Notebook

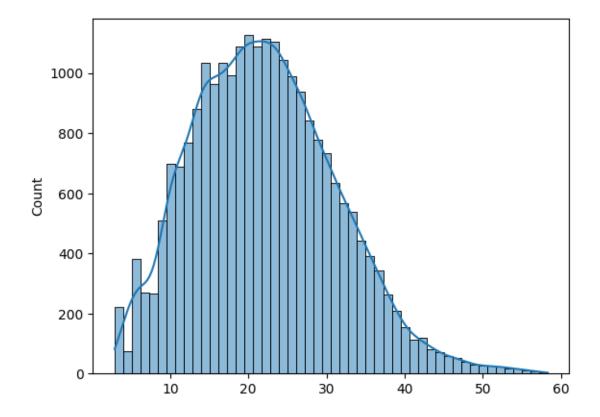
May 8, 2023

```
[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)
```

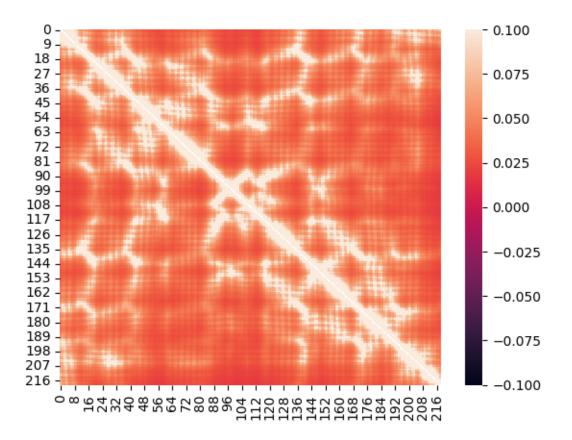
[2]: <Axes: ylabel='Count'>



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

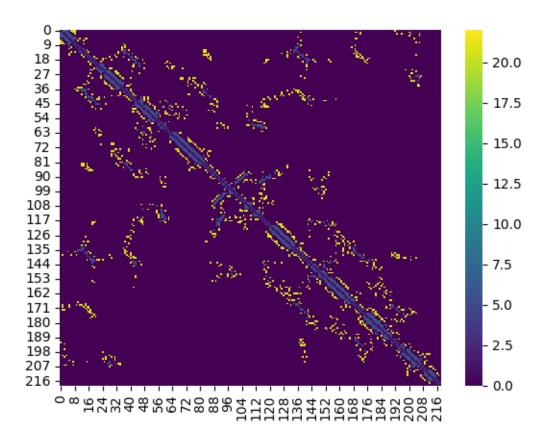
/tmp/ipykernel_1019/2899854611.py:2: RuntimeWarning: divide by zero encountered
in divide
 sns.heatmap(1./D)

[3]: <Axes: >



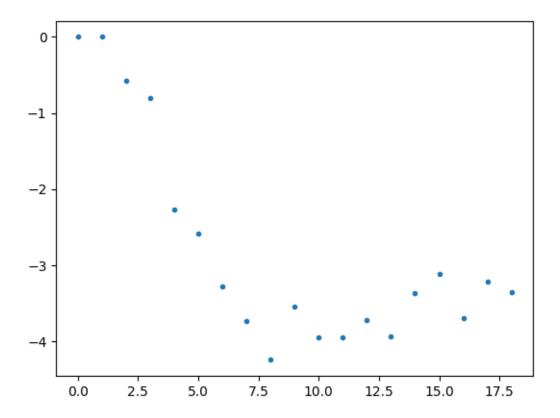
```
[4]: Net6 = (D < 6) * D
Net10 = (D > 10) * (D < 11) * D
N1 = (D < 11) * D
sns.heatmap(Net6 + 2 * Net10, cmap="viridis")</pre>
```

[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>]

