

Notebook

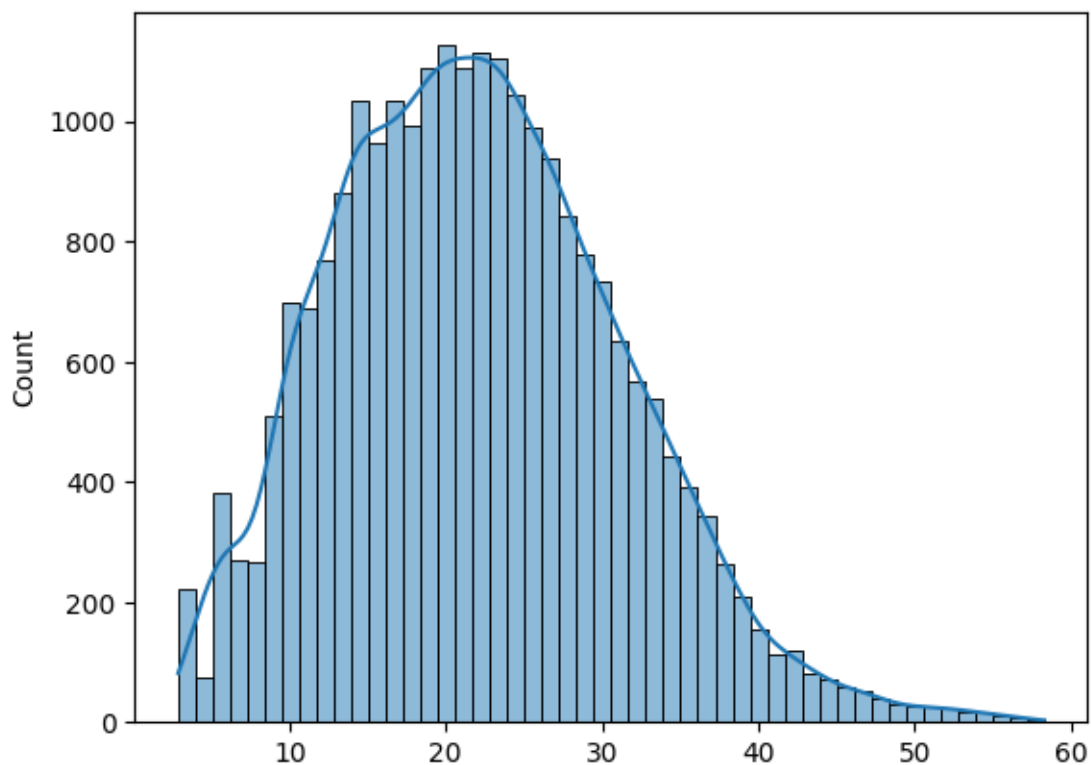
May 9, 2023

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

```
[2]: data = sp.io.loadmat("coord1PHP.mat")
protdist = data["protdist"][:, 0]
A = data["A"]
coord = data["coord"]
Nnode = A.shape[0]

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

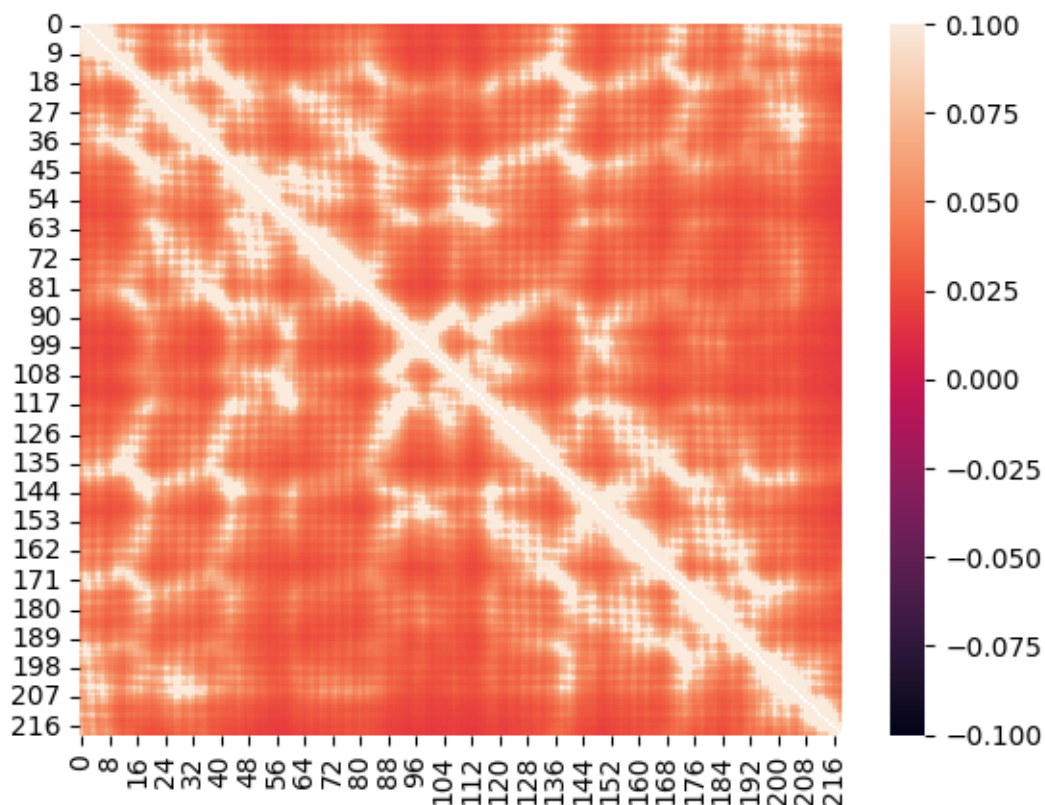
```
[2]: <Axes: ylabel='Count'>
```



```
[3]: D = sp.spatial.distance.squareform(protdist)
sns.heatmap(1.0 / D)
```

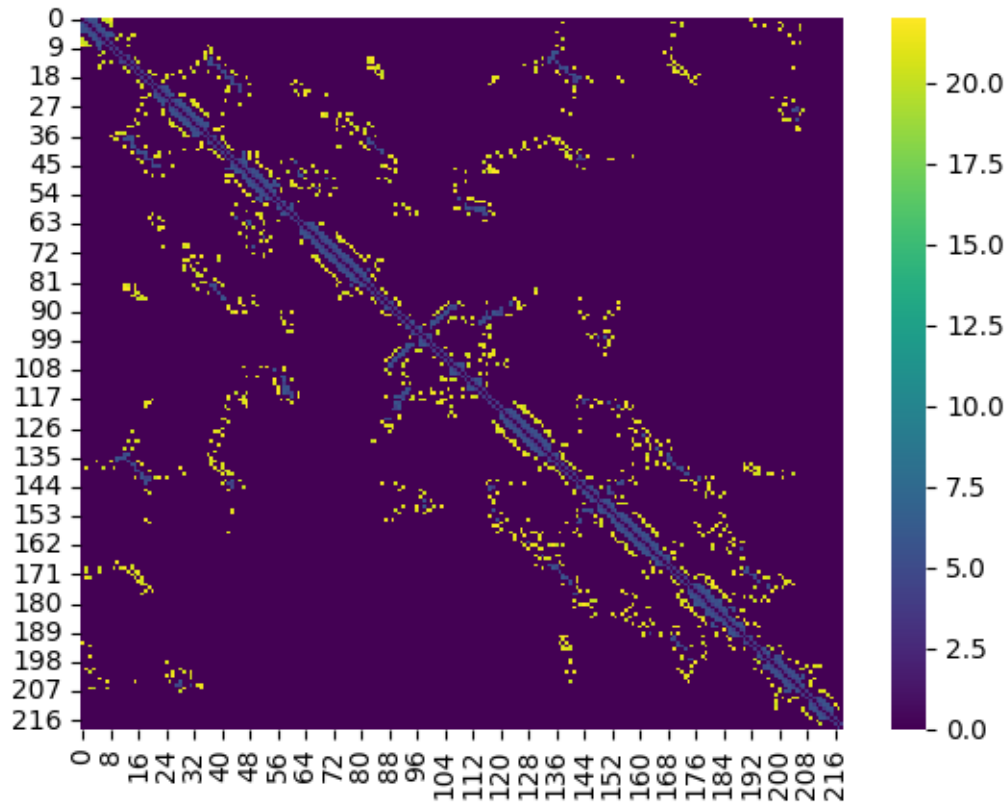
```
/tmp/ipykernel_1019/2899854611.py:2: RuntimeWarning: divide by zero encountered
in divide
  sns.heatmap(1./D)
```

[3]: <Axes: >



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

[4]: <Axes: >

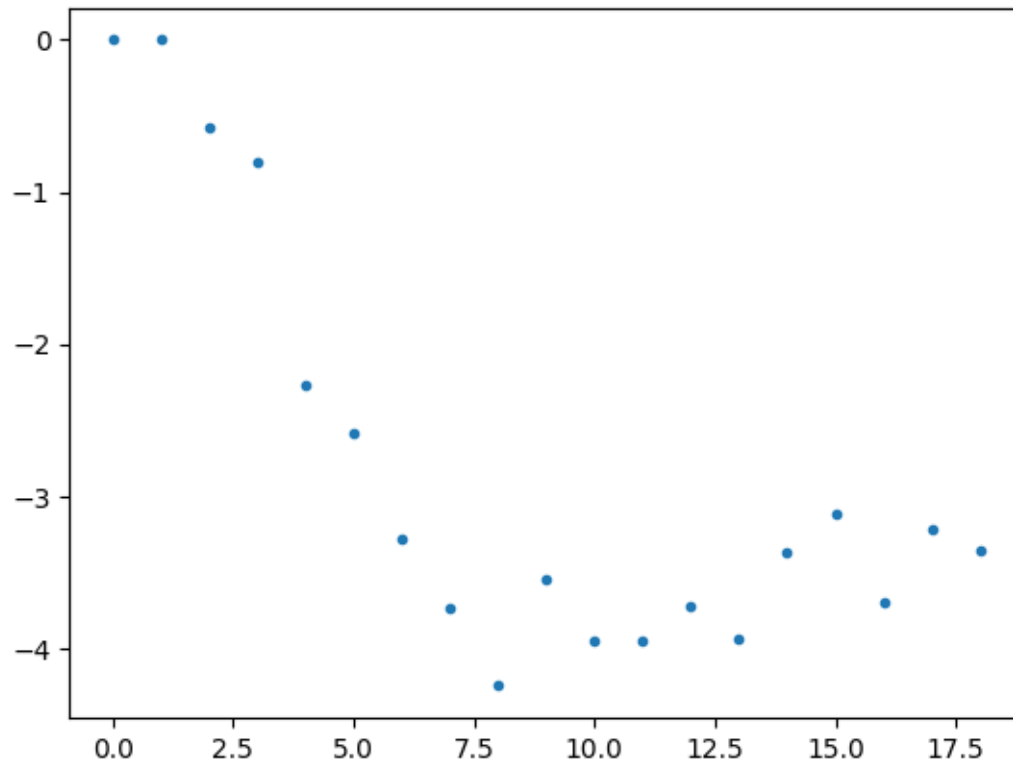


```
[5]: Kdiag = []

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

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

```
[5]: [<matplotlib.lines.Line2D at 0x7fa5a3550d90>]
```

