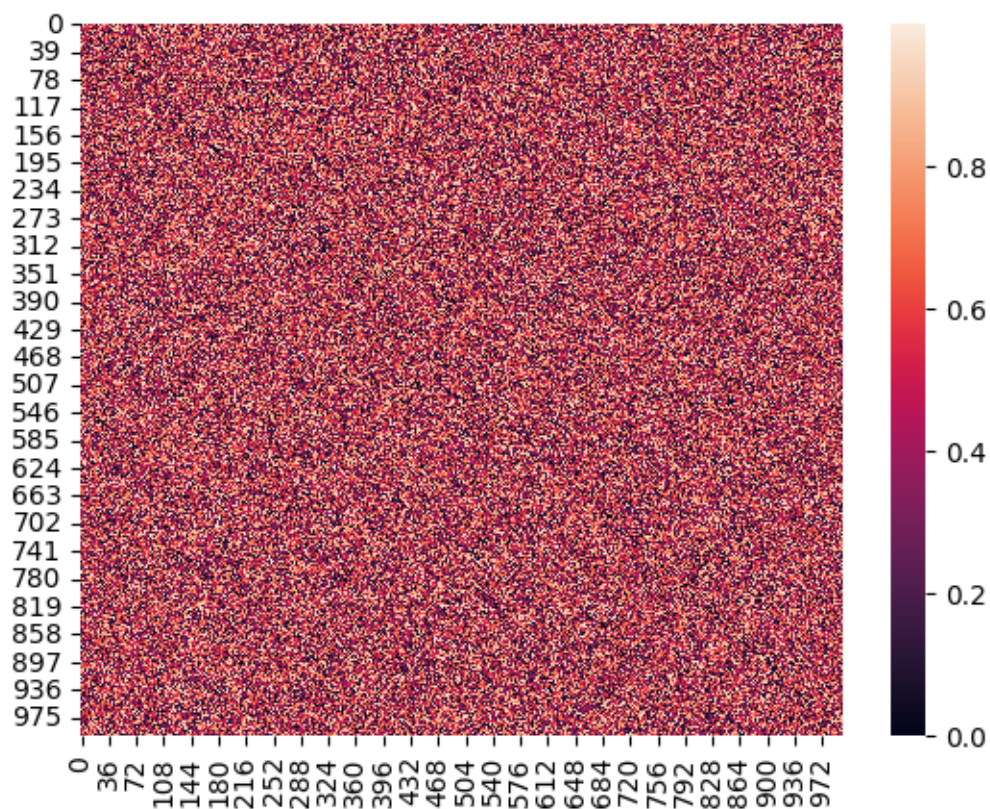
1.4 Semicircle law for ER network spectrum vs RMT (Random Matrix Theory)

```
[73]: Nnode = int(1e3)
Plink = 0.2 # link probability (canonical)

rr = np.triu(np.random.rand(Nnode, Nnode), k=1)
rr = rr + rr.T
np.fill_diagonal(rr, 0) # remove loops

# plot matrix with values
sns.heatmap(rr)
```

