leggi_pdb

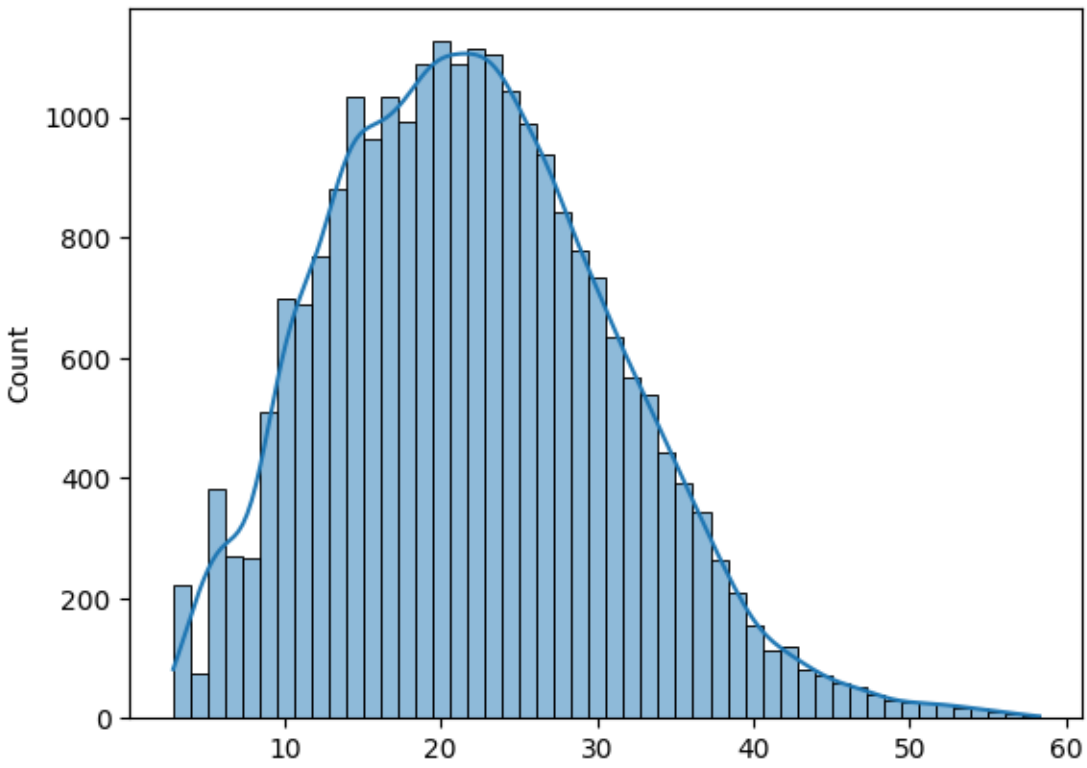
April 11, 2023

[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']
Nnode = A.shape[0]