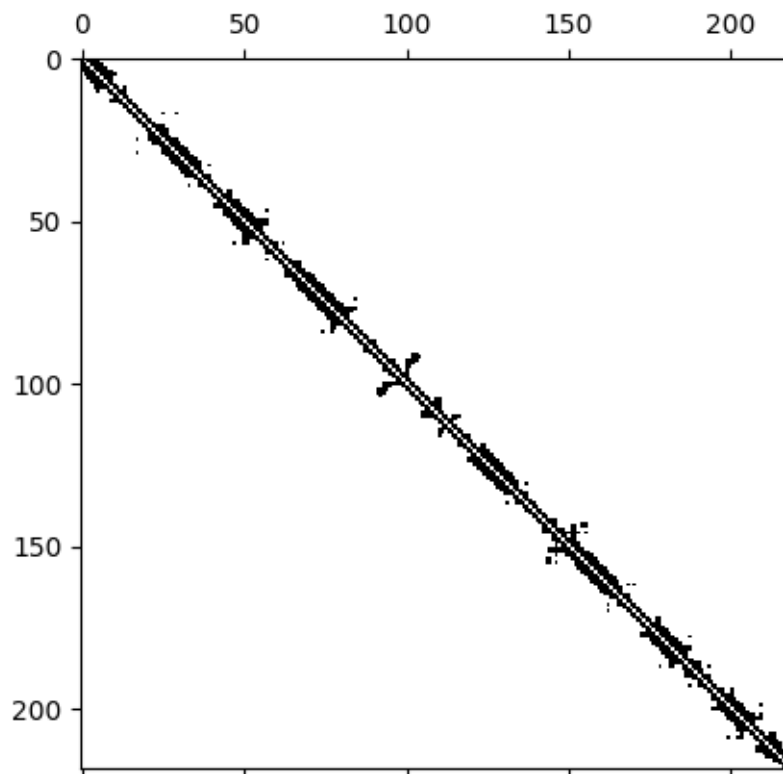


```
[6]: Nkd = 12
Ad = np.zeros((Nnode, Nnode), dtype=int)

for ind in range(-Nkd, Nkd + 1):
    Ad += np.diagflat(A.diagonal(ind), ind)

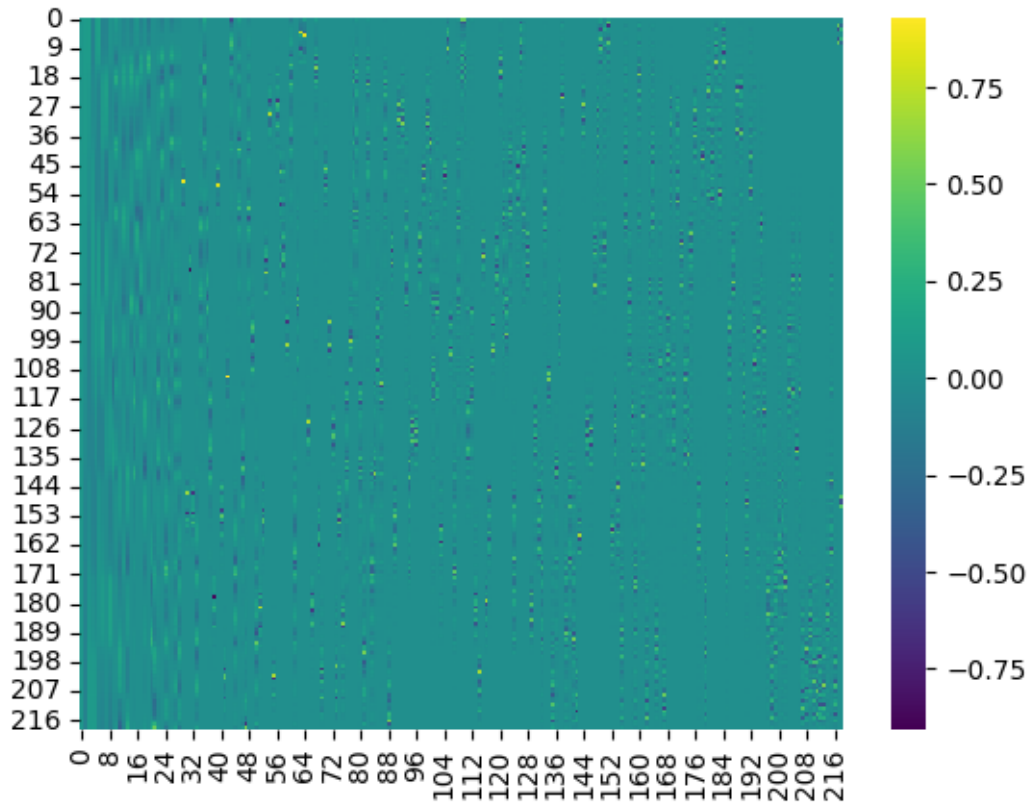
plt.spy(Ad)
```

```
[6]: <matplotlib.image.AxesImage at 0x7fa5a1a3e4a0>
```



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

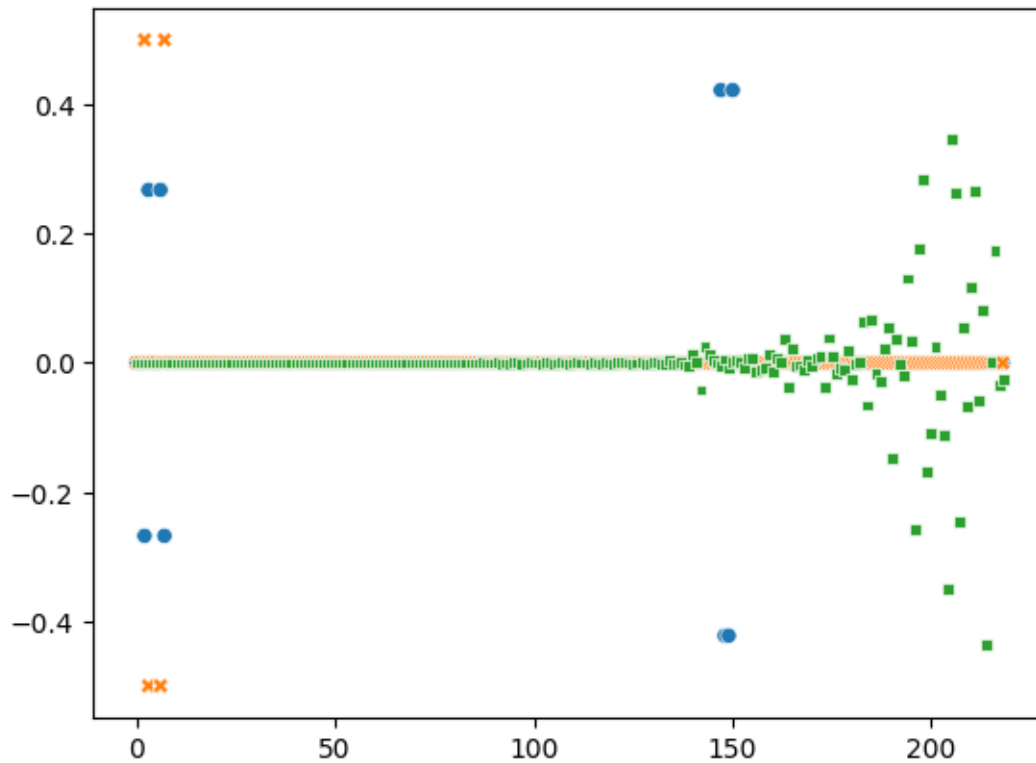
```
[7]: <Axes: >
```



We can clearly see that the components of the last eigenvectors are almost all zero and the non-zero ones are tiny and sparse.

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

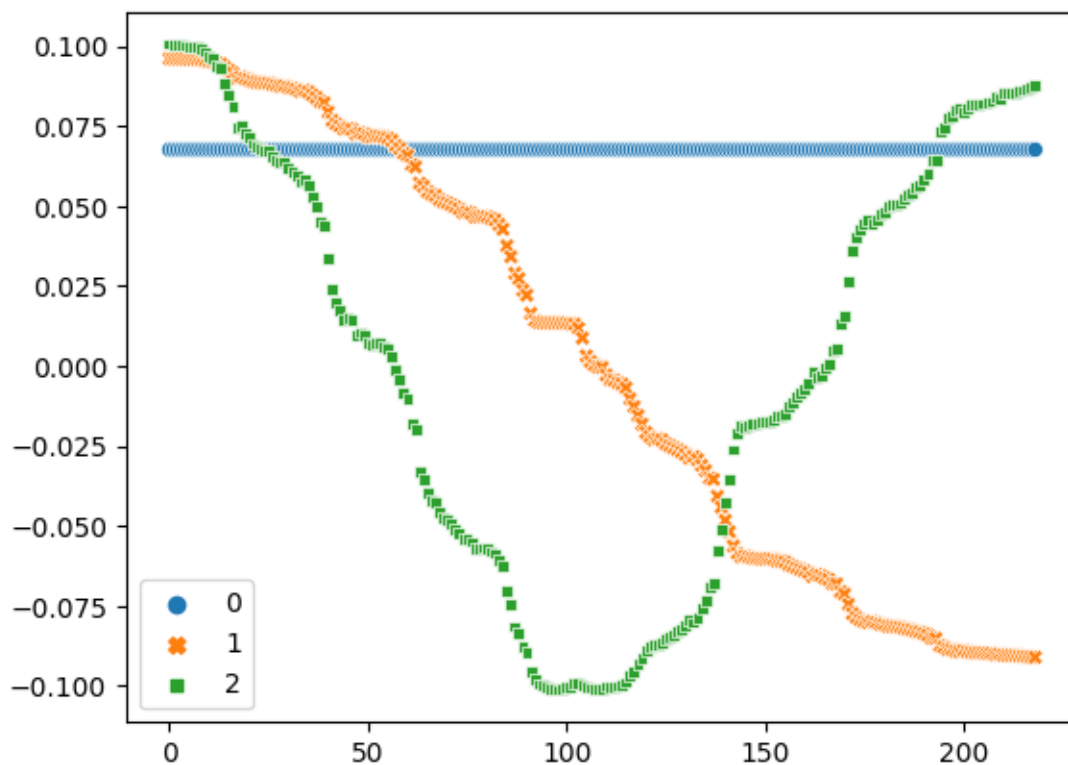
```
[47]: <Axes: >
```



On the other hand, plotting the first three eigenvalues we notice how continuous and far from zero their components are. So, the more we look at eigenvectors with small eigenvalues, the more we lose *smoothness*.

```
[15]: sns.scatterplot(VecAd[:, [0, 1, 2]])
```

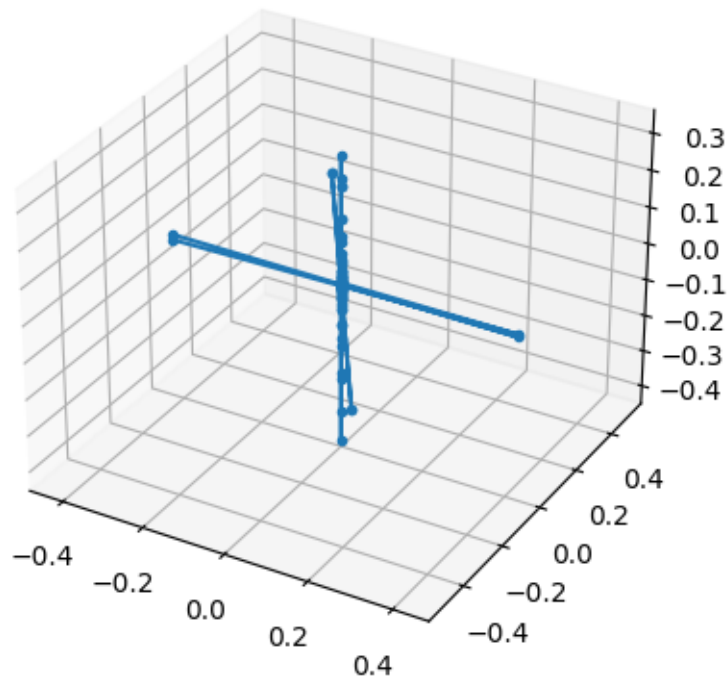
```
[15]: <Axes: >
```



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

ax.plot3D(VecAd[:, i1], VecAd[:, i2], VecAd[:, i3], marker=".")
```

```
[10]: [<mpl_toolkits.mplot3d.art3d.Line3D at 0x7fa5a1771450>]
```

```
[11]: 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(np.mean(K))
print(BC)
```

```
0.057588259732525154
10.0
{0: 0.0, 1: 0.01204099367300543, 2: 0.01401334954164753, 3:
0.0006162970922864942, 4: 0.003207949937519427, 5: 0.004760302926528808, 6:
0.015745067857777278, 7: 0.00021252745606001165, 8: 0.00021175435907414559, 9:
0.018880116457933395, 10: 0.00888257472519769, 11: 0.0023694854983744664, 12:
0.0094880906468599, 13: 0.02933047382010951, 14: 0.03252025074991718, 15:
0.030695451217927962, 16: 0.038462364866308704, 17: 0.08435553124496131, 18:
0.024875777266538317, 19: 0.01898044341253277, 20: 0.012672017990833909, 21:
0.03203780430616507, 22: 0.020321735104592082, 23: 0.002593975616196208, 24:
0.006316049722693714, 25: 0.035867958406912044, 26: 0.00886974262256941, 27:
0.018539458858847696, 28: 0.029567403288930073, 29: 0.05102375663848864, 30:
```

0.013992145898055398, 31: 0.021094277586248687, 32: 0.022239208860012256, 33:
0.026374887834566138, 34: 0.0026377886461965614, 35: 0.01576424530824187, 36:
0.01584612667926236, 37: 0.013458710054482643, 38: 0.020007909512706208, 39:
0.04026872767018317, 40: 0.04116080043864233, 41: 0.031038824591402815, 42:
0.049506359273908354, 43: 0.07907563229687638, 44: 0.04581152688258064, 45:
0.025131182388419635, 46: 0.03463129057560673, 47: 0.006967532365888618, 48:
0.03873656519658367, 49: 0.01664604905974633, 50: 0.025236811190241043, 51:
0.008069711606234008, 52: 0.012008750054378977, 53: 4.4476800585852575e-05, 54:
0.00032554028818180245, 55: 0.00352953253426607, 56: 0.004601901943844797, 57:
0.021729101317803156, 58: 0.0021898518685196278, 59: 0.007972611015039441, 60:
0.013490805530604694, 61: 0.015217894877977626, 62: 0.014595108310520391, 63:
0.005991598655525304, 64: 0.000977136686718743, 65: 8.779572871367042e-05, 66:
0.00713082915552444, 67: 0.006780980038972298, 68: 0.0015920870216777734, 69:
0.0016156416676844354, 70: 0.017791848819956543, 71: 0.013775533674461092, 72:
0.0033992464645559864, 73: 0.029584864415429072, 74: 0.013202010924415211, 75:
0.0029463454953501124, 76: 0.004832367770598038, 77: 0.008853984296002388, 78:
0.0017218174595826365, 79: 0.0004899953839856271, 80: 0.001831193396308073, 81:
0.0017018359316171938, 82: 0.013174651761843273, 83: 0.008101155134373013, 84:
0.021480055121599707, 85: 0.020440890091434388, 86: 0.013040609677003335, 87:
0.04160345196893862, 88: 0.006992795703025573, 89: 0.008885548648901715, 90:
0.018733337255943523, 91: 0.01669154396358291, 92: 0.014229311136340066, 93:
0.01950489924079859, 94: 0.0019413816919582165, 95: 0.0021947242902580753, 96:
0.0024969387352375494, 97: 0.0021155962689326803, 98: 0.005304111672620396, 99:
0.0018397665359675323, 100: 0.0017114368241285135, 101: 0.0012072615043293763,
102: 0.001706180488012439, 103: 0.001195931596923099, 104:
0.0025517284381880636, 105: 0.006450860097221825, 106: 0.0028488804030948564,
107: 0.02045802291555756, 108: 0.0010351101405947209, 109:
0.0013741651130016568, 110: 0.009067461233343422, 111: 0.0006701891739726152,
112: 0.0005098619105737825, 113: 0.00033585664354907725, 114:
0.004770191645450268, 115: 0.022265054141984365, 116: 0.023376925553120237, 117:
0.05343715784061073, 118: 0.029600132593646702, 119: 0.042523522001271324, 120:
0.016777053826530084, 121: 0.0031890514396772777, 122: 0.0017688215704714278,
123: 0.014933951218284551, 124: 0.019715521257656438, 125: 0.002870722798816541,
126: 0.004360841163996621, 127: 0.030222649717141236, 128: 0.012389527629766302,
129: 0.0034695083944923633, 130: 0.004949597107106605, 131:
0.028225526376477492, 132: 0.004902191941911185, 133: 0.003176831905893899, 134:
0.012982396688985891, 135: 0.005350926055501822, 136: 0.0224118403074471, 137:
0.030644829376982832, 138: 0.018367872687382557, 139: 0.022133454411966274, 140:
0.033270056279473895, 141: 0.07154977878028065, 142: 0.041442192285288816, 143:
0.02974603933453213, 144: 0.029360846576278316, 145: 0.015275114748458208, 146:
0.027027311139692832, 147: 5.4070162780407754e-05, 148: 0.009264316050508576,
149: 0.0012838785151195941, 150: 0.008944705451739204, 151:
0.018733382155081198, 152: 0.009906271919185744, 153: 0.008832610192563775, 154:
0.030530566891168946, 155: 0.021868919339924627, 156: 0.01964725405928555, 157:
0.012867587764840717, 158: 0.025817656809759486, 159: 0.014807401235733852, 160:
0.006212465003977074, 161: 0.010365547118589714, 162: 0.026389643147896703, 163:
0.006702678621782567, 164: 0.0005089854157410398, 165: 0.002790989419934251,
166: 0.0005390301918236331, 167: 0.0011757513436919313, 168:

```

0.013708967377539785, 169: 0.0062230404399575, 170: 0.01860456955123589, 171:
0.02017392603687551, 172: 0.02489230843891768, 173: 0.06003089293203244, 174:
0.041275892955877636, 175: 0.005132034272732839, 176: 0.007231489848532819, 177:
0.02289808314820412, 178: 0.02065485568164289, 179: 0.002516859061860833, 180:
0.031175919810288166, 181: 0.015741357790581067, 182: 0.002312050114904961, 183:
0.0008180224023849952, 184: 0.002463079947627114, 185: 0.0005371761968987288,
186: 0.009818127251788943, 187: 0.004417996363606854, 188:
0.0007952555789802801, 189: 0.0013435470994491983, 190: 0.024106549846167332,
191: 0.0029870143027755256, 192: 0.0181704925816694, 193: 0.00871654427885206,
194: 0.010426663364159735, 195: 0.001104736513914226, 196: 0.004940120084855866,
197: 0.006607756060464395, 198: 0.006847534005938651, 199: 0.017862210749160765,
200: 0.029517026611465137, 201: 0.029967784477801136, 202: 0.039952256576713335,
203: 0.03000062376678563, 204: 0.032254913533162385, 205: 0.027821596797377886,
206: 0.014042953740099047, 207: 0.005862523318016057, 208: 0.021187174675247094,
209: 0.05822620705972127, 210: 0.002464162745641879, 211: 0.005387054758404398,
212: 0.008261391650002588, 213: 0.028543381424905416, 214:
0.00011626432165053056, 215: 0.0066772402029717185, 216: 0.011572735134899446,
217: 4.2277935145647484e-05, 218: 0.0}

```

1 Permutation effects

```

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

```

```

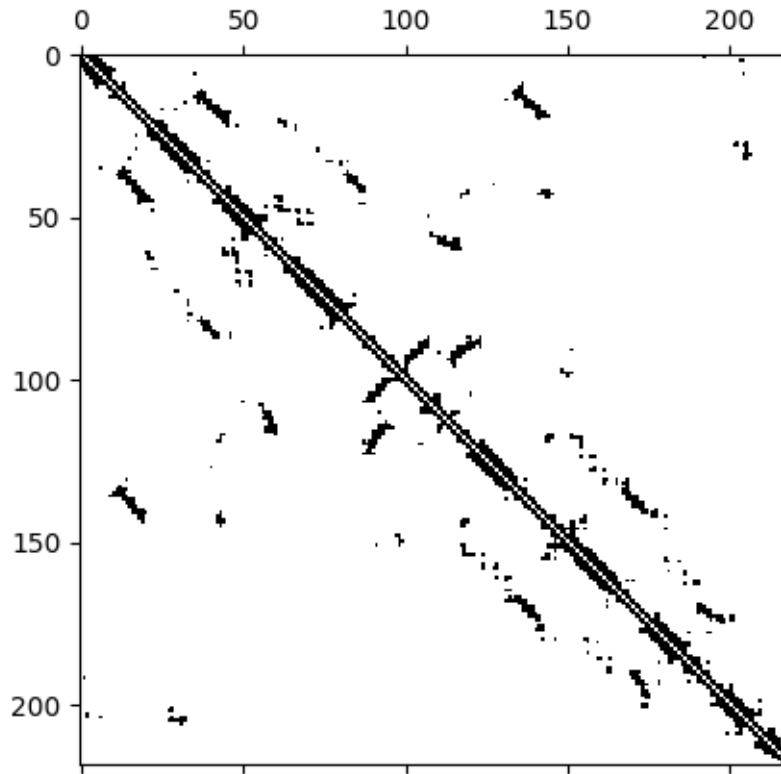
[29]: data = sp.io.loadmat('coord1PHP.mat')
A = data['A']
coord = data['coord']
Nnode = A.shape[0]
plt.spy(A)

```

```

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

```



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

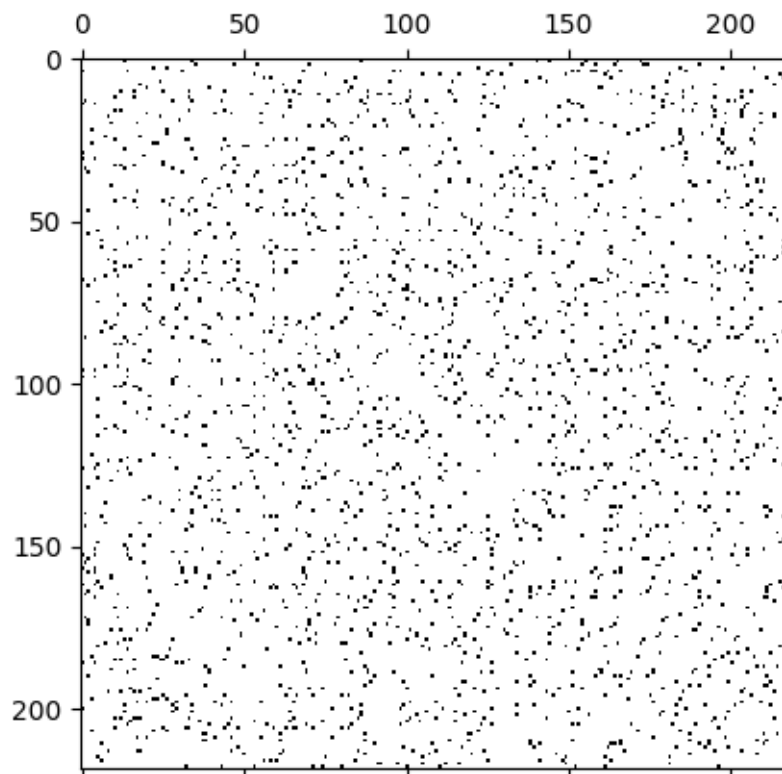
```
[23]: for ind in Index:
      PermMat[Index[ind], PermIndex[ind]] = 1
```

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)
```

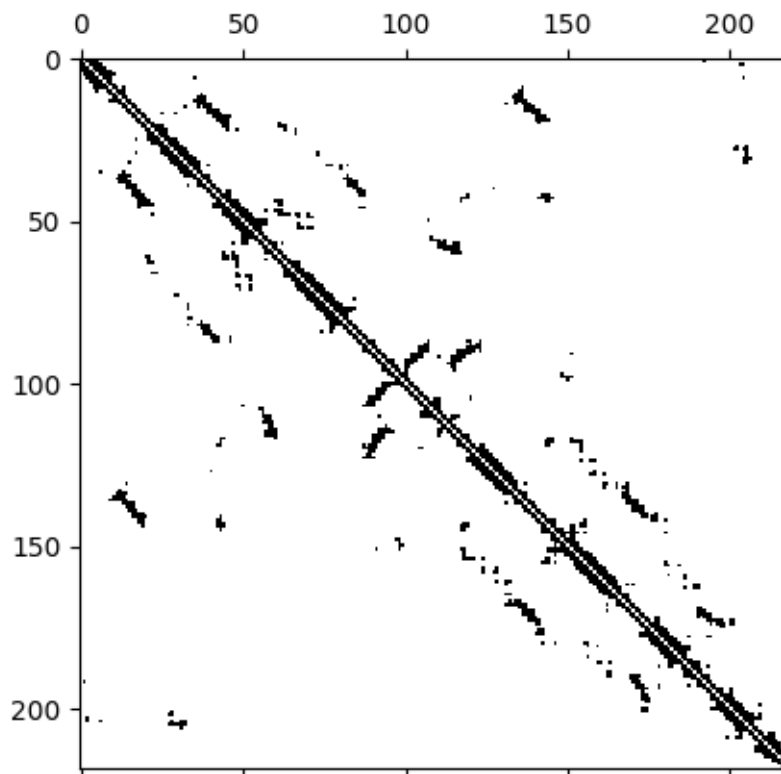
```
[25]: <matplotlib.image.AxesImage at 0x7fc8e8d9c190>
```



We can invert the permutation effect

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

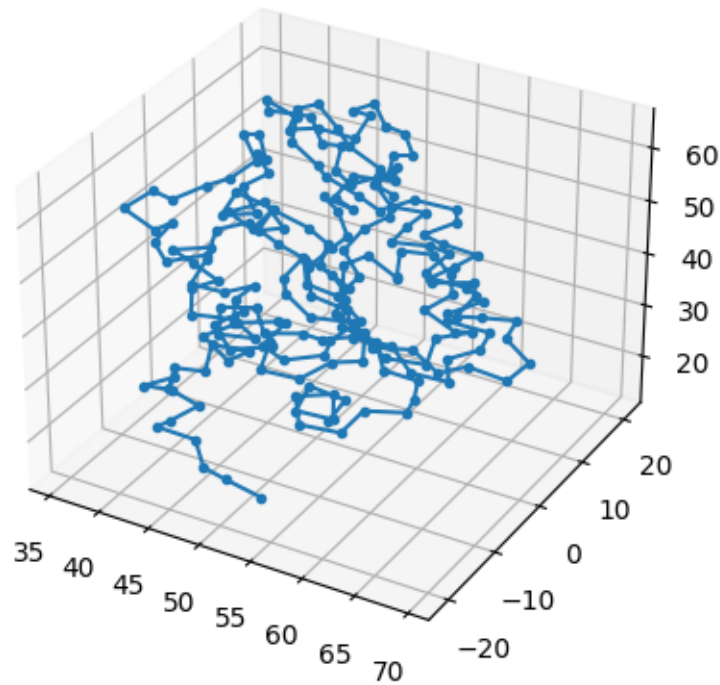
```
[26]: <matplotlib.image.AxesImage at 0x7fc8e8c082b0>
```



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]: [<matplotlib.mplot3d.art3d.Line3D at 0x7fc8e19db5b0>]
```



2 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

2.1 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

2.2 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)
```