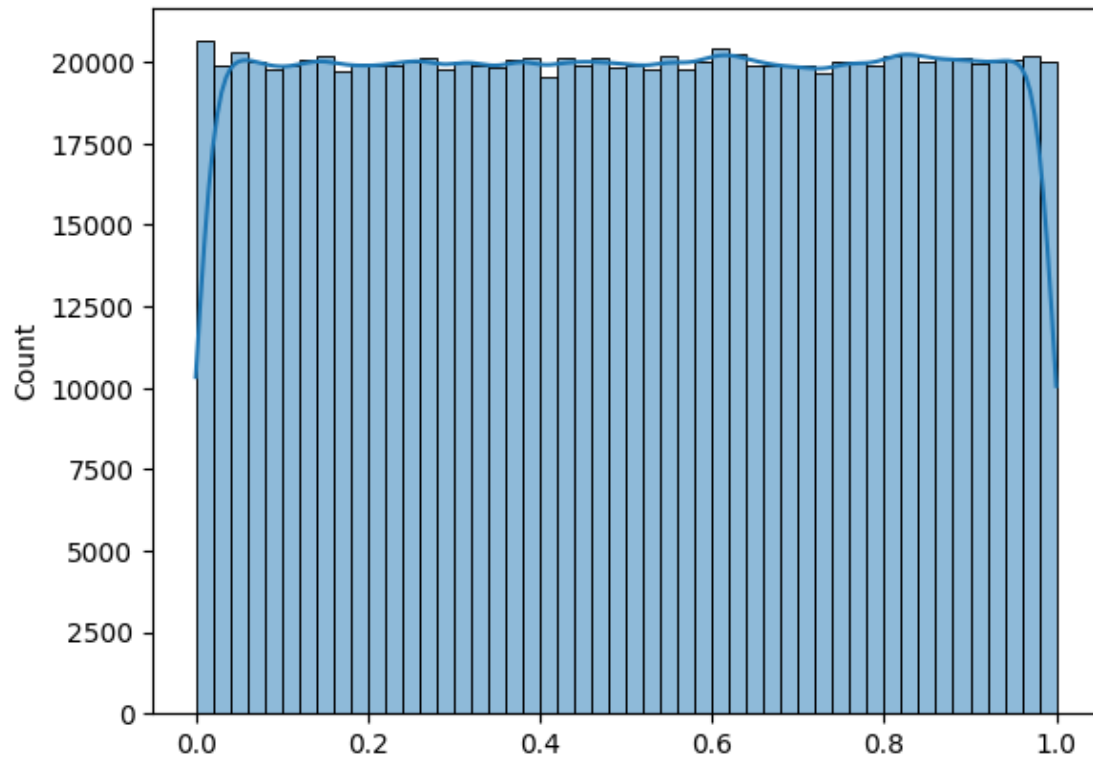
```
[73]: <Axes: >
```



Let's see also the histogram of coefficients

```
[74]: sns.histplot(data=rr.ravel(), bins=50, kde=True)
```

```
[74]: <Axes: ylabel='Count'>
```