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

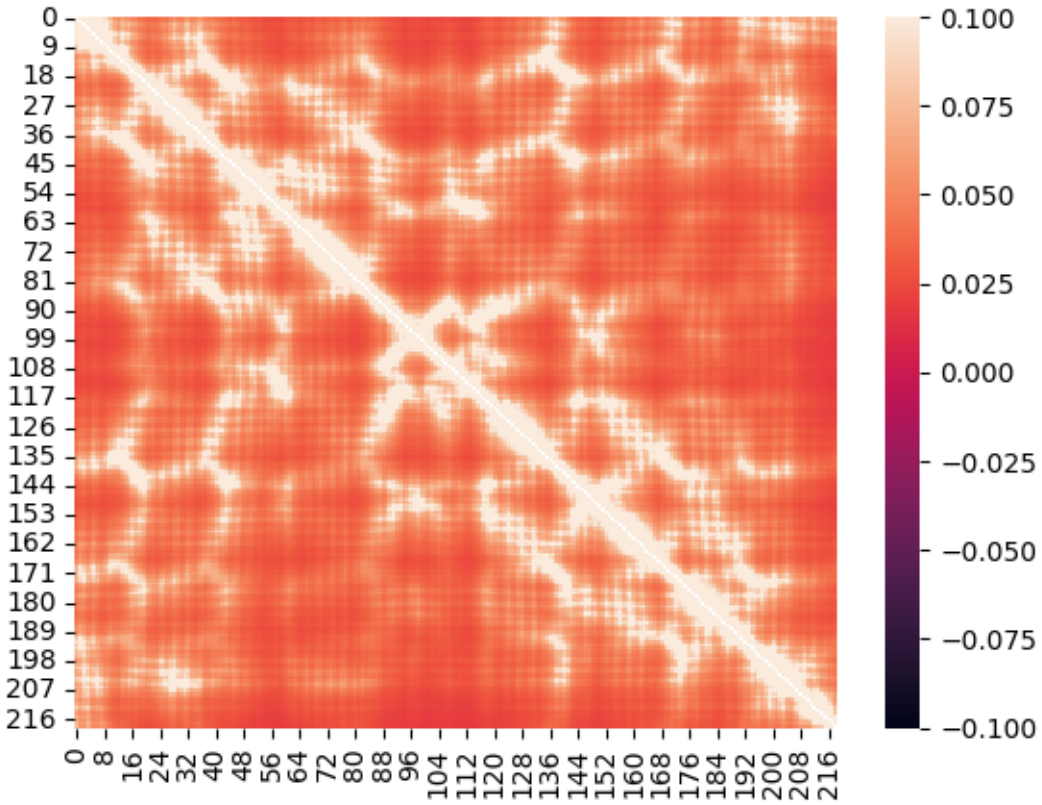
[2]:
```
<Axes: ylabel='Count'>
```



[3]:
```
D = sp.spatial.distance.squareform(protdist)
sns.heatmap(1./D)
```

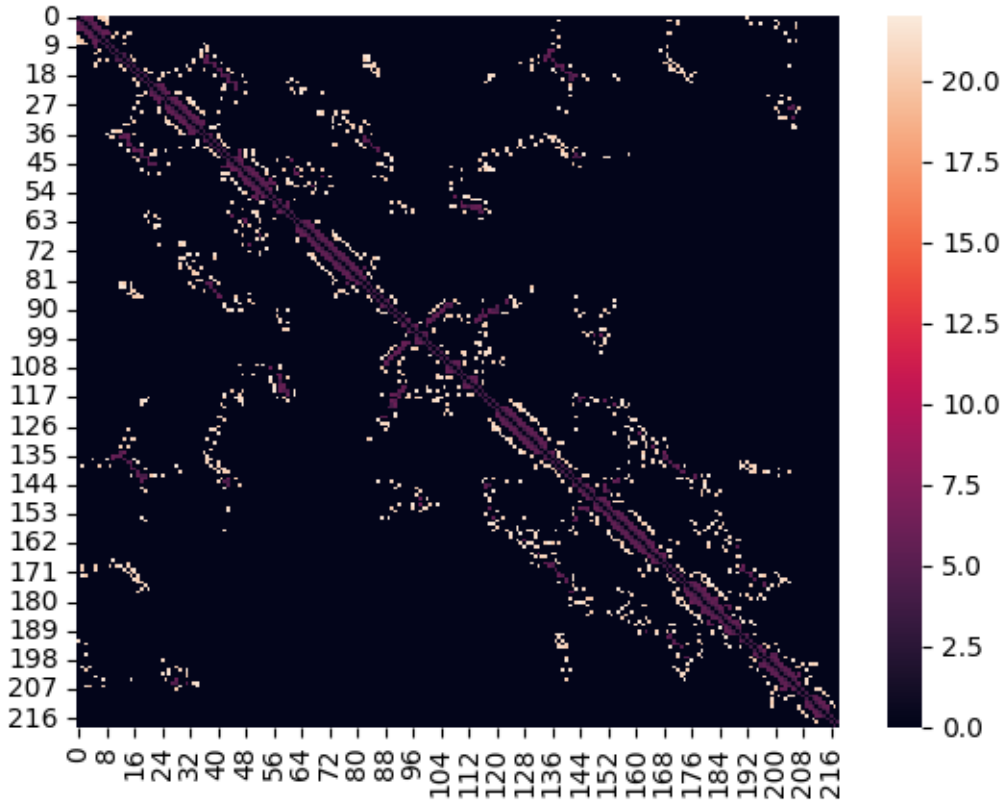
```
/tmp/ipykernel_3448/2899854611.py:2: RuntimeWarning: divide by zero encountered
in divide
  sns.heatmap(1./D)
```

[3]: <Axes: >



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

[4]: <Axes: >

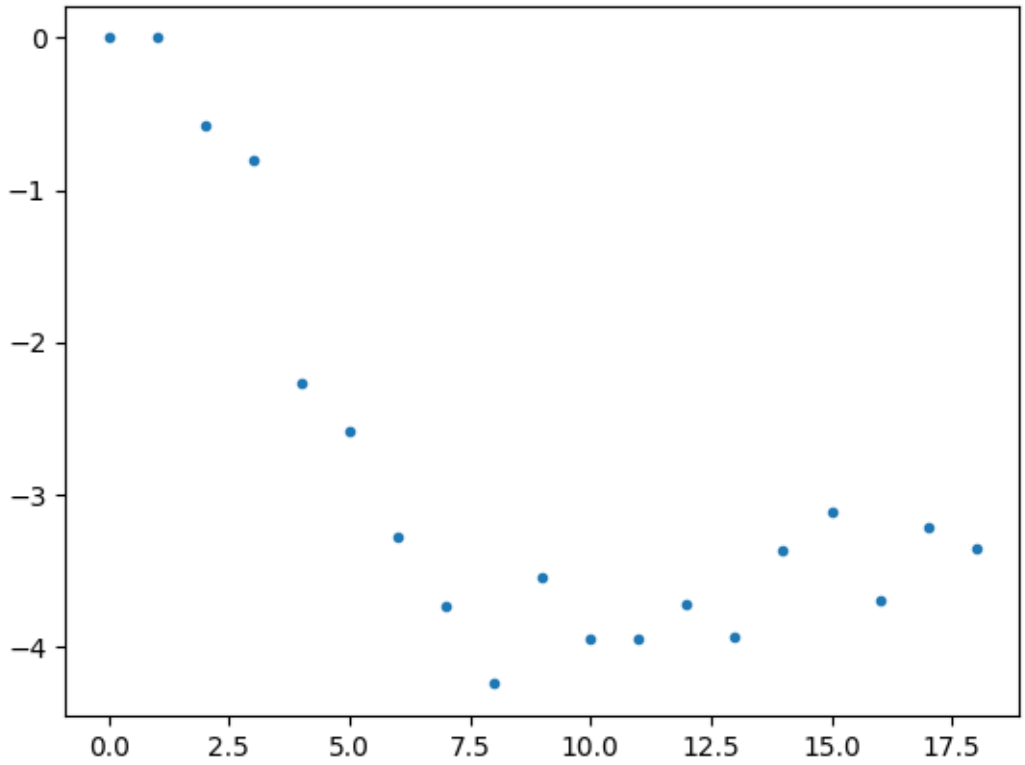


[5]:
```
Kdiag = []

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 0x7f98a7d73e20>]

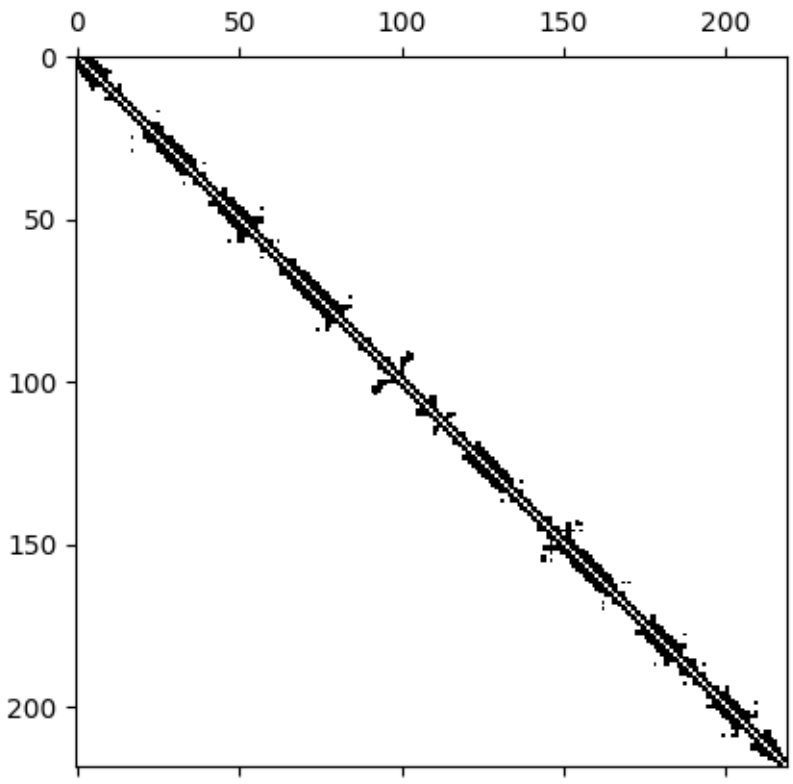


[6]:
```
Nkd = 12
Ad = np.zeros((Nnode, Nnode))