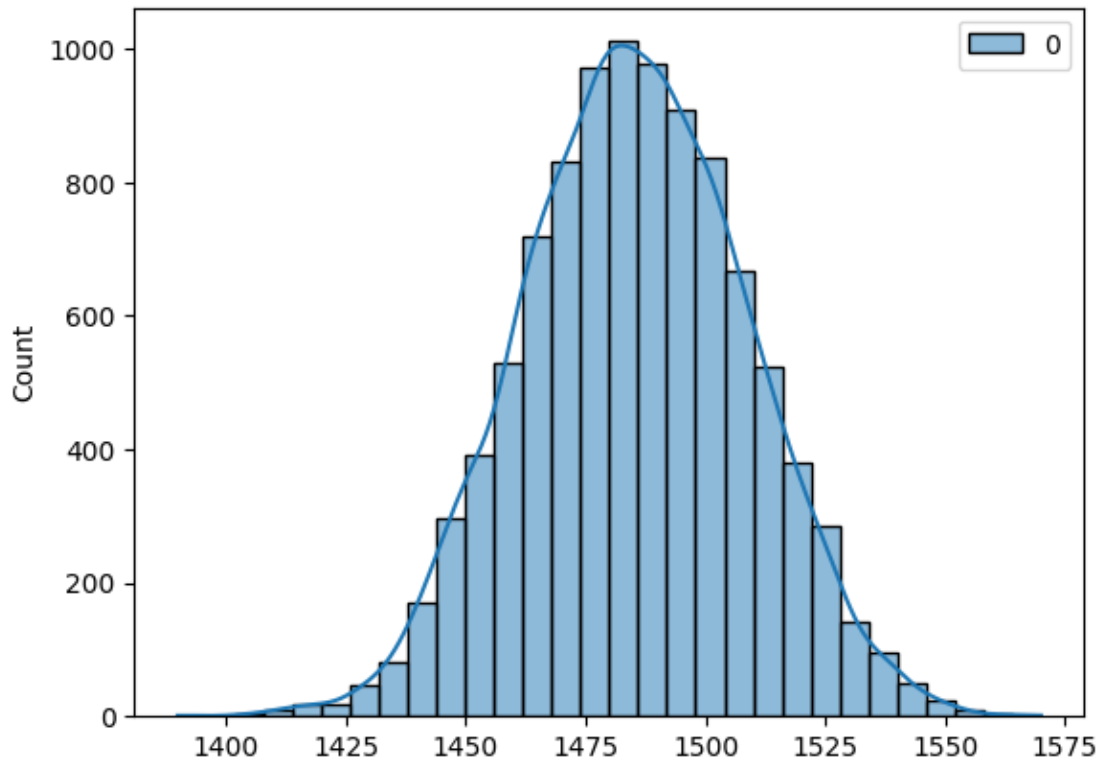
Average number of links: 1485.08

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

```

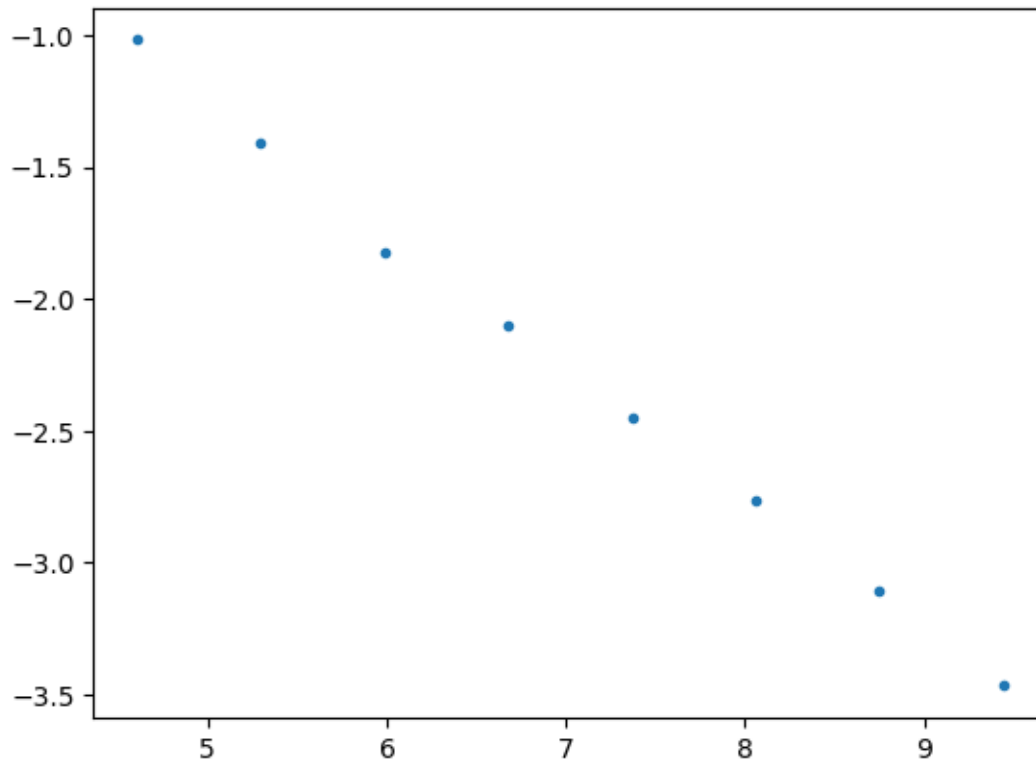
```

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>]
```



2.3 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

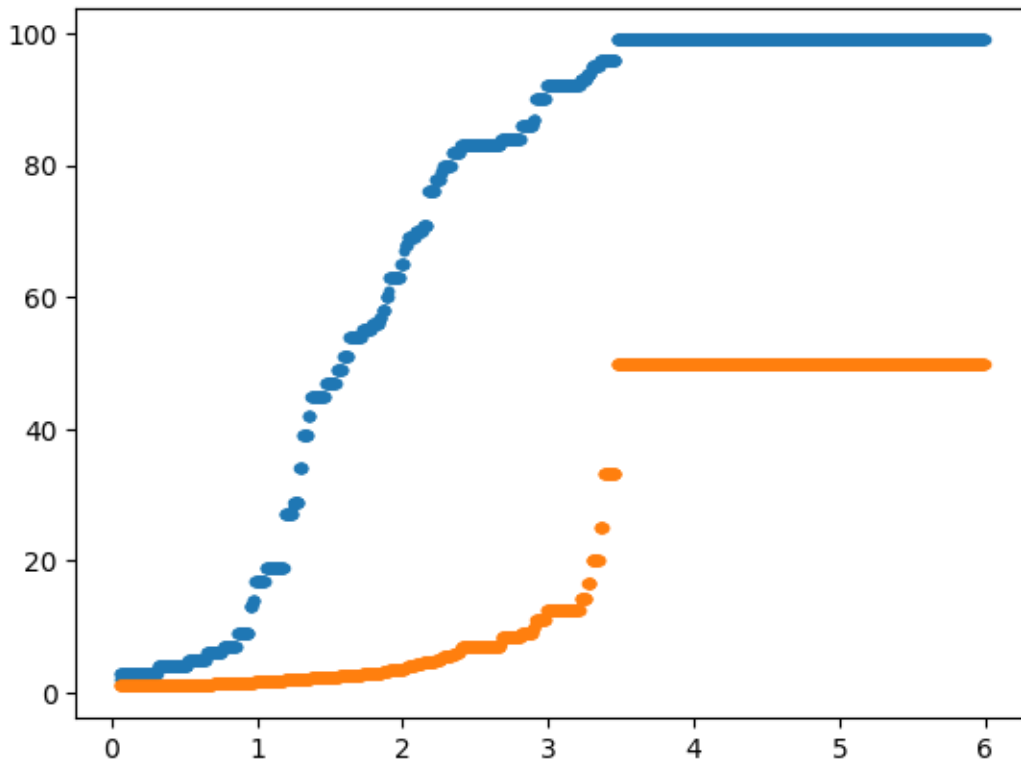
for index in xP:
    Net = nx.from_numpy_array(rr > 1 - index)
    CompList = nx.connected_components(Net)
    Comps = [len(x) for x in CompList]
    Rc[Cnt] = max(Comps)
```

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

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

```

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



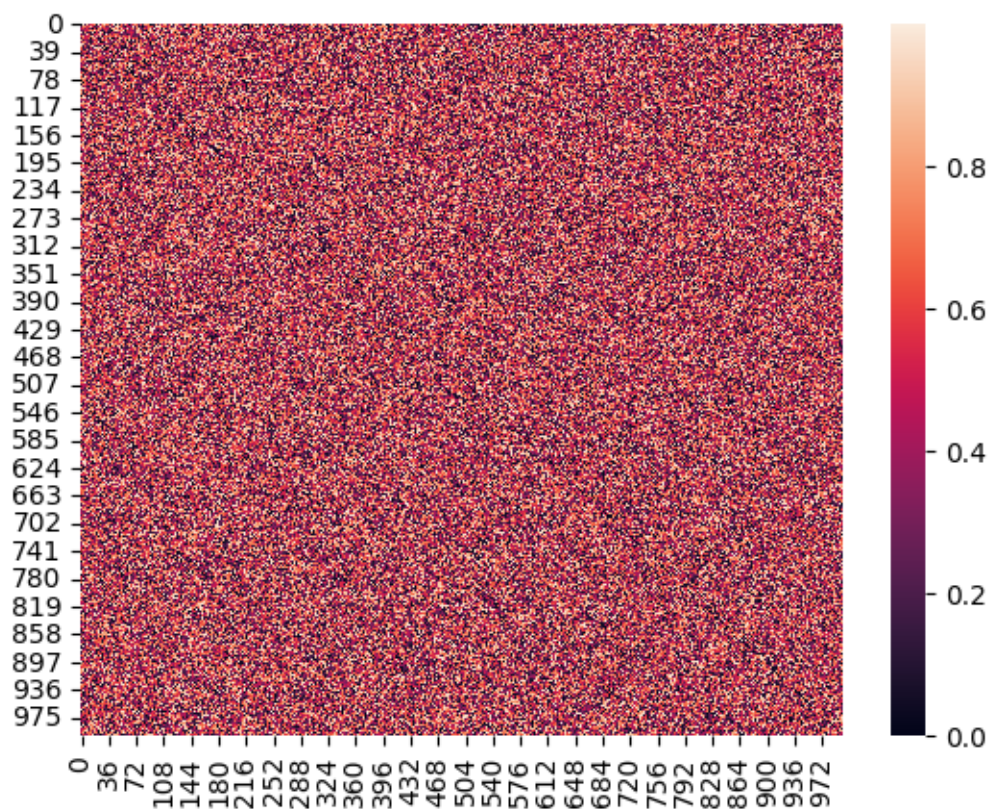
2.4 Semicircle law for ER network spectrum vs RMT (Random Matrix Theory)

```
[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)
```

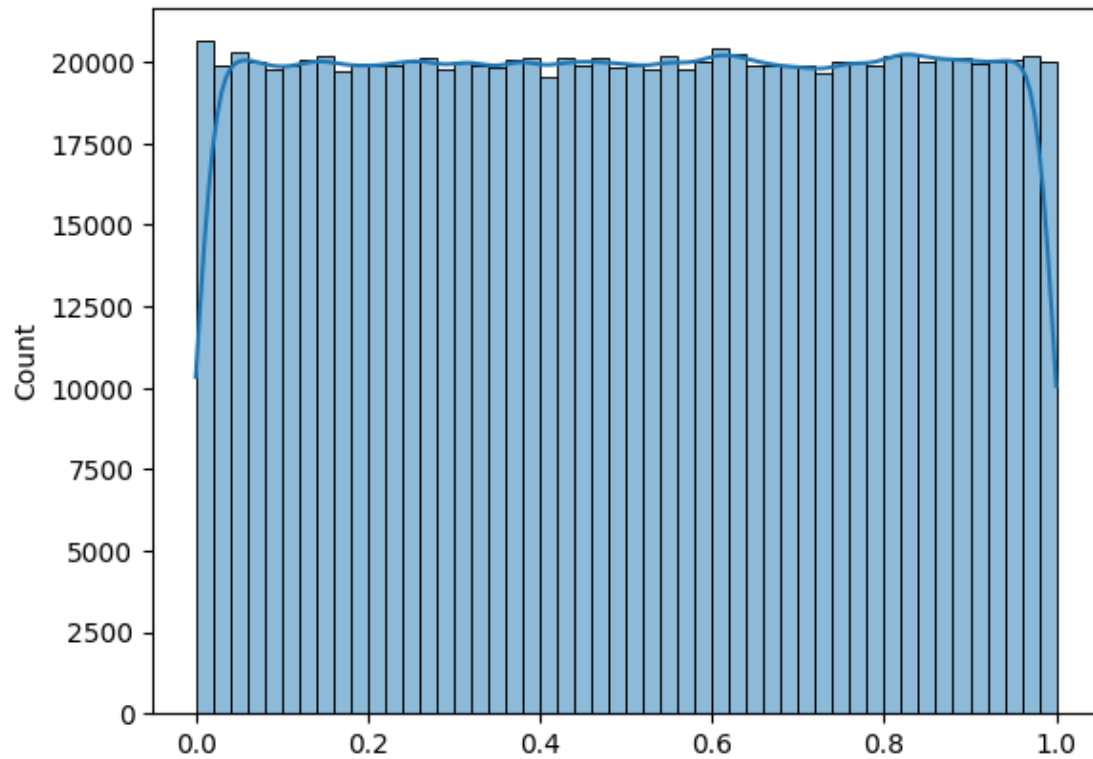
```
[73]: <Axes: >
```



Let's see also the histogram of coefficients

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

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

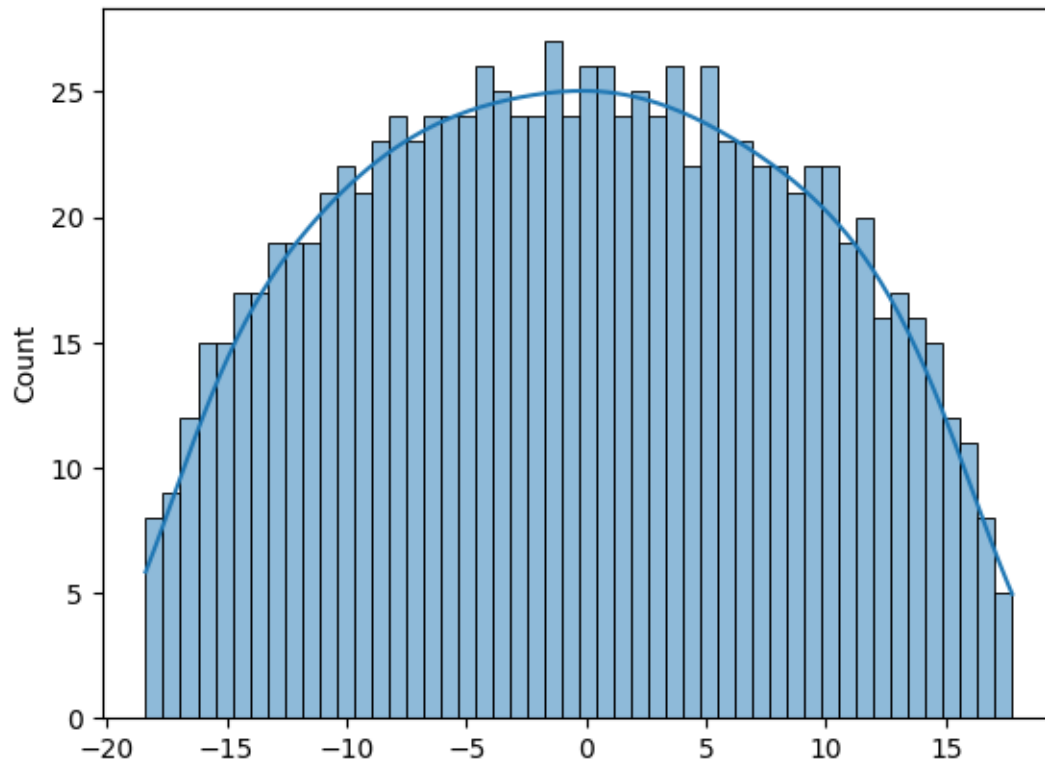


Now the eigenvalues and eigenvectors.

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'>
```

