Counting and generating tailored random graphs

DPG physics school on efficient algorithms in computational physics
Bad Honnef, September 2012

ACC Coolen

Institute for Mathematical and Molecular Biomedicine
King's College London

London Institute for Mathematical Sciences

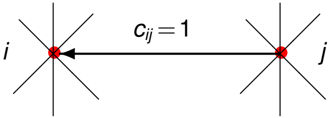
1. Background - tailored random graphs

networks/graphs:

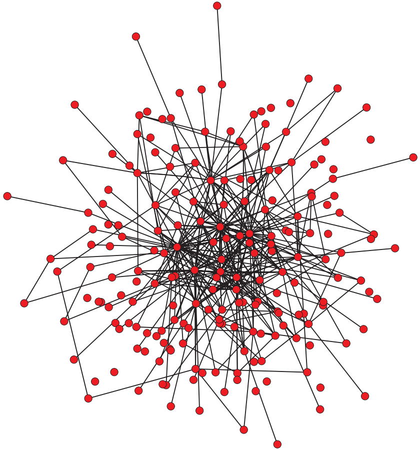
number of nodes: N
nodes (vertices): $i, j \in \{1, \ldots, N\}$

links (edges): $c_{ij} \in \{0, 1\}$
no self-links: $c_{ii} = 0$ for all i

graph: $\mathbf{c} = \{c_{ij}\}$



nondirected graph: $\forall(i, j): \ c_{ij} = c_{ji}$
directed graph: $\exists(i, j): \ c_{ij} \neq c_{ji}$



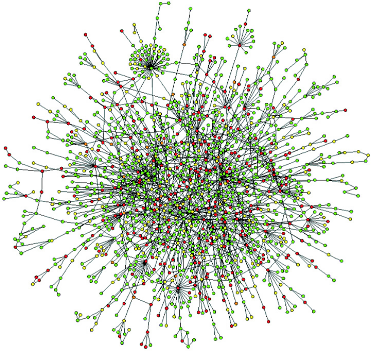
if we model real-world systems by graphs
we want these graphs to be realistic ...

Networks in cell biology

- **protein interaction networks**:

  nodes: proteins $i, j = 1 \ldots N$
  links: $c_{ij} = c_{ji} = 1$ if i can bind to j
  $c_{ij} = c_{ji} = 0$ otherwise

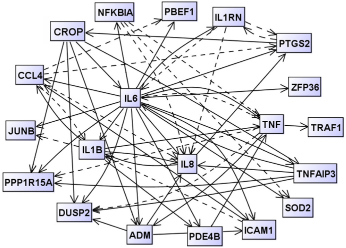
  nondirected graphs,
  $N \sim 10^4$, links/node ~ 7



- **gene regulation networks**:

  nodes: genes $i, j = 1 \ldots N$
  links: $c_{ij} = 1$ if j is transcription factor of i
  $c_{ij} = 0$ otherwise

  directed graphs,
  $N \sim 10^4$, links/node ~ 5

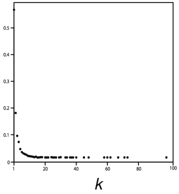


Quantify topology of nondirected graphs

- degrees,
  degree sequence: $k_i(\mathbf{c}) = \sum_j c_{ij}$, $\mathbf{k}(\mathbf{c}) = (k_1(\mathbf{c}), \ldots, k_N(\mathbf{c}))$

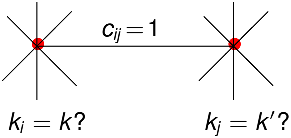
- degree distribution:

$$p(k|\mathbf{c}) = \frac{1}{N} \sum_{i=1}^{N} \delta_{k,k_i(\mathbf{c})}$$



- joint degree statistics
  of connected nodes

$$W(k,k'|\mathbf{c}) = \frac{1}{N\langle k\rangle} \sum_{ij} c_{ij} \delta_{k,k_i(\mathbf{c})} \delta_{k',k_j(\mathbf{c})}$$



normalisation:

$$\sum_{k,k'\geq 0} W(k,k'|\mathbf{c}) = \frac{1}{N\langle k\rangle} \sum_{ij} c_{ij} = \frac{1}{N\langle k\rangle} \sum_i k_i(\mathbf{c}) = 1$$

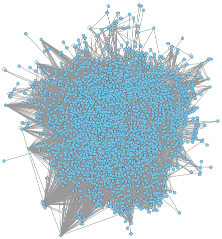
- relation between p and W:

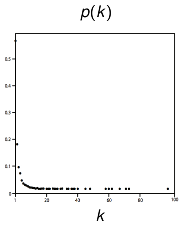
$$
\begin{aligned}
W(k|\mathbf{c}) &= \sum_{k'} W(k,k'|\mathbf{c}) = \frac{1}{N\langle k\rangle}\sum_{ij} c_{ij}\delta_{k,k_i(\mathbf{c})} \\
&= \frac{1}{N\langle k\rangle}\sum_{i} k_i(\mathbf{c})\delta_{k,k_i(\mathbf{c})} = \frac{k}{N\langle k\rangle}\sum_{i}\delta_{k,k_i(\mathbf{c})} = p(k|\mathbf{c})k/\langle k\rangle
\end{aligned}
$$

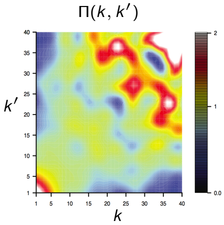
- hence maginals of W carry no info beyond degree statistics so focus on:

$$
\Pi(k,k'|\mathbf{c}) = \frac{W(k,k'|\mathbf{c})}{W(k|\mathbf{c})W(k'|\mathbf{c})}
$$

if $\exists(k,k')$ with $\Pi(k,k'|\mathbf{c}) \neq 1$:
structural information in degree correlations







H sapiens PIN
$N = 9306$
$\langle k\rangle = 7.53$

Quantify topology of directed graphs

links now become *arrows*

- degrees,
  degree sequences:

$$k_i^{\rm in}(\mathbf{c}) = \sum_j c_{ij}, \qquad \mathbf{k}^{\rm in}(\mathbf{c}) = (k_1^{\rm in}(\mathbf{c}),\ldots,k_N^{\rm in}(\mathbf{c}))$$

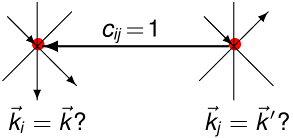
$$k_i^{\rm out}(\mathbf{c}) = \sum_j c_{ji}, \qquad \mathbf{k}^{\rm out}(\mathbf{c}) = (k_1^{\rm out}(\mathbf{c}),\ldots,k_N^{\rm out}(\mathbf{c}))$$

- degree distribution:

$$k_i \ \to\ \vec{k}_i = (k_i^{\rm in}, k_i^{\rm out}) \qquad\qquad p(\vec{k}|\mathbf{c}) = \frac{1}{N}\sum_i \delta_{\vec{k},\vec{k}_i(\mathbf{c})}$$

- joint in-out degree statistics
  of connected nodes

$$W(\vec{k},\vec{k}'|\mathbf{c}) = \frac{1}{N\langle k\rangle}\sum_{ij} c_{ij}\delta_{\vec{k},\vec{k}_i(\mathbf{c})}\delta_{\vec{k}',\vec{k}_j(\mathbf{c})}$$



note:

$$W(\vec{k},\vec{k}'|\mathbf{c}) - W(\vec{k}',\vec{k}|\mathbf{c}) = \frac{1}{N\langle k\rangle}\sum_{ij}(c_{ij}-c_{ji})\ \delta_{\vec{k},\vec{k}_i(\mathbf{c})}\delta_{\vec{k}',\vec{k}_j(\mathbf{c})} \ \neq 0$$

- relation between p and W:

$$
\begin{aligned}
W_1(\vec{k}|\mathbf{c}) &= \sum_{\vec{k}'} \frac{1}{N\langle k\rangle} \sum_{ij} c_{ij}\delta_{\vec{k},\vec{k}_i(\mathbf{c})}\delta_{\vec{k}',\vec{k}_j(\mathbf{c})} = \frac{1}{N\langle k\rangle} \sum_{ij} c_{ij}\delta_{\vec{k},\vec{k}_i(\mathbf{c})} \\
&= \frac{1}{N\langle k\rangle} \sum_{i} k_i^{\rm in}(\mathbf{c})\delta_{\vec{k},\vec{k}_i(\mathbf{c})} = \frac{k^{\rm in}}{N\langle k\rangle} \sum_{i} \delta_{\vec{k},\vec{k}_i(\mathbf{c})} = p(\vec{k}|\mathbf{c})k^{\rm in}/\langle k\rangle
\end{aligned}
$$

$$
\begin{aligned}
W_2(\vec{k}'|\mathbf{c}) &= \sum_{\vec{k}} \frac{1}{N\langle k\rangle} \sum_{ij} c_{ij}\delta_{\vec{k},\vec{k}_i(\mathbf{c})}\delta_{\vec{k}',\vec{k}_j(\mathbf{c})} = \frac{1}{N\langle k\rangle} \sum_{ij} c_{ij}\delta_{\vec{k}',\vec{k}_j(\mathbf{c})} \\
&= \frac{1}{N\langle k\rangle} \sum_{j} k_j^{\rm out}(\mathbf{c})\delta_{\vec{k}',\vec{k}_j(\mathbf{c})} = \frac{k^{\rm out\prime}(\mathbf{c})}{N\langle k\rangle} \sum_{j} \delta_{\vec{k}',\vec{k}_j(\mathbf{c})} = p(\vec{k}'|\mathbf{c})k^{\rm out\prime}/\langle k\rangle
\end{aligned}
$$

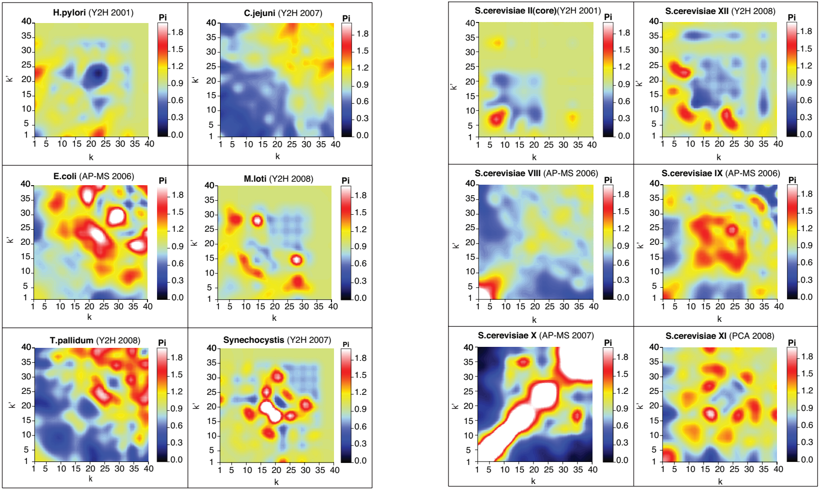
so focus on:

$$
\Pi(\vec{k},\vec{k}'|\mathbf{c}) = \frac{W(\vec{k},\vec{k}'|\mathbf{c})}{W_1(\vec{k}|\mathbf{c})W_2(\vec{k}'|\mathbf{c})}
$$

if $\exists(\vec{k},\vec{k}')$ with $\Pi(\vec{k},\vec{k}'|\mathbf{c}) \neq 1$:
structural information in degree correlations

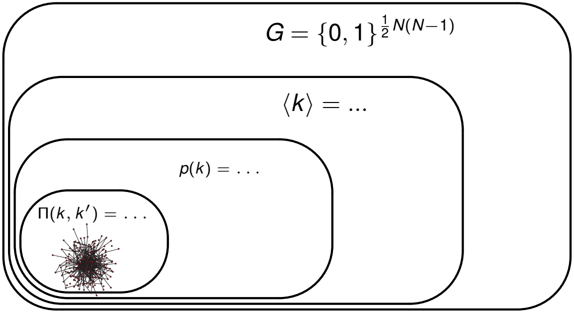
Information in degree correlations?

plot $\Pi(k,k') = W(k,k')/W(k)W(k')$
for protein interaction networks:



Graph classification
via increasingly detailed
feature prescription

e.g. directed graphs:



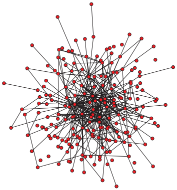
Tailored random graph ensembles

maximum entropy random graph ensembles,
$p(\mathbf{c})$ with prescribed values for $\langle k \rangle$, $p(k)$, $\Pi(k,k')$, ...