for index in range(-Nkd, Nkd):
    Ad += np.diag(np.diag(A, index), index)

plt.spy(Ad)
```

[6]: <matplotlib.image.AxesImage at 0x7f98a6289570>



[7]:
```
# valAd, vecAd = np.linalg.eig(sp.sparse.csgraph.laplacian(Ad))
# plt.plot(vecAd, '.')
```

[8]:
```
# i1 = Nnode - 1
# i2 = Nnode - 2
# i3 = Nnode - 3
# plt.plot(vecAd[:,[i1, i2, i3]], '.')
```

[9]:
```
# fig = plt.figure()
# ax = fig.add_subplot(projection='3d')
# plt.plot(vecAd[:,i1], vecAd[:,i2], vecAd[:,i3], '.')
```

PCM_permute

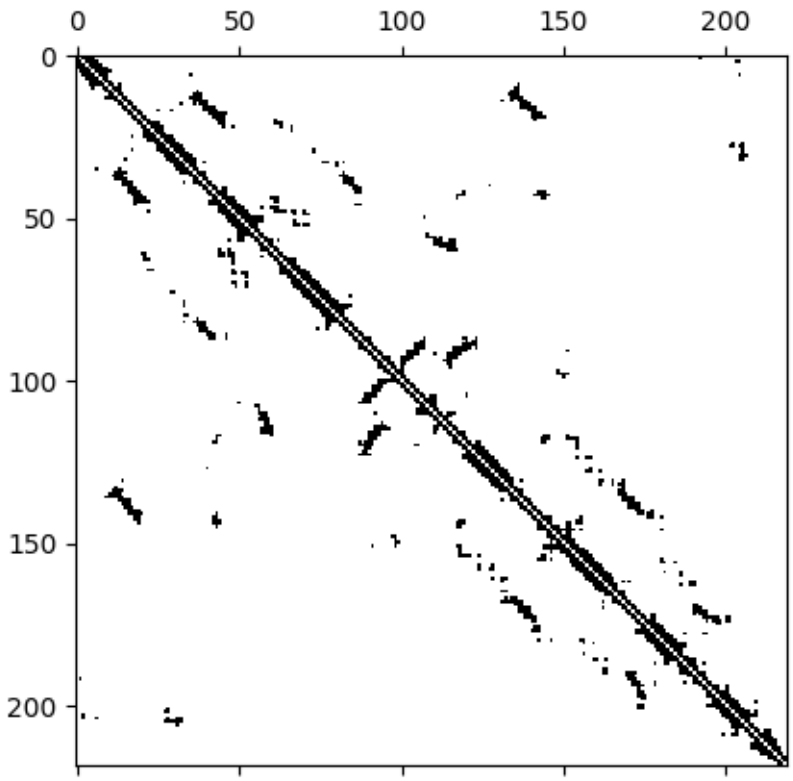
April 11, 2023

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))
```

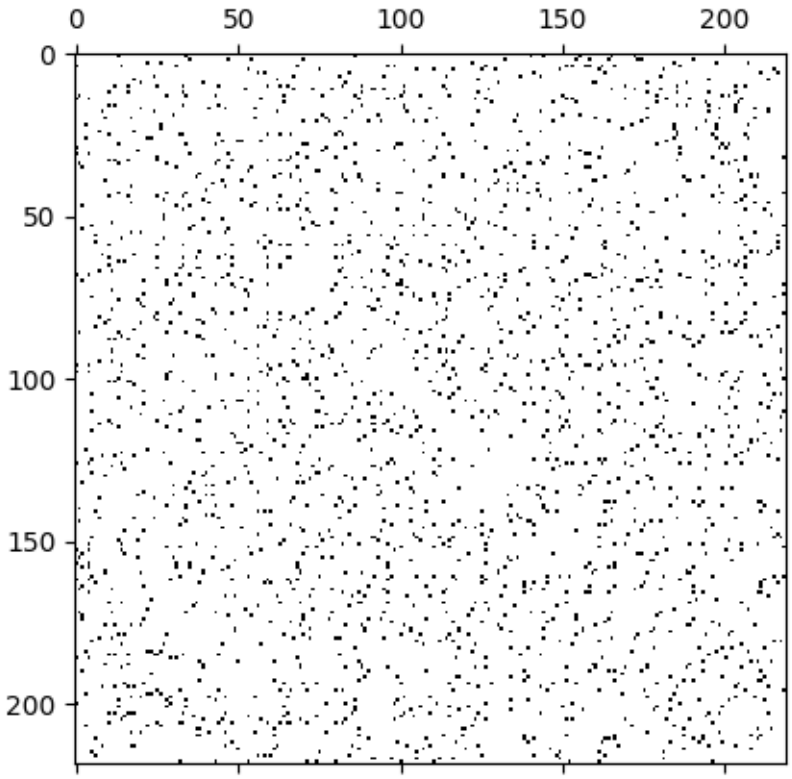
[23]:
```
for ind in Index:
    PermMat[Index[ind], PermIndex[ind]] = 1
```