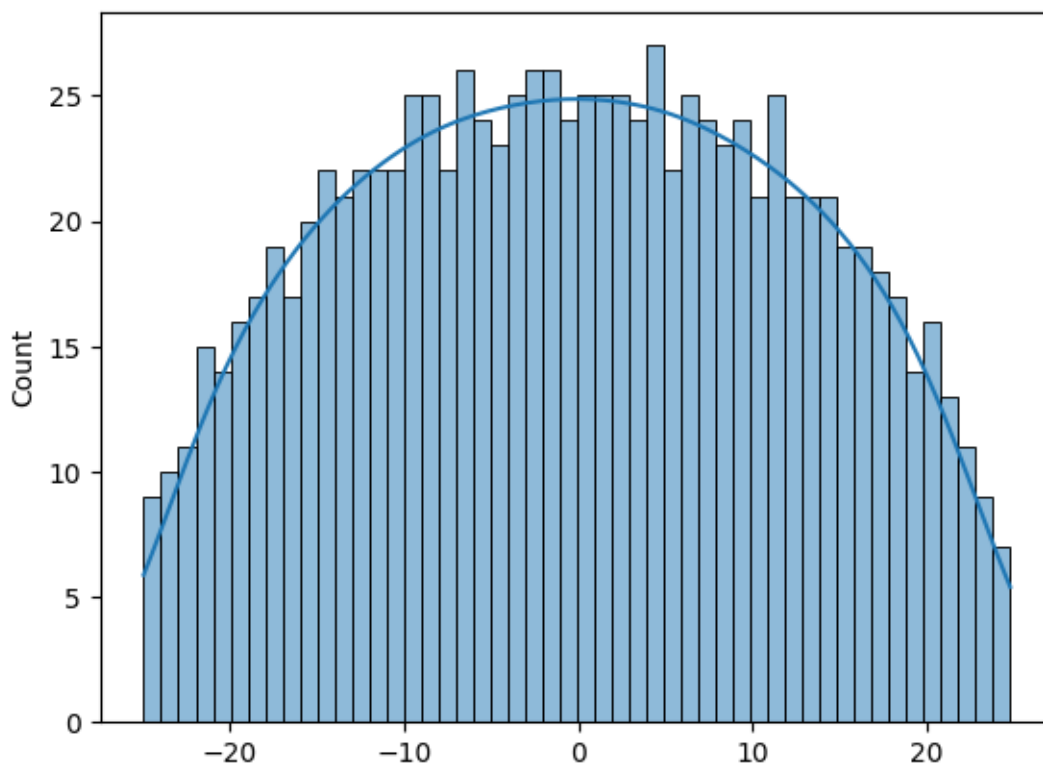



```
[76]: rr = np.triu(np.random.rand(Nnode, Nnode), k=1) > 1 - Plink
      rr = rr + rr.T
```

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

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

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

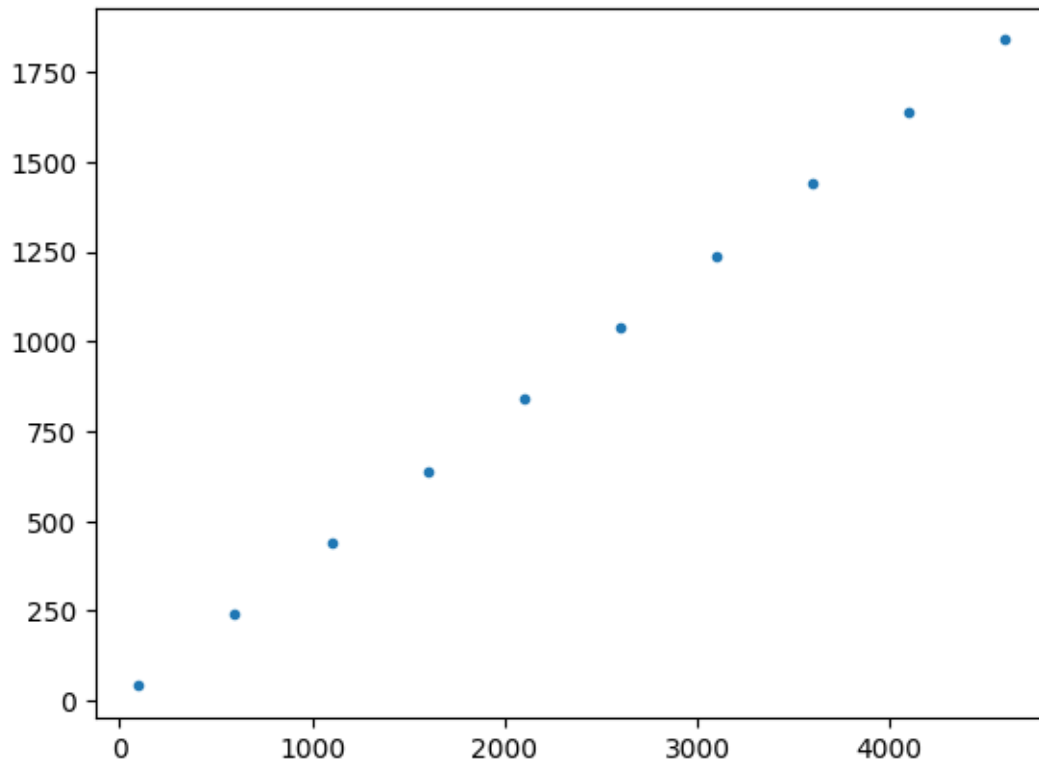


```
[83]: Cnt = 0
xx = np.arange(100, 5000, step=500)
vmax = []

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, '.')
```

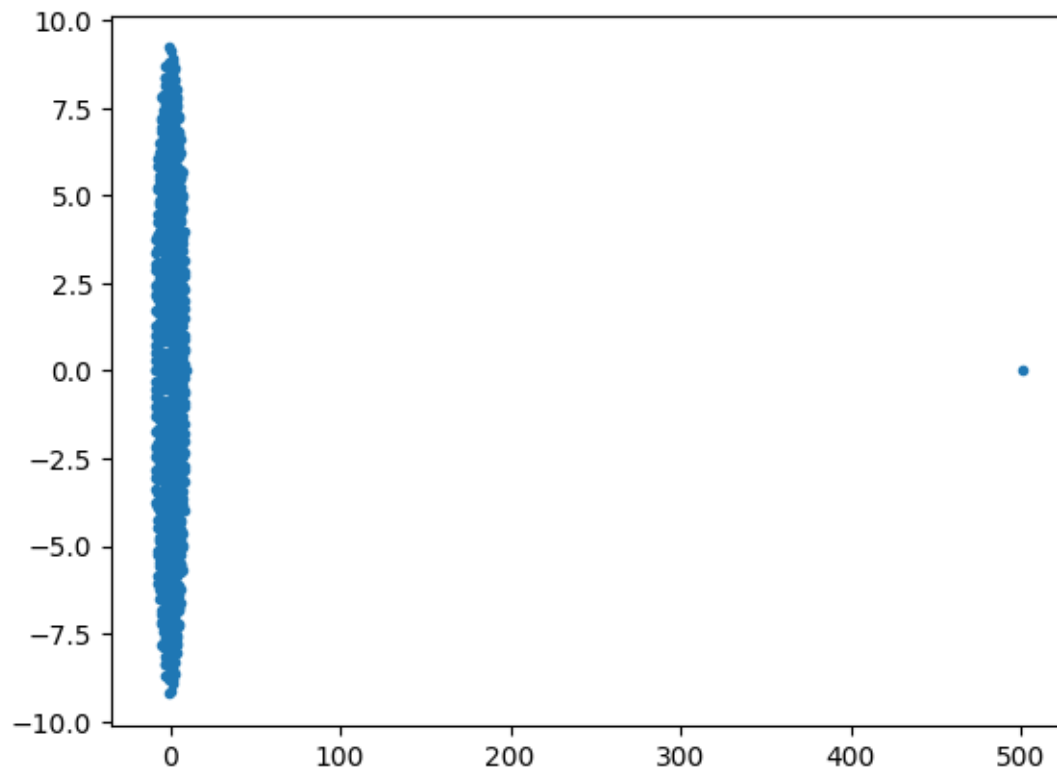
```
[83]: [<matplotlib.lines.Line2D at 0x7fafb8358f10>]
```



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

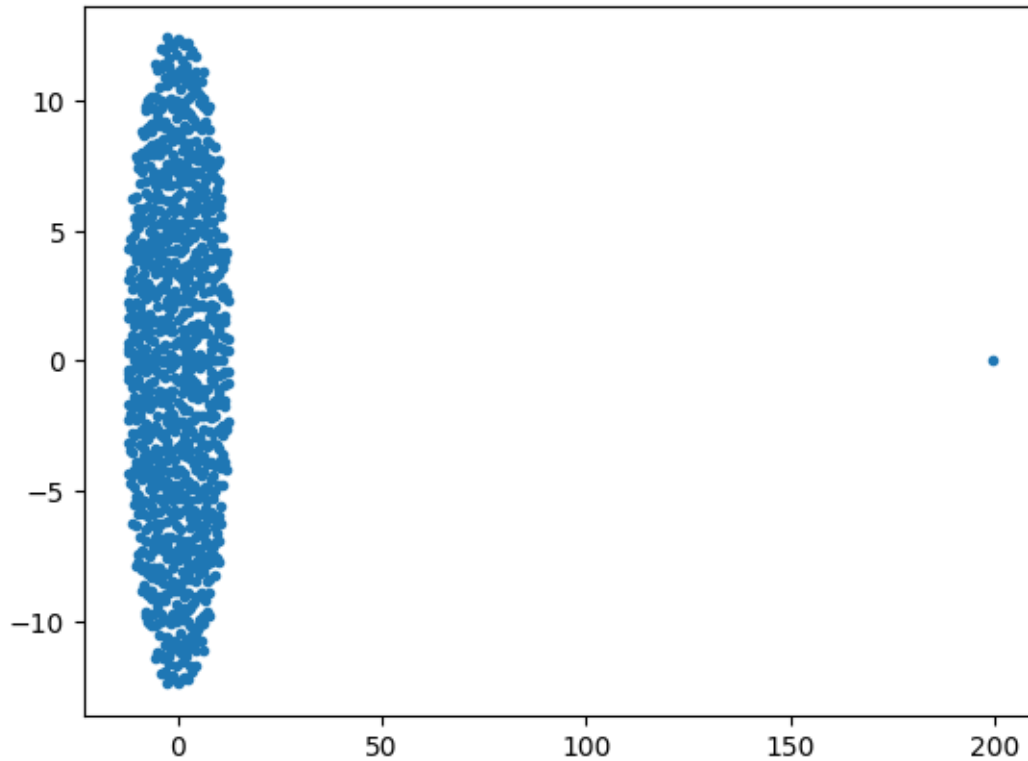
```
[80]: rr = np.random.rand(Nnode, Nnode)
      vv = np.linalg.eigvals(rr)
      vvr = np.real(vv)
      vvi = np.imag(vv)
      plt.plot(vvr, vvi, '.')
```

```
[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>]
```



```
[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[0]][0] != I[L[0]][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

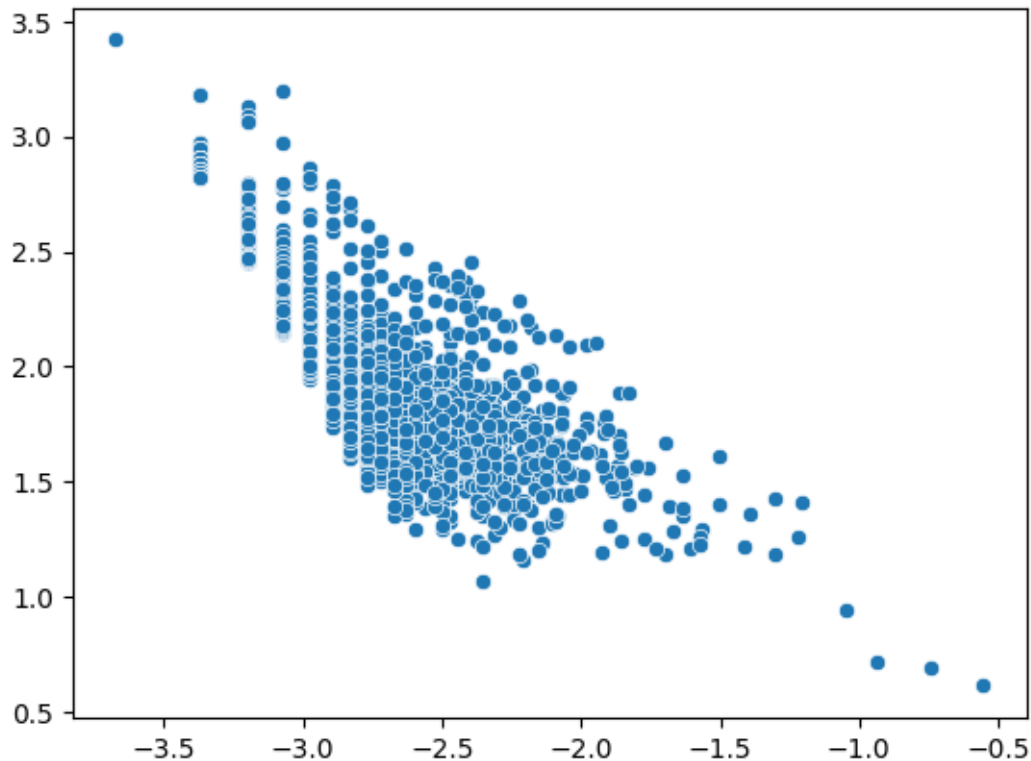
      sns.scatterplot(x=np.log10(Kyst), y=np.log10(Knn))