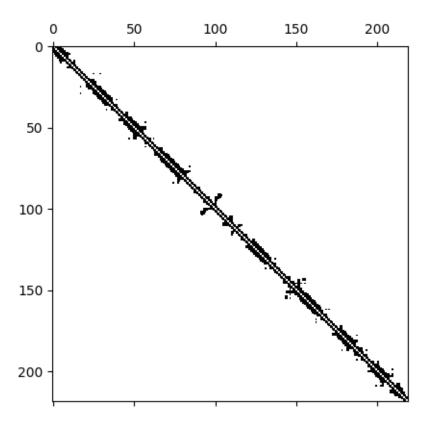


```
[6]: Nkd = 12
Ad = np.zeros((Nnode, Nnode), dtype=int)

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

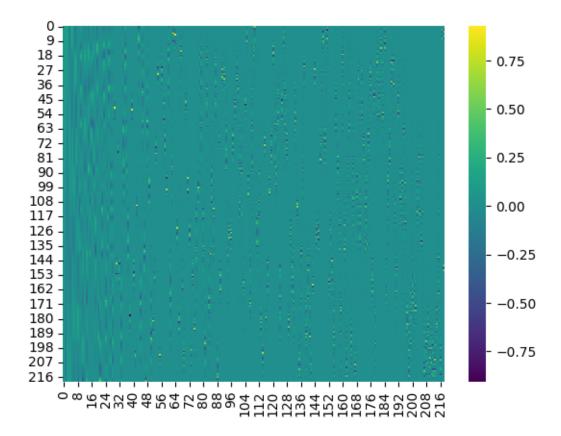
plt.spy(Ad)
```

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



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

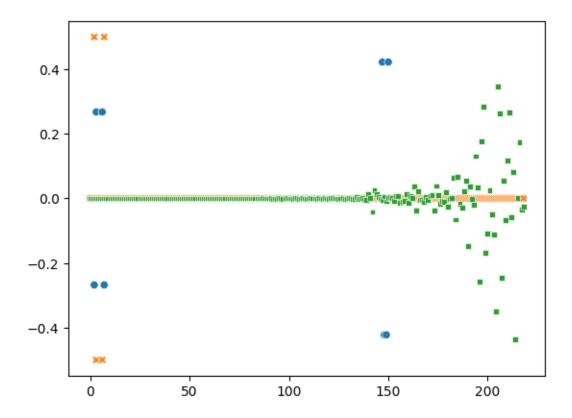
[7]: <Axes: >



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)
```

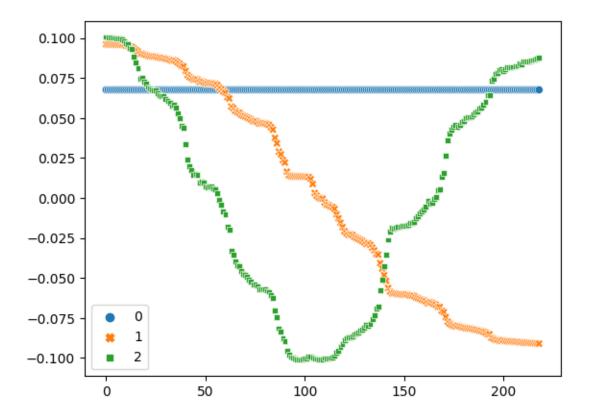
[47]: <Axes: >



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.

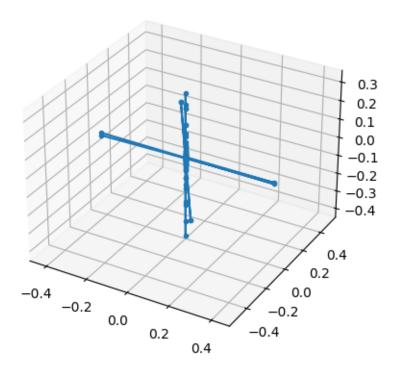
```
[15]: sns.scatterplot(VecAd[:, [0, 1, 2]])
```

[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: 0.012008750054378977
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: 0.013202010924415211
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:
```

