Controlled Markovian dynamics of structured graphs

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Outline

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1. Background - tailored random graphs
2. Generating tailored random graphs numerically
3. Constrained Markovian graph dynamics
4. Degree-constrained dynamics of nondirected graphs
5. Degree-constrained dynamics of directed graphs
6. Summary

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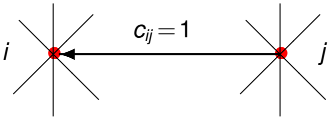
Background - tailored random graphs

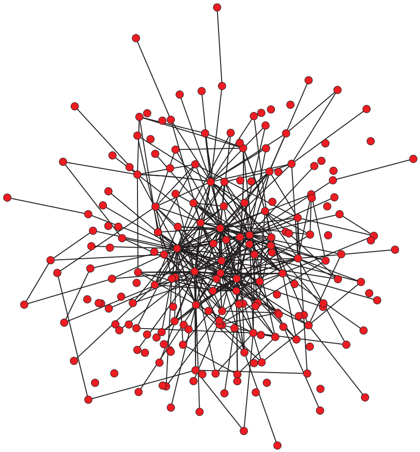
networks/graphs:

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





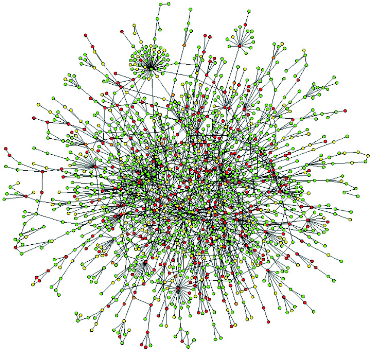
degrees: $k_i^{\rm in}(\mathbf{c}) = \sum_j c_{ij}, \quad k_i^{\rm out}(\mathbf{c}) = \sum_j c_{ji}$

$$\mathbf{k}^{\rm in}(\mathbf{c}) = (k_1^{\rm in}(\mathbf{c}), \ldots, k_N^{\rm in}(\mathbf{c})), \;\; \mathbf{k}^{\rm out}(\mathbf{c}) = \ldots$$

Networks in cellular biology

- **protein interaction networks**: (nondirected)

  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
  $N \sim 10^4$, about 7 links/node



- **gene regulation networks**: (directed)

  nodes: proteins $i, j = 1 \ldots N$
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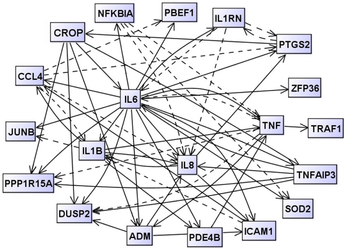

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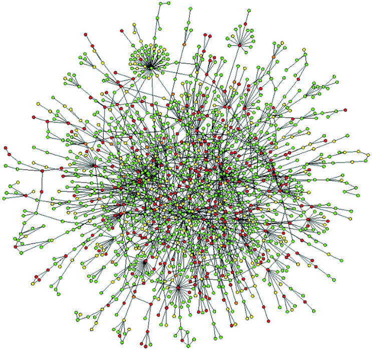

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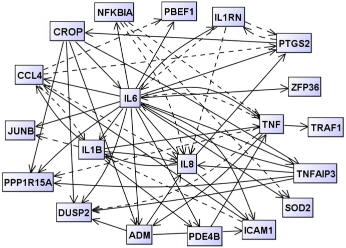
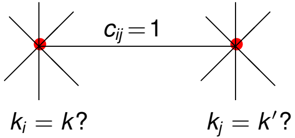


Quantify graph topology beyond degrees

joint degree statistics
of connected nodes

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



- $W(k|\mathbf{c}) = p(k|\mathbf{c})k/\langle k\rangle$
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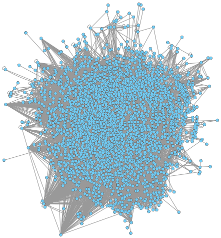
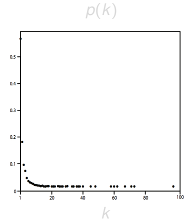
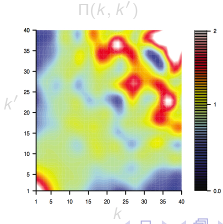
$$\Pi(k,k'|\mathbf{c}) = \frac{W(k,k'|\mathbf{c})}{W(k|\mathbf{c})W(k'|\mathbf{c})}$$

