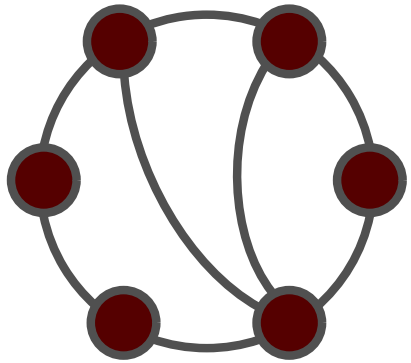
# Graph-tool package



graph-tool

Kristóf Furuglyás

Clustering with networks, 2020

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# Details

- Created by Tiago P. Peixoto
- Python-wrapped C++ core
- Boost Graph Library, Open MP
- Inferring internal structure
- Web of trust (N=39,796 vertices and E=301,498 edges)

| **Algorithm** | **graph-tool (16 threads)** | **graph-tool (1 thread)** | **igraph** | **NetworkX** |
|---|---|---|---|---|
| Single-source shortest path | 0.0023 s | 0.0022 s | 0.0092 s | 0.25 s |
| Global clustering | 0.011 s | 0.025 s | 0.027 s | 7.94 s |
| PageRank | 0.0052 s | 0.022 s | 0.072 s | 1.54 s |
| K-core | 0.0033 s | 0.0036 s | 0.0098 s | 0.72 s |
| Minimum spanning tree | 0.0073 s | 0.0072 s | 0.026 s | 0.64 s |
| Betweenness | 102 s (~1.7 mins) | 331 s (~5.5 mins) | 198 s (vertex) + 439 s (edge) (~ 10.6 mins) | 10297 s (vertex) 13913 s (edge) (~6.7 hours) |

# Drawbacks

- Increased time and memory required during compilation
- More resources needed
- igraph has bindings to R and C
- Non-trivial installation

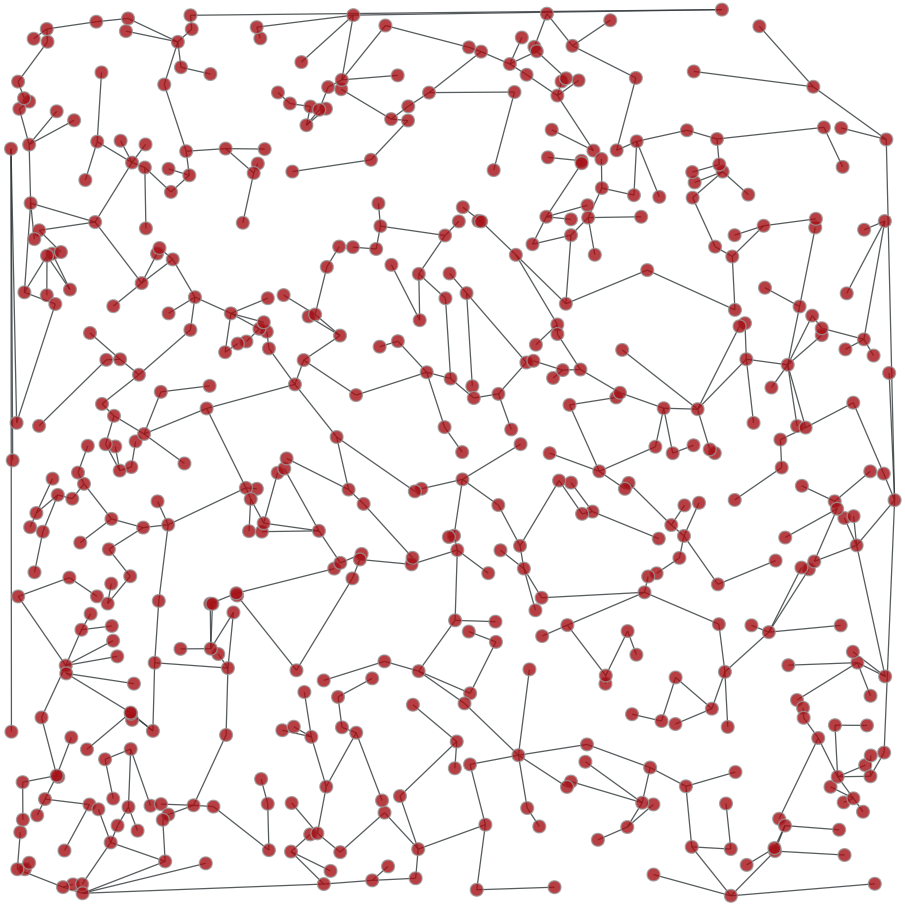
```
pip install networkx
jupyter notebook
```

Compared to

```
docker pull tiagopeixoto/graph-tool

docker run -p 8888:8888 -p 6006:6006 -it -u user -w /home/user -v /home/kfurug
lyas:/home/user tiagopeixoto/graph-tool bash

[user@c20b92b8c4bf ~]$ jupyter notebook --ip 0.0.0.0
```

# Other features

- Vertex, edge and graph properties
- Efficient "on the fly" filtering
- Powerful graph I/O
- Cairo and GTK+ based visualization



# Basic usage

In [1]:
```
from graph_tool.all import *
```

In [2]:
```
import numpy as np
import matplotlib.pyplot as plt
```

In [3]:
```
num_of_nodes, num_of_edges = 9, 18

def create_edges(num_of_nodes, num_of_edges, self_loops = False, multiedges = T
rue, weighted = True):
    edges_labels = {}
    while len(edges_labels.keys()) < num_of_edges:
        e_pair = tuple(np.random.choice(num_of_nodes, 2,self_loops))
        if multiedges or (e_pair not in list(edges_labels.keys()) and e_pair
[::-1] not in list(edges_labels.keys())):
            e_weight = np.random.rand() if weighted else 1
            edges_labels[e_pair] = e_weight
    return edges_labels
```

In [4]:
```
np.random.seed(0)
edges_labels = create_edges(num_of_nodes, num_of_edges)
```

In [5]:
```
g = Graph()

g.add_vertex(num_of_nodes);

for i,j in edges_labels.keys():
    g.add_edge(i,j)
```