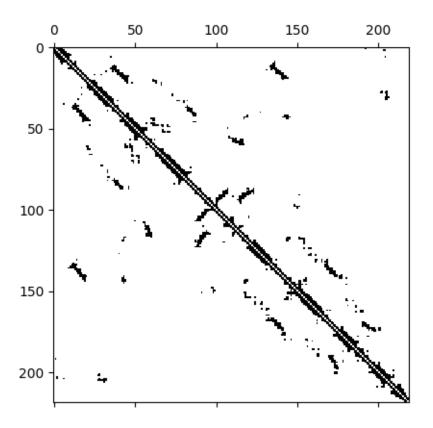
```
0.013708967377539785, 169: 0.0062230404399575, 170: 0.01860456955123589, 171:
0.02017392603687551, 172: 0.02489230843891768, 173: 0.06003089293203244, 174:
0.041275892955877636, 175: 0.005132034272732839, 176: 0.007231489848532819, 177:
0.02289808314820412, 178: 0.02065485568164289, 179: 0.002516859061860833, 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>



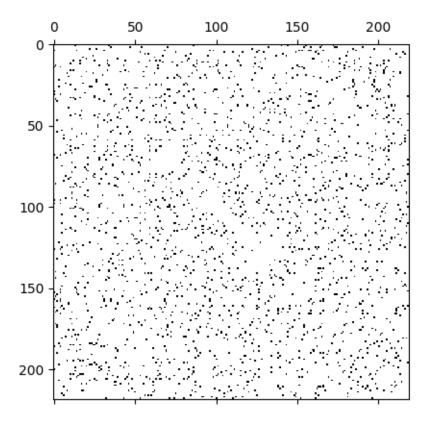
```
[22]: Index = np.arange(Nnode)
PermIndex = np.random.permutation(Nnode)
PermMat = np.zeros((Nnode, Nnode))
```

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

A faster method could be

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

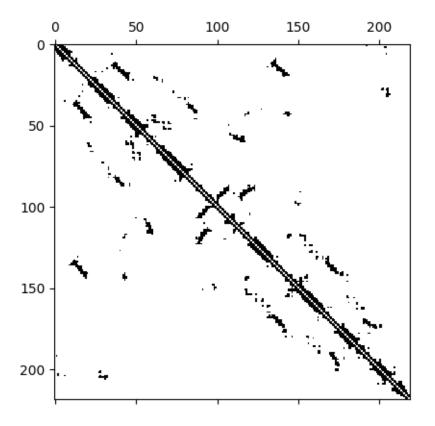
[25]: <matplotlib.image.AxesImage at 0x7fc8e8d9c190>



We can invert the permutation effect

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

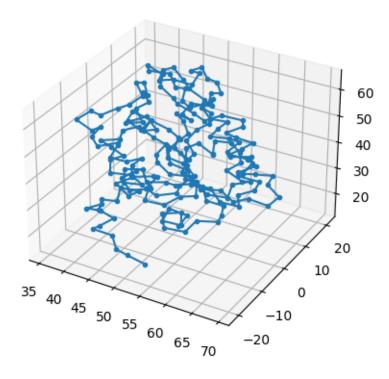
[26]: <matplotlib.image.AxesImage at 0x7fc8e8c082b0>



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>]



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 $\frac{1}{Nnode^2}$

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.

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)
```

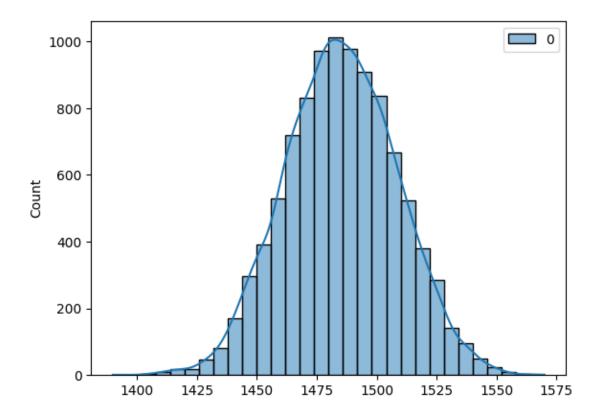
Let's see some stats

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.