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







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$N = 9306$
$\langle k\rangle = 7.53$

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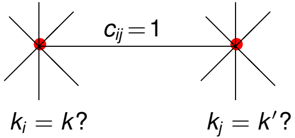

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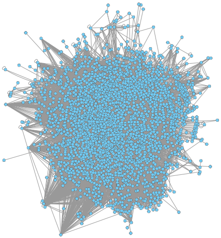

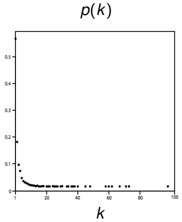

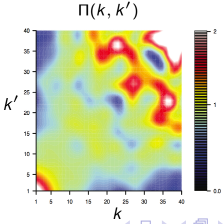

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for directed graphs:

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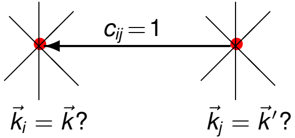

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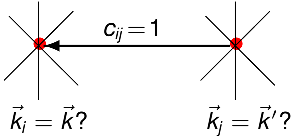

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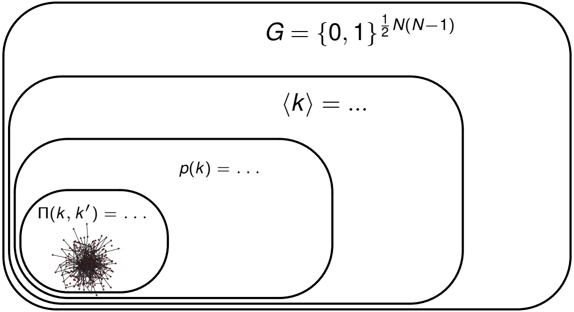
Graph classification
via increasingly detailed
measurements



we are led to study:

Tailored random graph ensembles

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

– proxies for real networks in stat mech process modelling
– complexity: how many networks exist with same features as **c**?
– hypothesis testing: graphs with controlled features as null models
– quantifying network dissimilarity

analytically in leading order in N

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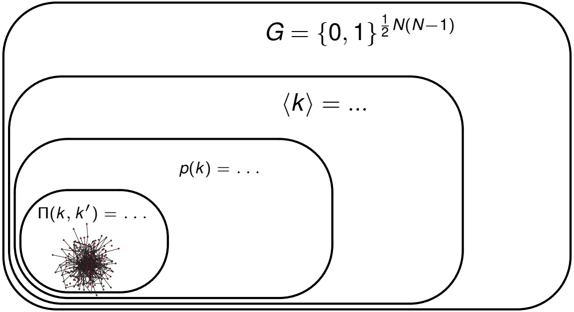

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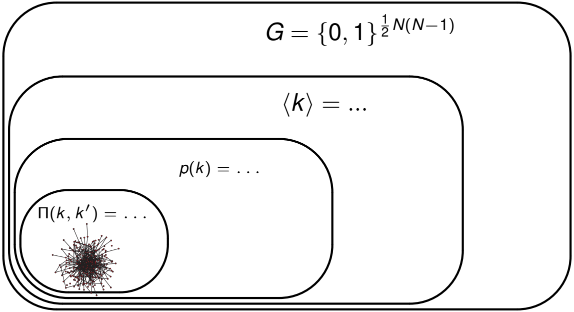

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effective nr of graphs in ensemble $p(\mathbf{c})$,
complexity of tailored random graphs

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

- nondirected graphs:

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

– write $\delta_{k_i,k_i(\mathbf{c})} = (2\pi)^{-1}\int_0^{2\pi}\mathrm{d}\omega_i\ \mathrm{e}^{\mathrm{i}\omega_i[k_i-k_i(\mathbf{c})]}$
– factorisation over bonds, sum over graphs
– write as path integral over $P(k,\omega) = N^{-1}\sum_i \delta_{k,k_i}\delta(\omega-\omega_i)$
– integration via steepest descent
– solve saddle-point equation analytically