```

```

[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]
```

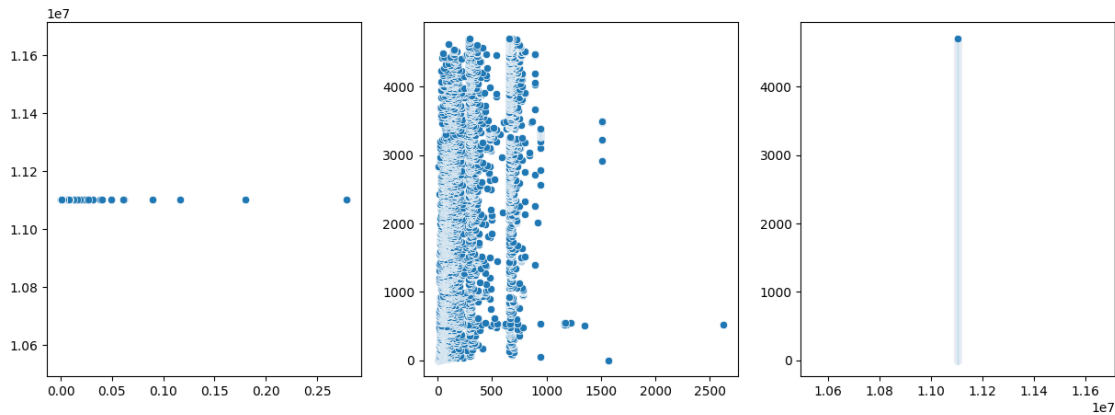
By shuffling we're actually creating another network with the same characteristic as the previous one: is it really the same network? Well, it depends. In some cases we actually lose information by shuffling, which means that links were not randomly generated in the original one, like in that case.

```
[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: >



3 Laplacian operator

3.1 Bi-clustering

Let's try first with some parameters that will affect clearly the second eigenvector's components.

```
[1]: Nb1 = 50
      Nb2 = 50
      Pb1 = 0.3
      Pb2 = 0.3
      P12 = 0.05
```

We can also try with parameters that will not show any effect, for example having too close probabilities or two different sizes of subnetworks.

```
[2]: # Nb1 = 50
      # Nb2 = 50
      # Pb1 = 0.3
      # Pb2 = 0.3
      # P12 = 0.15
```

```
[3]: # Nb1 = 20
      # Nb2 = 80
      # Pb1 = 0.3
      # Pb2 = 0.3
      # P12 = 0.05
```

Let's generate an ER random network with the variables we've just set up. We can clearly see the two highly connected networks.

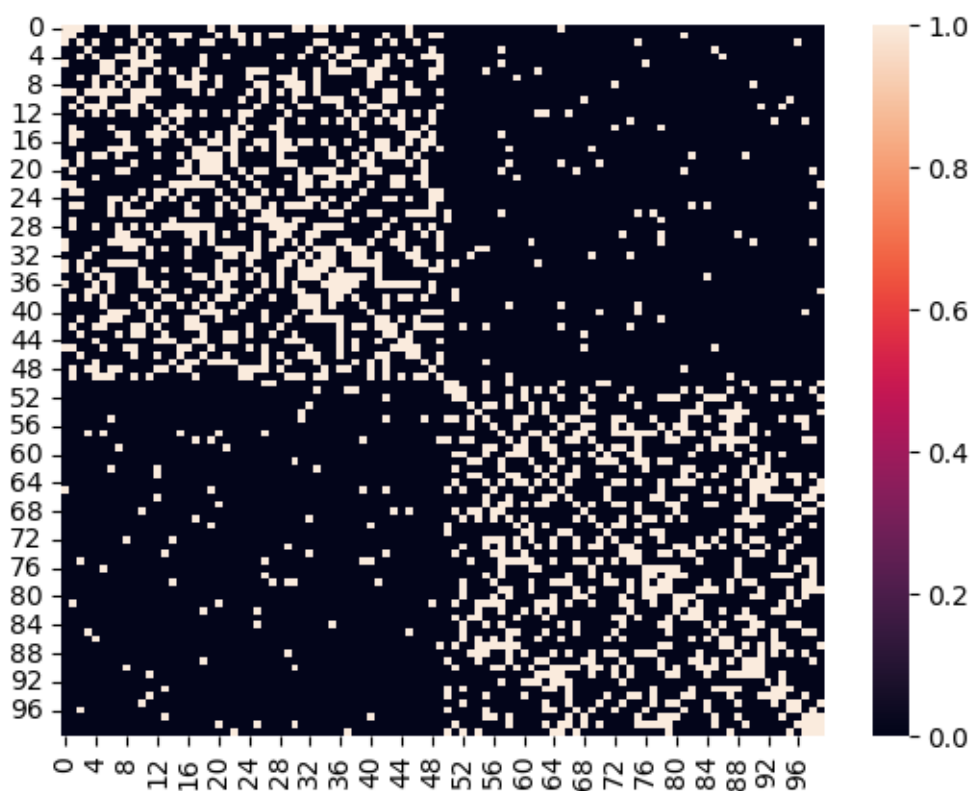

```
[4]: import numpy as np

Net = np.triu(np.random.rand(Nb1+Nb2, Nb1+Nb2), k=1)
Net[0:Nb1, Nb1:Nb1+Nb2] = Net[0:Nb1, Nb1:Nb1+Nb2] < P12
Net = Net + Net.T
Net[0:Nb1, 0:Nb1] = Net[0:Nb1, 0:Nb1] < Pb1
Net[Nb1:Nb1+Nb2, Nb1:Nb1+Nb2] = Net[Nb1:Nb1+Nb2, Nb1:Nb1+Nb2] < Pb2

import seaborn as sns

sns.heatmap(Net)
```

[4]: <Axes: >



```
[5]: import scipy as sp

ll = sp.sparse.csgraph.laplacian(Net, normed=False)

Val, Vec = np.linalg.eig(ll)
Val = np.sort(Val)
```

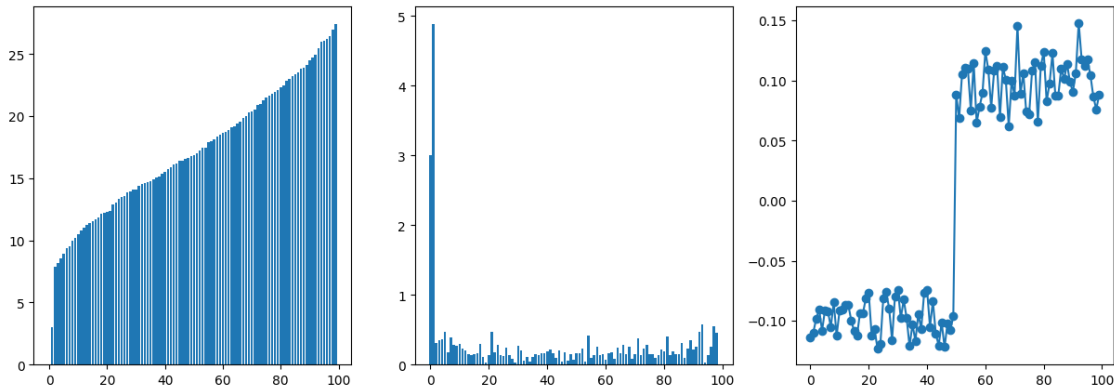
```

from matplotlib import pyplot as plt
fig, ax = plt.subplots(1, 3, figsize=(15, 5))

ax[0].bar(range(0, len(Val)), Val)
ax[1].bar(range(0, len(Val)-1), np.diff(Val))
ax[2].plot(Vec[:, 1], '-o')

```

[5]: [<matplotlib.lines.Line2D at 0x7fcd500dab30>]



3.2 Chain - 1D lattice

Usually the topological features of our graphs result in some spectral properties. For instance, we can see how the chain structure affects the eigenvalues and the eigenvector corresponding to the Fiedler number.

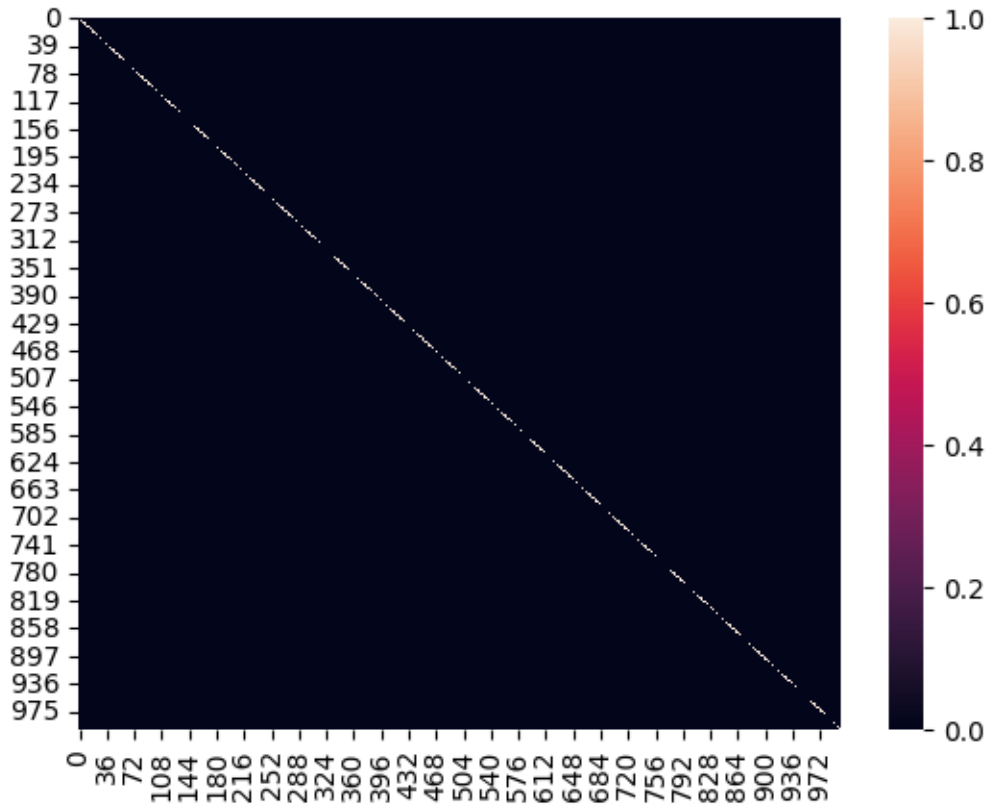
```

[6]: Nnode = 1000
aa = np.zeros((Nnode, Nnode))
aa += np.diag(np.ones(Nnode-1), k=1) + np.diag(np.ones(Nnode-1), k=-1)

sns.heatmap(aa)

```

[6]: <Axes: >



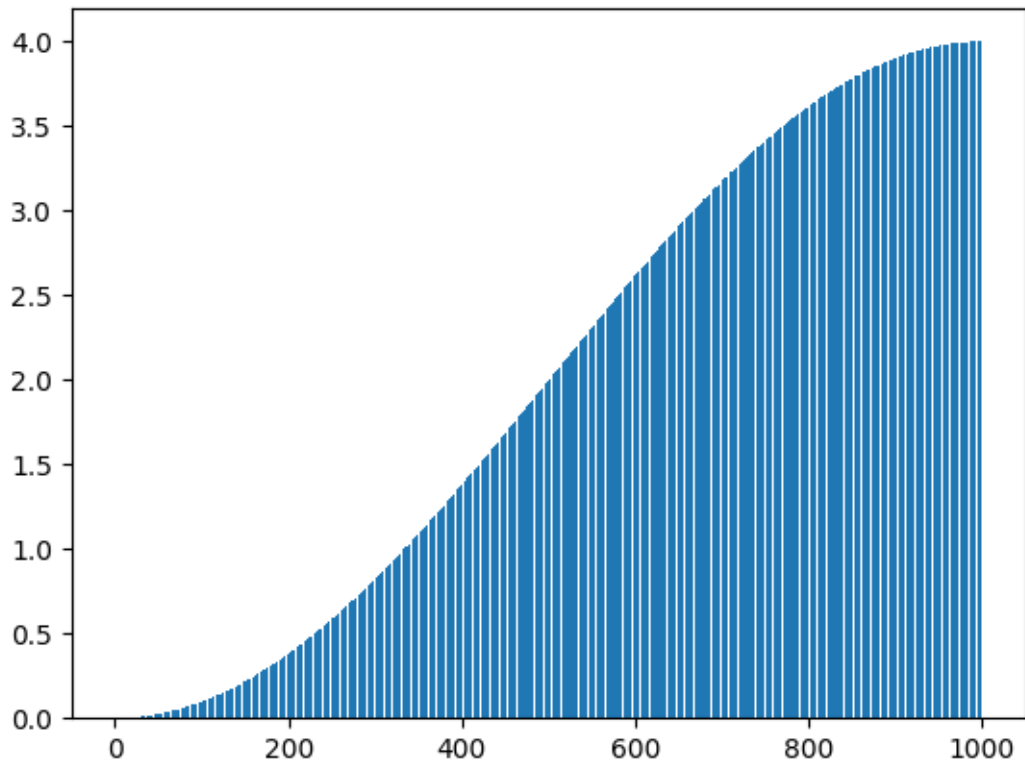
The adjacency matrix of a chain is very regular and the distribution of its eigenvalues is a monotonic function, then we have a way to label nodes.