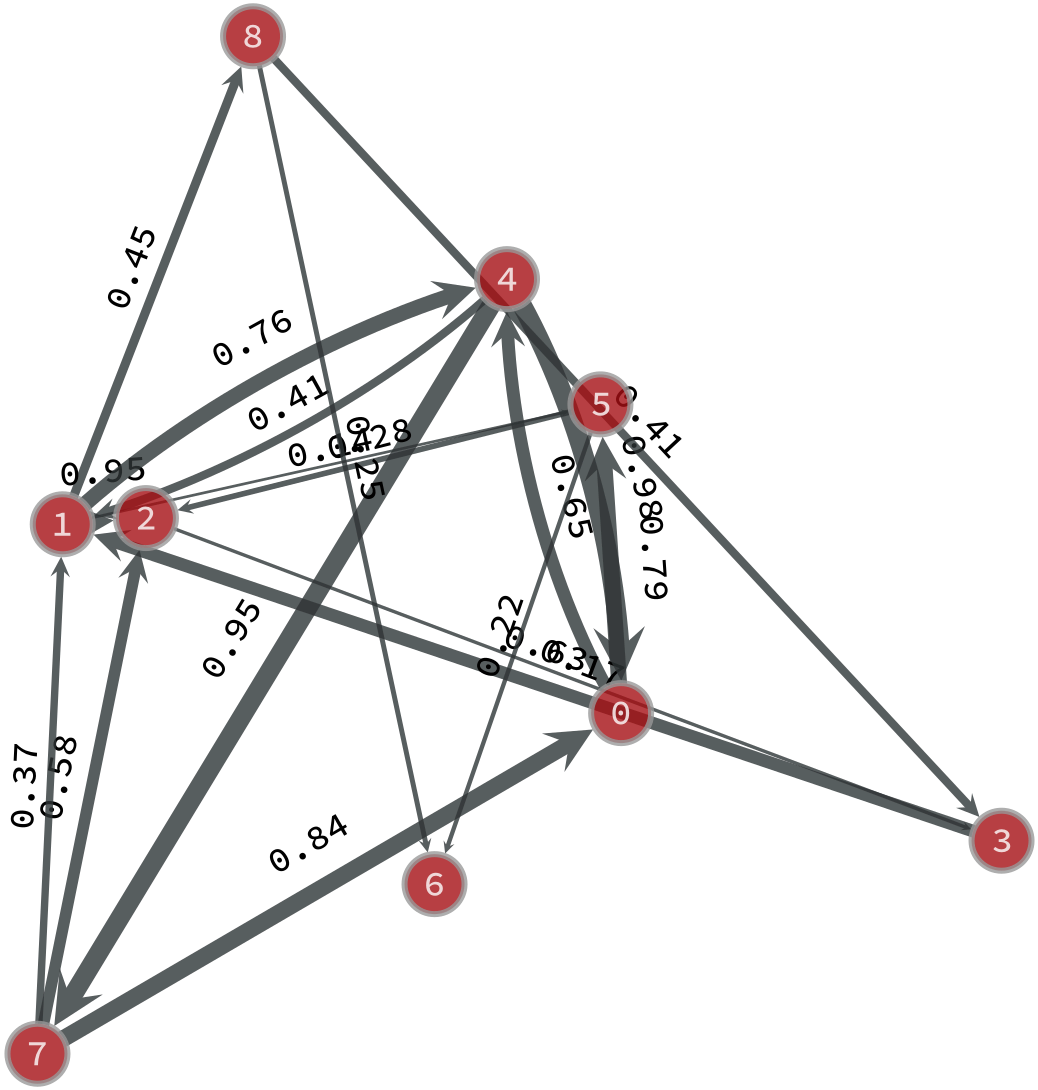
# Vertex, edge and graph properties

In [6]:
```
eprop_wei = g.new_edge_property("double")
eprop_str = g.new_edge_property("string")

for c,key in enumerate(edges_labels.keys()):
    e = list(g.edges())[c]
    eprop_wei[e] = edges_labels[key]*10
    eprop_str[e] = f"{edges_labels[key]:.2f}"
```

In [7]:
```
vprop_id = g.new_vertex_property("string")
for i in g.vertices():
    vprop_id[i] = str(i)
```

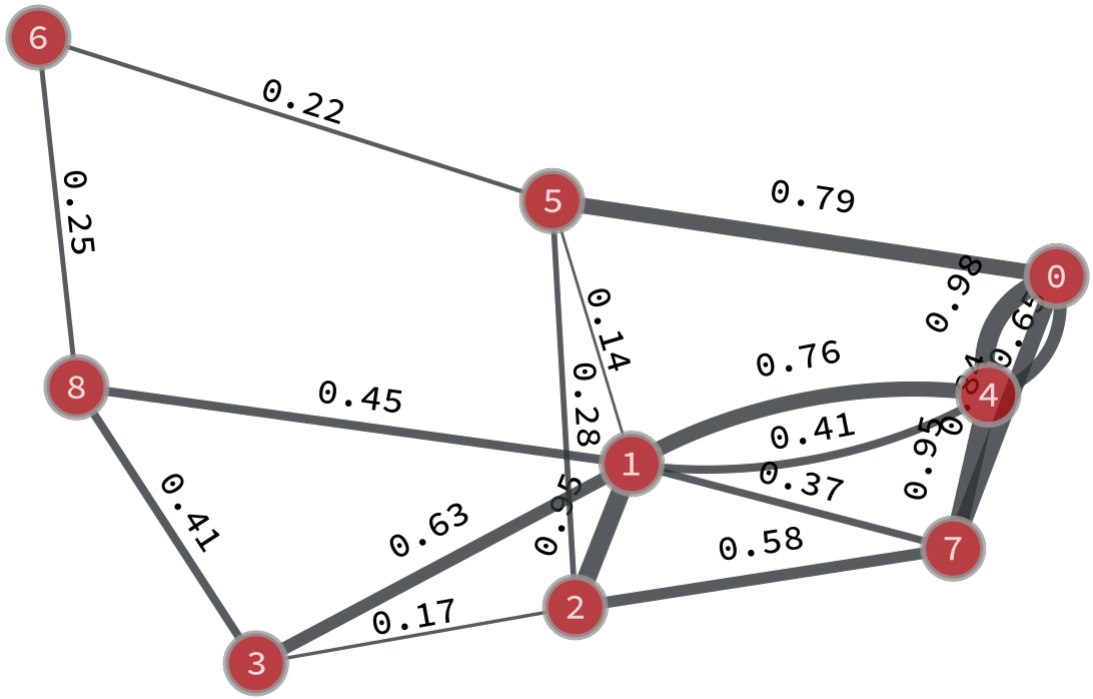
In [9]:

```
pos = random_layout(g)

graph_draw(g, pos,  vertex_text = vprop_id,
           vertex_size=30, edge_pen_width=eprop_wei,
           edge_text = eprop_str);
```



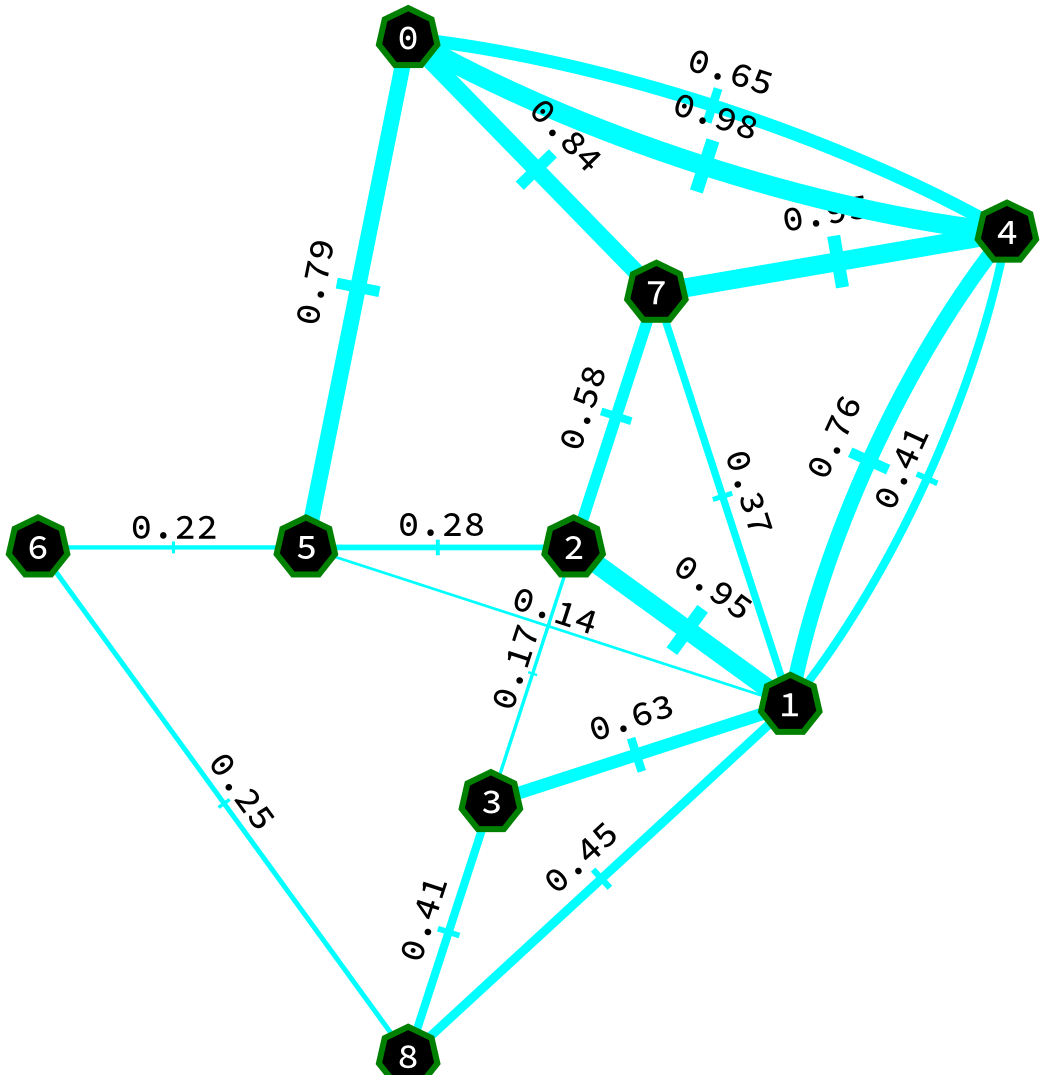
In [10]:

```
g.set_directed(False)
pos = arf_layout(g)
graph_draw(g, pos,  vertex_text = vprop_id,
                    vertex_size=30, edge_pen_width=eprop_wei, edge_text = eprop_
str, );
```



In [11]:

```
pos = radial_tree_layout(g, 2)

graph_draw(g, pos,  vertex_text = vprop_id,
                    vertex_size=30, edge_pen_width=eprop_wei, edge_text = eprop_
str,
              vertex_color = 'green', vertex_shape = "heptagon",vertex_fill_color
= 'k',
             edge_color = "cyan", edge_font_family= "cursive", edge_mid_marker = "
bar");
```