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

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with $\vec{k}_i(\mathbf{c}) = (k_i^{\rm in}(\mathbf{c}), k_i^{\rm out}(\mathbf{c}))$

similar methods ...
final result:

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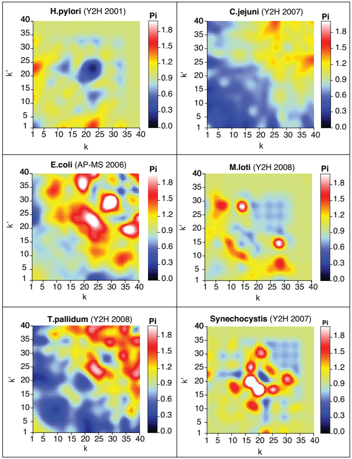
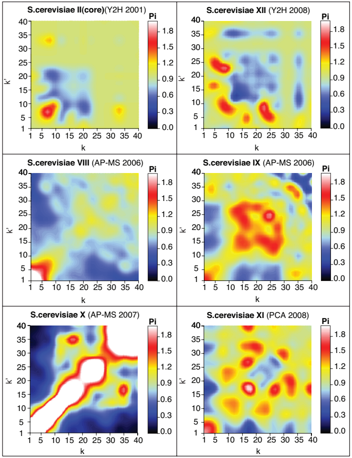
Information in degree correlations?

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





structural dissimilarity of graphs $\mathbf{c}_A$ and $\mathbf{c}_B$, based on
Information-theoretic distance between associated ensembles

$$D_{AB} = \frac{1}{2N} \sum_{\mathbf{c} \in G} \left\{ p(\mathbf{c}|p_A, W_A) \log \left[\frac{p(\mathbf{c}|p_A, W_A)}{p(\mathbf{c}|p_B, W_B)} \right] + p(\mathbf{c}|p_B, W_B) \log \left[\frac{p(\mathbf{c}|p_B, W_B)}{p(\mathbf{c}|p_A, W_A)} \right] \right\}$$

same methods as in calculating
Shannon entropy:

$$\begin{aligned} D_{AB} = {} & \frac{1}{2} \sum_k p_A(k) \log \left[\frac{p_A(k)}{p_B(k)} \right] + \frac{1}{2} \sum_k p_B(k) \log \left[\frac{p_B(k)}{p_A(k)} \right] \\ & + \frac{1}{4\langle k \rangle_A} \sum_{kk'} p_A(k) p_A(k') kk' \Pi_A(k,k') \log \left[\frac{\Pi_A(k,k')}{\Pi_B(k,k')} \right] \\ & + \frac{1}{4\langle k \rangle_B} \sum_{kk'} p_B(k) p_B(k') kk' \Pi_B(k,k') \log \left[\frac{\Pi_B(k,k')}{\Pi_A(k,k')} \right] \\ & + \frac{1}{2} \sum_k p_A(k) k \log \rho_{AB}(k) + \frac{1}{2} \sum_k p_B(k) k \log \rho_{BA}(k) \end{aligned}$$

with

$$\Pi(k,k') = W(k,k)/W(k)W(k'), \qquad \rho_{AB}(k) = \sum_{k'} \Pi_B(k,k') W_A(k') \rho_{AB}^{-1}(k')$$

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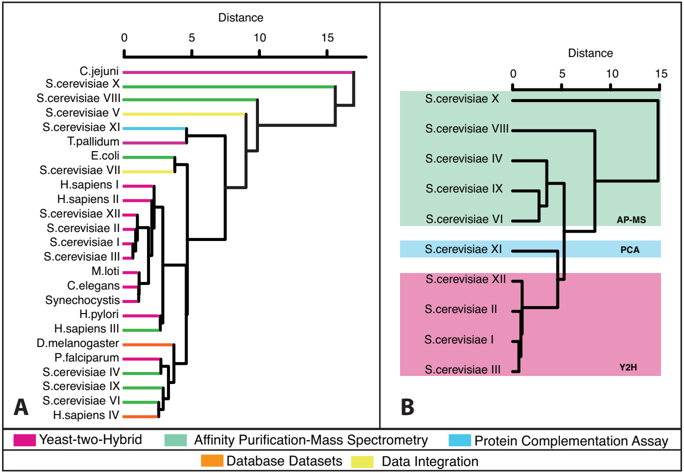
clustering of protein interaction networks with information-theoretic distance measure