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)
```

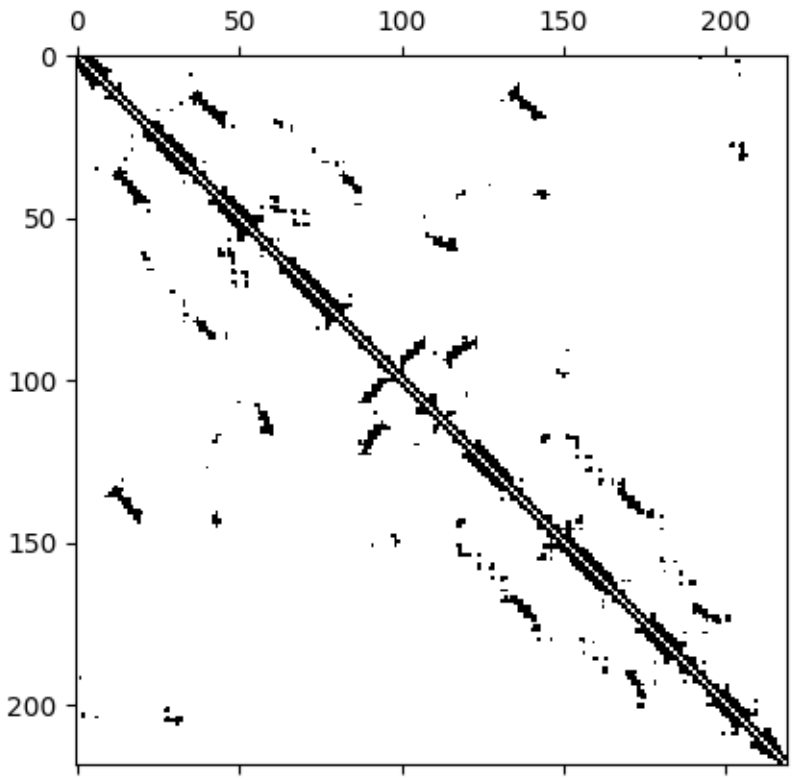
[25]:
```
<matplotlib.image.AxesImage at 0x7fc8e8d9c190>
```



We can invert the permutation effect

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

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

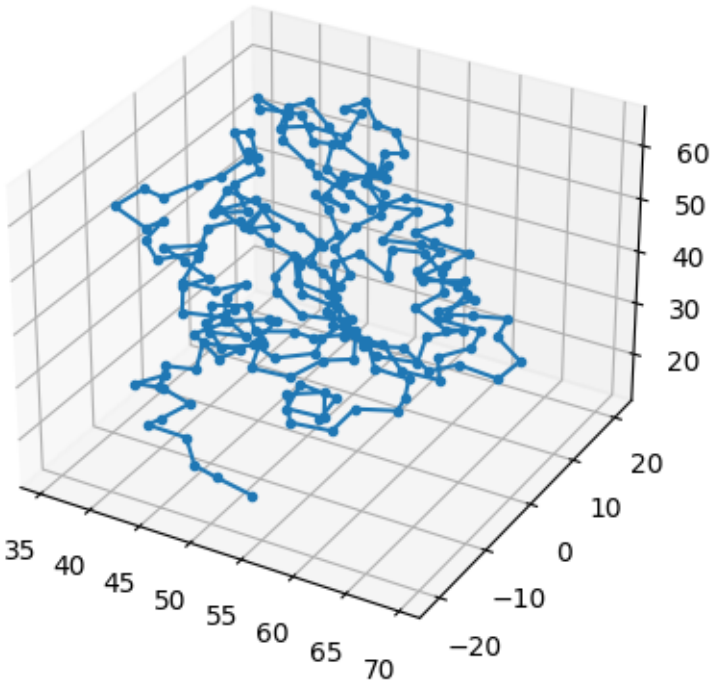


Let's try to visualize the 3d structure of the protein

[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>]


60
50
40
30
20
20
10
0
−10
−20
35
40
45
50
55
60
65
70

ER_networks

April 11, 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 $\frac{1}{Nnode^2}$

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.

[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

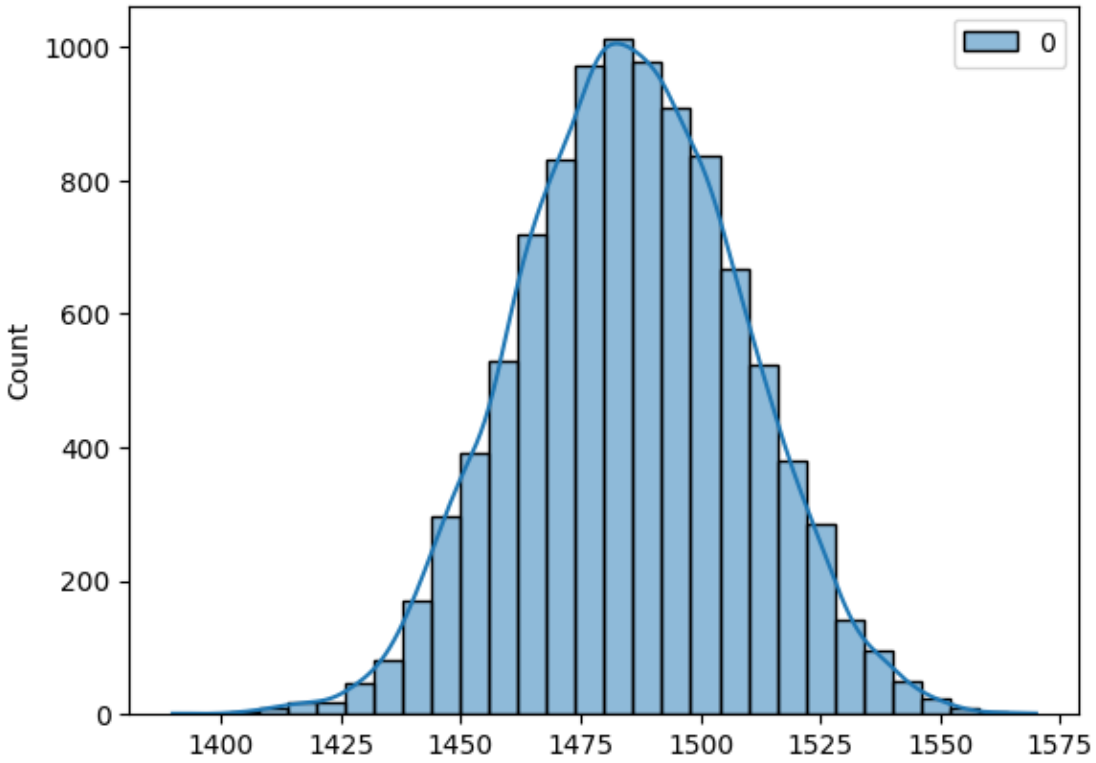
[65]:
```
print('Average number of links: {:.2f}'.format(np.mean(LinkS)))
print('Standard deviation: {:.2f}'.format(np.std(LinkS)))