# Nonparametric statistical inference [1]

- Goal: divide nodes into $B$ communities
- Partition $\mathbf{b} = \{b_i\}$ where $b_i \in [0, B-1]$
- Define probability that network $\mathbf{A}$ generated with $\theta$ parameters:

$$P\left(\mathbf{A} \mid \theta, \mathbf{b}\right)$$

- Bayesian posterior probability

$$P\left(\mathbf{b} \mid \mathbf{A}\right) = \frac{\sum_{\theta} P\left(\mathbf{A} \mid \theta, \mathbf{b}\right) P\left(\theta, \mathbf{b}\right)}{P\left(\mathbf{A}\right)}$$

- Evidence

$$P\left(\mathbf{A}\right) = \sum_{\theta, \mathbf{b}} P\left(\mathbf{A} \mid \theta, \mathbf{b}\right) P\left(\theta, \mathbf{b}\right)$$

# Nonparametric statistical inference

- "Hard constraints" = 1 possible set of parameters

$$P(\mathbf{b} \mid \mathbf{A}) = \frac{P(\mathbf{A} \mid \theta, \mathbf{b})\, P(\theta, \mathbf{b})}{P(\mathbf{A})}$$

- Either maximize posterior probability or
- Sampling different partitions acc. to post. probability

# Minimum description length (MDL)

$$P(\mathbf{b} \mid \mathbf{A}) = \frac{\exp(-\Sigma)}{P(\mathbf{A})},$$

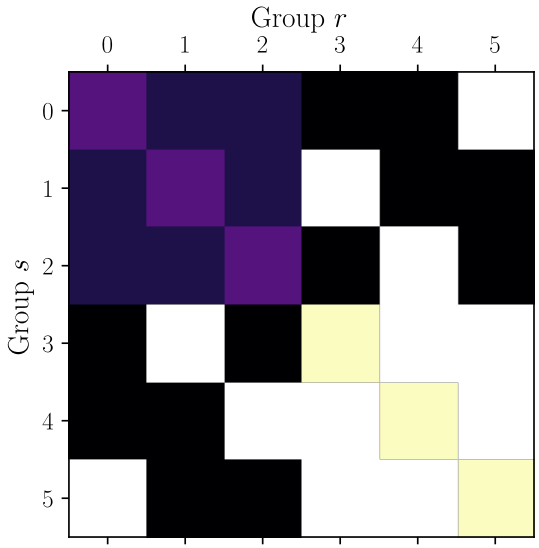
where **description length (entropy)** is

$$\Sigma = -\ln P(\mathbf{A} \mid \theta, \mathbf{b}) - \ln P(\theta, \mathbf{b}).$$

Measures the amount of information required to describe the data

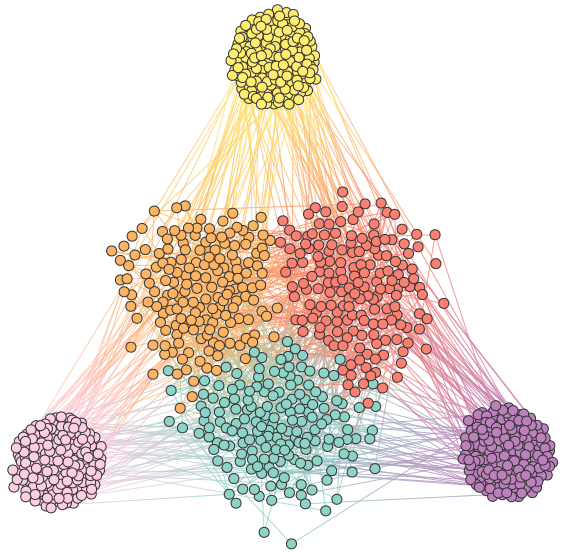
# Stochastic block model

- Generates based on microcanonical ensemble [2, 3]
- Parameters: matrix $\mathbf{e}$, $e_{ij}$ : edge count
- Only the $\mathbf{e}$ is constrained
- Degree-corrected model can be applied [4]
- Drawback: $B_{max} = \mathcal{O}\left(\sqrt{N}\right)$




(../../_images/sbm-example-ers.svg)

Matrix of edge counts $e$ between groups.

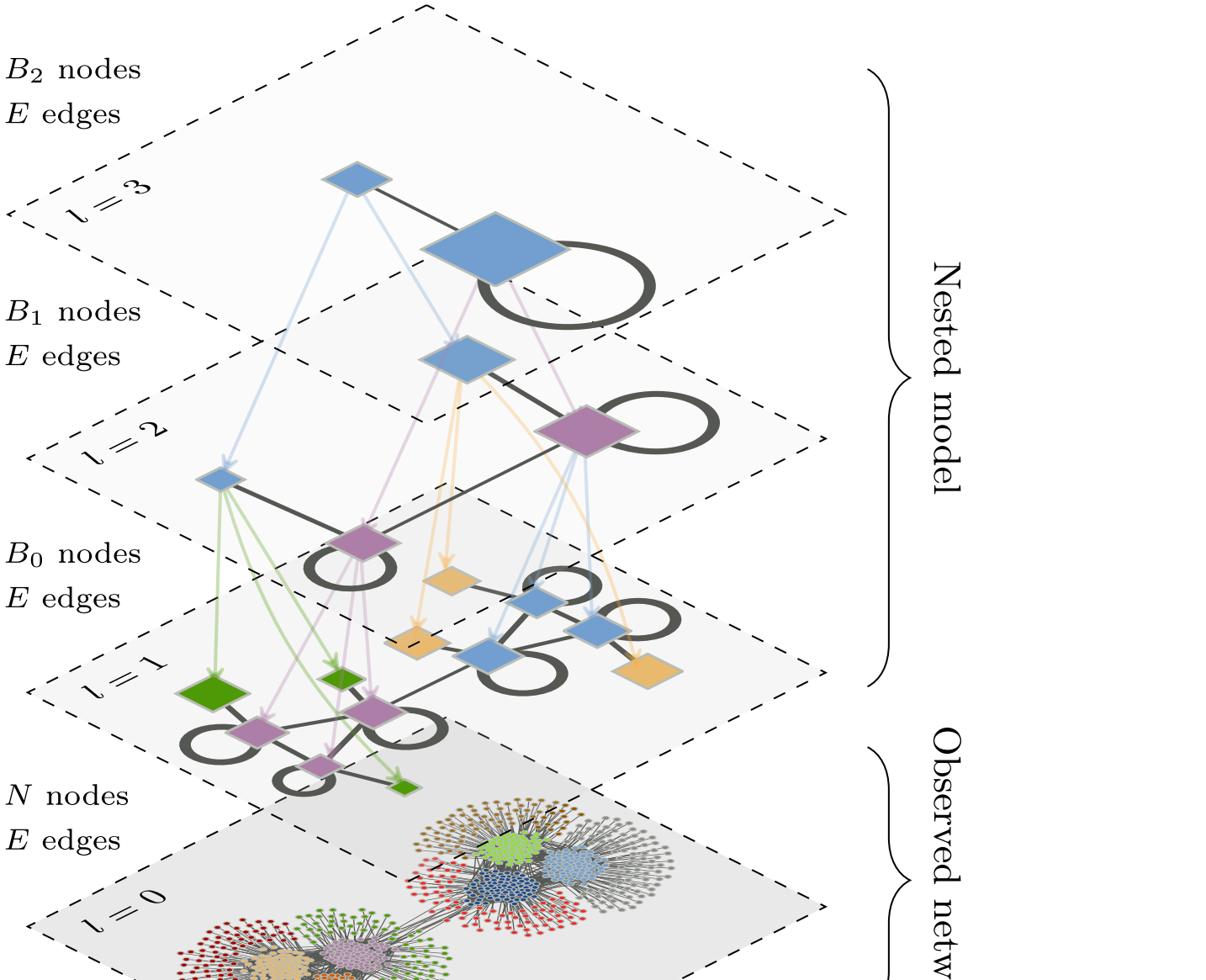


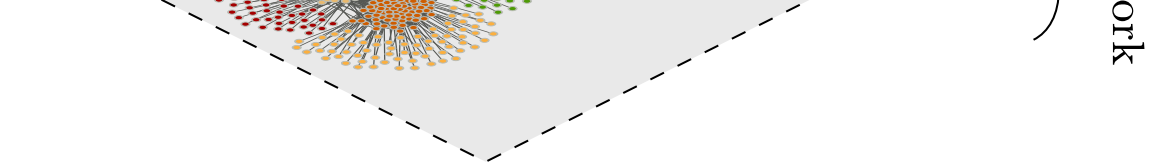
(../../_images/sbm-example.svg)

Generated network.

# Nested Stochastic Block Model

- Multilayer-description [5]
- Groups clustered into groups
- Recursive SBM [6]
- Benefit: $B_{max}^{nSBM} = \mathcal{O}\left(N/\log N\right)$ compared to $B_{max}^{SBM} = \mathcal{O}\left(\sqrt{N}\right)$






Example of a nested SBM with three levels.