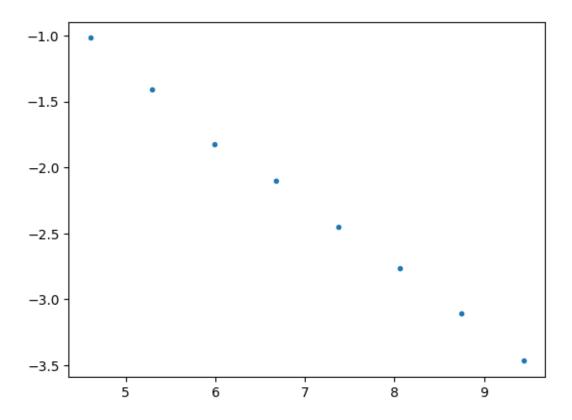
```
[66]: Pow = 4.21 # max network size
Pl = 0.1
Cnt = 0

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

```
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,_u
    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 $\lambda = xP * Nnode$

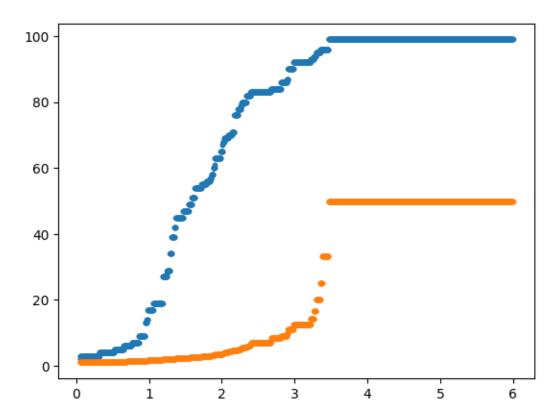
```
[71]: Rc = np.zeros(len(xP))
Rm = np.zeros(len(xP))
Cnt = 0

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>]



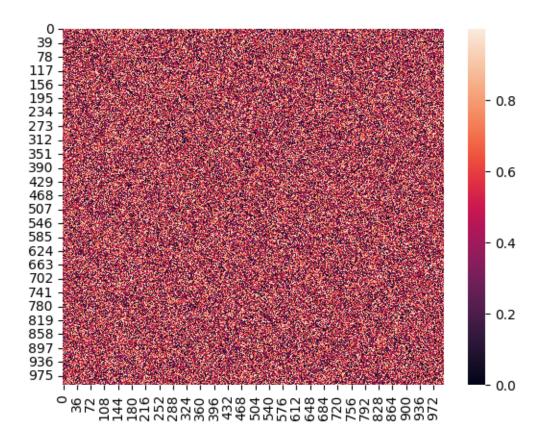
2.4 Semicircle law for ER network spectrum vs RMT (Random Matrix Theory)

```
[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)
```

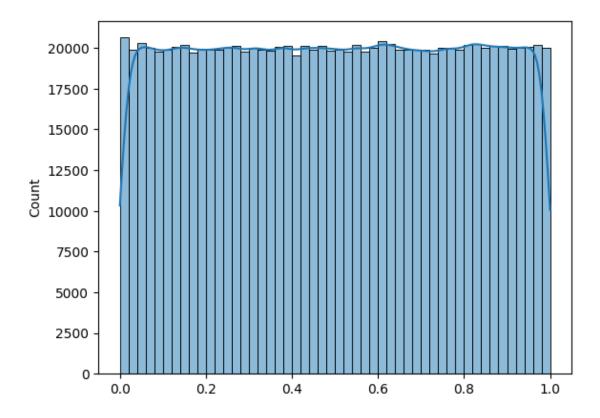
[73]: <Axes: >



Let's see also the histogram of coefficients

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

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

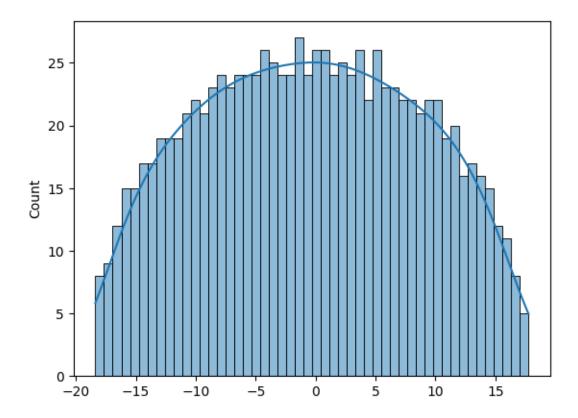


Now the eigenvalues and eigenvectors. $\,$

 ${\bf NOTE}$ 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'>

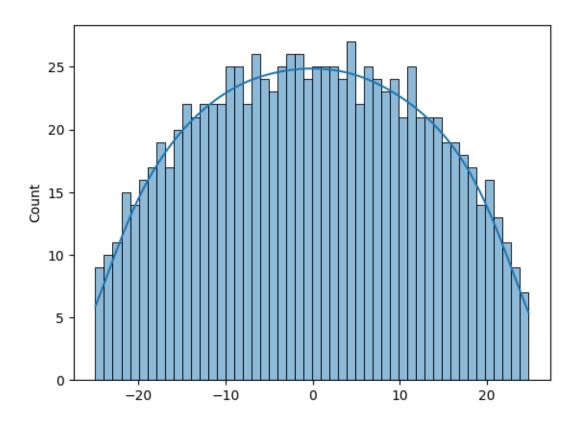