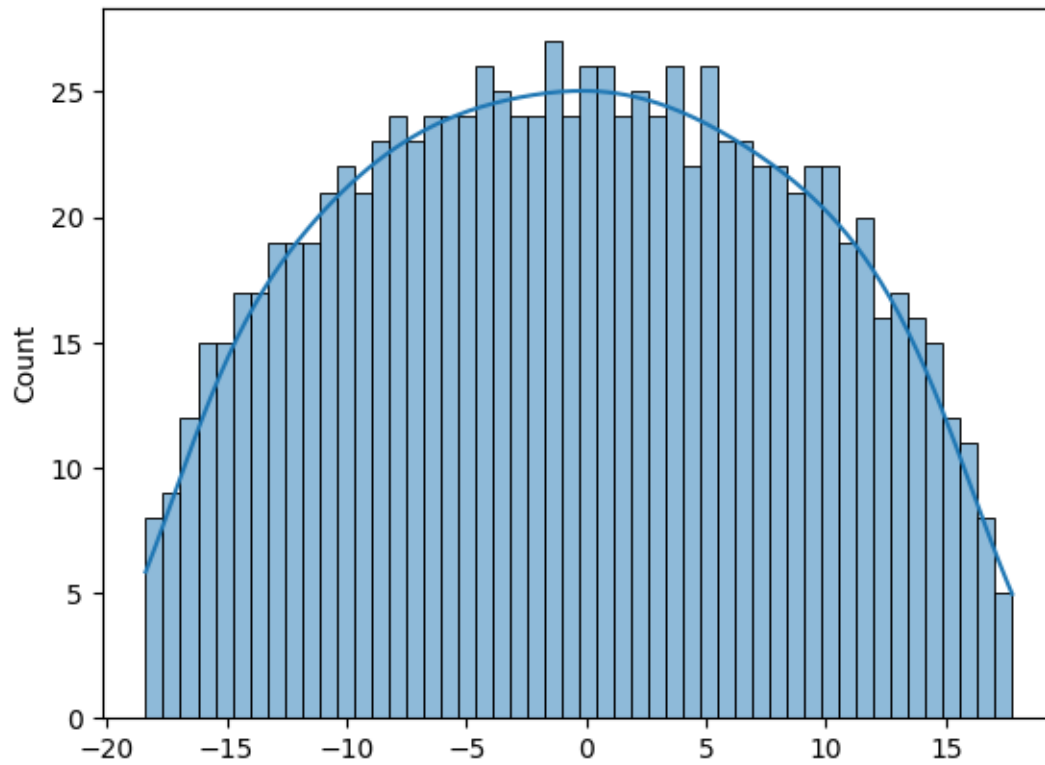



Now the eigenvalues and eigenvectors.

NOTE A symmetric ER network has a real semicircle spectrum

```
[75]: vv = np.linalg.eigvals(rr)
      sns.histplot(data=vv[vv < vv.max()], bins=50, kde=True)
```

```
[75]: <Axes: ylabel='Count'>
```

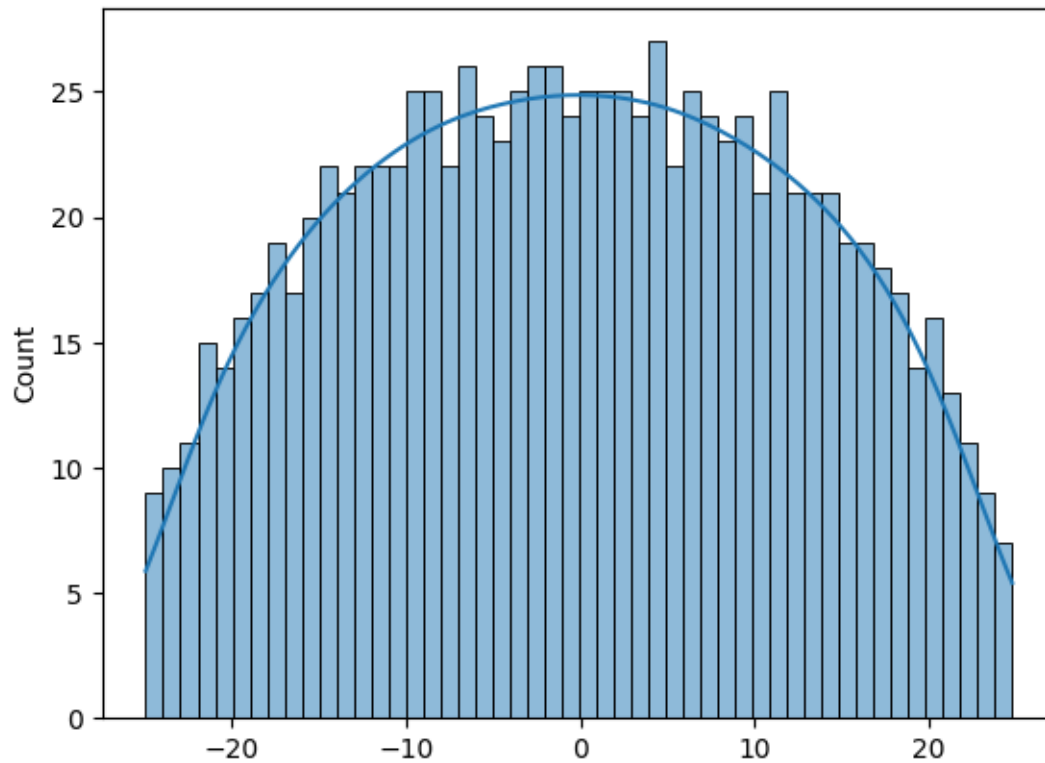


```
[76]: rr = np.triu(np.random.rand(Nnode, Nnode), k=1) > 1 - Plink
      rr = rr + rr.T
```

```
[77]: vv, vec = np.linalg.eig(rr)
```

```
[78]: sns.histplot(data=vv[vv < vv.max()], bins=50, kde=True)
```

```
[78]: <Axes: ylabel='Count'>
```