– proxies for real networks in stat mech models
– complexity: how many networks exist with same features as $\mathbf{c}$? counting
– hypothesis testing: graphs with controlled features as null models generating

$N = 1000$: $2^{\frac{1}{2}N(N-1)} \approx 10^{150,364}$ graphs
(universe has $\sim 10^{82}$ atoms ...)

random graph ensembles



(i) set G of allowed graphs,
(ii) probability measure $p(\mathbf{c})$ on G

- **Tailoring via hard constraints**

  (i) impose values for specific observables: $\Omega_\mu(\mathbf{c}) = \Omega_\mu$ for $\mu = 1 \ldots p$
  (ii) $p(\mathbf{c})$: all graphs that meet constraints are equally likely

$$p(\mathbf{c}|\mathbf{\Omega}) = \frac{\delta_{\mathbf{\Omega}(\mathbf{c}),\mathbf{\Omega}}}{\mathcal{N}(\mathbf{\Omega})}, \qquad \mathcal{N}(\mathbf{\Omega}) = \sum_{\mathbf{c}} \delta_{\mathbf{\Omega}(\mathbf{c}),\mathbf{\Omega}} \quad (\textit{nr of graphs in ensemble})$$

with $\mathbf{\Omega} = (\Omega_1, \ldots, \Omega_p)$

note 1:

$p(\mathbf{c})$ maximises Shannon entropy S on $G[\mathbf{\Omega}] = \{\mathbf{c}|\ \mathbf{\Omega}(\mathbf{c}) = \mathbf{\Omega}\}$

$$S = -\frac{1}{N\langle k\rangle} \sum_{\mathbf{c}} p(\mathbf{c}) \log p(\mathbf{c})$$

note 2:

$$\mathrm{e}^{N\langle k\rangle S[\mathbf{\Omega}]} = \mathrm{e}^{-\sum_{\mathbf{c}} p(\mathbf{c}) \log p(\mathbf{c})} = \mathrm{e}^{-\sum_{\mathbf{c}} \frac{\delta_{\mathbf{\Omega}(\mathbf{c}),\mathbf{\Omega}}}{\mathcal{N}(\mathbf{\Omega})} \left(\log \delta_{\mathbf{\Omega}(\mathbf{c}),\mathbf{\Omega}} - \log \mathcal{N}(\mathbf{\Omega})\right)} = \mathcal{N}(\mathbf{\Omega})$$

Tailoring via soft constraints

(i) impose *averages* for specific observables: $\Omega_\mu(\mathbf{c}) = \Omega_\mu$ for $\mu = 1 \ldots p$
(ii) $p(\mathbf{c})$: maximum entropy, subject to constraints

$$p(\mathbf{c}|\boldsymbol{\Omega}) = Z^{-1}(\boldsymbol{\Omega})\, \mathrm{e}^{\sum_\mu \omega_\mu(\boldsymbol{\Omega})\Omega_\mu(\mathbf{c})}, \qquad Z(\boldsymbol{\Omega}) = \sum_{\mathbf{c}} \mathrm{e}^{\sum_\mu \omega_\mu(\boldsymbol{\Omega})\Omega_\mu(\mathbf{c})}$$

parameters $\omega_\mu(\boldsymbol{\Omega})$:
to be solved from

$$\forall \mu: \quad \sum_{\mathbf{c}} p(\mathbf{c}|\boldsymbol{\Omega})\Omega_\mu(\mathbf{c}) = \Omega_\mu$$

note 1:

all graphs $\mathbf{c}$ can in principle emerge; those with $\boldsymbol{\Omega}(\mathbf{c}) \approx \boldsymbol{\Omega}$ are the most likely

note 2:

effective number of graphs $\mathcal{N}(\boldsymbol{\Omega})$ defined via entropy:

$$\mathcal{N}(\boldsymbol{\Omega}) = \mathrm{e}^{N\langle k\rangle S[\boldsymbol{\Omega}]}, \qquad S[\boldsymbol{\Omega}] = -\frac{1}{N\langle k\rangle}\sum_{\mathbf{c}\in G} p(\mathbf{c}|\boldsymbol{\Omega}) \log p(\mathbf{c}|\boldsymbol{\Omega})$$

note 3:

for observables $\boldsymbol{\Omega}(\mathbf{c})$ that are *macroscopic in nature and* $\mathcal{O}(N^0)$,
one will generally find deviations from $\boldsymbol{\Omega}(\mathbf{c}) = \boldsymbol{\Omega}$ to tend to zero as $N \to \infty$

Example 1a

nondirected graphs, $c_{ii} = 0$ for all i,
impose average connectivity via hard constraint,
$\Omega(\mathbf{c}) = \sum_{ij} c_{ij}$

- demand $\sum_{ij} c_{ij} = N\langle k\rangle$

$$p(\mathbf{c}|\langle k\rangle) = \frac{\delta_{\sum_{ij} c_{ij}, N\langle k\rangle}}{\mathcal{N}(\langle k\rangle)}, \qquad \mathcal{N}(\langle k\rangle) = \sum_{\mathbf{c}} \delta_{\sum_{ij} c_{ij}, N\langle k\rangle}$$

- calculate $\mathcal{N}(\langle k\rangle)$:

use $\delta_{nm} = (2\pi)^{-1} \int_{-\pi}^{\pi} \mathrm{d}\omega\ \mathrm{e}^{\mathrm{i}(n-m)\omega}$

$$\begin{aligned}
\mathcal{N}(\langle k\rangle) &= \int_{-\pi}^{\pi} \frac{\mathrm{d}\omega}{2\pi}\ \mathrm{e}^{\mathrm{i}\omega N\langle k\rangle} \sum_{\mathbf{c}} \mathrm{e}^{-\mathrm{i}\omega \sum_{ij} c_{ij}} = \int_{-\pi}^{\pi} \frac{\mathrm{d}\omega}{2\pi}\ \mathrm{e}^{\mathrm{i}\omega N\langle k\rangle} \prod_{i<j} \Big[\sum_{c_{ij}} \mathrm{e}^{-2\mathrm{i}\omega c_{ij}} \Big] \\
&= \int_{-\pi}^{\pi} \frac{\mathrm{d}\omega}{2\pi}\ \mathrm{e}^{\mathrm{i}\omega N\langle k\rangle} (1+\mathrm{e}^{-2\mathrm{i}\omega})^{\frac{1}{2}N(N-1)} \\
&= \sum_{\ell=0}^{\frac{1}{2}N(N-1)} \binom{\frac{1}{2}N(N-1)}{\ell} \int_{-\pi}^{\pi} \frac{\mathrm{d}\omega}{2\pi}\ \mathrm{e}^{\mathrm{i}\omega N\langle k\rangle - 2\mathrm{i}\ell\omega} = \binom{\frac{1}{2}N(N-1)}{\frac{1}{2}N\langle k\rangle} \\
&= \mathrm{e}^{\frac{1}{2}N\langle k\rangle \left[\log(N/\langle k\rangle)+1\right] + \mathcal{O}(\log N)} \qquad \textit{Stirling}:\quad n! = \mathrm{e}^{n\log n - n + \mathcal{O}(\log n)} \quad n\to\infty
\end{aligned}$$

Example 1b

nondirected graphs, $c_{ii}=0$ for all i,
impose average connectivity via soft constraint,
$\Omega(\mathbf{c})=\sum_{ij}c_{ij}$

- demand $\langle\sum_{ij}c_{ij}\rangle=N\langle k\rangle$

$$p(\mathbf{c}|\langle k\rangle)=\frac{1}{Z(\omega)}\mathrm{e}^{\omega\sum_{ij}c_{ij}},\qquad Z(\omega)=\sum_{\mathbf{c}}\mathrm{e}^{\omega\sum_{ij}c_{ij}}$$

$$\omega\ \textit{solved from}:\qquad \langle k\rangle=\frac{1}{Z(\omega)}\sum_{\mathbf{c}}\Big(\frac{1}{N}\sum_{k\ell}c_{k\ell}\Big)\mathrm{e}^{\omega\sum_{ij}c_{ij}}=\frac{\mathrm{d}}{\mathrm{d}\omega}\frac{1}{N}\log Z(\omega)$$

- calculate $Z(\omega)$ and ω:

$$\langle k\rangle=\frac{\mathrm{d}}{\mathrm{d}\omega}\frac{1}{N}\log(\mathrm{e}^{2\omega}+1)^{\frac{1}{2}N(N-1)}=(N-1)\frac{\mathrm{e}^{2\omega}}{\mathrm{e}^{2\omega}+1}$$

- Equivalently:

$$\begin{aligned}p(\mathbf{c}|\langle k\rangle)&=\frac{1}{Z(\omega)}\prod_{i<j}\mathrm{e}^{2\omega c_{ij}}=\frac{1}{Z(\omega)}\prod_{i<j}\Big[\mathrm{e}^{2\omega}\delta_{c_{ij},1}+\delta_{c_{ij},0}\Big]\\&=\prod_{i<j}\frac{\mathrm{e}^{2\omega}\delta_{c_{ij},1}+\delta_{c_{ij},0}}{\mathrm{e}^{2\omega}+1}=\prod_{i<j}\Big[\frac{\mathrm{e}^{2\omega}}{\mathrm{e}^{2\omega}+1}\delta_{c_{ij},1}+\frac{1}{\mathrm{e}^{2\omega}+1}\delta_{c_{ij},0}\Big]\end{aligned}$$

Example 2a

nondirected graphs, $c_{ii}=0$ for all i,
impose degree sequence via hard constraint,
$\Omega_i(\mathbf{c})=\sum_j c_{ij},\quad i=1\ldots N$

- demand: $\sum_j c_{ij}=k_i$ for all i

$$p(\mathbf{c}|\mathbf{k})=\frac{\prod_i \delta_{\sum_j c_{ij},k_i}}{\mathcal{N}(\mathbf{k})},\qquad \mathcal{N}(\mathbf{k})=\sum_{\mathbf{c}}\prod_i \delta_{\sum_j c_{ij},k_i}$$

- calculate $\mathcal{N}(\mathbf{k})$:

  use $\delta_{nm}=(2\pi)^{-1}\int_{-\pi}^{\pi}\mathrm{d}\omega\ \mathrm{e}^{\mathrm{i}(n-m)\omega}$

$$\mathcal{N}(\mathbf{k}) = \int_{-\pi}^{\pi}\prod_i\Big(\frac{\mathrm{d}\omega_i}{2\pi}\ \mathrm{e}^{\mathrm{i}\omega_i k_i}\Big)\sum_{\mathbf{c}}\mathrm{e}^{-\mathrm{i}\sum_i\omega_i\sum_j c_{ij}} = \int_{-\pi}^{\pi}\frac{\mathrm{d}\boldsymbol{\omega}\mathrm{e}^{\mathrm{i}\boldsymbol{\omega}\cdot\mathbf{k}}}{(2\pi)^N}\prod_{i<j}\Big[\sum_{c_{ij}}\mathrm{e}^{-\mathrm{i}(\omega_i+\omega_j)c_{ij}}\Big]$$

$$= \int_{-\pi}^{\pi}\frac{\mathrm{d}\boldsymbol{\omega}\ \mathrm{e}^{\mathrm{i}\boldsymbol{\omega}\cdot\mathbf{k}}}{(2\pi)^N}\prod_{i<j}(1+\mathrm{e}^{-\mathrm{i}(\omega_i+\omega_j)})=?$$

possible (leading orders in N),
but no longer obvious ...