# Inferring best partition

Goal is to **minimize description length** [7]

a.k.a **entropy**

$$P\left(\mathbf{b} \mid \mathbf{A}\right) = \frac{\exp(-\Sigma)}{P\left(\mathbf{A}\right)}, \text{ where } \Sigma = -\ln P\left(\mathbf{A} \mid \theta, \mathbf{b}\right) - \ln P\left(\theta, \mathbf{b}\right).$$

where $\boldsymbol{\theta} = \boldsymbol{e}$ for the traditional SBM and $\boldsymbol{\theta} = \{\boldsymbol{e}, \boldsymbol{k}\}$ for the degree-corrected model. For the former one

$$P(\boldsymbol{A}|\boldsymbol{e}, \boldsymbol{b}) = \frac{\prod_{r<s} e_{rs}! \prod_r e_{rr}!!}{\prod_r n_r^{e_r}} \times \frac{1}{\prod_{i<j} A_{ij}! \prod_i A_{ii}!!},$$

$$P(\boldsymbol{A}|\boldsymbol{e}, \boldsymbol{b}) = \frac{\prod_{rs} e_{rs}!}{\prod_r n_r^{e_r}} \times \frac{1}{\prod_{ij} A_{ij}!},$$

For the latter one:

$$P(\boldsymbol{A}|\boldsymbol{e},\boldsymbol{b},\boldsymbol{k}) = \frac{\prod_{r<s} e_{rs}!\prod_r e_{rr}!!}{\prod_r e_r!} \times \frac{\prod_i k_i!}{\prod_{i<j} A_{ij}!\prod_i A_{ii}!!},$$

$$P(\boldsymbol{A}|\boldsymbol{e},\boldsymbol{b},\boldsymbol{k}) = \frac{\prod_{rs} e_{rs}!}{\prod_r e_r^+!\prod_r e_r^-!} \times \frac{\prod_i k_i^+!\prod_i k_i^-!}{\prod_{ij} A_{ij}!},$$

Using Markov chain Monte Carlo (MCMC)

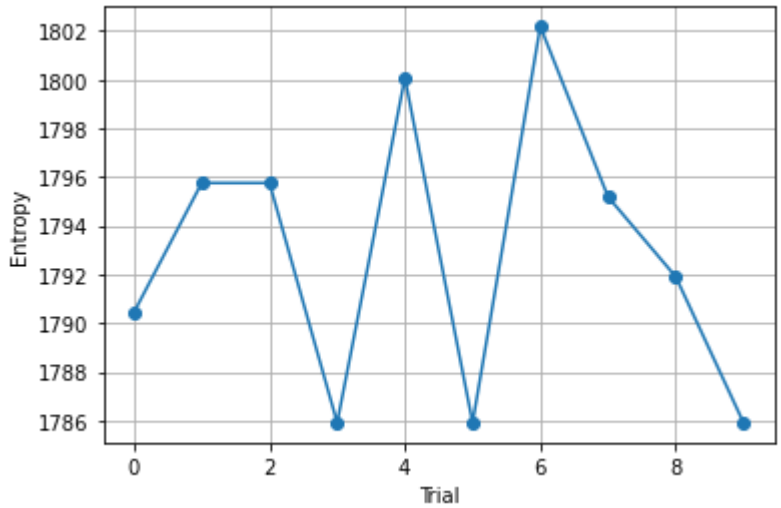
```
minimize_blockmodel_dl()
minimize_nested_blockmodel_dl()
```

In [12]:
```
g = collection.data["football"]
print(g)

for k in g.graph_properties.keys():
    print(k+":",  g.gp[k])
```

```
<Graph object, undirected, with 115 vertices and 613 edges, 4 internal vertex
properties, 2 internal graph properties, at 0x7f7137009d90>
readme: The file football.gml contains the network of American football games
between Division IA colleges during regular season Fall 2000, as compiled
by M. Girvan and M. Newman.  The nodes have values that indicate to which
conferences they belong.  The values are as follows:

  0 = Atlantic Coast
  1 = Big East
  2 = Big Ten
  3 = Big Twelve
  4 = Conference USA
  5 = Independents
  6 = Mid-American
  7 = Mountain West
  8 = Pacific Ten
  9 = Southeastern
 10 = Sun Belt
 11 = Western Athletic

If you make use of these data, please cite M. Girvan and M. E. J. Newman,
Community structure in social and biological networks,
Proc. Natl. Acad. Sci. USA 99, 7821-7826 (2002).

Correction: Two edges were erroneously duplicated in this data set, and
have been removed (21 SEP 2014)

description: American College football: network of American football games bet
ween Division IA colleges during regular season Fall 2000. Please cite M. Girv
an and M. E. J. Newman, Proc. Natl. Acad. Sci. USA 99, 7821-7826 (2002). Retri
eved from `Mark Newman's website <http://www-personal.umich.edu/~mejn/netdata/
>`_. This file also contains corrections made by T. S. Evans, available `here
```

<http://figshare.com/articles/American_College_Football_Network_Files/93179>`
_. Thus, please also cite T.S. Evans, "Clique Graphs and Overlapping Communiti
es" J.Stat.Mech. (2010) P12037 [arXiv:1009.0638]

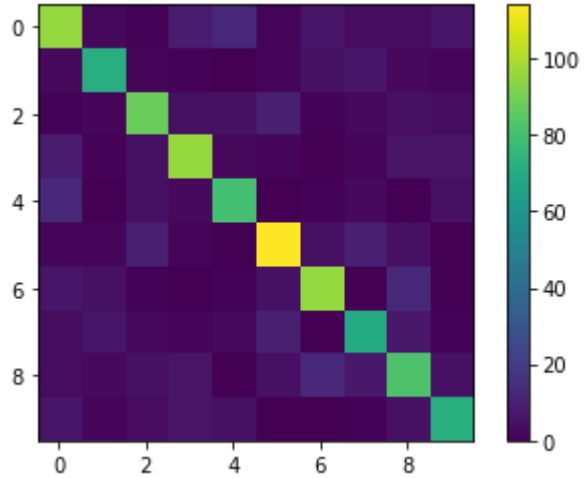
In [13]:
```
states = [minimize_blockmodel_dl(g) for _ in range(10)]
entropies = [state.entropy() for state in states]
# minimize_blockmodel_dl(g)  returns BlockState object
plt.plot(range(10), entropies, '-o')
plt.xlabel("Trial"), plt.ylabel("Entropy"), plt.grid()
state = states[np.argmin(entropies)]
```



In [14]:
```
b = state.get_blocks()
r = b[10]   # group membership of vertex 10
print(r)
```

```
3
```

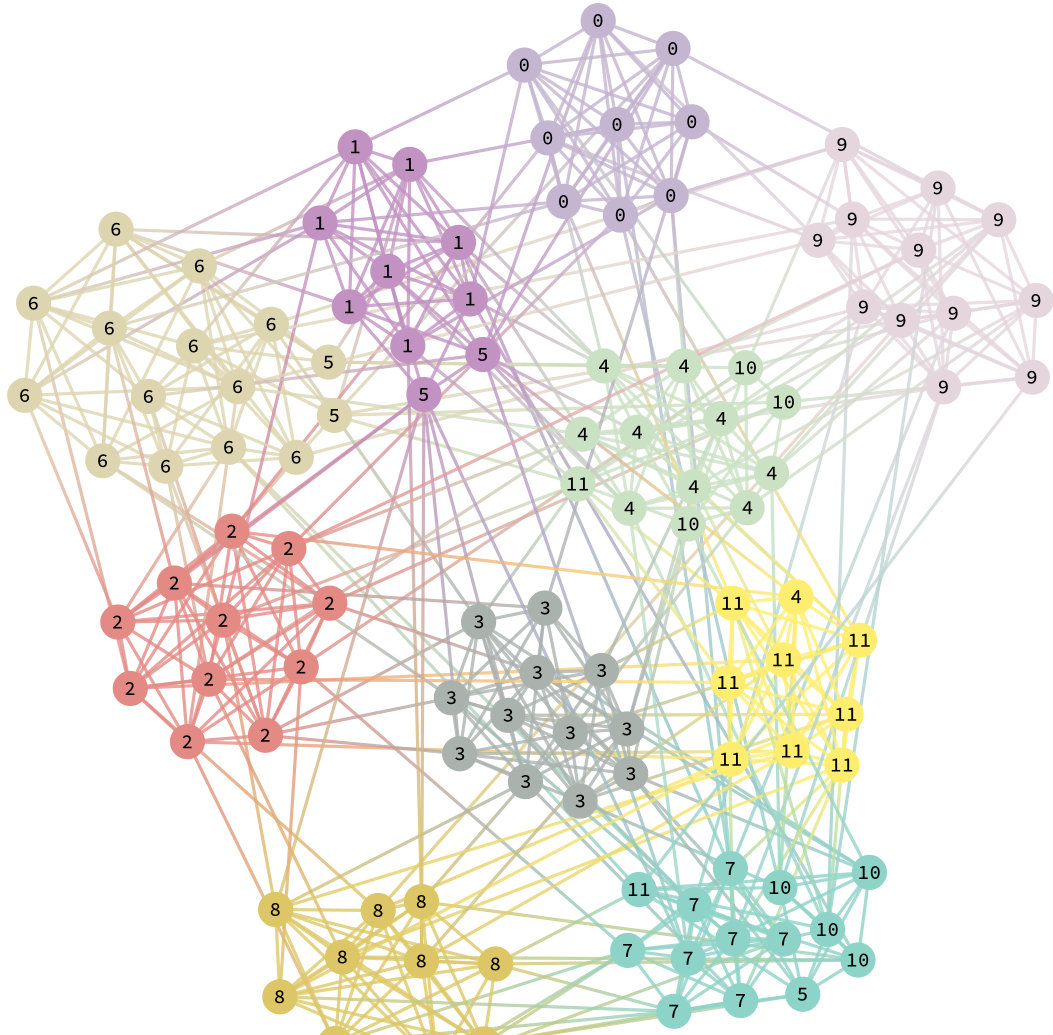
In [15]:
```
e = state.get_matrix()
im = plt.imshow(e.todense())
plt.colorbar(im);
```