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 = []
```

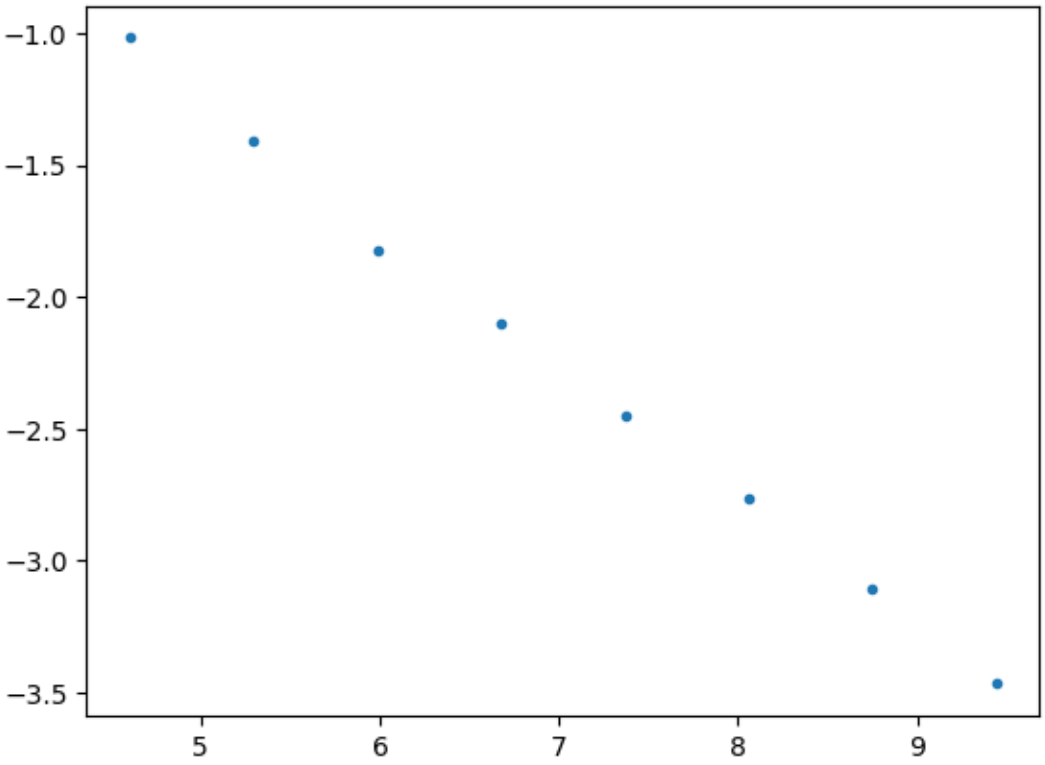
[67]:
```
for index in np.arange(2, Pow, step=0.3):
    Nnodes.append(int(10**index))
    NetC = sp.sparse.triu(sp.sparse.rand(Nnodes[Cnt], Nnodes[Cnt], density=Pl,␣
 ↪format='csr'), k=1)
    NetC = NetC + NetC.T
    K = sum(NetC).todense()
    M.append(np.mean(K))
    S.append(np.std(K))
    CV.append(np.std(K)/np.mean(K))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

```
    # 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 $\lambda = xP * Nnode$

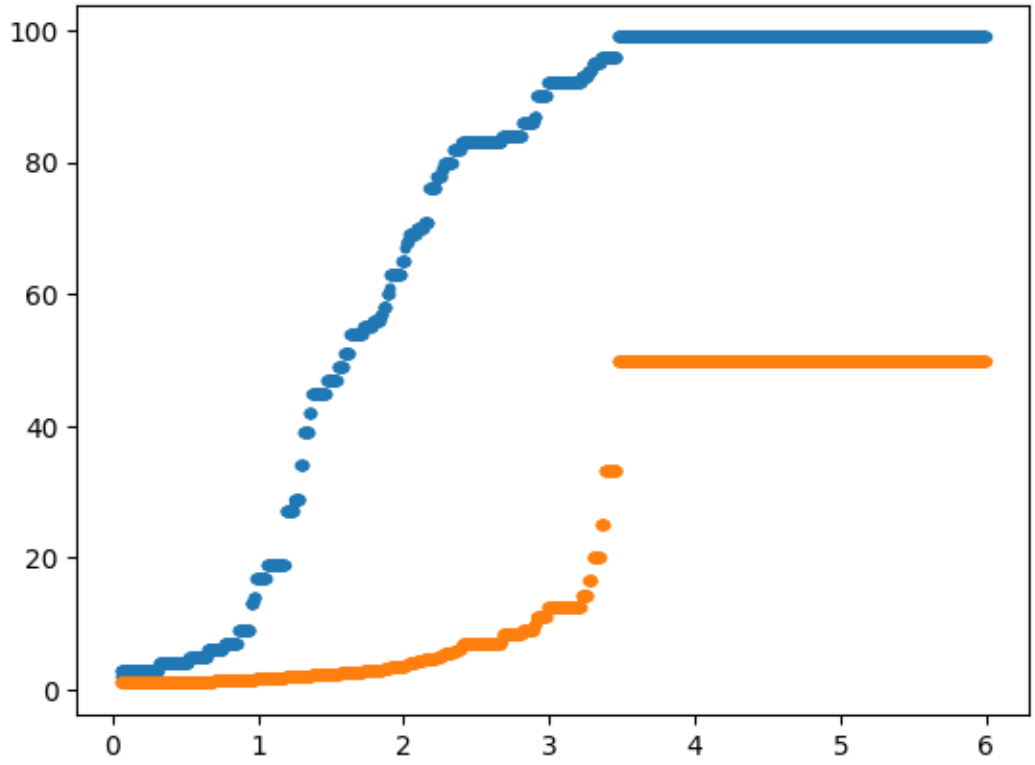
[71]:
```
Rc = np.zeros(len(xP))
Rm = np.zeros(len(xP))
Cnt = 0

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>]