Example 2b

nondirected graphs, $c_{ii} = 0$ for all i,
impose degree sequence via soft constraint,
$\Omega_i(\mathbf{c}) = \sum_j c_{ij}, \quad i = 1 \ldots N$

- demand: $\langle \sum_j c_{ij} \rangle = k_i$ for all i

$$p(\mathbf{c}|\mathbf{k}) = \frac{1}{Z(\boldsymbol{\omega})} \mathrm{e}^{\sum_i \omega_i \sum_j c_{ij}}, \qquad Z(\boldsymbol{\omega}) = \sum_{\mathbf{c}} \mathrm{e}^{\sum_i \omega_i \sum_j c_{ij}}$$

$$\boldsymbol{\omega} \textit{ solved from}: \qquad \forall m: \quad k_m = \frac{1}{Z(\boldsymbol{\omega})} \sum_{\mathbf{c}} \Big(\sum_n c_{mn} \Big) \mathrm{e}^{\sum_i \omega_i \sum_j c_{ij}} = \frac{\partial}{\partial \omega_m} \log Z(\boldsymbol{\omega})$$

- calculate $Z(\boldsymbol{\omega})$ and $\boldsymbol{\omega}$:

$$\begin{aligned} k_m &= \frac{\partial}{\partial \omega_m} \log \sum_{\mathbf{c}} \mathrm{e}^{\sum_{i<j} c_{ij}(\omega_i+\omega_j)} = \frac{\partial}{\partial \omega_m} \log \prod_{i<j} \Big[\sum_{c_{ij}} \mathrm{e}^{c_{ij}(\omega_i+\omega_j)} \Big] \\ &= \sum_{i<j} \frac{\partial}{\partial \omega_m} \log(1+\mathrm{e}^{\omega_i+\omega_j}) = \frac{1}{2} \sum_{i \neq j} (\delta_{im}+\delta_{jm}) \frac{\mathrm{e}^{\omega_i+\omega_j}}{1+\mathrm{e}^{\omega_i+\omega_j}} = \sum_{i \neq m} \frac{\mathrm{e}^{\omega_i+\omega_m}}{1+\mathrm{e}^{\omega_i+\omega_m}} \end{aligned}$$

N transcendental eqns to be solved ...

Example 3a

nondirected graphs, $c_{ii} = 0$ for all i,
impose degree sequence and kernel $W(k, k')$ via hard constraint,

$\Omega_i(\mathbf{c}) = \sum_j c_{ij}, \quad i, j = 1 \dots N,$
$\Omega_{kk'}(\mathbf{c}) = \sum_{ij} c_{ij}\delta_{k,\sum_\ell c_{i\ell}}\delta_{k',\sum_\ell c_{j\ell}}, \quad k, k' \in \mathbb{N}$

- demand: $\sum_j c_{ij} = k_i$ for all i, and
  $\sum_{ij} c_{ij}\delta_{k,\sum_\ell c_{i\ell}}\delta_{k',\sum_\ell c_{j\ell}} = N\langle k\rangle W(k, k')$ for all (k, k')
  (with $\langle k\rangle = N^{-1}\sum_i k_i$)

$$p(\mathbf{c}|\mathbf{k}, W) = \frac{\left[\prod_i \delta_{\sum_j c_{ij}, k_i}\right]\left[\prod_{k,k'} \delta_{\sum_{ij} c_{ij}\delta_{k,k_i}\delta_{k',k_j}, N\langle k\rangle W(k,k')}\right]}{\mathcal{N}(\mathbf{k}, W)},$$

$$\mathcal{N}(\mathbf{k}, W) = \sum_{\mathbf{c}}\left[\prod_i \delta_{\sum_j c_{ij}, k_i}\right]\left[\prod_{k,k'} \delta_{\sum_{ij} c_{ij}\delta_{k,k_i}\delta_{k',k_j}, N\langle k\rangle W(k,k')}\right]$$

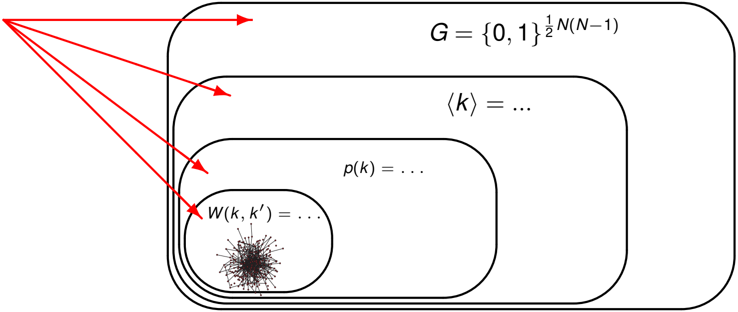
- calculate $\mathcal{N}(\mathbf{k}, W)$:

$$\mathcal{N}(\mathbf{k}, W) = \int_{-\pi}^{\pi}\prod_i\left(\frac{\mathrm{d}\omega_i}{2\pi}\mathrm{e}^{\mathrm{i}\omega_i k_i}\right)\left(\prod_{k,k'}\frac{\mathrm{d}\psi_{kk'}}{2\pi}\mathrm{e}^{\mathrm{i}\psi_{kk'}N\langle k\rangle W(k,k')}\right)$$
$$\times \sum_{\mathbf{c}} \mathrm{e}^{-\mathrm{i}\sum_i \omega_i \sum_j c_{ij} - \mathrm{i}\sum_{kk'}\psi_{kk'}\sum_{ij} c_{ij}\delta_{k,k_i}\delta_{k',k_j}}$$

doable, but increasingly complicated....

2. Counting tailored graphs

how many graphs in each family?



entropy and complexity

properties of Shannon entropy (information theory)

- **effective nr of graphs** in ensemble $p(\mathbf{c}|\star)$:
  ($\star$: imposed observables)

$$\mathcal{N}(\star)=e^{N\langle k\rangle S(\star)},\qquad S(\star)=-\frac{1}{N\langle k\rangle}\sum_{\mathbf{c}} p(\mathbf{c}|\star)\log p(\mathbf{c}|\star)\quad (\textit{entropy per link})$$

- $S(\star)$: proportional to the average nr of bits one needs to specify
  to identify a member graph **c** in the ensemble

- **complexity of graphs** in ensemble $p(\mathbf{c}|\star)$:

$$\mathcal{C}(\star)=S(\emptyset)-S(\star)$$

$\emptyset$: no constraints
nondirected, $c_{ii}=0\ \forall i$:

$$p(\mathbf{c}|\emptyset)=2^{-\frac{1}{2}N(N-1)},\qquad S(\emptyset)=-\frac{1}{N\langle k\rangle}\log 2^{-\frac{1}{2}N(N-1)}=\frac{N-1}{2\langle k\rangle}\log 2$$

$\exists$ many graphs with feature $\star$: graphs with $\star$ have low complexity
$\exists$ few graphs with feature $\star$: graphs with $\star$ have high complexity

Entropy calculation for nondirected graphs

with controlled degree statistics and degree correlations

$$P(\mathbf{c}|p,W)=$$

$$\sum_{k_1\ldots k_N}\prod_i p(k_i)\;\overbrace{\frac{\prod_i \delta_{k_i,k_i(\mathbf{c})}}{Z(\mathbf{k},W)}}^{\textit{hard degree constraint}}\;\overbrace{\prod_{i<j}\Big[\frac{\langle k\rangle}{N}\frac{W(k_i,k_j)}{p(k_i)p(k_j)}\delta_{c_{ij},1}+\Big(1-\frac{\langle k\rangle}{N}\frac{W(k_i,k_j)}{p(k_i)p(k_j)}\Big)\delta_{c_{ij},0}\Big]}^{\textit{soft degree correlation constraint}}$$

$$Z(\mathbf{k},W)=\sum_{\mathbf{c}}\Big[\prod_i \delta_{k_i,k_i(\mathbf{c})}\Big]\prod_{i<j}\Big[\frac{\langle k\rangle}{N}\frac{W(k_i,k_j)}{p(k_i)p(k_j)}\delta_{c_{ij},1}+\Big(1-\frac{\langle k\rangle}{N}\frac{W(k_i,k_j)}{p(k_i)p(k_j)}\Big)\delta_{c_{ij},0}\Big]$$

to calculate for large N:

$$S(\mathbf{k},W) \;=\; -\frac{1}{N\langle k\rangle}\sum_{\mathbf{c}}P(\mathbf{c}|p,W)\log P(\mathbf{c}|p,W)$$

- short-hands:

$$Q(k,k')=W(k,k')/p(k)p(k')$$

$$w(\mathbf{c})=\prod_{i<j}\Big[\frac{\langle k\rangle}{N}Q(k_i,k_j)\delta_{c_{ij},1}+\Big(1-\frac{\langle k\rangle}{N}Q(k_i,k_j)\Big)\delta_{c_{ij},0}\Big]$$

normalised :

$$\sum_{\mathbf{c}}w(\mathbf{c})=\prod_{i<j}\sum_{c_{ij}}\Big[\frac{\langle k\rangle}{N}Q(k_i,k_j)\delta_{c_{ij},1}+\Big(1-\frac{\langle k\rangle}{N}Q(k_i,k_j)\Big)\delta_{c_{ij},0}\Big]=1$$

- in terms of new measure w:

$$w(\mathbf{c}) = \prod_{i<j} \Big[\frac{\langle k\rangle}{N} Q(k_i,k_j)\delta_{c_{ij},1} + \Big(1-\frac{\langle k\rangle}{N} Q(k_i,k_j)\Big)\delta_{c_{ij},0} \Big]$$

$$P(\mathbf{c}|p,W) = \sum_{\mathbf{k}} \Big[\prod_i p(k_i)\Big] \frac{w(\mathbf{c})\delta_{\mathbf{k},\mathbf{k}(\mathbf{c})}}{Z(\mathbf{k},W)}, \qquad Z(\mathbf{k},W) = \langle \delta_{\mathbf{k},\mathbf{k}(\mathbf{c})}\rangle_w$$

- use $0\log 0 = 0$:

$$\begin{aligned}
S(\mathbf{k},W) &= -\frac{1}{N\langle k\rangle} \sum_{\mathbf{c}} \sum_{\mathbf{k}} \Big[\prod_i p(k_i)\Big] \frac{w(\mathbf{c})\delta_{\mathbf{k},\mathbf{k}(\mathbf{c})}}{Z(\mathbf{k},W)} \log\Big[\sum_{\mathbf{k}'} \Big(\prod_i p(k_i')\Big) \frac{w(\mathbf{c})\delta_{\mathbf{k}',\mathbf{k}(\mathbf{c})}}{Z(\mathbf{k}',W)}\Big] \\
&= -\frac{1}{N\langle k\rangle} \sum_{\mathbf{c}} \sum_{\mathbf{k}} \Big[\prod_i p(k_i)\Big] \frac{w(\mathbf{c})\delta_{\mathbf{k},\mathbf{k}(\mathbf{c})}}{Z(\mathbf{k},W)} \log\Big[\Big(\prod_i p(k_i)\Big) \frac{w(\mathbf{c})}{Z(\mathbf{k},W)}\Big] \\
&= -\frac{1}{N\langle k\rangle} \sum_{\mathbf{k}} \Big[\prod_i p(k_i)\Big] \Big[\sum_{\mathbf{c}} \frac{w(\mathbf{c})\delta_{\mathbf{k},\mathbf{k}(\mathbf{c})}}{Z(\mathbf{k},W)}\Big] \Big[\sum_i \log p(k_i) - \log Z(\mathbf{k},W)\Big] \\
&\quad -\frac{1}{N\langle k\rangle} \sum_{\mathbf{k}} \Big[\prod_i p(k_i)\Big] \frac{\sum_{\mathbf{c}} w(\mathbf{c})\delta_{\mathbf{k},\mathbf{k}(\mathbf{c})} \log w(\mathbf{c})}{Z(\mathbf{k},W)}
\end{aligned}$$

$$= \frac{1}{N\langle k\rangle} \sum_{\mathbf{k}} \Big[\prod_i p(k_i)\Big] \underbrace{\Big\{ \log\langle \delta_{\mathbf{k},\mathbf{k}(\mathbf{c})}\rangle_w - \frac{\langle \delta_{\mathbf{k},\mathbf{k}(\mathbf{c})} \log w(\mathbf{c})\rangle_w}{\langle \delta_{\mathbf{k},\mathbf{k}(\mathbf{c})}\rangle_w} \Big\}}_{\text{doable...}} - \underbrace{\frac{1}{\langle k\rangle} \sum_k p(k)\log p(k)}_{\text{trivial...}}$$

left to calculate : $A(\mathbf{k})=\frac{1}{N}\log\langle\delta_{\mathbf{k},\mathbf{k}(\mathbf{c})}\rangle_w \qquad B(\mathbf{k})=\frac{1}{N}\frac{\langle\delta_{\mathbf{k},\mathbf{k}(\mathbf{c})}\log w(\mathbf{c})\rangle_w}{\langle\delta_{\mathbf{k},\mathbf{k}(\mathbf{c})}\rangle_w}$

measure : $w(\mathbf{c})=\prod_{i<j}\left[\frac{\langle k\rangle}{N}Q(k_i,k_j)\delta_{c_{ij},1}+\Big(1-\frac{\langle k\rangle}{N}Q(k_i,k_j)\Big)\delta_{c_{ij},0}\right]$