```
[7]: ll = sp.sparse.csgraph.laplacian(aa, normed=False)
```

```
Val, Vec = np.linalg.eig(ll)
ind = np.argsort(Val)
Val = Val[ind]
Vec = Vec[:, ind]

plt.bar(range(0, len(Val)), Val)
```

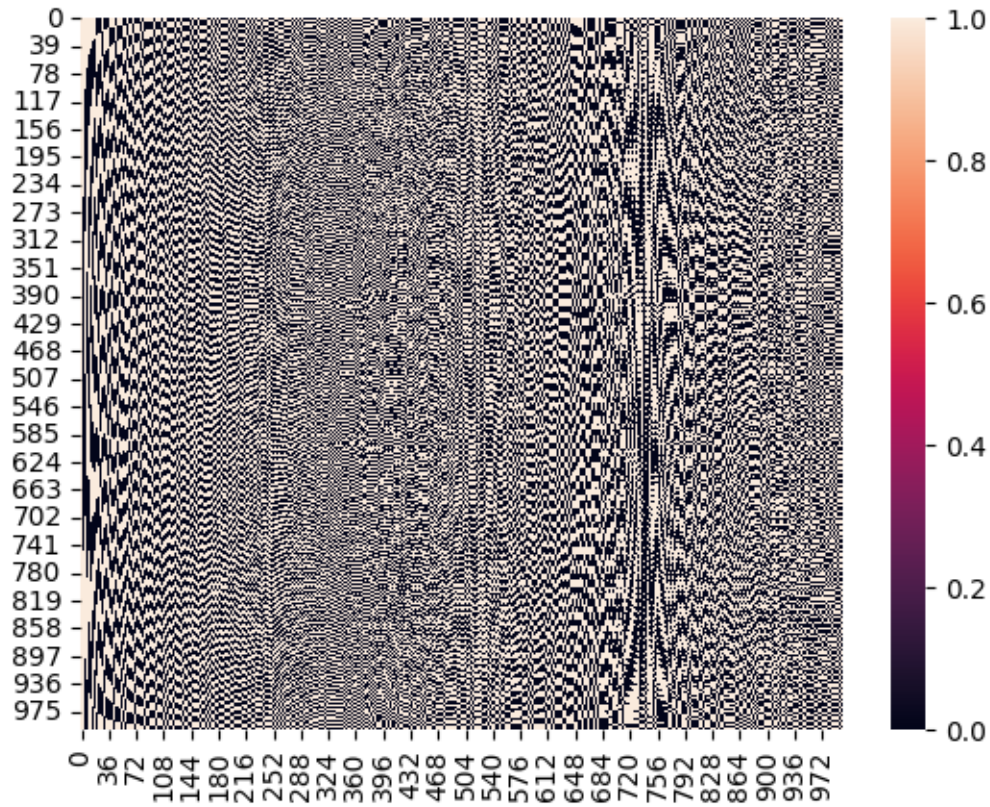
```
[7]: <BarContainer object of 1000 artists>
```



Moreover, plotting the matrix of eigenvectors we can see a sort of periodicity in their values.

```
[8]: sns.heatmap(Vec>0)
```

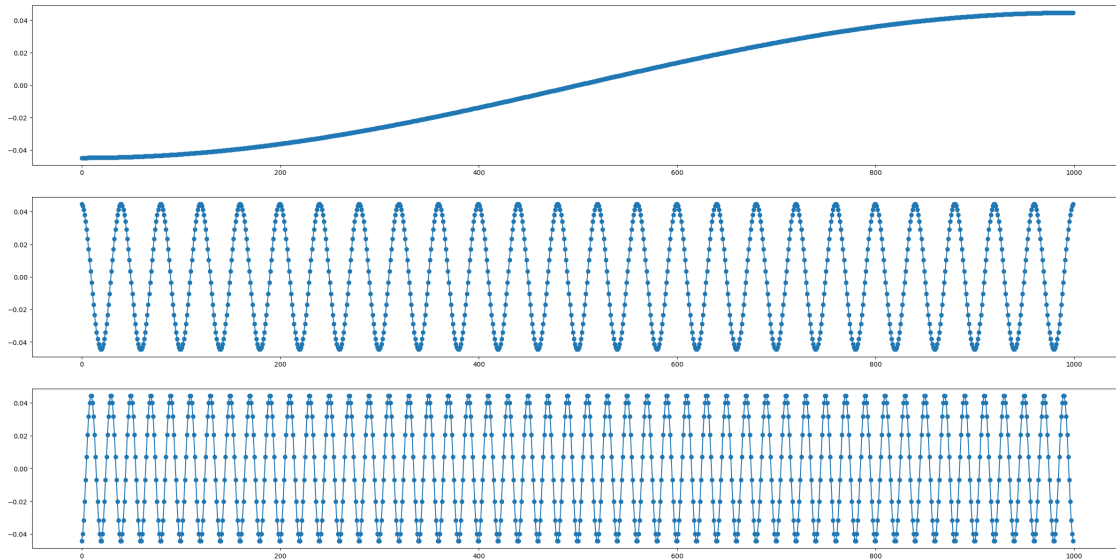
```
[8]: <Axes: >
```



```
[9]: fig, ax = plt.subplots(3, 1, figsize=(30, 15))
```

```
ax[0].plot(Vec[:, 1], '-o')
ax[1].plot(Vec[:, 50], '-o')
ax[2].plot(Vec[:, 100], '-o')
```

```
[9]: [<matplotlib.lines.Line2D at 0x7fcd4c6e9180>]
```



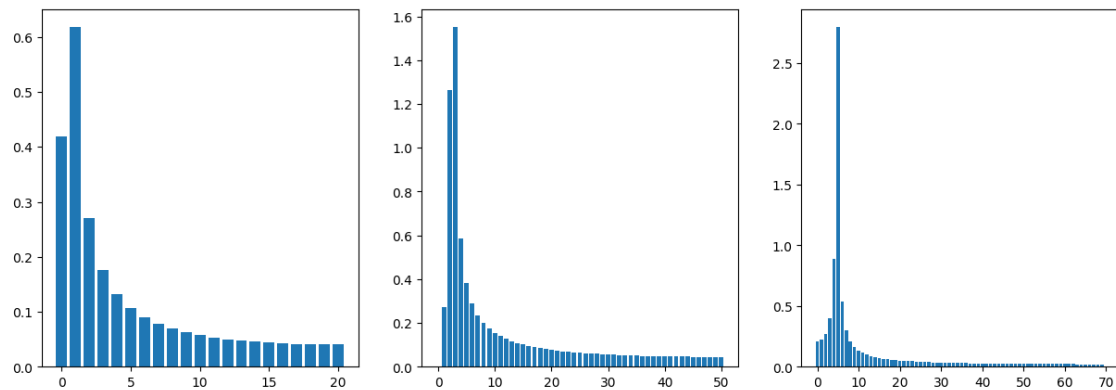
As all good physicist do, periodic signals MUST be decomposed with Fourier, so here we go. We can notice that we need to be in the thermodynamic limit in order to obtain the pure delta function (in the frequency domain).

```
[10]: ff1 = np.fft.rfft(Vec[:, 20], n=20*2)
      ff2 = np.fft.rfft(Vec[:, 50], n=50*2)
      ff3 = np.fft.rfft(Vec[:, 69], n=69*2)

      fig, ax = plt.subplots(1, 3, figsize=(15, 5))

      ax[0].bar(np.arange(len(ff1)), np.abs(ff1))
      ax[1].bar(np.arange(len(ff2)), np.abs(ff2))
      ax[2].bar(np.arange(len(ff3)), np.abs(ff3))
```

```
[10]: <BarContainer object of 70 artists>
```

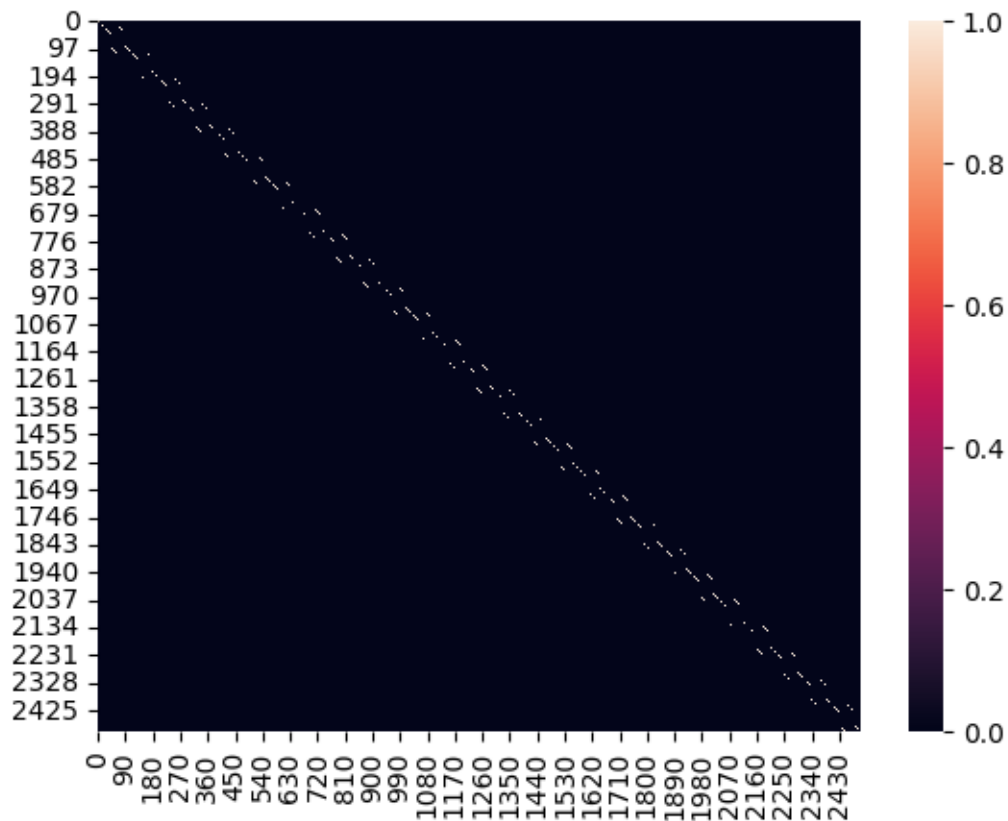


3.3 2D lattice

```
[11]: def reticolo2d(N, P):  
    # N = lattice side  
    # P = number of nearest neighbors  
    Nq = N*N  
    A = sp.sparse.lil_matrix((Nq, Nq))  
  
    for i1 in range(Nq):  
        for i2 in range(i1, Nq):  
            if (i2-i1) <= P and i2 != i1 and i1 % N > 0:  
                A[i1, i2] = 1  
            elif (i2 - i1) == N:  
                A[i1, i2] = 1  
  
    A = A + A.T  
    return A
```

```
[12]: Net = reticolo2d(50, 1)  
  
sns.heatmap(Net.toarray())
```

[12]: <Axes: >



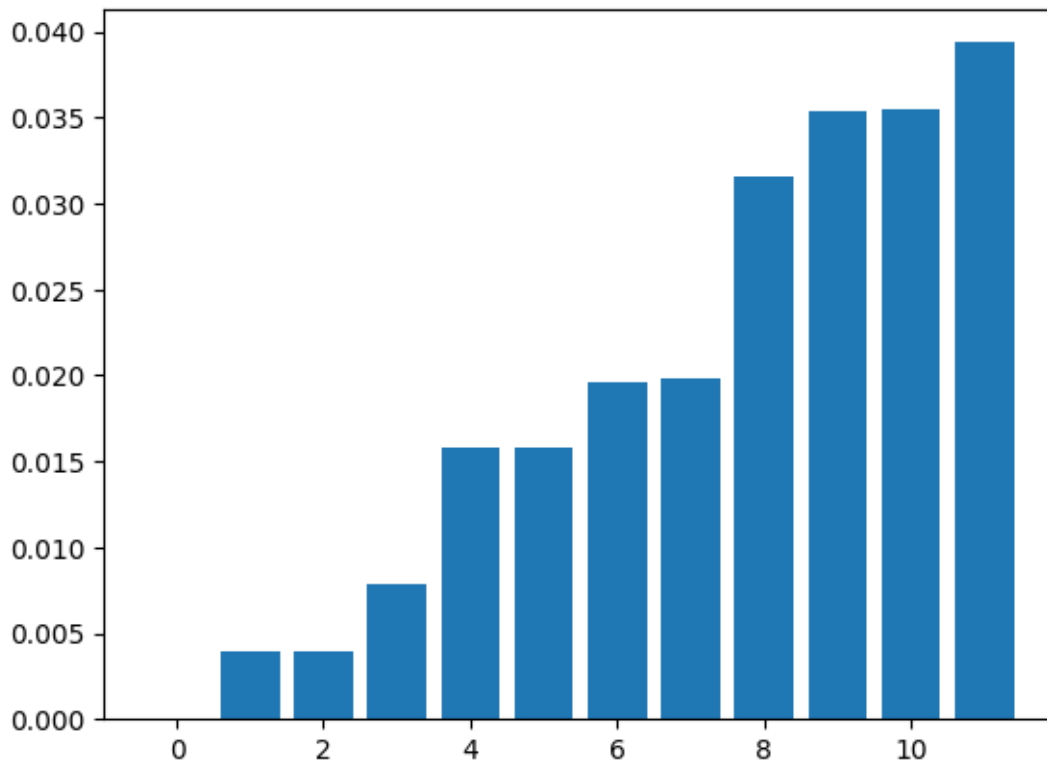
```
[13]: l1 = sp.sparse.csgraph.laplacian(Net.toarray(), normed=False)

Val, Vec = np.linalg.eig(l1)
ind = np.argsort(Val)
Val = Val[ind]
Vec = Vec[:, ind]
```

Plotting the eigenvalues in a bar plot we notice how there are many with multiplicity 2.