In [16]:

```
print(f"Modularity of found partition: {modularity(g, b):.4f}")
print(f"GN modularity of found partition (from prev lesson): {0.599629027407790
1:.4f}")
print(f"GN modularity of original partition: {modularity(g, g.vp.value_tsevan
s):.4f}" )
state.draw(pos=g.vp.pos,vertex_text= g.vp['value']);
```

```
Modularity of found partition: 0.6044
GN modularity of found partition (from prev lesson): 0.5996
GN modularity of original partition: 0.5744
```



# Nested model

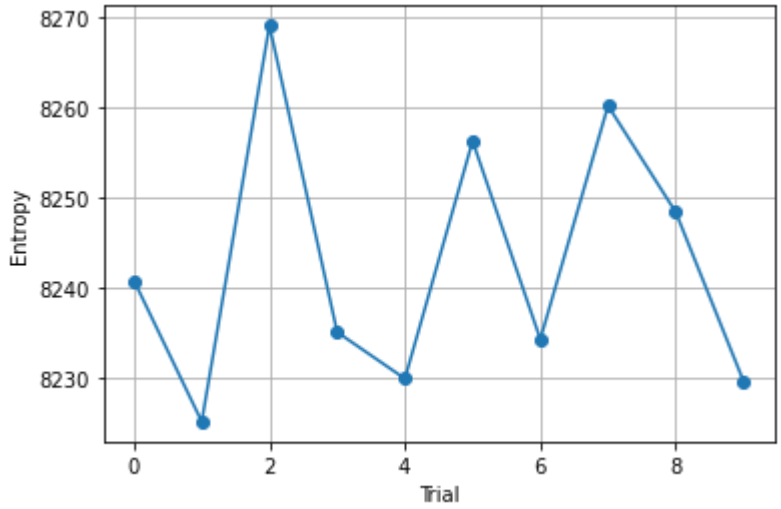
In [39]:
```
g = collection.data["celegansneural"]
print(g)

for k in g.graph_properties.keys():
    print(k+":",  g.gp[k])
```

```
<Graph object, directed, with 297 vertices and 2359 edges, 2 internal vertex p
roperties, 1 internal edge property, 2 internal graph properties, at 0x7f7135d
b30d0>
```

In [44]:

```
states = [minimize_nested_blockmodel_dl(g) for _ in range(10)]
entropies = [state.entropy() for state in states]
# minimize_blockmodel_dl(g)  returns BlockState object
plt.plot(range(10), entropies, '-o')
plt.xlabel("Trial"), plt.ylabel("Entropy"), plt.grid()
state = states[np.argmin(entropies)]
cel_ent = state.entropy().copy()
```

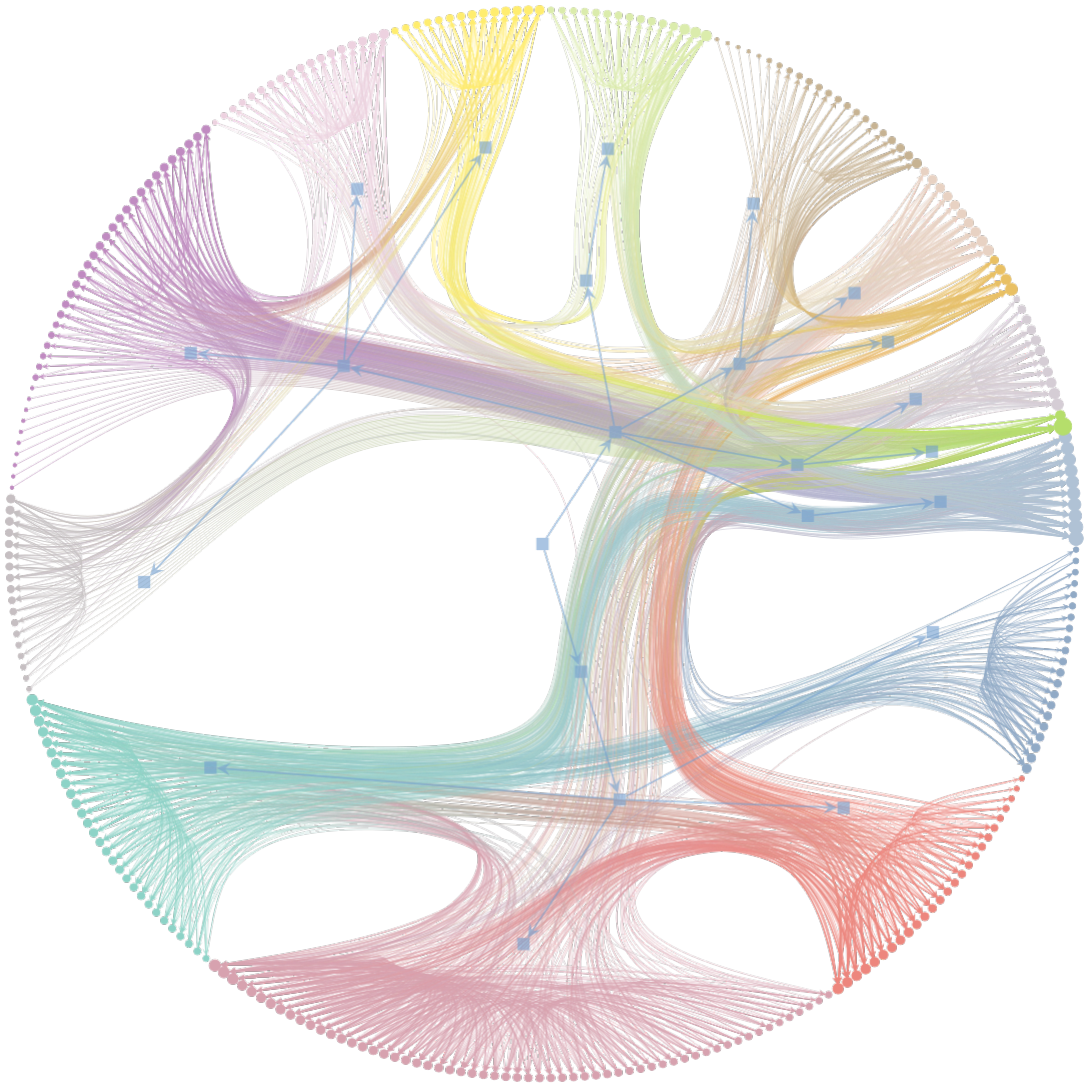
```
---------------------------------------------------------------------------
AttributeError                            Traceback (most recent call last)
<ipython-input-44-13e4f2eadfee> in <module>
      5 plt.xlabel("Trial"), plt.ylabel("Entropy"), plt.grid()
      6 state = states[np.argmin(entropies)]
----> 7 cel_ent = state.entropy().copy()

AttributeError: 'float' object has no attribute 'copy'
```



In [19]:

```
state.print_summary()
state.draw();
```

```
l: 0, N: 297, B: 15
l: 1, N: 15, B: 6
l: 2, N: 6, B: 2
l: 3, N: 2, B: 1
```