- degree constraints: $\delta_{\mathbf{k},\mathbf{k}(\mathbf{c})}=\int_{-\pi}^{\pi}\prod_i\left[\frac{\mathrm{d}\omega_i}{2\pi}\mathrm{e}^{\mathrm{i}\omega_i(k_i-\sum_j c_{ij})}\right]$
- sum over graphs:

$$A(\mathbf{k})=\frac{1}{N}\log\int\frac{\mathrm{d}\boldsymbol{\omega}\ \mathrm{e}^{\mathrm{i}\boldsymbol{\omega}\cdot\mathbf{k}}}{(2\pi)^N}\prod_{i<j}\Big[1+\frac{\langle k\rangle}{N}Q(k_i,k_j)[\mathrm{e}^{-\mathrm{i}(\omega_i+\omega_j)}-1]\Big]$$

$$B(\mathbf{k})=\frac{\mathrm{e}^{-NA(\mathbf{k})}}{N}\int\frac{\mathrm{d}\boldsymbol{\omega}\ \mathrm{e}^{\mathrm{i}\boldsymbol{\omega}\cdot\mathbf{k}}}{(2\pi)^N}\sum_{\mathbf{c}}\prod_{i<j}\left[\frac{\langle k\rangle}{N}Q(k_i,k_j)\delta_{c_{ij},1}\mathrm{e}^{-(\omega_i+\omega_j)}+\Big(1-\frac{\langle k\rangle}{N}Q(k_i,k_j)\Big)\delta_{c_{ij},0}\right]$$

$$\times\sum_{\ell<m}\log\left[\frac{\langle k\rangle}{N}Q(k_\ell,k_m)\delta_{c_{\ell m},1}+\Big(1-\frac{\langle k\rangle}{N}Q(k_\ell,k_m)\Big)\delta_{c_{\ell m},0}\right]$$

$$=\mathrm{e}^{-NA(\mathbf{k})}\int\frac{\mathrm{d}\boldsymbol{\omega}\ \mathrm{e}^{\mathrm{i}\boldsymbol{\omega}\cdot\mathbf{k}}}{(2\pi)^N}\prod_{i<j}\Big[1+\frac{\langle k\rangle}{N}Q(k_i,k_j)[\mathrm{e}^{-\mathrm{i}(\omega_i+\omega_j)}-1]\Big]$$

$$\times\frac{1}{N}\sum_{\ell<m}\Big\{\log\Big[\frac{\langle k\rangle}{N}Q(k_\ell,k_m)\Big]-\frac{\langle k\rangle}{N}Q(k_\ell,k_m)\Big\}+\mathcal{O}(\frac{1}{N})$$

- $B(\mathbf{k})$: easy for large N

$$B(\mathbf{k}) = \frac{1}{N}\sum_{\ell<m}\Big\{\log\Big[\frac{\langle k\rangle}{N}Q(k_\ell,k_m)\Big] - \frac{\langle k\rangle}{N}Q(k_\ell,k_m)\Big\} + \mathcal{O}(\frac{1}{N}) \qquad \textit{done}!$$

- $A(\mathbf{k})$: still nontrivial

$$A(\mathbf{k}) = \frac{1}{N}\log\underbrace{\int\frac{\mathrm{d}\boldsymbol{\omega}}{(2\pi)^N}\;\mathrm{e}^{\mathrm{i}\sum_i\omega_i k_i+\frac{1}{2}\sum_{ij}\frac{\langle k\rangle}{N}Q(k_i,k_j)[\mathrm{e}^{-\mathrm{i}(\omega_i+\omega_j)}-1]}}_{\textit{integral over } \boldsymbol{\omega}?} + \mathcal{O}(\frac{1}{N})$$

introduce path integral over
all functions $\frac{1}{N}\sum_i\delta_{k,k_i}\delta(\omega-\omega_i)$

$$1 = \prod_{k,\omega}\int \mathrm{d}P(k,\omega)\delta\Big[P(k,\omega) - \frac{1}{N}\sum_i\delta_{k,k_i}\delta(\omega-\omega_i)\Big]$$

$$= \prod_{k,\omega}\int\frac{\mathrm{d}P(k,\omega)\mathrm{d}\hat{P}(k,\omega)}{2\pi}\;\mathrm{e}^{\mathrm{i}\hat{P}(k,\omega)\big[P(k,\omega)-\frac{1}{N}\sum_i\delta_{k,k_i}\delta(\omega-\omega_i)\big]}$$

$$= \lim_{\Delta\to 0}\int\Big[\prod_{k,\omega}\frac{\mathrm{d}P(k,\omega)\mathrm{d}\hat{P}(k,\omega)}{2\pi/N\Delta}\Big]\mathrm{e}^{\mathrm{i}N\Delta\sum_{k,\omega}\hat{P}(k,\omega)\big[P(k,\omega)-\frac{1}{N}\sum_i\delta_{k,k_i}\delta(\omega-\omega_i)\big]}$$

$$= \int\{\mathrm{d}P\mathrm{d}\hat{P}\}\;\mathrm{e}^{\mathrm{i}N\sum_k\int\mathrm{d}\omega\;\hat{P}(k,\omega)P(k,\omega)-\mathrm{i}\sum_i\hat{P}(k_i,\omega_i)}$$

- in terms of path integral:

$$A(\mathbf{k}) = \frac{1}{N}\log\int\{\mathrm{d}P\mathrm{d}\hat{P}\}\ \mathrm{e}^{N\Psi[P,\hat{P}]} + \mathcal{O}(\frac{1}{N})$$

$$\Psi[P,\hat{P}] = \mathrm{i}\sum_k\int\!\mathrm{d}\omega\ \hat{P}(k,\omega)P(k,\omega) + \frac{1}{N}\sum_i\log\int\frac{\mathrm{d}\omega}{2\pi}\ \mathrm{e}^{\mathrm{i}\omega k_i - \mathrm{i}\hat{P}(k_i,\omega)}$$
$$+\frac{1}{2}\langle k\rangle\sum_{kk'}\int\!\mathrm{d}\omega\mathrm{d}\omega' P(k,\omega)P(k',\omega')Q(k,k')[\mathrm{e}^{-\mathrm{i}(\omega+\omega')} - 1]$$

- large N:

$$\frac{1}{N}\sum_i\log\int\frac{\mathrm{d}\omega}{2\pi}\ \mathrm{e}^{\mathrm{i}\omega k_i - \mathrm{i}\hat{P}(k_i,\omega)} \ \to\ \sum_k p(k)\log\int\frac{\mathrm{d}\omega}{2\pi}\ \mathrm{e}^{\mathrm{i}\omega k - \mathrm{i}\hat{P}(k,\omega)}$$

integral $\int\{\mathrm{d}P\mathrm{d}\hat{P}\}\ldots$ via steepest descent,
functional saddle-point eqns $\delta\Psi/\delta P = \delta\Psi/\delta\hat{P} = 0$,
can be solved analytically

Shannon entropy per bond
final result for nondirected graphs

$$P(\mathbf{c}) = \sum_{\mathbf{k}} \Big[\prod_i \mathrm{d}k_i\; p(k_i)\Big] \frac{\prod_i \delta_{k_i,k_i(\mathbf{c})}}{Z(\mathbf{k},W)} \prod_{i<j} \Big[\frac{\langle k\rangle}{N}\frac{W(k_i,k_j)}{p(k_i)p(k_j)}\delta_{c_{ij},1} + \Big(1-\frac{\langle k\rangle}{N}\frac{W(k_i,k_j)}{p(k_i)p(k_j)}\Big)\delta_{c_{ij},0}\Big]$$

$$S = \underbrace{\frac{1}{2}[1+\log(\frac{N}{\langle k\rangle})]}_{Erdos-Renyi\;\;entropy} - \Big\{ \underbrace{\frac{1}{\langle k\rangle}\sum_k p(k)\log[\frac{p(k)}{\pi(k)}]}_{degree\;\;complexity} + \underbrace{\frac{1}{2}\sum_{k,k'} W(k,k')\log\Big[\frac{W(k,k')}{W(k)W(k')}\Big]}_{wiring\;\;complexity} \Big\} + \epsilon_N$$

$\lim_{N\to\infty} \epsilon_N = 0$

$\pi(\ell) = \mathrm{e}^{-\langle k\rangle}\langle k\rangle^{\ell}/\ell!$
degree distr of Erdös-Renyi graphs

degree complexity: proportional to Kullback-Leibler distance (so ≥ 0)
wiring complexity: proportional to mutual information (so ≥ 0)

Shannon entropy per bond
final result for directed graphs:
$\vec{k}_i = (k_i^{\rm in}, k_i^{\rm out})$

$$p(\mathbf{c}) = \sum_{\vec{\mathbf{k}}} \prod_i \left[{\rm d}\vec{k}_i \, p(\vec{k}_i) \right] \frac{\prod_i \delta_{\vec{k}_i, \vec{k}_i(\mathbf{c})}}{Z(\vec{\mathbf{k}}, W)} \prod_{i<j} \left[\frac{\langle k \rangle}{N} \frac{W(\vec{k}_i, \vec{k}_j)}{p(\vec{k}_i) p(\vec{k}_j)} \delta_{c_{ij},1} + \left(1 - \frac{\langle k \rangle}{N} \frac{W(\vec{k}_i, \vec{k}_j)}{p(\vec{k}_i) p(\vec{k}_j)} \right) \delta_{c_{ij},0} \right]$$

$$S = \underbrace{1 + \log(\frac{N}{\langle k \rangle})}_{\text{directed ER entropy}} - \Big\{ \underbrace{\frac{1}{\langle k \rangle} \sum_{\vec{k}} p(\vec{k}) \log[\frac{p(\vec{k})}{\pi(k^{\rm in})\pi(k^{\rm out})}]}_{\text{degree complexity}} + \underbrace{\sum_{\vec{k}, \vec{k}'} W(\vec{k}, \vec{k}') \log\left[\frac{W(\vec{k}, \vec{k}')}{W(\vec{k}) W(\vec{k}')} \right]}_{\text{wiring complexity}} \Big\} + \epsilon_N$$

$\lim_{N\to\infty} \epsilon_N = 0$

$\pi(\ell) = {\rm e}^{-\langle k \rangle} \langle k \rangle^\ell / \ell!$
$\pi(k^{\rm in})\pi(k^{\rm out})$: degree distr of directed Erdös-Renyi graphs

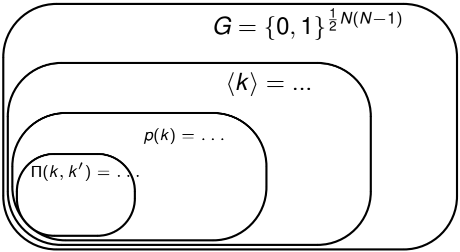
degree complexity: proportional to Kullback-Leibler distance (so ≥ 0)
wiring complexity: proportional to mutual information (so ≥ 0)

3. Generating tailored random graphs numerically

next:

generate
tailored random graphs

from these families
numerically ...



typical questions

G: all nondirected N-node graphs
$G[\mathbf{k}] \subset G$: all nondirected N-node graphs with degrees $\mathbf{k}$

how to generate

- random $\mathbf{c} \in G$, with specified probability $p(\mathbf{c})$
- random $\mathbf{c} \in G[\mathbf{k}]$, with uniform probability
- random $\mathbf{c} \in G[\mathbf{k}]$, with specified probability $p(\mathbf{c})$

similar for directed graphs ...

why is the generation of graphs a nontrivial issue?

- many users underestimate/misjudge what the real problem is:

  sampling the space of all graphs with given features: usually easy ...
  sampling them with required probabilities: nontrivial!

- many ad-hoc graph generation algorithms that *appear* sensible, but without proper analysis of which measure they converge to

- in cellular biology graphs are often used as 'null models', against which to test hypotheses on observed features in signalling networks

  if these null models are *biased*,
  the hypothesis test is fundamentally flawed ...