```
[14]: plt.bar(range(0, len(Val[0:12])), Val[0:12])
```

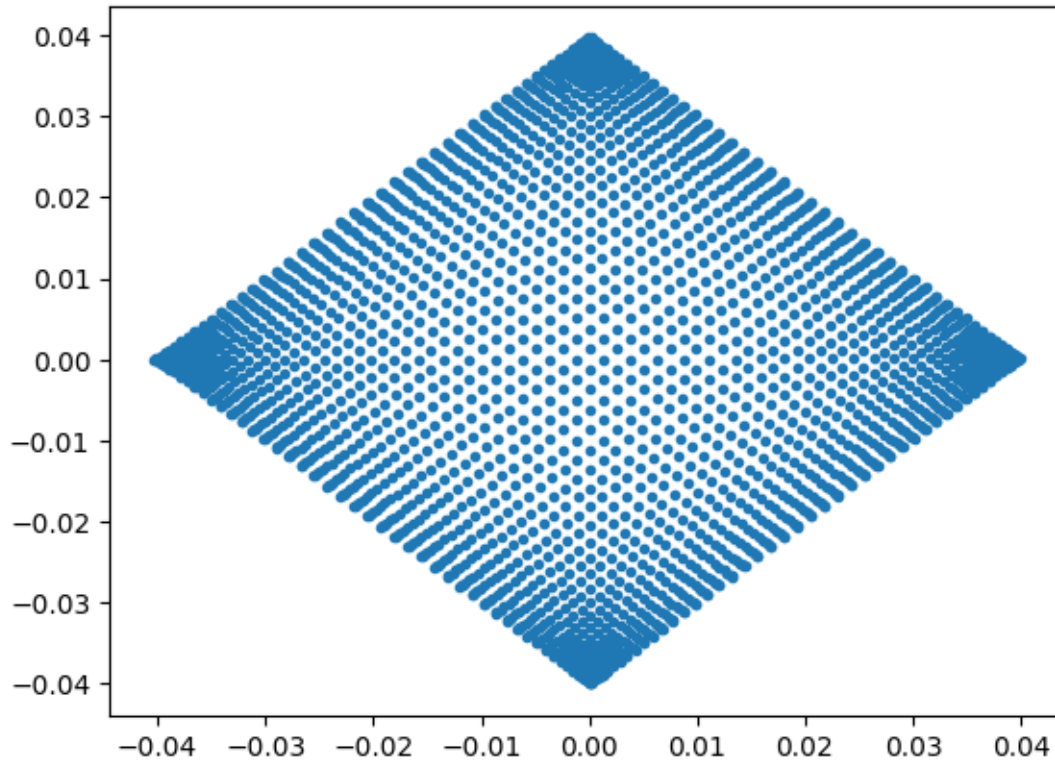
```
[14]: <BarContainer object of 12 artists>
```



Here is a weird thing: plotting a pair of eigenvectors with the same eigenvalue will result in the reticle itself. Notice how, due to the finite dimension of it, we've also border effects: in the thermodynamic limit they'll vanish (at least theoretically).

```
[15]: plt.plot(Vec[:, 1], Vec[:, 2], '.')
```

```
[15]: [<matplotlib.lines.Line2D at 0x7fcd4c20b400>]
```

4 Open network models generation

4.1 Exponential network

We now want to build an exponential network with no preferential attachment effects.

```
[28]: import networkx as nx
import scipy as sp
import numpy as np
from tqdm.notebook import trange

N = int(5e3) # number of nodes/steps
M = 4 # links per step

A = sp.sparse.lil_matrix((N, N), dtype=int)

for ind in trange(M+1, N):
    rr = np.random.permutation(ind-1)
    A[ind, rr[:M]] = 1
    A[rr[:M], ind] = 1
```

```
Net = nx.from_scipy_sparse_array(A)
```

```
0%|          | 0/4995 [00:00<?, ?it/s]
```

Let's study some statistics about it.

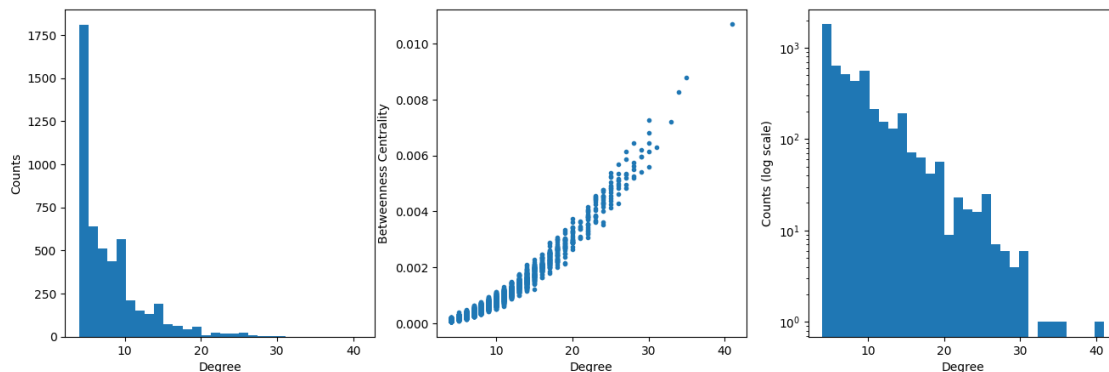
```
[2]: K = [d for n, d in Net.degree()]
```

```
BC = nx.betweenness_centrality(Net)
```

```
[7]: from matplotlib import pyplot as plt

fig, ax = plt.subplots(1, 3, figsize=(16, 5))
ax[0].hist(K[1:], bins=30)
ax[0].set_xlabel('Degree')
ax[0].set_ylabel('Counts')
ax[1].plot(K[1:], list(BC.values())[1:], '.')
ax[1].set_xlabel('Degree')
ax[1].set_ylabel('Betweenness Centrality')
ax[2].set_yscale('log')
ax[2].hist(K[1:], bins=30)
ax[2].set_xlabel('Degree')
ax[2].set_ylabel('Counts (log scale)')
```

```
[7]: Text(0, 0.5, 'Counts (log scale)')
```



4.2 “B-A” Barabasi-Alberts model

Let's now see what happens with preferential attachment.

In *networkx* one can easily generate a Barabasi-Alberts network with a dedicated function. We can see how the Degree is distributed according to a power law.

```
[5]: import networkx as nx
from matplotlib import pyplot as plt
```

```

import numpy as np

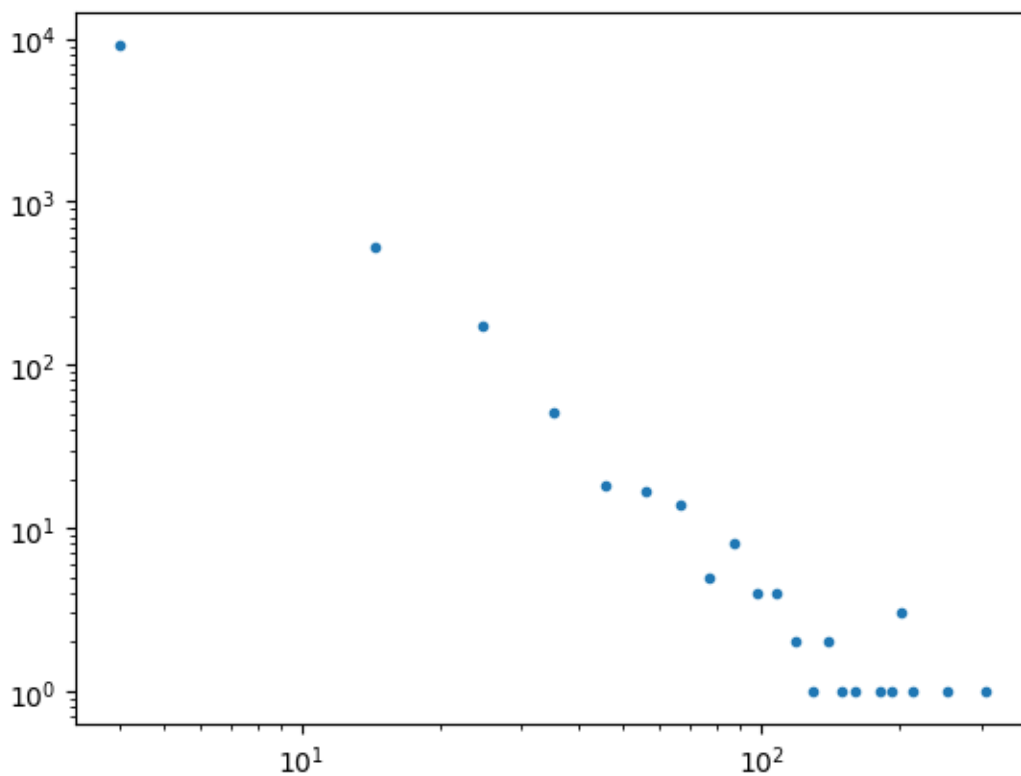
N = int(1e4) # number of nodes/steps
M = 4 # links per step

Net = nx.barabasi_albert_graph(N, M)

K = [d for n, d in Net.degree()]

fig, ax = plt.subplots()
Y, X, patches = ax.hist(K[1:], bins=30)
X = np.delete(X, -1)
ax.cla()
ax.set_xscale('log')
ax.set_yscale('log')
ax.plot(X[Y > 0], Y[Y > 0], '.')
```

[5]: [<matplotlib.lines.Line2D at 0x7ff57d1a1ab0>]



```
[6]: BC = nx.betweenness centrality(Net)

CC = nx.clustering(Net)
```

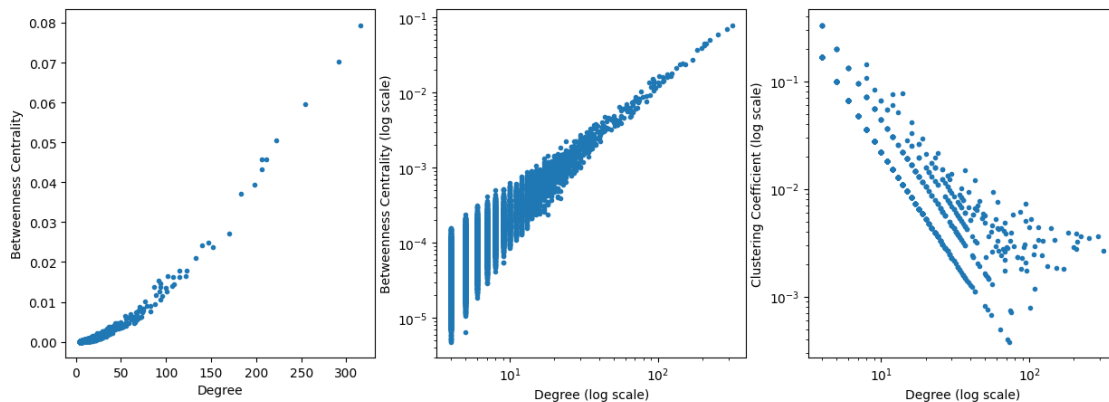
Moreover, we can see that despite this is a Barabasi-Alberts network, the relationship between Betweenness Centrality and Degree remains quadratic.

```
[7]: from matplotlib import pyplot as plt

fig, ax = plt.subplots(1, 3, figsize=(15, 5))

ax[0].set_xlabel('Degree')
ax[0].set_ylabel('Betweenness Centrality')
ax[0].plot(K, list(BC.values()), '.')
ax[1].set_xscale('log')
ax[1].set_yscale('log')
ax[1].set_xlabel('Degree (log scale)')
ax[1].set_ylabel('Betweenness Centrality (log scale)')
ax[1].plot(K, list(BC.values()), '.')
ax[2].set_xscale('log')
ax[2].set_yscale('log')
ax[2].set_xlabel('Degree (log scale)')
ax[2].set_ylabel('Clustering Coefficient (log scale)')
ax[2].plot(K, list(CC.values()), '.')
```

```
[7]: [<matplotlib.lines.Line2D at 0x7ff57aaf7370>]
```



4.3 Duplication - divergence model

As before, *networkx* provides us a magic function that will do all the hard work

```
[16]: import networkx as nx
```

```

N = int(5e3)
p = 0.5

Net = nx.duplication_divergence_graph(N, p)

```

```

[17]: K = [d for n, d in Net.degree()]
BC = nx.betweenness_centrality(Net)
CC = nx.clustering(Net)
Kn = nx.average_neighbor_degree(Net)

```

As we can see, the betweenness centrality trend remained quadratic.

```

[18]: from matplotlib import pyplot as plt

fig, ax = plt.subplots(1, 4, figsize=(23, 5))

ax[0].set_xlabel('Degree')
ax[0].set_ylabel('Betweenness Centrality')
ax[0].plot(K, list(BC.values()), '.')
ax[1].set_xlabel('Degree')
ax[1].set_ylabel('Average Neighbor Degree')
ax[1].plot(K, list(Kn.values()), '.')
ax[2].set_xlabel('Degree')
ax[2].set_ylabel('Clustering Coefficient')
ax[2].plot(K, list(CC.values()), '.')
ax[3].set_xscale('log')
ax[3].set_yscale('log')
ax[3].set_xlabel('Degree (log scale)')
ax[3].set_ylabel('Clustering Coefficient (log scale)')
ax[3].plot(K, list(CC.values()), '.')

```

```

[18]: [<matplotlib.lines.Line2D at 0x7fd486476530>]

```