# Trade-off between memory usage and computation time [8]

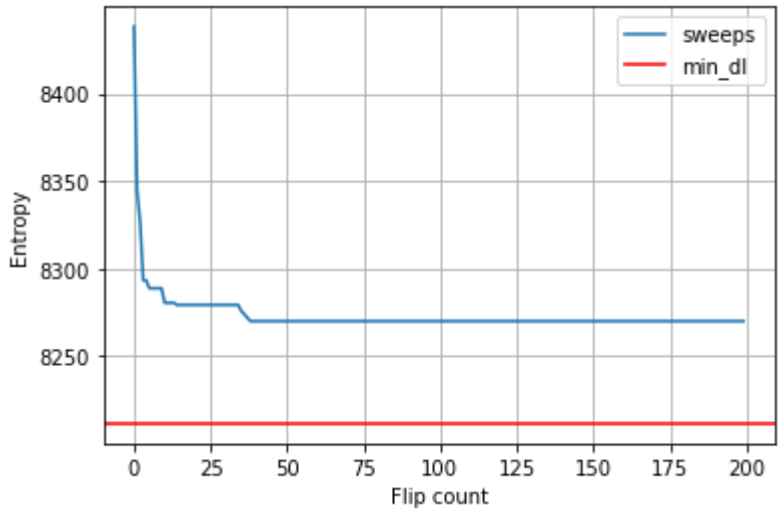
In [59]:
```
g = collection.data["celegansneural"]

state = NestedBlockState(g)
state.print_summary()
state.entropy()
```

```
l: 0, N: 297, B: 1
l: 1, N: 1, B: 1
l: 2, N: 1, B: 1
l: 3, N: 1, B: 1
l: 4, N: 1, B: 1
l: 5, N: 1, B: 1
l: 6, N: 1, B: 1
l: 7, N: 1, B: 1
l: 8, N: 1, B: 1
l: 9, N: 1, B: 1
```

Out[59]:
```
9468.527791619807
```

```
entropies = []
for _ in range(200): # this should be sufficiently large
    state.multiflip_mcmc_sweep(beta=np.inf, niter=10)
    entropies.append(state.entropy())
state.print_summary()
plt.plot(range(200), entropies, label = "sweeps")
plt.axhline(cel_ent,color = "red", label = 'min_dl', )
plt.xlabel("Flip count"), plt.ylabel("Entropy"), plt.grid(), plt.legend();
```

```
l: 0, N: 297, B: 11
l: 1, N: 11, B: 4
l: 2, N: 4, B: 1
l: 3, N: 1, B: 1
l: 4, N: 1, B: 1
l: 5, N: 1, B: 1
l: 6, N: 1, B: 1
l: 7, N: 1, B: 1
l: 8, N: 1, B: 1
l: 9, N: 1, B: 1
```



## Simulated annealing

In [61]:
```
state = NestedBlockState(g)
mcmc_anneal(state, beta_range=(1, 10), niter=500, mcmc_equilibrate_args=dict(fo
rce_niter=10))
state.print_summary()
print(f"Entropy: {state.entropy()}, with MDL: {cel_ent}")
```

```
l: 0, N: 297, B: 21
l: 1, N: 21, B: 7
l: 2, N: 7, B: 2
l: 3, N: 2, B: 1
l: 4, N: 1, B: 1
l: 5, N: 1, B: 1
l: 6, N: 1, B: 1
l: 7, N: 1, B: 1
l: 8, N: 1, B: 1
l: 9, N: 1, B: 1
Entropy: 8150.537898604023, with MDL: 8211.603988675375
```

Combinations like `minimize_nested_blockmodel_dl` $\rightarrow$ `mcmc_anneal` could give better results.

## Model selection

In [23]:
```
g = collection.data["celegansneural"]

state_ndc = minimize_nested_blockmodel_dl(g, deg_corr=False)
state_dc  = minimize_nested_blockmodel_dl(g, deg_corr=True)

print("Non-degree-corrected DL:\t", state_ndc.entropy())
print("Degree-corrected DL:\t\t", state_dc.entropy())
```

```
Non-degree-corrected DL:         8529.502159049163
Degree-corrected DL:             8216.06947699617
```

In [24]:
```
g = collection.data["football"]

state_ndc = minimize_nested_blockmodel_dl(g, deg_corr=False)
state_dc  = minimize_nested_blockmodel_dl(g, deg_corr=True)

print("Non-degree-corrected DL:\t", state_ndc.entropy())
print("Degree-corrected DL:\t\t", state_dc.entropy())
```

```
Non-degree-corrected DL:         1733.5256851451725
Degree-corrected DL:             1780.5767169430787
```

# Sampling from the posterior distribution

- More than one fit with similar post. prob.
- Attempting to move nodes into different groups
- Suitable for large networks (linear on # edges, indep of groups)

In [26]:
```
g = collection.data["lesmis"]

state = BlockState(g, B=1)   # This automatically initializes the state with a
partition
                             # into one group. The user could also pass a hi
gher number
                             # to start with a random partition of a given s
ize, or pass a
                             # specific initial partition using the 'b' para
meter.

# Now we run 1,000 sweeps of the MCMC. Note that the number of groups
# is allowed to change, so it will eventually move from the initial
# value of B=1 to whatever is most appropriate for the data.
print(f"Initial dl: {state.entropy()}")
dS, nattempts, nmoves = state.multiflip_mcmc_sweep(niter=10000)

print("Change in description length:", dS)
print("Number of vertex moves attempts:", nattempts)
print("Number of accepted vertex moves:", nmoves)
print(f"Final dl: {state.entropy()}")
```

```
Initial dl: 787.4999819793873
Change in description length: -71.4314895705073
Number of vertex moves attempts: 3571289
Number of accepted vertex moves: 449625
Final dl: 716.0684924088499
```

In [27]:
```
# We will accept equilibration if 10 sweeps are completed without a
# record breaking event, 2 consecutive times.
state = BlockState(g, B=1)
mcmc_equilibrate(state, wait=1000, nbreaks=2, mcmc_args=dict(niter=10))
```

Out[27]:
```
(698.9506193551209, 9157858, 1117729)
```

In [28]:

```
# We will first equilibrate the Markov chain
mcmc_equilibrate(state, wait=1000, mcmc_args=dict(niter=10))

bs = [] # collect some partitions

def collect_partitions(s):
    global bs
    bs.append(s.b.a.copy())

# Now we collect partitions for exactly 100,000 sweeps, at intervals
# of 10 sweeps:
mcmc_equilibrate(state, force_niter=10000, mcmc_args=dict(niter=10),
                         callback=collect_partitions)

# Disambiguate partitions and obtain marginals
pmode = PartitionModeState(bs, converge=True)
pv = pmode.get_marginal(g)

# Now the node marginals are stored in property map pv. We can
# visualize them as pie charts on the nodes:
state.draw(pos=g.vp.pos, vertex_shape="pie", vertex_pie_fractions=pv,)
```

Out[28]: <VertexPropertyMap object with value type 'vector<double>', for Graph 0x7f7136fe3340, at 0x7f7135d54be0>

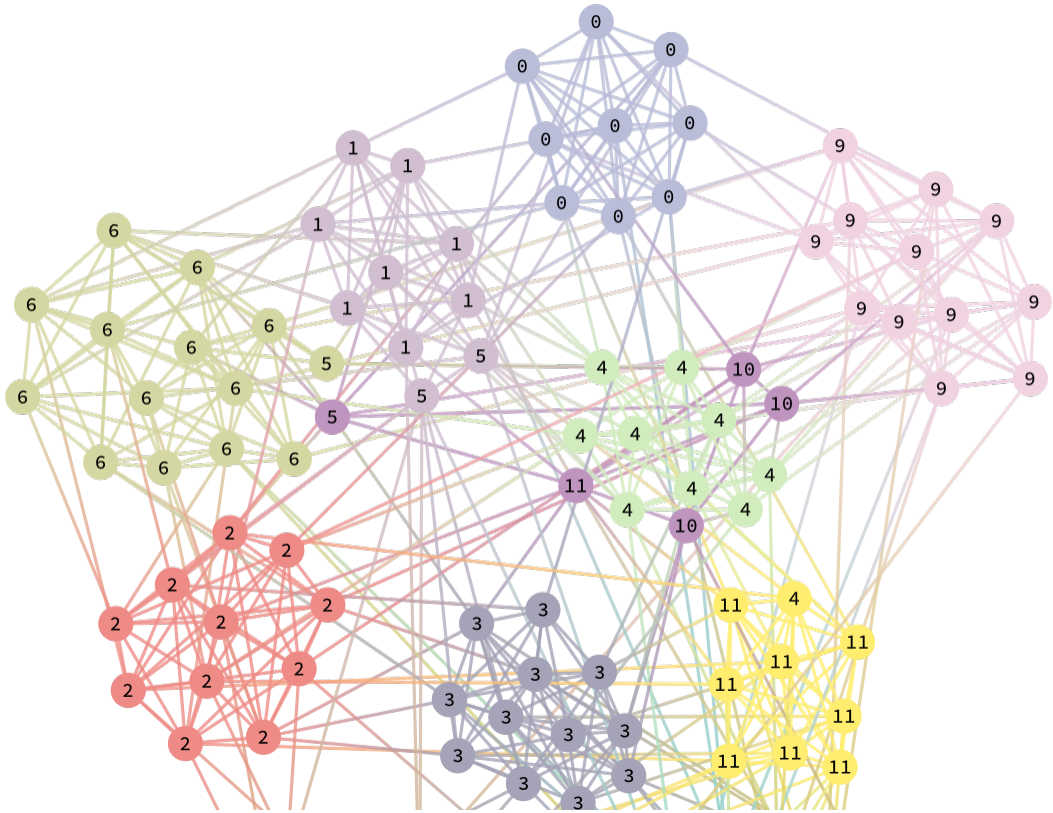
# Assortative community structure

- Planted partition model [9]