Fundamental limitations

since $\mathcal{N} = \exp(N\langle k\rangle S)$:
entropy crisis when S becomes zero
(nr of graphs with imposed features vanishes)

- nondirected:

$$S \approx \frac{1}{2}[1+\log(\frac{N}{\langle k\rangle})] - \frac{1}{\langle k\rangle}\sum_k p(k)\log[\frac{p(k)}{\pi(k)}] - \frac{1}{2}\sum_{k,k'} W(k,k')\log\left[\frac{W(k,k')}{W(k)W(k')}\right]$$

so graphs exist if

$$N > \langle k\rangle\, \mathrm{e}^{\frac{2}{\langle k\rangle}\sum_k p(k)\log[\frac{p(k)}{\pi(k)}] + \sum_{k,k'} W(k,k')\log\left[\frac{W(k,k')}{W(k)W(k')}\right] - 1}$$

- directed:

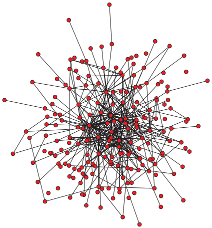
$$S \approx 1+\log(\frac{N}{\langle k\rangle}) - \frac{1}{\langle k\rangle}\sum_{\vec{k}} p(\vec{k})\log[\frac{p(\vec{k})}{\pi(k^{\rm in})\pi(k^{\rm out})}] - \sum_{\vec{k},\vec{k}'} W(\vec{k},\vec{k}')\log\left[\frac{W(\vec{k},\vec{k}')}{W(\vec{k})W(\vec{k}')}\right]\Big\}$$

so graphs exist if

$$N > \langle k\rangle\, \mathrm{e}^{\frac{1}{\langle k\rangle}\sum_{\vec{k}} p(\vec{k})\log[\frac{p(\vec{k})}{\pi(k^{\rm in})\pi(k^{\rm out})}] + \sum_{\vec{k},\vec{k}'} W(\vec{k},\vec{k}')\log\left[\frac{W(\vec{k},\vec{k}')}{W(\vec{k})W(\vec{k}')}\right] - 1}$$

trivial case: no constraints
standard Glauber/MCMC dynamics

(Metropolis et al 1953)



objective: generate random nondirected $\mathbf{c} \in \{0,1\}^{\frac{1}{2}N(N-1)}$
with specified probabilities $p(\mathbf{c})$

strategy: start from any graph $\mathbf{c}$
propose random moves $c_{ij} \to 1-c_{ij}$ (giving $\mathbf{c} \to F_{ij}\mathbf{c}$),

define acceptance probabilities $A(F_{ij}\mathbf{c}|\mathbf{c})$
via detailed balance condition

$$A(F_{ij}\mathbf{c}|\mathbf{c})p(\mathbf{c}) = A(\mathbf{c}|F_{ij}\mathbf{c})p(F_{ij}\mathbf{c}) \quad \to \quad A(\mathbf{c}'|\mathbf{c}) = \Big[1 + p(\mathbf{c})/p(\mathbf{c}')\Big]^{-1}$$

stochastic process is ergodic,
and converges to the distribution $p(\mathbf{c})$

practicalities:
equilibration can take a *very long* time,
so monitor Hamming distances

(trivially generalised
to directed graphs)

Matching algorithm

(Bender and Canfield, 1978)

objective: generate random nondirected graph $\mathbf{c} \in \{0,1\}^{\frac{1}{2}N(N-1)}$ with specified degree sequence $\mathbf{k} = (k_1, \ldots, k_N)$

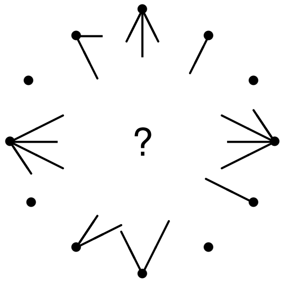
strategy: stochastic growth dynamics, starting from graph with no links

- initialisation: $c_{ij} = 0$ for all (i,j)

repeat:

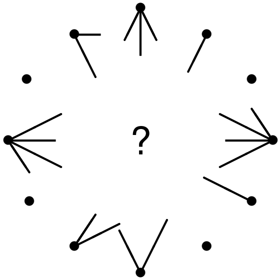
- pick at random two nodes (i,j)
- if $\sum_\ell c_{i\ell} < k_i$ and $\sum_\ell c_{j\ell} < k_j$:
  connect i and j
  $c_{ij} = 0 \;\rightarrow\; c_{ij} = 1$

terminate if $\sum_j c_{ij} = k_i$ for all i



(trivially generalised to directed graphs)

Matching algorithm
limitations and problems ...



- major limitation:

  cannot control graph probabilities, just aims to generate $\mathbf{c} \in G[\mathbf{k}]$ with equal probs

- inconvenience: convergence not guaranteed

  process can 'hang' before $\sum_j c_{ij} = k_i$ for all i if one remaining 'stub' requires self-loops (happens more often when there are 'hubs', i.e. nodes with large degree)

  – monitor the evolving degrees, to test for this
  – if process 'hangs': reject and start over again from empty graph

- sampling bias:

  if process 'hangs', users often don't reject the graph but do 'backtracking' (for CPU reasons), this creates correlations between graph realisations

  even if we reject rather than backtrack: no proof published yet that sampling measure $p(\mathbf{c})$ is flat ...

Edge switching algorithm

(Seidel, 1976)

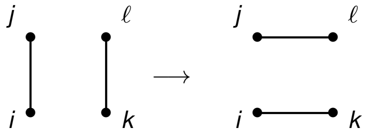
objective: generate random nondirected graph $\mathbf{c} \in \{0,1\}^{\frac{1}{2}N(N-1)}$
with specified degree sequence $\mathbf{k} = (k_1, \ldots, k_N)$

strategy: degree-preserving randomisation ('shuffling') process,
starting from any graph $\mathbf{k} = (k_1, \ldots, k_N)$

- initialisation: $c_{ij} = c_{ij}^0$ for all (i,j),
  where $\mathbf{c}^0$ is some graph
  with the correct degrees

repeat:

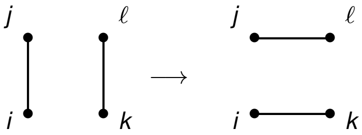
- pick at random four nodes (i,j,k,ℓ)
  that are *pairwise connected*
- carry out an 'edge swap'
  (or 'Seidel switch), see diagram
  (preserves all degrees!)



terminate if stochastic process has equilibrated

Edge switching algorithm

limitations and problems ...



- major limitation:

  cannot control graph probabilities, aims to generate $\mathbf{c} \in G[\mathbf{k}]$ with equal probs

- inconvenience: need for a 'seed graph' with the correct degrees $\mathbf{k} = (k_1, \ldots, k_N)$

- sampling bias:

  edge swaps are ergodic on $G[\mathbf{k}]$ (Taylor, 1981), but sampling is *not uniform*!

  nr of possible moves depends on state **c**!

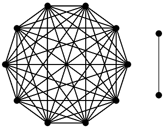
  result:
  stationary state of Markov chain favours high-mobility graphs

many possible moves *only one move ...*

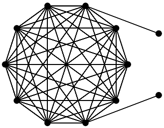
dangerous for scale-free graphs ...

target:
uniform measure $p(\mathbf{c})$
on $G[\mathbf{k}]$

1 *graph*
$n(\mathbf{c}) = (N-2)(N-3)$



$(N-2)(N-3)$ *graphs*
$n(\mathbf{c}) = 2(N-3)$



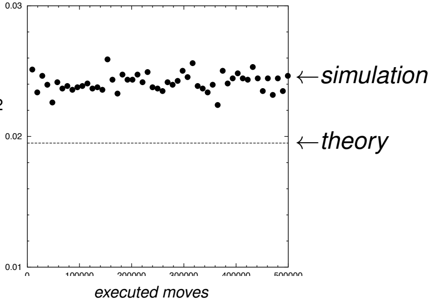
for flat measure:

$$\langle n(\mathbf{c})\rangle = \frac{(N-2)(N-3) + (N-2)(N-3).2(N-3)}{1+(N-2)(N-3)}$$
$$= \frac{(N-2)(N-3)[1+2(N-3)]}{1+(N-2)(N-3)}$$

$N = 100$:
$\langle n(\mathbf{c})\rangle/N^2 \approx 0.0195$

'accept all'
edge swapping:

$\overline{n(\mathbf{c})}/N^2$



4. Constrained Markovian graph dynamics

need to study graph dynamics more systematically ...

Monte Carlo processes for constrained graphs

- constraints:
  $G[\star] \subseteq G$: all $\mathbf{c} \in G$ that satisfy constraints $\star$

- stochastic graph dynamics as a Markov chain,
  transition probabilities $W(\mathbf{c}|\mathbf{c}')$ for the move $\mathbf{c}' \to \mathbf{c}$
  $n \in \mathbb{N}$: algorithmic time

$$\forall \mathbf{c} \in G[\star]: \qquad p_{n+1}(\mathbf{c}) = \sum_{\mathbf{c}' \in G[\star]} W(\mathbf{c}|\mathbf{c}')p_n(\mathbf{c}')$$

- allowed moves (exclude identity):

  Φ: set of allowed moves $F: G_F[\star] \to G[\star]$
  $G_F[\star]$: those $\mathbf{c} \in G[\star]$ on which F can act

  all moves are auto-invertible: $(\forall F \in \Phi): \; F^2 = 1\!\!1$
  Φ is ergodic on $G[\star]$

MCMC objective

construct transition probs $W(\mathbf{c}|\mathbf{c}')$, based on moves $F \in \Phi$, such that process converges to $p(\mathbf{c}) = Z^{-1} e^{-H(\mathbf{c})}$ on $G[\star]$

$$W(\mathbf{c}|\mathbf{c}') = \sum_{F\in\Phi} q(F|\mathbf{c}') \Big[\delta_{\mathbf{c},F\mathbf{c}'} A(F\mathbf{c}'|\mathbf{c}') + \delta_{\mathbf{c},\mathbf{c}'}[1 - A(F\mathbf{c}'|\mathbf{c}')]\Big]$$

$$q(F|\mathbf{c}): \quad \textit{move proposal probability}$$
$$A(\mathbf{c}|\mathbf{c}'): \quad \textit{move acceptance probability}$$

- graph mobility $n(\mathbf{c})$:

$$n(\mathbf{c}) = \sum_{F\in\Phi} I_F(\mathbf{c}), \qquad I_F(\mathbf{c}) = \begin{cases} 1 & \textit{if } \mathbf{c} \in G_F[\star] \\ 0 & \textit{if } \mathbf{c} \notin G_F[\star] \end{cases}$$

- detailed balance condition:

$$(\forall F\in\Phi)(\forall \mathbf{c}\in G[\star]): \qquad q(F|\mathbf{c})A(F\mathbf{c}|\mathbf{c})\mathrm{e}^{-H(\mathbf{c})} = q(F|F\mathbf{c})A(\mathbf{c}|F\mathbf{c})\mathrm{e}^{-H(F\mathbf{c})}$$

if allowed F equally probable:
$q(F|\mathbf{c}) = I_F(\mathbf{c})/n(\mathbf{c})$

$$(\forall F\in\Phi)(\forall \mathbf{c}\in G_F[\star]): \qquad \frac{1}{n(\mathbf{c})}A(F\mathbf{c}|\mathbf{c})\mathrm{e}^{-H(\mathbf{c})} = \frac{1}{n(F\mathbf{c})}A(\mathbf{c}|F\mathbf{c})\mathrm{e}^{-H(F\mathbf{c})}$$

canonical Markov chain

ergodic auto-invertible moves $F \in \Phi$,
convergence to $p(\mathbf{c}) = Z^{-1} e^{-H(\mathbf{c})}$ on $G[\star]$
for acceptance probabilities

$$A(\mathbf{c}|\mathbf{c}') = \frac{n(\mathbf{c}')\mathrm{e}^{-\frac{1}{2}[H(\mathbf{c})-H(\mathbf{c}')]}}{n(\mathbf{c}')e^{-\frac{1}{2}[H(\mathbf{c})-H(\mathbf{c}')]} + n(\mathbf{c})\mathrm{e}^{\frac{1}{2}[H(\mathbf{c})-H(\mathbf{c}')]}}$$

conventional edge-swapping?
$(\forall \mathbf{c}, \mathbf{c}') : \; A(\mathbf{c}|\mathbf{c}') = 1$

$$(\forall F, \mathbf{c}) : \; \frac{A(F\mathbf{c}|\mathbf{c})\mathrm{e}^{-H(\mathbf{c})}}{n(\mathbf{c})} = \frac{A(\mathbf{c}|F\mathbf{c})\mathrm{e}^{-H(F\mathbf{c})}}{n(F\mathbf{c})} \quad \rightarrow \quad (\forall F, \mathbf{c}) : \; \frac{\mathrm{e}^{-H(\mathbf{c})}}{n(\mathbf{c})} = \frac{\mathrm{e}^{-H(F\mathbf{c})}}{n(F\mathbf{c})}$$

corresponds to
$H(\mathbf{c}) = -\log n(\mathbf{c})$,
so would give

$$\textit{sampling bias}: \quad p(\mathbf{c}) = \frac{n(\mathbf{c})}{\sum_{\mathbf{c}' \in G[\star]} n(\mathbf{c}')}$$