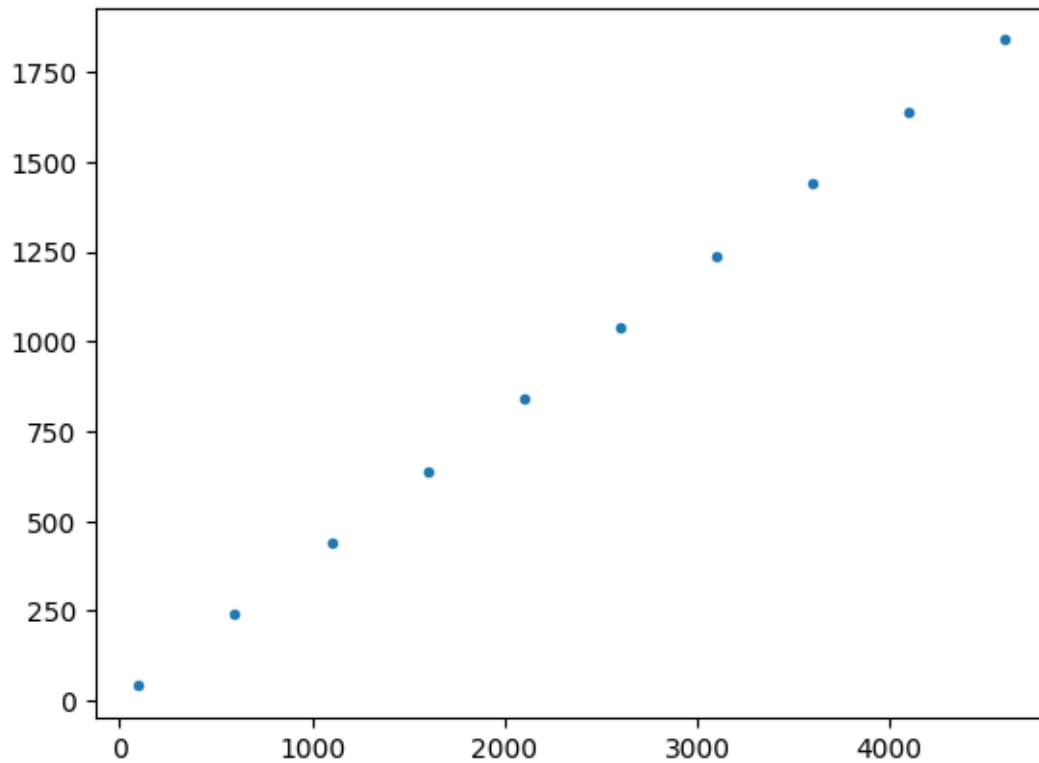


```
[83]: Cnt = 0
xx = np.arange(100, 5000, step=500)
vmax = []

for index in xx:
    rr = rand_canonical_f(index, Plink)
    vv = np.linalg.eigvals(rr)
    vmax.append(np.max(vv))
    Cnt += 1

plt.plot(xx, vmax, '.')
```