In [65]:

```
g = collection.data["football"]

state = PPBlockState(g)
# Now we run 1,000 sweeps of the MCMC with zero temperature.
state.multiflip_mcmc_sweep(beta=np.inf, niter=1000)
print(modularity(g, state.get_blocks()))
state.draw(pos=g.vp.pos,vertex_text= g.vp['value'])
```

```
0.6005165407471079
```



# Network reconstruction

- Generative models can make predictions [10]
- Repair or replace edges
- $\boldsymbol{\mathcal{D}}$ observed data

$$P(\boldsymbol{A}, \boldsymbol{b}|\boldsymbol{\mathcal{D}}) = \frac{P(\boldsymbol{\mathcal{D}}|\boldsymbol{A})P(\boldsymbol{A}, \boldsymbol{b})}{P(\boldsymbol{\mathcal{D}})}$$

- Marginal probability of edge $\{i, j\}$

$$\pi_{ij} = \sum_{\boldsymbol{A},\boldsymbol{b}} A_{ij} P(\boldsymbol{A}, \boldsymbol{b}|\boldsymbol{\mathcal{D}}).$$

- Best estimate

$$\hat{A}_{ij} = \begin{cases} 1 & \text{if } \pi_{ij} > \frac{1}{2}, \\ 0 & \text{if } \pi_{ij} < \frac{1}{2}. \end{cases}$$

- `MeasuredBlockState` $\rightarrow$ `MixedMeasuredBlockState` $\rightarrow$ `UncertainBlockState`

# Measured networks

- $\boldsymbol{n}$: number of measurements
- $\boldsymbol{x}$: number of observations
- $p$: probability of missing edge occurrence
- $q$: probability of spurious edge occurrence

$$P(\boldsymbol{x}|\boldsymbol{n},\boldsymbol{A},\boldsymbol{p},\boldsymbol{q}) = \prod_{i<j} \binom{n_{ij}}{x_{ij}} \left[(1-p_{ij})^{x_{ij}} p_{ij}^{n_{ij}-x_{ij}}\right]^{A_{ij}} \left[q_{ij}^{x_{ij}} (1-q_{ij})^{n_{ij}-x_{ij}}\right]^{1-A_{ij}}$$

.

- $p$ and $q$ are generally not known $\longrightarrow$ integrated likelihood

$$P(\boldsymbol{x}|\boldsymbol{n},\boldsymbol{A},\alpha,\beta,\mu,\nu) = \int P(\boldsymbol{x}|\boldsymbol{n},\boldsymbol{A},p,q) P(p|\alpha,\beta) P(q|\mu,\nu)\, \mathrm{d}p\, \mathrm{d}q$$

In [30]:
```
g = collection.data["lesmis"].copy()

# pretend we have measured and observed each edge twice

n = g.new_ep("int", 2)   # number of measurements
x = g.new_ep("int", 2)   # number of observations

e = g.edge(11, 36)
x[e] = 1                 # pretend we have observed edge (11, 36) only once

e = g.add_edge(15, 73)
n[e] = 2                 # pretend we have measured non-edge (15, 73) twice,
x[e] = 1                 # but observed it as an edge once.
```

In [31]:
```
# We inititialize MeasuredBlockState, assuming that each non-edge has
# been measured only once (as opposed to twice for the observed
# edges), as specified by the 'n_default' and 'x_default' parameters.

state = MeasuredBlockState(g, n=n, n_default=1, x=x, x_default=0)

# We will first equilibrate the Markov chain
mcmc_equilibrate(state, wait=1000, mcmc_args=dict(niter=10))
```

Out[31]:
```
(1035.6463478081441, 10881739, 2640325)
```

In [32]:
```
# Now we collect the marginals for exactly 100,000 sweeps, at
# intervals of 10 sweeps:

u = None                # marginal posterior edge probabilities
bs = []                 # partitions
cs = []                 # average local clustering coefficient

def collect_marginals(s):
   global u, bs, cs
   u = s.collect_marginal(u)
   bstate = s.get_block_state()
   bs.append(bstate.levels[0].b.a.copy())
   cs.append(local_clustering(s.get_graph()).fa.mean())
```

In [33]:
```
mcmc_equilibrate(state, force_niter=10000, mcmc_args=dict(niter=10),
                     callback=collect_marginals)

eprob = u.ep.eprob
print("Posterior probability of edge (11, 36):", eprob[u.edge(11, 36)])
print("Posterior probability of non-edge (15, 73):", eprob[u.edge(15, 73)])
print("Estimated average local clustering: %g ± %g" % (np.mean(cs), np.std(c
s)))
```

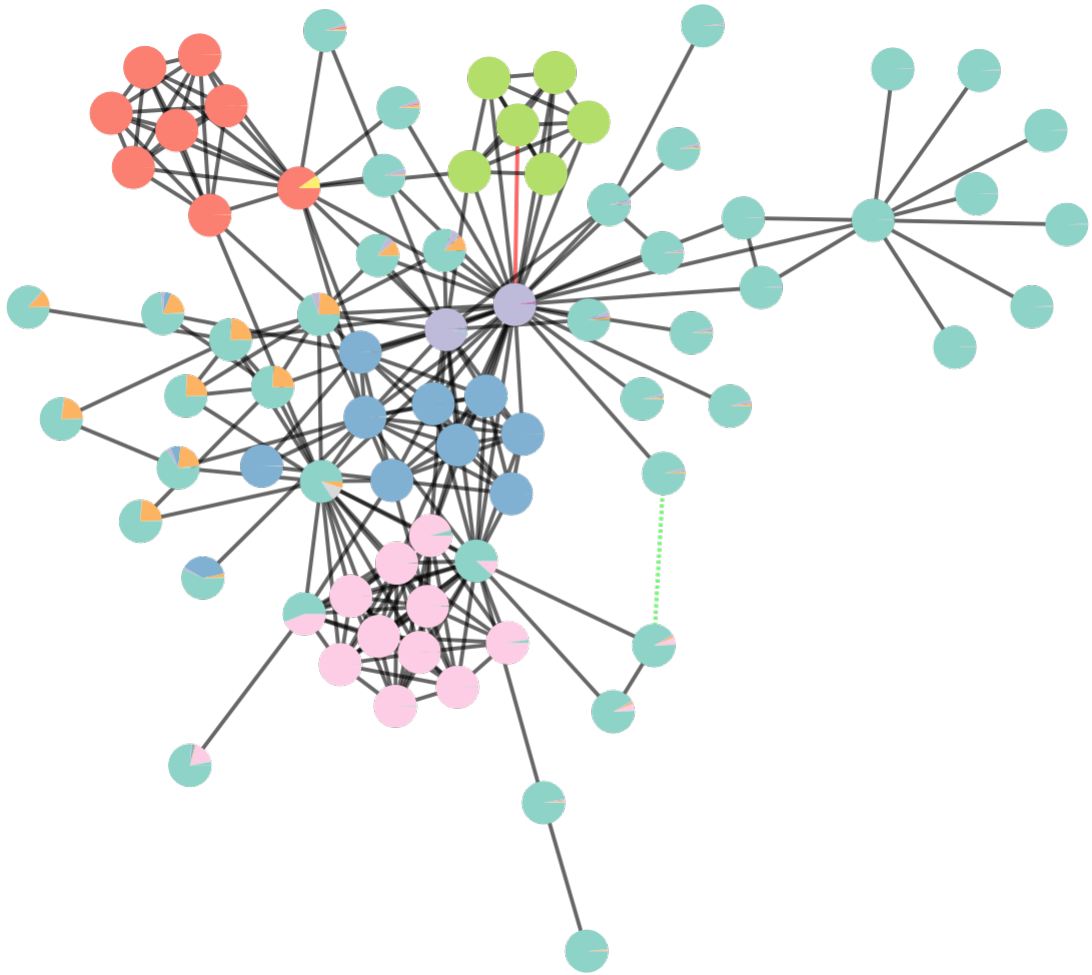
```
Posterior probability of edge (11, 36): 0.7044704470447045
Posterior probability of non-edge (15, 73): 0.0349034903490349
Estimated average local clustering: 0.57169 ± 0.00336791
```