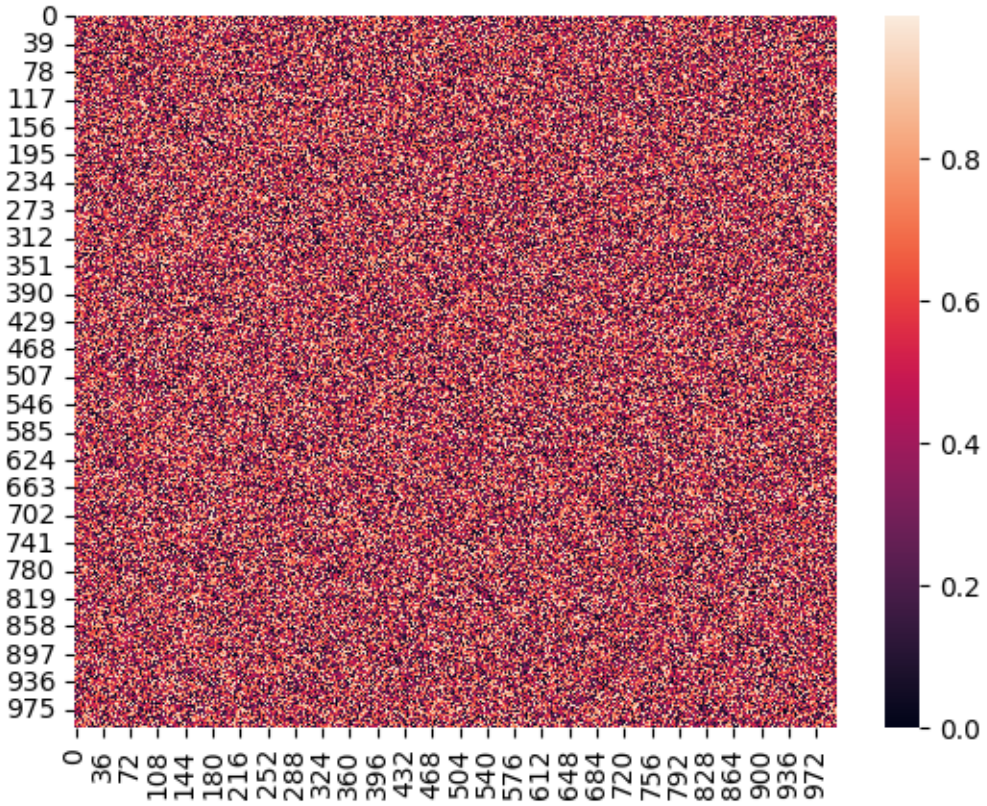
1.4 Semicircle law for ER network spectrum vs RMT (Random Matrix Theory)

[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)
```

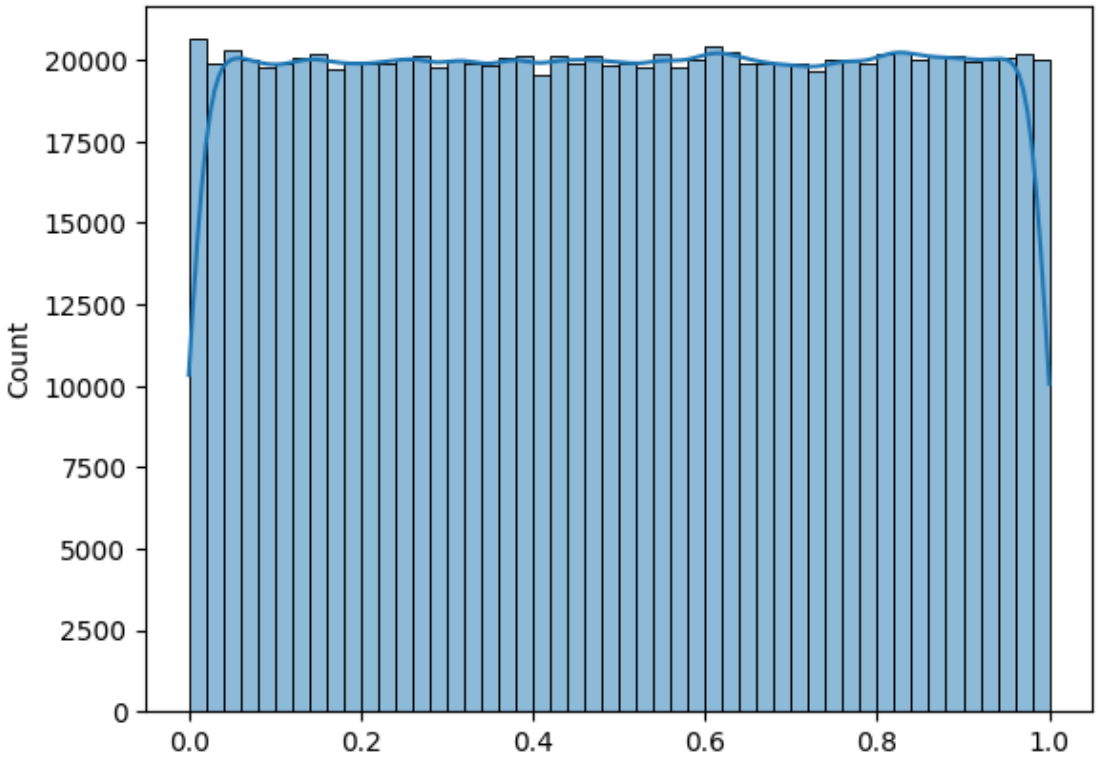
[73]: <Axes: >



Let's see also the histogram of coefficients

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

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

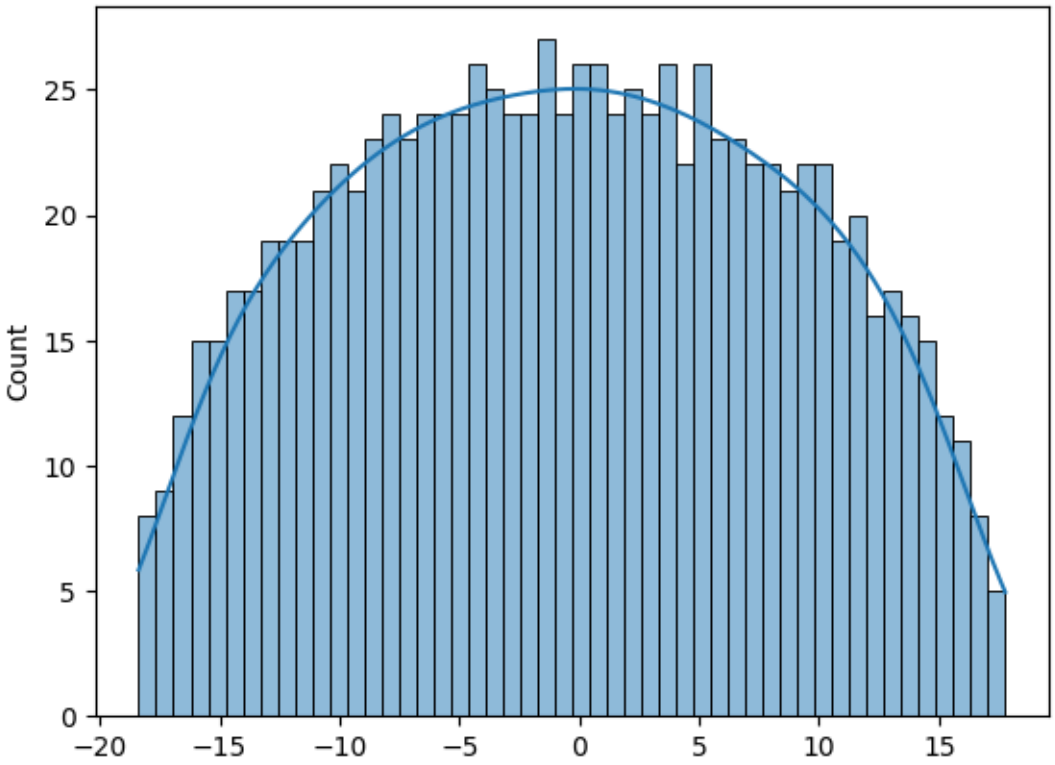


Now the eigenvalues and eigenvectors.

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'>
```