Master equation representation of the process

$$\textit{Markov chain}: \quad p_{n+1}(\mathbf{c}) = \sum_{\mathbf{c}'} W(\mathbf{c}|\mathbf{c}')p_n(\mathbf{c}')$$

- from integer to real times:

  continuous time process, $p_t(\mathbf{c})$, $t \in [0, \infty\rangle$
  via *random durations* of MC steps,
  $\pi_n(t)$: prob that n MC steps have been made at time t

$$p_t(\mathbf{c}) = \sum_{n\geq 0} \pi_n(t)p_n(\mathbf{c})$$

  choose $\pi_m(t) = (t/\tau)^m \mathrm{e}^{-t/\tau}/m!$:
  so $\langle m\rangle = t/\tau$

$$\tau\frac{\mathrm{d}}{\mathrm{d}t}\pi_0(t) = -\pi_0(t) \qquad \tau\frac{\mathrm{d}}{\mathrm{d}t}\pi_{m>0}(t) = \pi_{m-1}(t) - \pi_m(t)$$

$$\begin{aligned}\tau\frac{\mathrm{d}}{\mathrm{d}t}p_t(\mathbf{c}) &= \sum_{n>0} \pi_{n-1}(t)p_n(\mathbf{c}) - \sum_{n\geq 0} \pi_n(t)p_n(\mathbf{c}) \\ &= \sum_{\mathbf{c}'} W(\mathbf{c}|\mathbf{c}')p_t(\mathbf{c}') - p_t(\mathbf{c})\end{aligned}$$

- work out details (not done here), using $\Delta_F U(\mathbf{c}) = U(F\mathbf{c}) - U(\mathbf{c})$

$$\tau \frac{\mathrm{d}}{\mathrm{d}t} p_t(\mathbf{c}) = \sum_{F\in\Phi} I_F(\mathbf{c}) \left\{ \frac{w_F^+(\mathbf{c})}{n(F\mathbf{c})} p_t(F\mathbf{c}) - \frac{w_F^-(\mathbf{c})}{n(\mathbf{c})} p_t(\mathbf{c}) \right\}$$

$$\text{`}\textit{edge swap}' \ \textit{rates}: \qquad w_F^{\pm}(\mathbf{c}) = \frac{1}{2} \pm \frac{1}{2} \tanh\left[\frac{1}{2}\Delta_F[H(\mathbf{c}) + \log n(\mathbf{c})]\right]$$

(very similar to master eqn for spin dynamics)

expectation values of observables, $\langle f(\mathbf{c})\rangle = \sum_{\mathbf{c}} p_t(\mathbf{c}) f(\mathbf{c})$:

$$\tau \frac{\mathrm{d}}{\mathrm{d}t} \langle f(\mathbf{c})\rangle = \sum_F \left\langle \frac{I_F(\mathbf{c})}{n(\mathbf{c})} w_F^-(\mathbf{c}) \Delta_F f(\mathbf{c}) \right\rangle$$

Convergence of the process

to show: $\lim_{t\to\infty} p_t(\mathbf{c}) = \mathrm{e}^{-H(\mathbf{c})}/Z$ for all $\mathbf{c}$

requires only:

(i) $(\forall \mathbf{c}):\ \frac{\mathrm{d}}{\mathrm{d}t} p_t(\mathbf{c}) = \sum_{\mathbf{c}'} W(\mathbf{c}|\mathbf{c}')p_t(\mathbf{c}') - p_t(\mathbf{c})$

(ii) $(\forall \mathbf{c},\mathbf{c}'):\ W(\mathbf{c}|\mathbf{c}')\mathrm{e}^{-H(\mathbf{c}')} = W(\mathbf{c}'|\mathbf{c})\mathrm{e}^{-H(\mathbf{c})}$

(iii) ergodicity: $(\forall \mathbf{c},\mathbf{c}')(\exists \ell \in \mathbb{N}):\ W^{\ell}(\mathbf{c}|\mathbf{c}') > 0$

Proof (standard but nice ...)

- define a quantity to act Lyapunov function

$$\textit{let}\quad \hat{p}(\mathbf{c}) = Z^{-1}\mathrm{e}^{-H(\mathbf{c})}, \qquad L(t) = \sum_{\mathbf{c}\in G[\star]} p_t(\mathbf{c}) \log[p_t(\mathbf{c})/\hat{p}(\mathbf{c})]$$

$L(t)$ is a Kullback-Leibler distance (information theory),
$L(t) \geq 0$ for all t, $L(t) = 0$ if and only if $p_t = \hat{p}$
so we need to show only: $\lim_{t\to\infty} L(t) = 0$

$$L(t) = \sum_{\mathbf{c}} p_t(\mathbf{c})\Big[\log p_t(\mathbf{c}) + H(\mathbf{c})\Big] + \log Z$$

- evolution of $L(t)$:

$$\tau\frac{\mathrm{d}}{\mathrm{d}t}L(t) = \tau\frac{\mathrm{d}}{\mathrm{d}t}\sum_{\mathbf{c}} p_t(\mathbf{c})[\log p_t(\mathbf{c})+H(\mathbf{c})]$$

$$= \sum_{\mathbf{c}}\Big[\log p_t(\mathbf{c})+H(\mathbf{c})+1\Big]\Big[\sum_{\mathbf{c}'} W(\mathbf{c}|\mathbf{c}')p_t(\mathbf{c}') - p_t(\mathbf{c})\Big]$$

$$= \sum_{\mathbf{c}\mathbf{c}'}\Big[\log p_t(\mathbf{c})+H(\mathbf{c})+1\Big]\Big[W(\mathbf{c}|\mathbf{c}')p_t(\mathbf{c}') - W(\mathbf{c}'|\mathbf{c})p_t(\mathbf{c})\Big]$$

$$= \frac{1}{2}\sum_{\mathbf{c}\mathbf{c}'}\Big[\Big(\log p_t(\mathbf{c})+H(\mathbf{c})\Big)-\Big(\log p_t(\mathbf{c}')+H(\mathbf{c}')\Big)\Big]\Big[W(\mathbf{c}|\mathbf{c}')p_t(\mathbf{c}')-W(\mathbf{c}'|\mathbf{c})p_t(\mathbf{c})\Big]$$

use detailed balance:

$$W(\mathbf{c}'|\mathbf{c}) = \mathrm{e}^{H(\mathbf{c})}\Big(W(\mathbf{c}'|\mathbf{c})\mathrm{e}^{-H(\mathbf{c})}\Big) = \mathrm{e}^{H(\mathbf{c})}\Big(W(\mathbf{c}|\mathbf{c}')\mathrm{e}^{-H(\mathbf{c}')}\Big)$$

now, with $\phi(\mathbf{c}) = H(\mathbf{c})+\log p_t(\mathbf{c})$:

$$\tau\frac{\mathrm{d}}{\mathrm{d}t}L(t) = \frac{1}{2}\sum_{\mathbf{c}\mathbf{c}'} W(\mathbf{c}|\mathbf{c}')\mathrm{e}^{-H(\mathbf{c}')}\Big[\phi(\mathbf{c})-\phi(\mathbf{c}')\Big]\Big[\mathrm{e}^{H(\mathbf{c}')}p_t(\mathbf{c}')-\mathrm{e}^{H(\mathbf{c})}p_t(\mathbf{c})\Big]$$

$$= \frac{1}{2}\sum_{\mathbf{c}\mathbf{c}'} W(\mathbf{c}|\mathbf{c}')\mathrm{e}^{-H(\mathbf{c}')}\Big[\phi(\mathbf{c})-\phi(\mathbf{c}')\Big]\Big[\mathrm{e}^{\phi(\mathbf{c}')}-\mathrm{e}^{\phi(\mathbf{c})}\Big] \;\leq\; 0$$

$(e^x-e^y)(x-y)\geq 0$, equality only if $x=y$

since $\mathrm{d}L/\mathrm{d}t \leq 0$ and $L(t) \geq 0$:
$\lim_{t\to\infty} \mathrm{d}L/\mathrm{d}t = 0$

last step, stationarity: $\frac{\mathrm{d}}{\mathrm{d}t} L(t) = 0$

$$(\forall \mathbf{c}, \mathbf{c}') : \qquad W(\mathbf{c}|\mathbf{c}') = 0 \quad \textit{or} \quad H(\mathbf{c}) + \log p(\mathbf{c}) = H(\mathbf{c}') + \log p(\mathbf{c}')$$
$$(\forall \mathbf{c}, \mathbf{c}') : \qquad W(\mathbf{c}|\mathbf{c}') = 0 \quad \textit{or} \quad p(\mathbf{c}) \mathrm{e}^{H(\mathbf{c})} = p(\mathbf{c}') \mathrm{e}^{H(\mathbf{c}')}$$

since process is ergodic:

any state $\mathbf{c}$ can be reached from any $\mathbf{c}'$
by a sequence of intermediate states
with nonzero transition probabilities,

hence

$$p(\mathbf{c}) \mathrm{e}^{H(\mathbf{c})} = \textit{const} \quad \Rightarrow \quad p(\mathbf{c}) = Z^{-1} \mathrm{e}^{-H(\mathbf{c})} = \hat{p}(\mathbf{c})$$

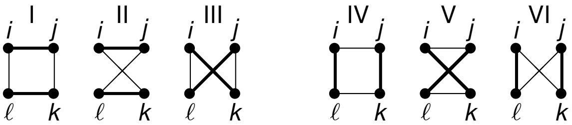
bookkeeping of elementary moves

- constraints: imposed degrees, so graph set is $G[\mathbf{k}]$

  ergodic set Φ of admissible moves:
  edge swaps $F: G_F[\mathbf{k}] \to G[\mathbf{k}]$

  $\{(i,j,k,\ell) \in \{1,\ldots,N\}^4 |\ i<j<k<\ell\}$, ordered node quadruplets

  possible edge swaps to act on (i,j,k,ℓ):



- group into pairs (I,IV), (II,V), and (III,VI)
  auto-invertible swaps: $F_{ijk\ell;\alpha}$, with $i<j<k<\ell$ and $\alpha \in \{1,2,3\}$

  $I_{ijk\ell;\alpha}(\mathbf{c}) = 1$:

$$F_{ijk\ell;\alpha}(\mathbf{c})_{qr} = 1 - c_{qr} \quad \text{for } (q,r) \in \mathcal{S}_{ijk\ell;\alpha}$$
$$F_{ijk\ell;\alpha}(\mathbf{c})_{qr} = c_{qr} \quad \text{for } (q,r) \notin \mathcal{S}_{ijk\ell;\alpha}$$

$$\mathcal{S}_{ijk\ell;1} = \{(i,j),(k,\ell),(i,\ell),(j,k)\}, \quad \mathcal{S}_{ijk\ell;2} = \{(i,j),(k,\ell),(i,k),(j,\ell)\}$$
$$\mathcal{S}_{ijk\ell;3} = \{(i,k),(j,\ell),(i,\ell),(j,k)\}$$

to implement the Markov chain,
need **analytical formula for the graph mobility**