# Maximum marginal posterior estimate

In [34]:
```
# The maximum marginal posterior estimator can be obtained by
# filtering the edges with probability larger than .5

u = GraphView(u, efilt=u.ep.eprob.fa > .5)

# Mark the recovered true edges as red, and the removed spurious edges as green
ecolor = u.new_ep("vector<double>", val=[0, 0, 0, .6])
for e in u.edges():
    if g.edge(e.source(), e.target()) is None or (e.source(), e.target()) == (1
1, 36):
        ecolor[e] = [1, 0, 0, .6]
for e in g.edges():
    if u.edge(e.source(), e.target()) is None:
        ne = u.add_edge(e.source(), e.target())
        ecolor[ne] = [0, 1, 0, .6]
```

In [35]:
```
# Duplicate the internal block state with the reconstructed network
# u, for visualization purposes.

bstate = state.get_block_state()
bstate = bstate.levels[0].copy(g=u)

# Disambiguate partitions and obtain marginals
pmode = PartitionModeState(bs, converge=True)
pv = pmode.get_marginal(u)
```

In [36]:
```
edash = u.new_ep("vector<double>")
edash[u.edge(15, 73)] = [.1, .1, 0]
bstate.draw(pos=u.own_property(g.vp.pos), vertex_shape="pie", vertex_pie_fracti
ons=pv,
            edge_color=ecolor, edge_dash_style=edash, edge_gradient=None,)
```

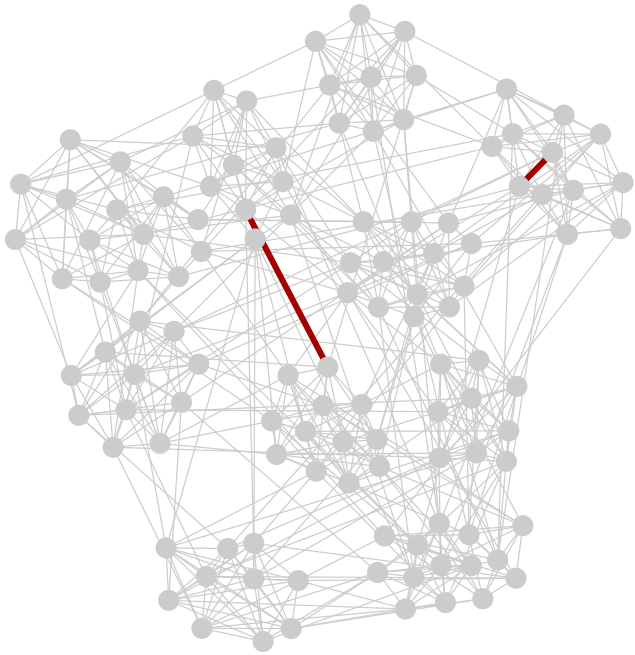


# Edge prediction as binary classification

- Fit generative model and compute edge/non-edge scores ($\boldsymbol{A}$ and $\delta\boldsymbol{A}$, respectively)
- Get probabilities of edges

$$P(\delta\boldsymbol{A}|\boldsymbol{A}) \propto \sum_{\boldsymbol{b}} \frac{P(\boldsymbol{A} \cup \delta\boldsymbol{A}|\boldsymbol{b})}{P(\boldsymbol{A}|\boldsymbol{b})} P(\boldsymbol{b}|\boldsymbol{A})$$

-$P(\delta\boldsymbol{A}|\boldsymbol{A}, \boldsymbol{b})$ can be obtained by `get_edges_prob`



Two non-existing edges in the football network (in red): $(101, 102)$ in the middle, and $(17, 56)$ in the upper right region of the figure. 

In [37]:

```
g = collection.data["football"]

missing_edges = [(101, 102), (17, 56)]

L = 10

state = minimize_nested_blockmodel_dl(g, deg_corr=True)

bs = state.get_bs()                         # Get hierarchical partition.
bs += [np.zeros(1)] * (L - len(bs))         # Augment it to L = 10 with
                                            # single-group levels.

state = state.copy(bs=bs, sampling=True)

probs = ([], [])

def collect_edge_probs(s):
    p1 = s.get_edges_prob([missing_edges[0]], entropy_args=dict(partition_dl=Fa
lse))
    p2 = s.get_edges_prob([missing_edges[1]], entropy_args=dict(partition_dl=Fa
lse))
    probs[0].append(p1)
    probs[1].append(p2)

# Now we collect the probabilities for exactly 100,000 sweeps
mcmc_equilibrate(state, force_niter=10000, mcmc_args=dict(niter=10),
                 callback=collect_edge_probs)


def get_avg(p):
   p = np.array(p)
   pmax = p.max()
   p -= pmax
   return pmax + np.log(np.exp(p).mean())

p1 = get_avg(probs[0])
p2 = get_avg(probs[1])
```

```
p_sum = get_avg([p1, p2]) + np.log(2)

l1 = p1 - p_sum
l2 = p2 - p_sum

print("likelihood-ratio for %s: %g" % (missing_edges[0], np.exp(l1)))
print("likelihood-ratio for %s: %g" % (missing_edges[1], np.exp(l2)))
```

```
likelihood-ratio for (101, 102): 0.365437
likelihood-ratio for (17, 56): 0.634563
```

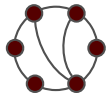
# Summary

- Graph-tool is C++ based, Python-wrapped
- (n)SBM calculations
- Inference of best partition
- Sampling from posterior distribution
- Network reconstruction

Ad:

- Hannu Reittu, Ilkka Norros, Tomi Räty, Marianna Bolla and Fülöp Bazsó : Regular decomposition of large graphs: foundation of a sampling approach to stochastic block model fitting. Data Science and Engineering 4 (1): pp. 44-60, 2019. https://doi.org/10.1007/s41019-019-0084-x (https://doi.org/10.1007/s41019-019-0084-x)

- Hannu Reittu, Fülöp Bazsó and Robert Weiss Regular Decomposition of Multivariate Time Series and Other Matrices, Structural, Syntactic, and Statistical Pattern Recognition, Lecture Notes in Computer Science , Volume 8621, 2014, pp 424-433



graph-tool

# Thank you for your attention!

## Sources:


- [1]: Tiago P. Peixoto, “Bayesian stochastic blockmodeling”, Advances in Network Clustering and Blockmodeling, edited by P. Doreian, V. Batagelj, A. Ferligoj, (Wiley, New York, 2019) DOI: 10.1002/9781119483298.ch11
- [2]: Paul W. Holland, Kathryn Blackmond Laskey, Samuel Leinhardt, “Stochastic blockmodels: First steps”, Social Networks Volume 5, Issue 2, Pages 109-137 (1983). DOI: 10.1016/0378-8733(83)90021-7
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- [4]: Brian Karrer, M. E. J. Newman “Stochastic blockmodels and community structure in networks”, Phys. Rev. E 83, 016107 (2011). DOI: 10.1103/PhysRevE.83.016107
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- [7]: Tiago P. Peixoto, “Efficient Monte Carlo and greedy heuristic for the inference of stochastic block models”, Phys. Rev. E 89, 012804 (2014).
- [8]: Tiago P. Peixoto, “Merge-split Markov chain Monte Carlo for community detection”, Phys. Rev. E 102, 012305 (2020), DOI: 10.1103/PhysRevE.102.012305
- [9]: Lizhi Zhang, Tiago P. Peixoto, “Statistical inference of assortative community structures”, arXiv: 2006.14493
- [10]: Tiago P. Peixoto, “Reconstructing networks with unknown and heterogeneous errors”, Phys. Rev. X 8 041011 (2018). DOI: 10.1103/PhysRevX.8.041011
- [11]: Aaron Clauset, Cristopher Moore, M. E. J. Newman, “Hierarchical structure and the prediction of missing links in networks”, Nature 453, 98-101 (2008). DOI: 10.1038/nature06830
- [12]: Roger Guimerà, Marta Sales-Pardo, “Missing and spurious interactions and the reconstruction of complex networks”, PNAS vol. 106 no. 52 (2009). DOI: 10.1073/pnas.0908366106



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*This presentation is partly based on graph-tool’s [cookbook (https://graph-tool.skewed.de/static/doc/demos/index.html)](https://graph-tool.skewed.de/static/doc/demos/index.html).*

Clustering with networks, 2020