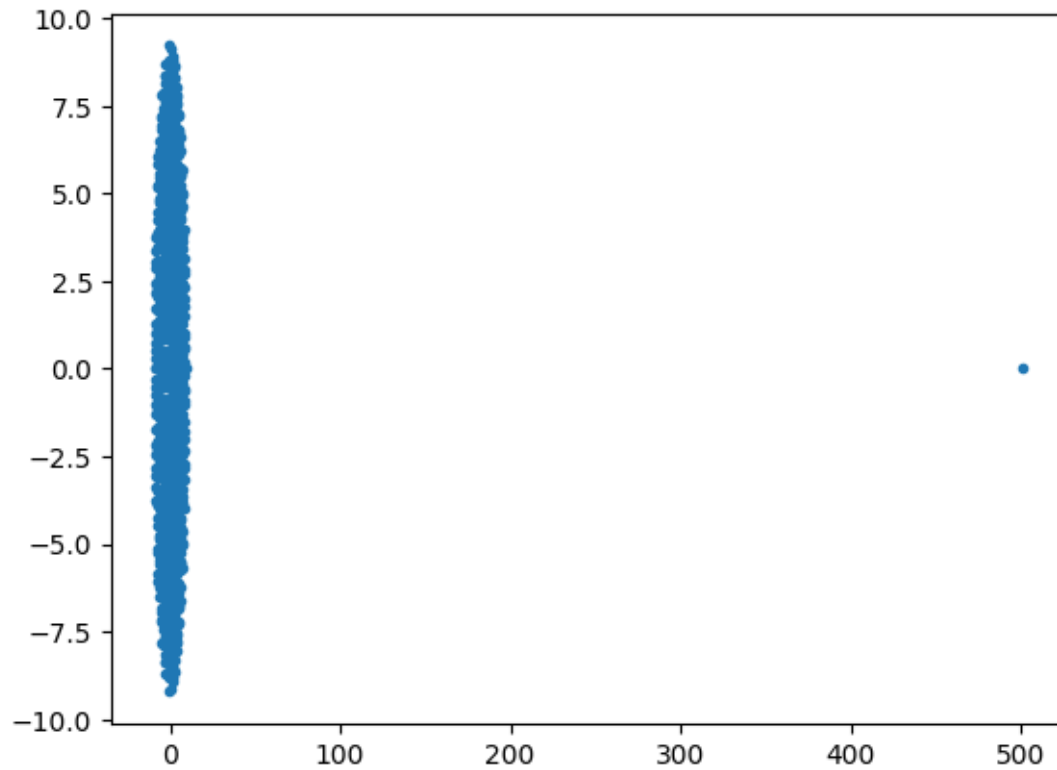
```
[83]: [<matplotlib.lines.Line2D at 0x7fafb8358f10>]
```



For a directed random matrix we'll have a complex circular spectrum

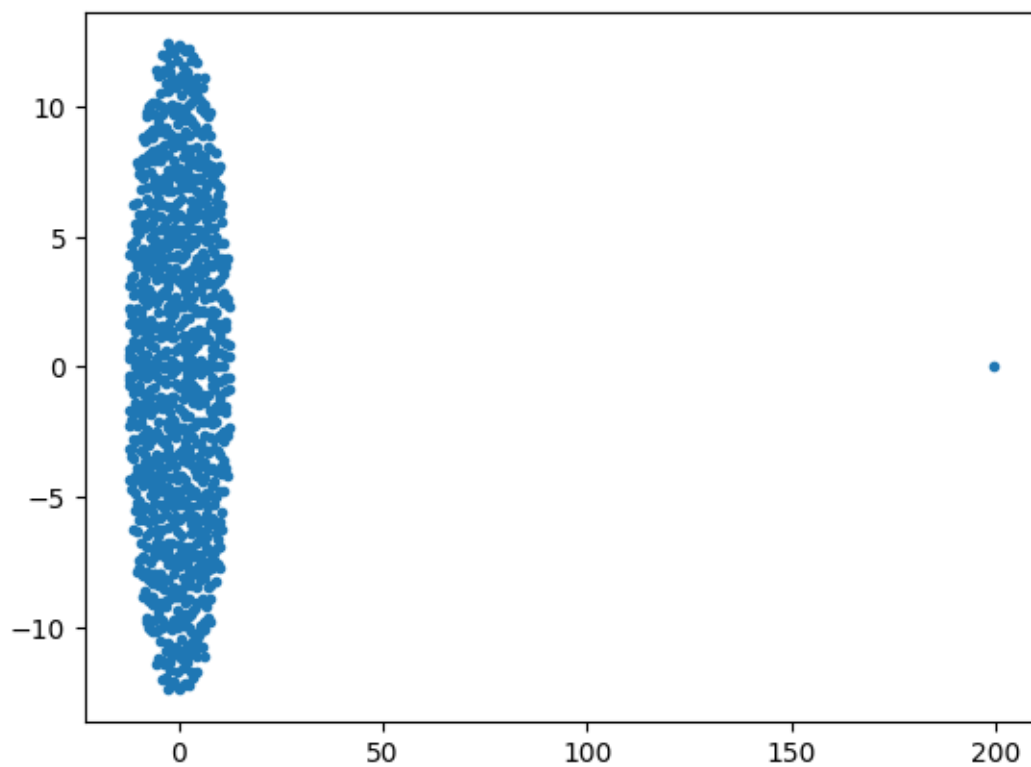
```
[80]: rr = np.random.rand(Nnode, Nnode)
      vv = np.linalg.eigvals(rr)
      vvr = np.real(vv)
      vvi = np.imag(vv)
      plt.plot(vvr, vvi, '.')
```

```
[80]: [<matplotlib.lines.Line2D at 0x7fafb83ea710>]
```



```
[81]: rr = np.random.rand(Nnode, Nnode) > 1 - Plink
      np.fill_diagonal(rr, 0)
      vv = np.linalg.eigvals(rr)
      vvr = np.real(vv)
      vvi = np.imag(vv)
      plt.plot(vvr, vvi, '.')
```

```
[81]: [<matplotlib.lines.Line2D at 0x7fafb84633d0>]
```