$n(\mathbf{c}) = \sum_{i<j<k<\ell}^{N} \sum_{\alpha=1}^{3} I_{ijk\ell;\alpha}(\mathbf{c})$

$$\begin{aligned}
I_{ijk\ell;1}(\mathbf{c}) &= c_{ij}c_{k\ell}(1-c_{i\ell})(1-c_{jk}) + (1-c_{ij})(1-c_{k\ell})c_{i\ell}c_{jk} \\
I_{ijk\ell;2}(\mathbf{c}) &= c_{ij}c_{k\ell}(1-c_{ik})(1-c_{j\ell}) + (1-c_{ij})(1-c_{k\ell})c_{ik}c_{j\ell} \\
I_{ijk\ell;3}(\mathbf{c}) &= c_{ik}c_{j\ell}(1-c_{i\ell})(1-c_{jk}) + (1-c_{ik})(1-c_{j\ell})c_{i\ell}c_{jk}
\end{aligned}$$

combinatorial problem:
$(\overline{\delta}_{ij} = 1-\delta_{ij})$

$$\begin{aligned}
n(\mathbf{c}) &= \sum_{i<j<k<\ell} \overbrace{\Big(I_{ijk\ell;1(\mathbf{c})} + I_{ijk\ell;2(\mathbf{c})} + I_{ijk\ell;3(\mathbf{c})}\Big)}^{\textit{invariant under all permutations of } (i,j,k,\ell)} \\
&= \frac{1}{4!}\sum_{ijk\ell} \overline{\delta}_{ij}\overline{\delta}_{ik}\overline{\delta}_{i\ell}\overline{\delta}_{jk}\overline{\delta}_{j\ell}\overline{\delta}_{k\ell} \sum_{\alpha=1}^{3} I_{ijk\ell;\alpha(\mathbf{c})} && (\textit{permutation invariance}) \\
&= \frac{1}{4}\sum_{ijk\ell} \overline{\delta}_{ij}\overline{\delta}_{ik}\overline{\delta}_{i\ell}\overline{\delta}_{jk}\overline{\delta}_{j\ell}\overline{\delta}_{k\ell} c_{ij}c_{k\ell}(1-c_{i\ell})(1-c_{jk}) && (\textit{permutation, inversion}) \\
&= \frac{1}{4}\sum_{ijk\ell} \overline{\delta}_{ik}\overline{\delta}_{i\ell}\overline{\delta}_{jk}\overline{\delta}_{j\ell} c_{ij}c_{k\ell}(1-c_{i\ell})(1-c_{jk}) && (\textit{no diagonal entries})
\end{aligned}$$

work out remaining terms explicitly ...

$$n(\mathbf{c}) = \underbrace{\frac{1}{4}N^2\langle k\rangle^2 + \frac{1}{4}N\langle k\rangle - \frac{1}{2}N\langle k^2\rangle}_{invariant} + \underbrace{\frac{1}{4}\mathrm{Tr}(\mathbf{c}^4) + \frac{1}{2}\mathrm{Tr}(\mathbf{c}^3) - \frac{1}{2}\sum_{ij} k_i c_{ij} k_j}_{state\ dependent}$$

Examples:

- Fully connected graphs:
  $k_i = N-1$ for all i, $\mathrm{Tr}(\mathbf{c}^4) = (N-1)[(N-1)^3+1]$, $\mathrm{Tr}(\mathbf{c}^3) = N(N-1)(N-2)$
  formula: $n(\mathbf{c}) = 0$ *(ok by inspection)*

- Periodic chains $c_{ij} = \delta_{i,j-1} + \delta_{i,j+1}$ (mod N), $N \geq 4$:
  $k_i = 2$ for all i, $\mathrm{Tr}(\mathbf{c}^4) = 6N$, $\mathrm{Tr}(\mathbf{c}^3) = 0$
  formula: $n(\mathbf{c}) = N(N-4)$ *(ok by inspection)*

- Two isolated links $c_{12} = c_{21} = c_{34} = c_{43} = 1$, all other $c_{ij} = 0$:
  $k_1 = k_2 = k_3 = k_4 = 1$, $k_{i>4} = 0$, $\mathrm{Tr}(\mathbf{c}^4) = 4$, $\mathrm{Tr}(\mathbf{c}^3) = 0$
  formula: $n(\mathbf{c}) = 2$ *(ok by inspection)*

- Regular random graphs with $p(k) = \delta_{k,2}$:
  use eigenvalue distribution of $\mathbf{c}$ (Dorogovtsev 2003),
  formula: $n(\mathbf{c}) = N(N-4) + o(N)$

$$n(\mathbf{c}) = \underbrace{\frac{1}{4}N^2\langle k\rangle^2 + \frac{1}{4}N\langle k\rangle - \frac{1}{2}N\langle k^2\rangle}_{invariant} + \underbrace{\frac{1}{4}\mathrm{Tr}(\mathbf{c}^4) + \frac{1}{2}\mathrm{Tr}(\mathbf{c}^3) - \frac{1}{2}\sum_{ij} k_i c_{ij} k_j}_{state\ dependent}$$

practicalities

how to avoid calculating $n(\mathbf{c})$ at each iteration step,

- use simple bounds:

$$\frac{N}{4}\Big(N\langle k\rangle^2+\langle k\rangle-\langle k^2\rangle\Big) - \frac{N}{2}\langle k^2\rangle k_{\rm max} \leq n(\mathbf{c}) \leq \frac{N}{4}\Big(N\langle k\rangle^2+\langle k\rangle-\langle k^2\rangle\Big)$$

  state-dependent part can be ignored if $\langle k^2\rangle k_{\rm max}/\langle k\rangle^2 \ll N$

- (i) calculate $n(\mathbf{c})$ only at time $n=0$

  (ii) update $n(\mathbf{c})$ dynamically, by calculating at each step change $\Delta_{ijk\ell;\alpha} n(\mathbf{c})$ for executed move $F_{ijk\ell;\alpha}$

  e.g.

$$\Delta_{ijk\ell;\alpha}\mathrm{Tr}(\mathbf{c}^3) = 6 \sum_{(a,b)\in S_{ijk\ell;\alpha},\ a<b} (1-2c_{ab}) \sum_{v\notin\{i,j,k,\ell\}} c_{bv}c_{va}$$

$$\Delta_{ijk\ell;\alpha}\mathrm{Tr}(\mathbf{c}^4) = \textit{ more complicated but explicit formula ...}$$

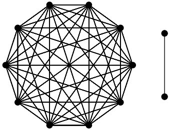
Example:

target =
uniform measure on $G[\mathbf{k}]$

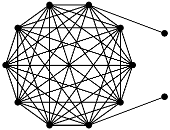
$N = 100$

naive versus correct
acceptance probabilities

many possible moves



only <u>one</u> move ...

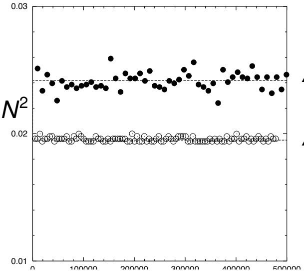


predictions:

$p(\mathbf{c}) = \textit{constant}$:
$\overline{n(\mathbf{c})}/N^2 \approx 0.0195$

$p(\mathbf{c}) = n(\mathbf{c})/Z$:
$\overline{n(\mathbf{c})}/N^2 \approx 0.0242$

$\overline{n(\mathbf{c})}/N^2$



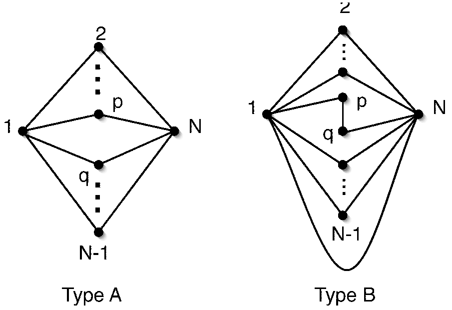
executed moves

$A(\mathbf{c}|\mathbf{c}') = 1$

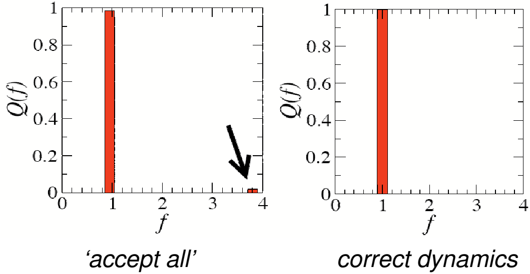
$A(\mathbf{c}|\mathbf{c}') = [1 + \frac{n(\mathbf{c})}{n(\mathbf{c}')}]^{-1}$

Example

graph type A: $n(\mathbf{c}) = K(K-1)$
graph type B: $n(\mathbf{c}) = 2(K-1)$

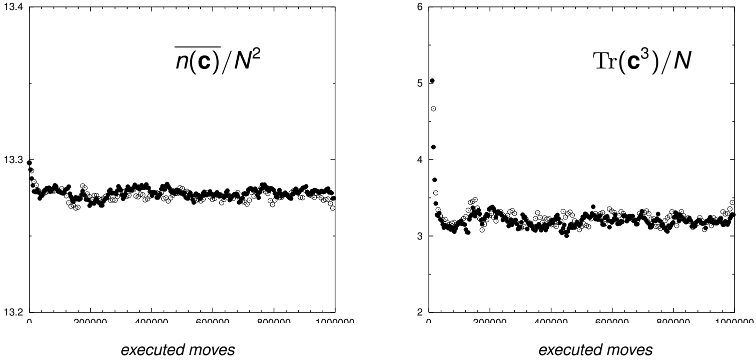


measure distribution $Q(f)$ of (rescaled) frequencies at which graphs are visited



Example

human protein interaction network
$N = 9463$, $\langle k \rangle \approx 7.4$

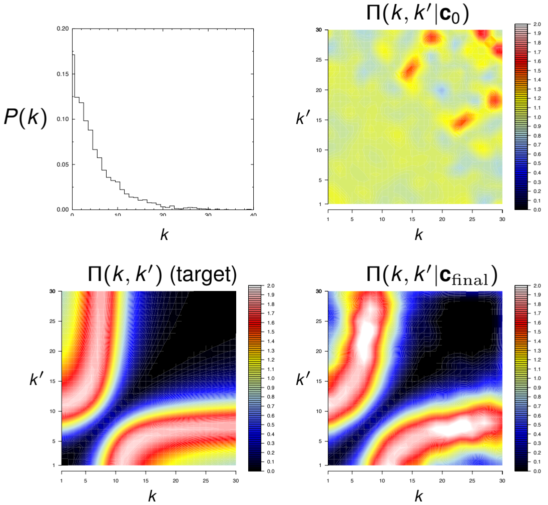


●: 'accept all' edge swap dynamics
o: correct edge swap dynamics

(so no serious harm done yet ...)

Example

target = degree-correlated measure on $G[\mathbf{k}]$



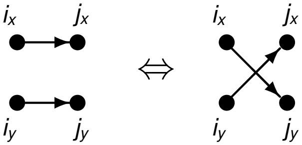
$N = 4000$,
$\overline{k} = 5$

$$\Pi(k,k') = \frac{(k-k')^2}{[\beta_1 - \beta_2 k + \beta_3 k^2][\beta_1 - \beta_2 k' + \beta_3 k'^2]}$$

bookkeeping of elementary moves

- constraints: imposed in-out degrees, so graph set is $G[\mathbf{k}^{\rm in},\mathbf{k}^{\rm out}]$

  set Φ of admissible moves:
  directed edge swaps $F: G_F[\mathbf{k}^{\rm in},\mathbf{k}^{\rm out}] \to G[\mathbf{k}^{\rm in},\mathbf{k}^{\rm out}]$



- auto-invertible edge-swaps:
  Let $\Lambda = \{(i,j)\in N^2 |\ c_{ji}=1\}$

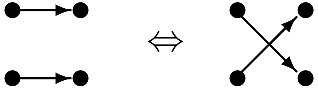
$$I_{(i_x,j_x),(i_y,j_y);\square} = \begin{cases} 1 & \textit{if } (i_x,j_x),(i_y,j_y)\in\Lambda \text{ and } (i_x,j_y),(i_y,j_x)\notin\Lambda \\ 0 & \text{otherwise} \end{cases}$$

If $I_{(i_x,j_x),(i_y,j_y);\square}=1$:

$$\begin{aligned} F_{(i_x,j_x),(i_y,j_y);\square}(\mathbf{c})_{ij} &= 1-c_{ij} && \text{if } i\in\{i_x,i_y\} \text{ and } j\in\{j_x,j_y\} \\ F_{(i_x,j_x),(i_y,j_y);\square}(\mathbf{c})_{ij} &= c_{ij} && \text{otherwise} \end{aligned}$$

for **nondirected** graphs:
edge swaps are *ergodic* set of moves
(Taylor, 1981 – proof based on Lyapunov function)

for **directed** graphs:
are edge swaps *ergodic* set of moves?