```
[76]: rr = np.triu(np.random.rand(Nnode, Nnode), k=1) > 1 - Plink
rr = rr + rr.T
```

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

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

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

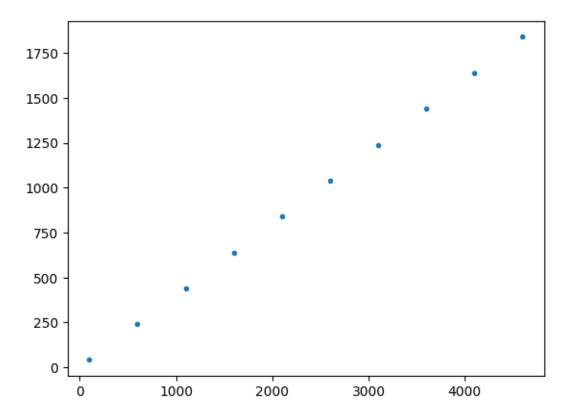


```
[83]: Cnt = 0
    xx = np.arange(100, 5000, step=500)
    vmax = []

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, '.')
```

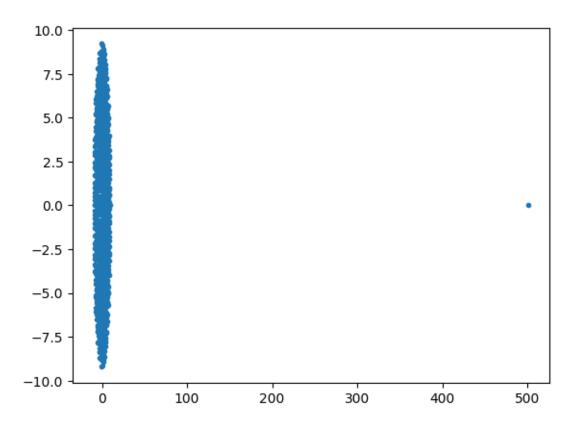
[83]: [<matplotlib.lines.Line2D at 0x7fafb8358f10>]



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

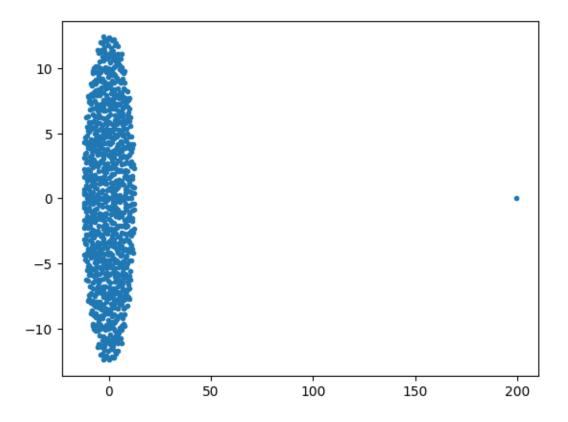
```
[80]: rr = np.random.rand(Nnode, Nnode)
vv = np.linalg.eigvals(rr)
vvr = np.real(vv)
vvi = np.imag(vv)
plt.plot(vvr, vvi, '.')
```

[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>]

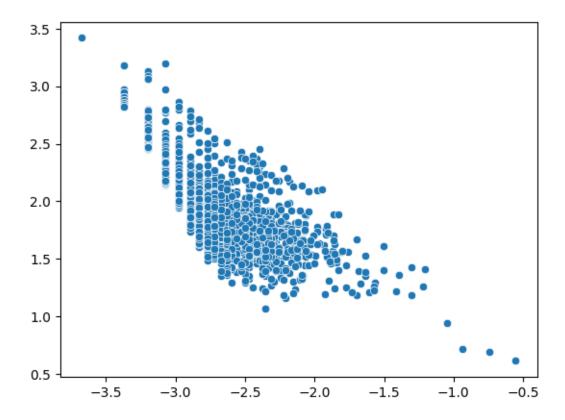