real_net_analysis

April 15, 2023

```
[9]: import scipy as sp
import numpy as np
import networkx as nx
from tqdm import tqdm # necessary because shuffling takes a while

def shuffle_net_sym_f(Net, Nsh):
    # Nsh = number of shuffles (* number of links)
    Shuf = Net
    I = list(nx.edges(Shuf))
    Nl = len(I)
    for ind in tqdm(range(Nl * Nsh)):
        L = np.random.randint(Nl, size = 2)
        while L[0] == L[1]:
            L[1] = np.random.randint(Nl)

        if Shuf.has_edge(I[L[0]][0], I[L[0]][1]) and Shuf.has_edge(I[L[1]][0], I[L[1]][1]) and (Shuf.has_edge(I[L[0]][0], I[L[1]][1]) == False) and (Shuf.has_edge(I[L[1]][0], I[L[0]][1]) == False) and (I[L[1]][0] != I[L[0]][1]) and (I[L[0]][0] != I[L[1]][1]) and (I[L[1]][0] != I[L[1]][1]):
            # delete links
            Shuf.remove_edge(I[L[0]][0], I[L[0]][1])
            Shuf.remove_edge(I[L[1]][0], I[L[1]][1])
            if Shuf.has_edge(I[L[0]][1], I[L[0]][0]):
                Shuf.remove_edge(I[L[0]][1], I[L[0]][0])
            if Shuf.has_edge(I[L[1]][1], I[L[1]][0]):
                Shuf.remove_edge(I[L[1]][1], I[L[1]][0])
            # shuffle links
            Shuf.add_edge(I[L[0]][0], I[L[1]][1])
            Shuf.add_edge(I[L[1]][1], I[L[0]][0])
            Shuf.add_edge(I[L[1]][0], I[L[0]][1])
            Shuf.add_edge(I[L[0]][1], I[L[1]][0])
            # remap links
            I = list(nx.edges(Shuf))
            Nl = len(I)
    return Shuf
```

```
[10]: data = sp.io.loadmat('Yeast_DIP.mat')
      YSTnet = data['YSTnet']
```

Let's process the network, which is not symmetrized with loops

```
[11]: Ndir = np.sum(YSTnet - YSTnet.T)
      Nloop = YSTnet.trace()

      print(Ndir)
      print(Nloop)

      YSTnet.setdiag(0)
      YSTnetSym = YSTnet + YSTnet.T

      GraphYST = nx.from_scipy_sparse_array(YSTnetSym)
```