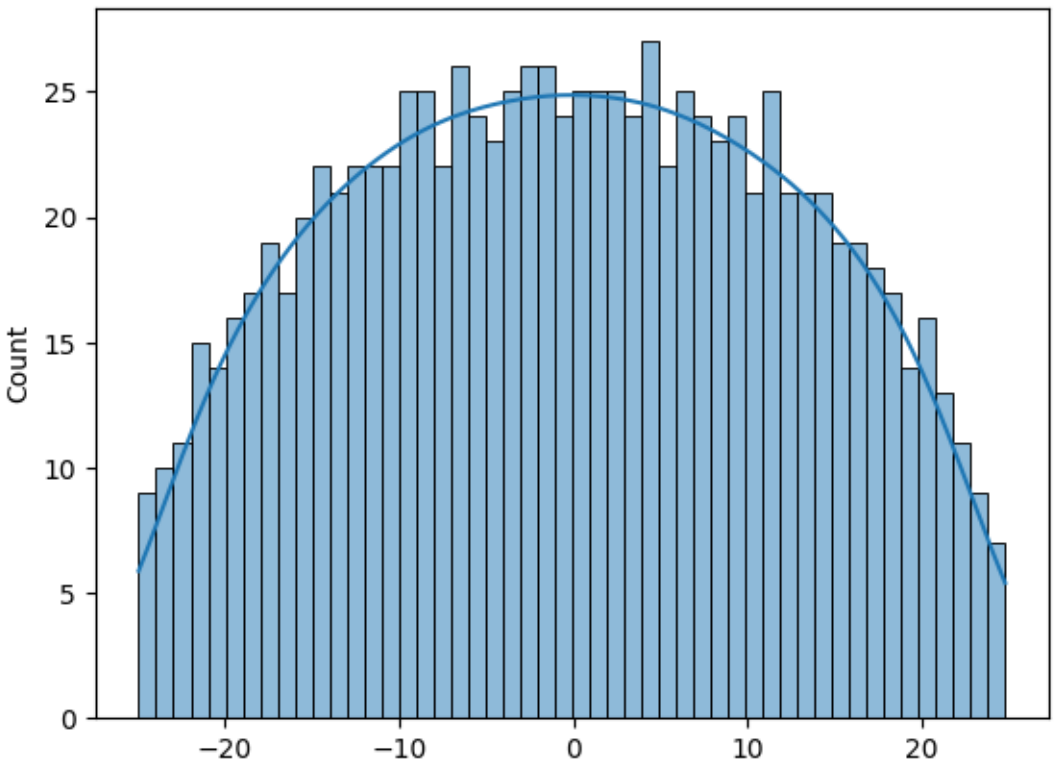


[76]:
```
rr = np.triu(np.random.rand(Nnode, Nnode), k=1) > 1 - Plink
rr = rr + rr.T
```

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

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

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

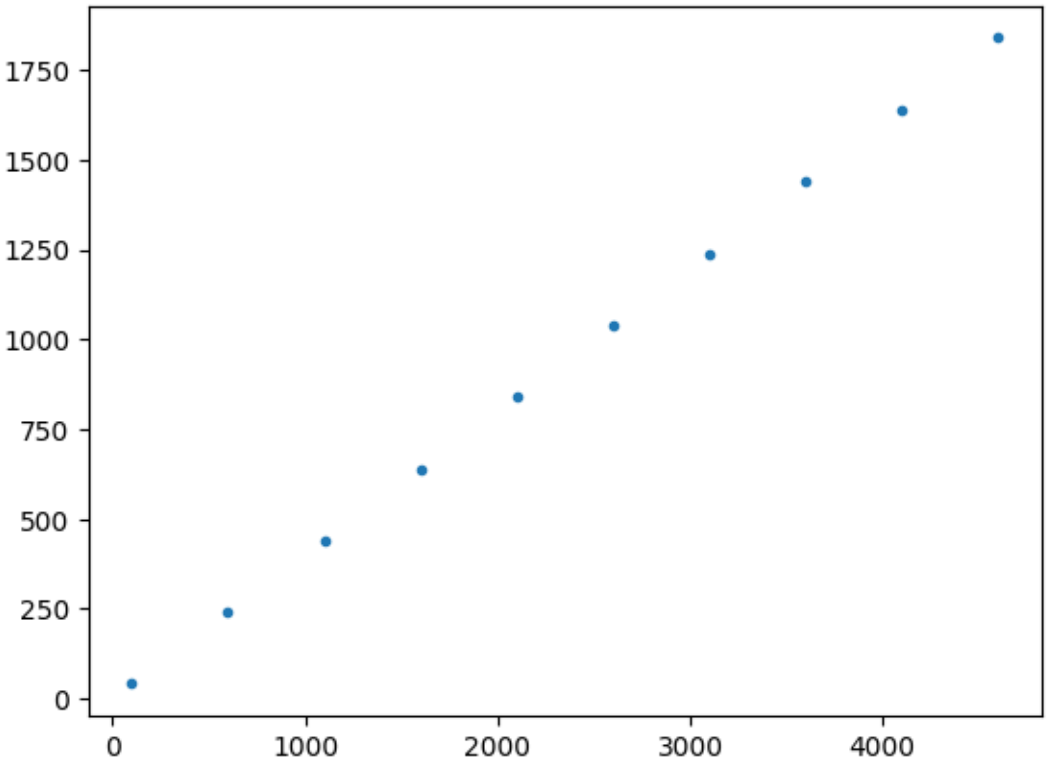


[83]:
```
Cnt = 0
xx = np.arange(100, 5000, step=500)
vmax = []

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, '.')
```