```
[9]: import scipy as sp
     import numpy as np
     import networkx as nx
     from tqdm import tqdm # necessary because shuffling takes a while
     def shuffle_net_sym_f(Net, Nsh):
         # Nsh = number of shuffles (* number of links)
         Shuf = Net
         I = list(nx.edges(Shuf))
         Nl = len(I)
         for ind in tqdm(range(Nl * Nsh)):
             L = np.random.randint(N1, size = 2)
             while L[0] == L[1]:
                  L[1] = np.random.randint(N1)
             if Shuf.has_edge(I[L[0]][0], I[L[0]][1]) and Shuf.has_edge(I[L[1]][0], __
      \BoxI[L[1]][1]) and (Shuf.has_edge(I[L[0]][0], I[L[1]][1]) == False) and (Shuf.
      \neghas_edge(I[L[1]][0], I[L[0]][1]) == False) and (I[L[1]][0] != I[L[0]][1])_u
      \hookrightarrow and (I[L[0]][0] != I[L[1]][1]) and (I[L[0]][0] != I[L[0]][1]) and
      \hookrightarrow (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))
                  N1 = 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
```

[13]: <Axes: >

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



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 enought but it__

stakes about 2 hours and half to run
```

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

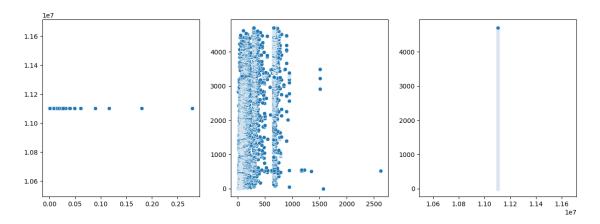
By shuffling we're actually creating another network with the same characteristic as the previous one: is it really the same network? Well, it depends. In some cases we actually lose information by shuffling, which means that links were not randomly generated in the original one, like in that case.

```
[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
```

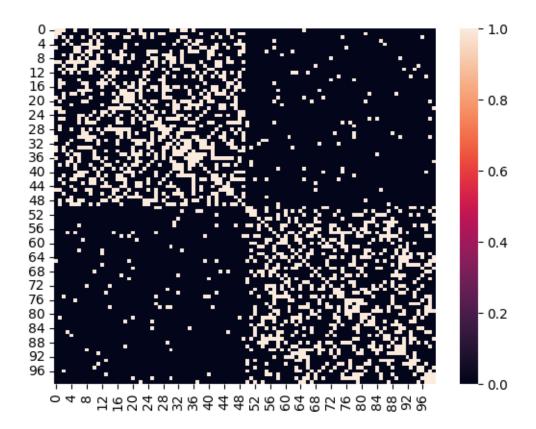
Let's generate an ER random network with the variables we've just set up. We can clearly see the two highly connected networks.

```
[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)</pre>
```