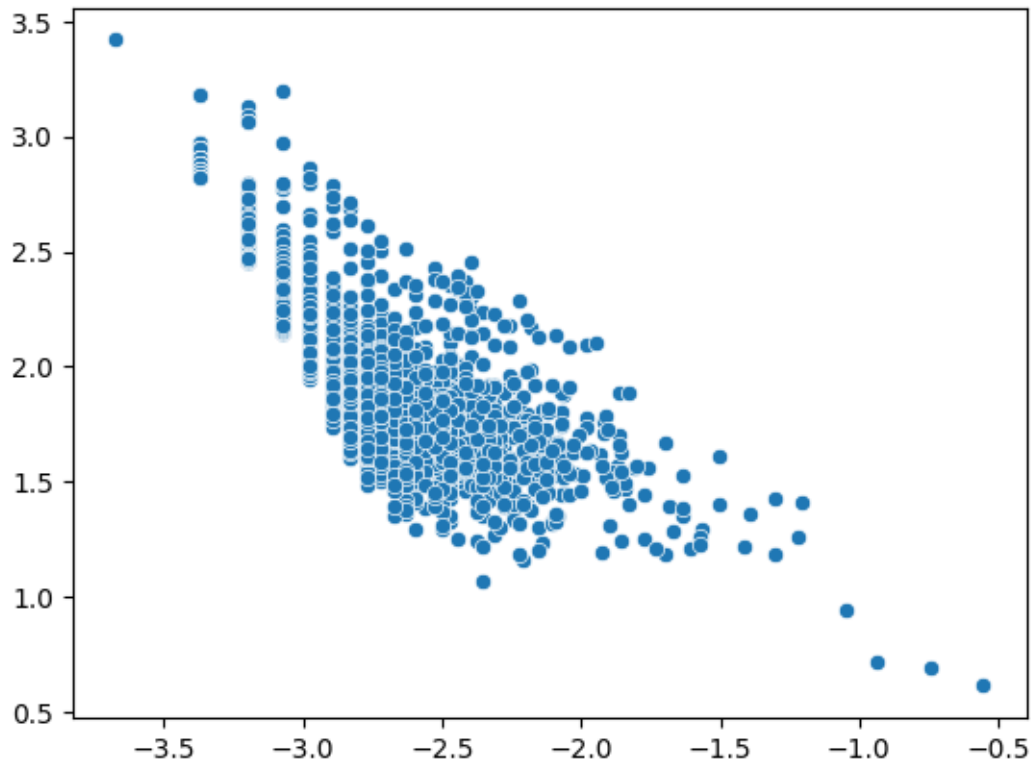
```
0.0
4713.0
```

```
[12]: Kyst = nx.degree_centrality(GraphYST)
      Kyst = np.array(list(Kyst.values()))
      Knn = np.divide(YSTnetSym * Kyst, Kyst)
```

```
[13]: import seaborn as sns

      sns.scatterplot(x=np.log10(Kyst), y=np.log10(Knn))
```

```
[13]: <Axes: >
```

Let's shuffle links - microcanonical ensemble. **NOTE:** microcanonical shuffle does not work with few iterations.

```
[14]: YSTshuf = shuffle_net_sym_f(GraphYST, 50) # maybe 50 is not enough but it
      ↪ takes about 2 hours and half to run
```

```
100%|          | 976400/976400 [1:08:31<00:00, 237.49it/s]
```

```
[15]: YSTshufK = np.sum(YSTshuf, axis = 0)
      KnnS = np.divide(YSTshuf * YSTshufK, YSTshufK)

      from matplotlib import pyplot as plt

      fig, ax = plt.subplots(ncols=3, figsize=(15, 5))
      sns.scatterplot(x=Kyst, y=YSTshufK, ax=ax[0])
      sns.scatterplot(x=Knn, y=KnnS, ax=ax[1])
      sns.scatterplot(x=YSTshufK, y=KnnS, ax=ax[2])
```

```
[15]: <Axes: >
```