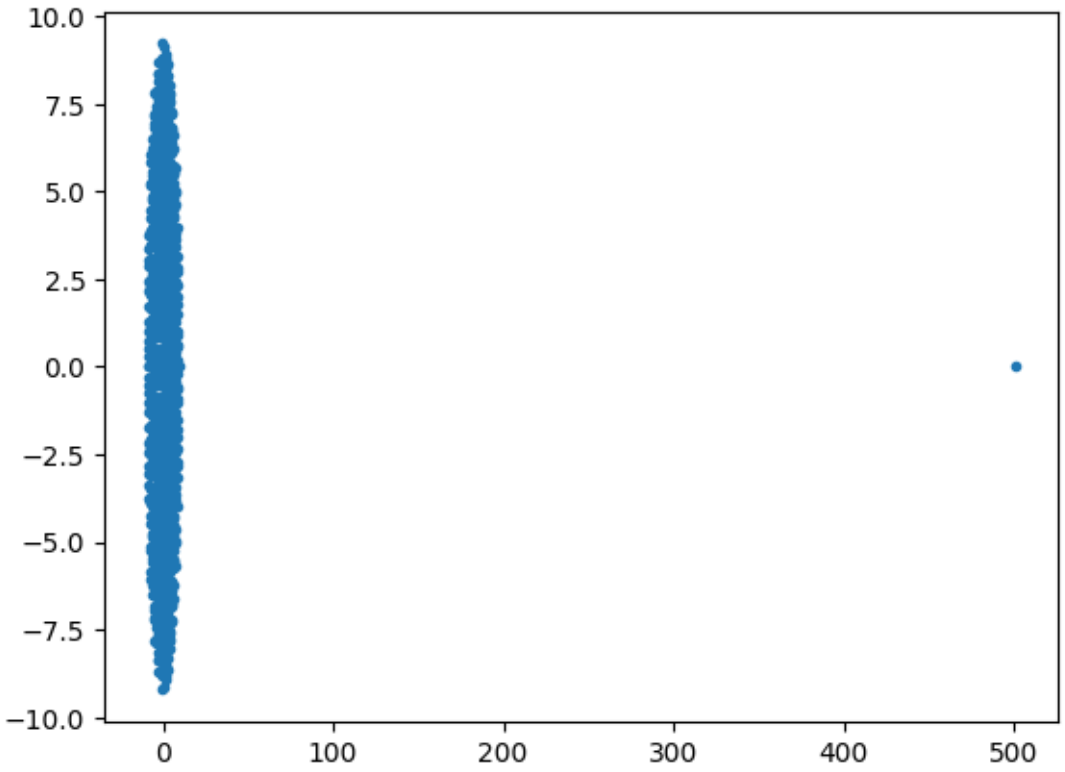
[83]: [<matplotlib.lines.Line2D at 0x7fafb8358f10>]



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

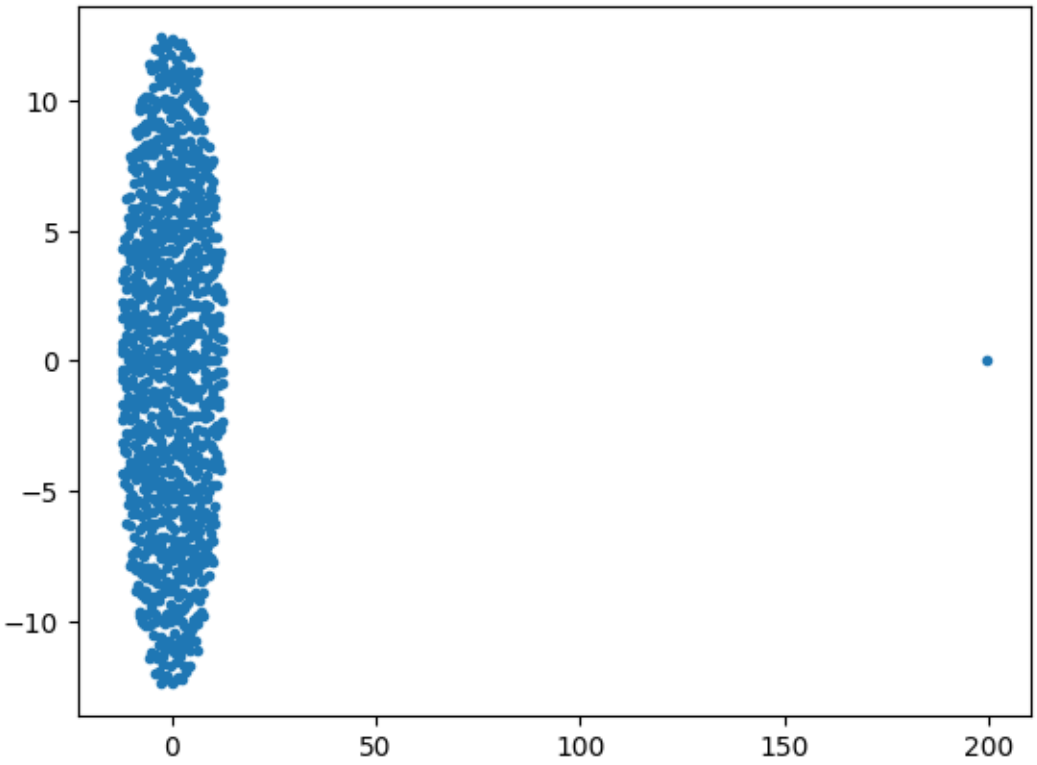
[80]:
```
rr = np.random.rand(Nnode, Nnode)
vv = np.linalg.eigvals(rr)
vvr = np.real(vv)
vvi = np.imag(vv)
plt.plot(vvr, vvi, '.')
```

[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>]


10
5
0
−5
−10
0
50
100
150
200