[4]: <Axes: >



```
[5]: import scipy as sp

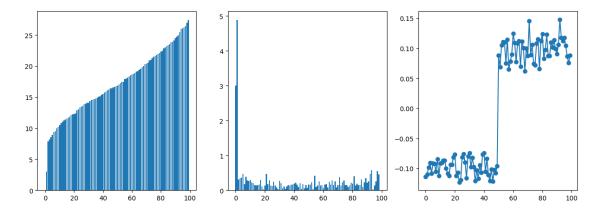
11 = sp.sparse.csgraph.laplacian(Net, normed=False)

Val, Vec = np.linalg.eig(11)
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>]

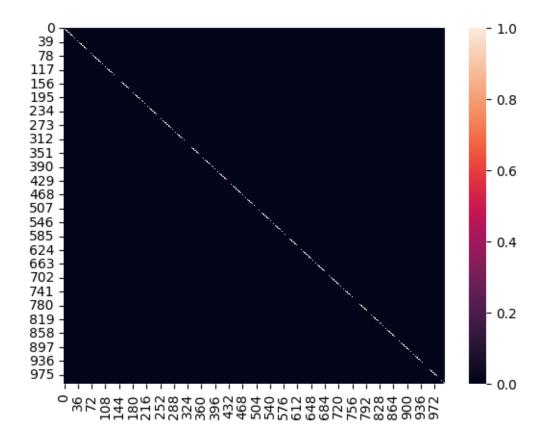


3.2 Chain - 1D lattice

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: >



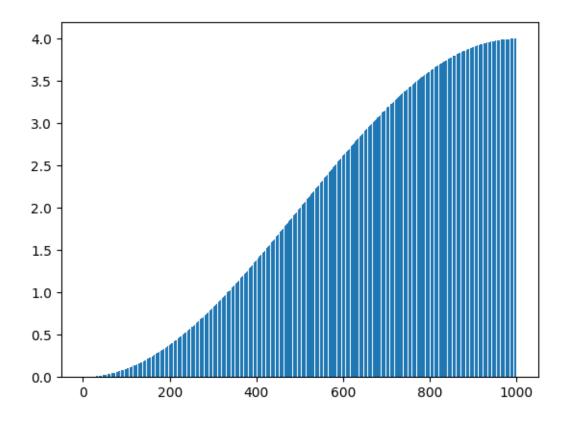
The adjacency matrix of a chain is very regular and the distribution of its eigenvalues is a monotonic function, then we have a way to label nodes.

```
[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)
```

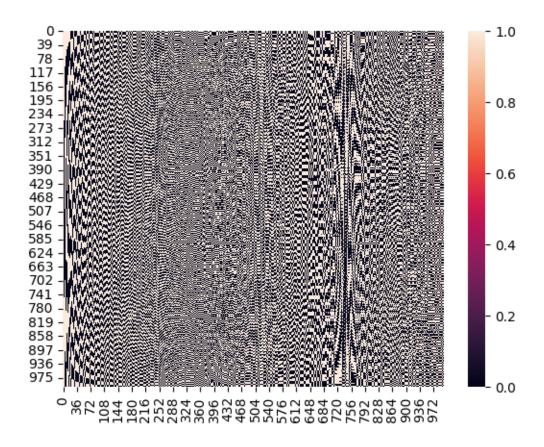
[7]: <BarContainer object of 1000 artists>



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

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

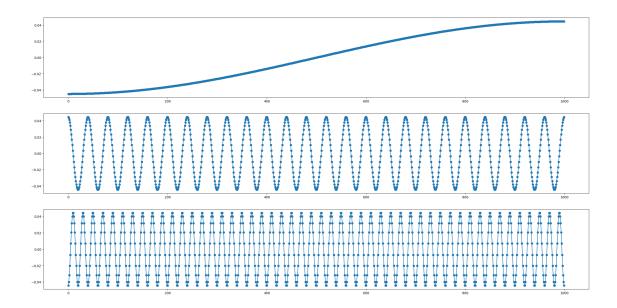
[8]: <Axes: >



```
[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>]



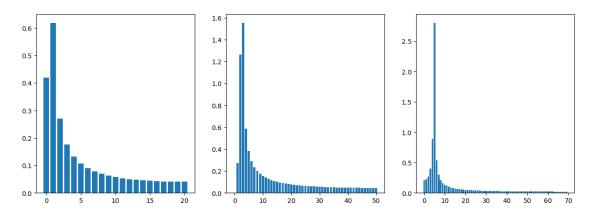
As all good physicist do, periodic signals MUST be decomposed with Fourier, so here we go. We can notice that we need to be in the thermodynamic limit in order to obtain the pure delta function (in the frequency domain).

```
[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))
```