Rao, 1996:

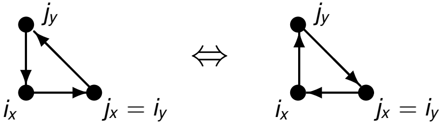
unless self-interactions are allowed,
edge swaps *not ergodic for directed graphs*

proof:
by counterexample

these two $N = 3$ graphs
are both in $G[\mathbf{k}^{\rm in}, \mathbf{k}^{\rm out}]$,
with $\mathbf{k}^{\rm in} = \mathbf{k}^{\rm out} = (1, 1, 1)$

but *no edge swap maps one to the other*

further move type required
to restore ergodicity:
3-loop reversal



$$I_{(i_x,j_x),(i_y,j_y);\triangle} = \begin{cases} 1 & \textit{if } (i_x,j_x),(i_y,j_y),(j_y,i_x) \in \Lambda \;\; \textit{and} \;\; x_j = y_i \\ & \textit{and} \;\; (j_x,i_x),(j_y,i_y),(i_x,j_y) \notin \Lambda \\ 0 & \text{otherwise} \end{cases}$$

$$\begin{aligned} F_{(i_x,j_x),(i_y,j_y);\triangle}(\mathbf{c})_{ij} &= 1 - c_{ij} \quad \textit{for } (i,j) \in \mathcal{S}_{i_x,j_x,j_y} \\ F_{(i_x,j_x),(i_y,j_y);\triangle}(\mathbf{c})_{ij} &= c_{ij} \quad\quad\;\; \textit{for } (i,j) \notin \mathcal{S}_{i_x,j_x,j_y} \end{aligned}$$

$$\mathcal{S}_{abc} = \{(a,b),(b,c),(c,a),(b,a),(c,b),(a,c)\}$$

to implement the Markov chain,
need to calculate graph mobility **analytically**:

$$\begin{aligned} n(\mathbf{c}) &= n_\square(\mathbf{c}) + n_\triangle(\mathbf{c}) \\ &= \sum_{(i_x,j_x),(i_y,j_y)\in\Lambda} I_{(i_x,j_x),(i_y,j_y);\square} + \sum_{(i_x,j_x),(i_y,j_y)\in\Lambda} I_{(i_x,j_x),(i_y,j_y);\triangle} \end{aligned}$$

$$\begin{aligned} I_{(i_x,j_x),(i_y,j_y);\square} &= c_{i_x,j_x} c_{i_y,j_y} (1-c_{i_x,j_y})(1-c_{i_y,j_x}) \\ I_{(i_x,j_x),(i_y,j_y);\triangle} &= \delta_{x_j,y_i}\; c_{i_x,j_x} c_{i_y,j_y} c_{j_y,i_x} (1-c_{j_x,i_x})(1-c_{j_y,i_y})(1-c_{i_x,j_y}) \end{aligned}$$

combinatorial problem again easily solved:

$$n_\square(\mathbf{c}) = \underbrace{\frac{1}{2}N^2\langle k\rangle^2 - \sum_j k_j^{\rm in} k_j^{\rm out}}_{invariant} + \underbrace{\frac{1}{2}{\rm Tr}(\mathbf{c}^2) + \frac{1}{2}{\rm Tr}(\mathbf{c}^\dagger\mathbf{c}\mathbf{c}^\dagger\mathbf{c}) + {\rm Tr}(\mathbf{c}^2\mathbf{c}^\dagger) - \sum_{ij} k_i^{\rm in} c_{ij} k_j^{\rm out}}_{state\ dependent}$$

$$n_\triangle(\mathbf{c}) = \underbrace{\frac{1}{3}{\rm Tr}(\mathbf{c}^3) - {\rm Tr}(\hat{\mathbf{c}}\mathbf{c}^2) + {\rm Tr}(\hat{\mathbf{c}}^2\mathbf{c}) - \frac{1}{3}{\rm Tr}(\hat{\mathbf{c}}^3)}_{state\ dependent}$$

with: $(\mathbf{c}^\dagger)_{ij} = c_{ji}$, $\hat{\mathbf{c}}_{ij} = c_{ij}c_{ji}$

$$n_\square(\mathbf{c}) = \frac{1}{2}N^2\langle k\rangle^2 - \sum_j k_j^{\rm in}k_j^{\rm out} + \frac{1}{2}{\rm Tr}(\mathbf{c}^2) + \frac{1}{2}{\rm Tr}(\mathbf{c}^\dagger\mathbf{c}\mathbf{c}^\dagger\mathbf{c}) + {\rm Tr}(\mathbf{c}^2\mathbf{c}^\dagger) - \sum_{ij} k_i^{\rm in}c_{ij}k_j^{\rm out}$$

$$n_\triangle(\mathbf{c}) = \frac{1}{3}{\rm Tr}(\mathbf{c}^3) - {\rm Tr}(\hat{\mathbf{c}}\mathbf{c}^2) + {\rm Tr}(\hat{\mathbf{c}}^2\mathbf{c}) - \frac{1}{3}{\rm Tr}(\hat{\mathbf{c}}^3)$$

practicalities

how to avoid calculating $n_\square(\mathbf{c})$ and $n_\triangle(\mathbf{c})$ at each iteration step,

- use simple bounds on $n_\square(\mathbf{c})$ and $n_\triangle(\mathbf{c})$,
  state-dependent part can be ignored if

$$\frac{1}{\langle k\rangle} + \frac{2}{\langle k\rangle^2}\Big(k_{\rm max}^{\rm in}\langle k^{{\rm out}\ 2}\rangle + k_{\rm max}^{\rm out}\langle k^{{\rm in}\ 2}\rangle\Big) \ll N$$

- (i) calculate $n_\square(\mathbf{c})$ and $n_\triangle(\mathbf{c})$ only at time $n=0$
  (ii) update $n_\square(\mathbf{c})$ and $n_\triangle(\mathbf{c})$ dynamically, by calculating at each step change $\Delta_{ijk\ell;\alpha}n_\square(\mathbf{c})$ and $\Delta_{ijk\ell;\alpha}n_\triangle(\mathbf{c})$ for executed move $F_{ijk\ell;\alpha}$

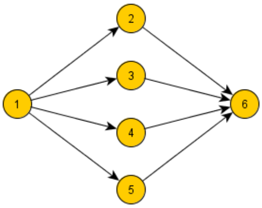
Example

$(k_1^{\rm in}, k_1^{\rm out}) = (0, N-2)$

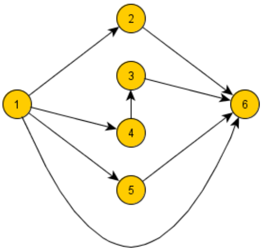
$i = 2 \ldots N-1$:
$(k_i^{\rm in}, k_i^{\rm out}) = (1, 1)$

$(k_N^{\rm in}, k_N^{\rm out}) = (N-2, 0)$

$(N-2)(N-3)$ moves



$2N-7$ moves



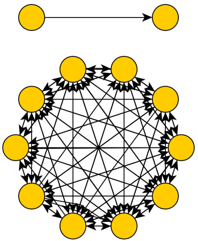
predicted values versus
equilibrated dynamics for $\overline{n(\mathbf{c})}/N^2$:

	prediction for $p(\mathbf{c}) = const$	dynamics with $A(\mathbf{c}\|\mathbf{c}') = 1$	dynamics with $A(\mathbf{c}\|\mathbf{c}') = [1 + \frac{n(\mathbf{c})}{n(\mathbf{c}')}]^{-1}$
$N = 17$:	27.87	33.59	27.87
$N = 27$:	47.92	58.32	47.95

Example

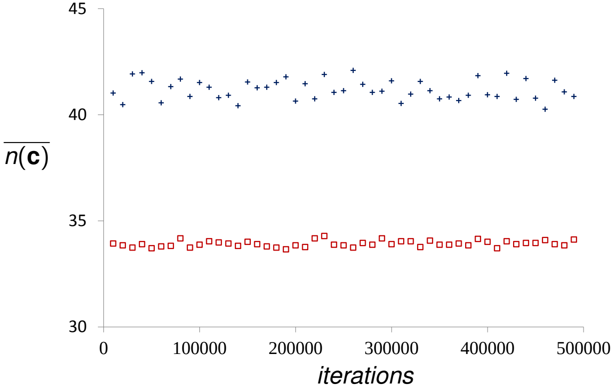
fully connected 'core' of $N-2$ nodes, plus two extra nodes

$N = 20$, target: flat measure



'accept all' edge swapping:
$\overline{n(\mathbf{c})})\rangle \approx 41.09$
predicted: 41.03

edge swapping with correct acceptance probabilities:
$\overline{n(\mathbf{c})} \approx 33.92$
predicted: 33.89



Looking ahead ...

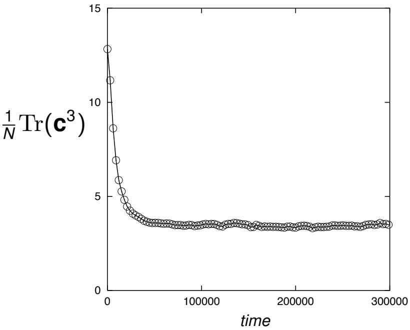
- direct generalisations and extensions:
  – weigthed graphs: $c_{ij} \in \mathbb{R}$
  – generalised degrees: $k_{i\ell}(\mathbf{c}) = \sum_j (\mathbf{c}^\ell)_{ij}$

- study the edge-swap relaxation dynamics?
  (evolution of macroscopic observables $\psi(\mathbf{c})$)

- new macroscopic characterisations
  beyond $p(k)$ and $W(k, k')$?

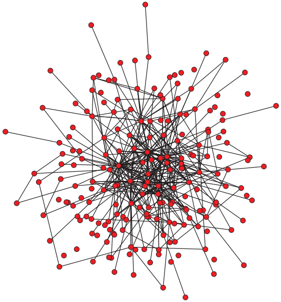
tailored graph ensembles characterised by statistics of **short loops** ...

(in addition to degrees and degree correlations)



all our current analytical techniques work only for locally tree-like graphs ...

simplest graph ensemble with short loops (Strauss ensemble)



$\overline{k}$: average nr of links per node
$\overline{m}$: average nr of triangles per node

$$p(\mathbf{c}) = \frac{1}{Z(u,v)}\, \mathrm{e}^{u\sum_{ij} c_{ij} + v\sum_{ijk} c_{ij}c_{jk}c_{ki}}$$

$$\overline{k} = \sum_{\mathbf{c}} p(\mathbf{c}) \frac{1}{N}\sum_{ij} c_{ij}, \qquad \overline{m} = \sum_{\mathbf{c}} p(\mathbf{c}) \frac{1}{N}\sum_{ijk} c_{ij}c_{jk}c_{ki}$$

generating function:
$\phi(u,v) = N^{-1}\log Z(u,v)$

$$\overline{k} = \frac{\partial}{\partial u}\phi(u,v), \qquad \overline{m} = \frac{\partial}{\partial v}\phi(u,v), \qquad S = \phi(u,v) - u\overline{k} - v\overline{m}$$

$$\phi(u,v) = \frac{1}{N}\log \sum_{\mathbf{c}} \mathrm{e}^{u\sum_{ij} c_{ij} + v\sum_{ijk} c_{ij}c_{jk}c_{ki}} \;=\; ?$$

some references

network reviews

R Albert and AL Barabasi, Rev Mod Phys 74, 2002
SN Dorogovtsev, AV Goltsev, and JFF Mendes, Rev Mod Phys 80, 2008
ACC Coolen, F Fraternali, A Annibale, L Fernandes and J Kleinjung, in Handbook of Statistical Systems Biology, Wiley, 2011

entropies of tailored graph ensembles

A Annibale, ACC Coolen, L P Fernandes, F Fraternali, J Kleinjung, J Phys A 42, 2009
ES Roberts, T Schlitt and ACC Coolen, J Phys A 44, 2011

graph dynamics and generation

R Taylor, in Combinatorial Mathematics VIII, Springer Lect Notes Math 884, 1981
AR Rao, R Jana, and S Bandyopadhya, Indian J of Statistics 58, 1996
ACC Coolen, A De Martino and A Annibale, J Stat Phys 136, 2009
K Roberts and ACC Coolen, Phys Rev E 85, 2012

websites

www.mth.kcl.ac.uk/∼tcoolen
www.mth.kcl.ac.uk/∼tcoolen/Summerschool2012