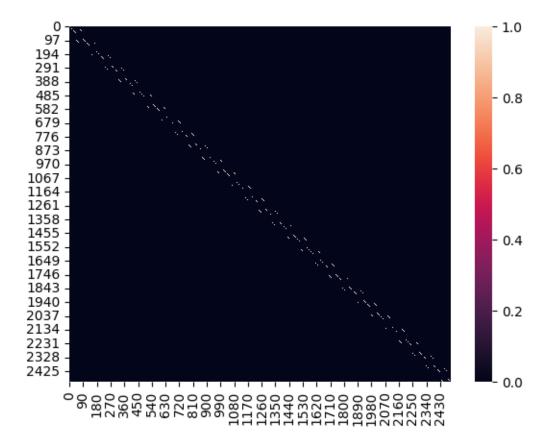
[10]: <BarContainer object of 70 artists>



3.3 2D lattice

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

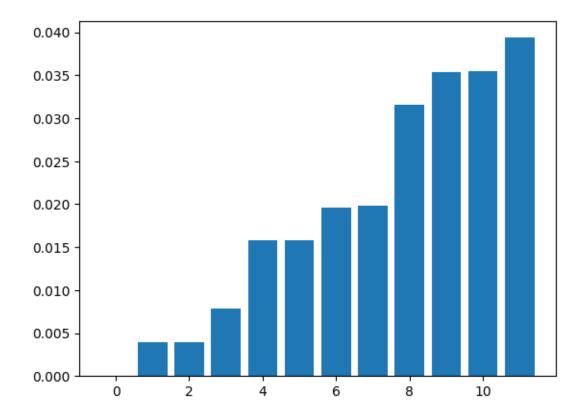
[12]: <Axes: >



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])
```

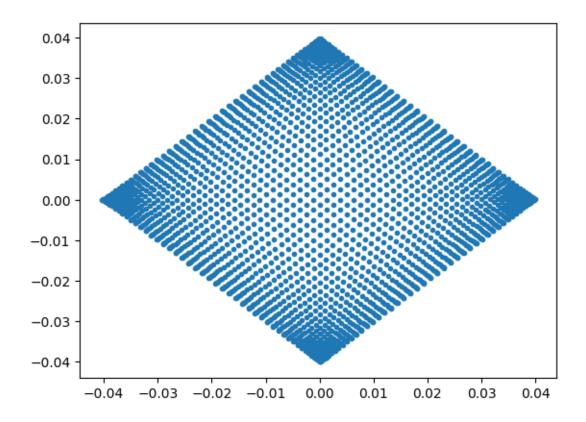
[14]: <BarContainer object of 12 artists>



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.

```
[1]: 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]

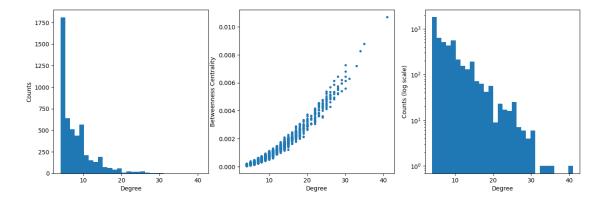
Let's study some statistics about it.

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

BC = nx.betweenness_centrality(Net)
```

```
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.

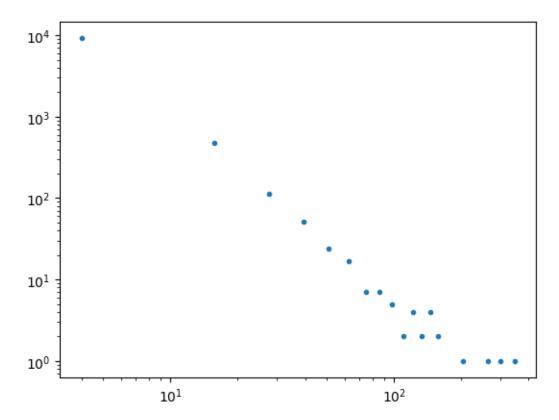
In *networkx* one can easily generate a Barabasi-Alberts network with a dedicated function. We can see how the Degree is distributed according a power law.

```
[9]: 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], '.')
```

[9]: [<matplotlib.lines.Line2D at 0x7f5c51d52da0>]



```
[10]: BC = nx.betweenness_centrality(Net)
```

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

```
[13]: from matplotlib import pyplot as plt
fig, ax = plt.subplots(1, 2, figsize=(10, 5))
```

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

[13]: Text(0, 0.5, 'Betweenness Centrality (log scale)')