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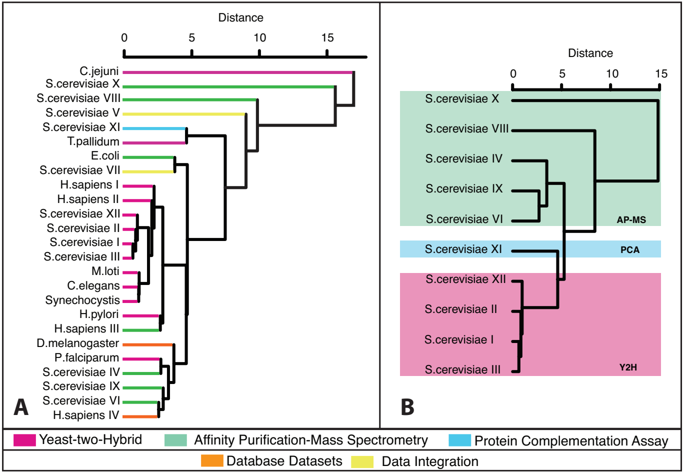

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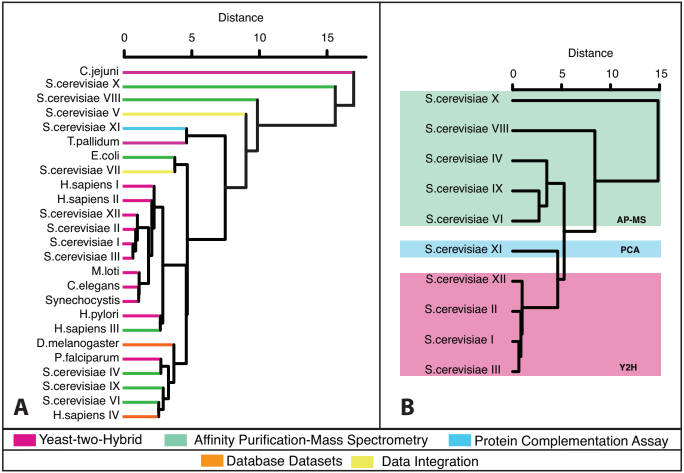
clustering of protein interaction networks with information-theoretic distance measure



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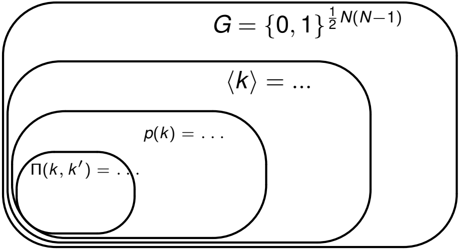


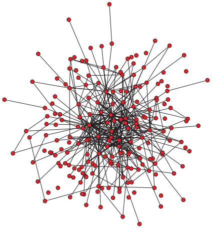
finally: let us

generate tailored random graphs

from the above families
numerically ...

Generating tailored random graphs numerically

$G[\mathbf{k}]$: all nondirected graphs $\mathbf{c}$ with degrees $\mathbf{k}$



how to generate

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

available approaches

- matching algorithm (Bender & Canfield, 1978)
  builds one random graph $\mathbf{c}$ with specified degrees $\mathbf{k}$
  (assign k_i 'stubs' to each node i, then randomly connect pairs of 'stubs')
- edge switching algorithm (Seidel, 1976; Taylor, 1981)
  ergodic Markov process in $G[\mathbf{k}]$
  $\mathbf{c} \rightarrow \mathbf{c}' \rightarrow \mathbf{c}'' \rightarrow \ldots$

– sampling all graphs in $G[\mathbf{k}]$: in principle easy
– main problem: sampling with **correct probabilities**
– matching and edge switching: both **biased** (yet widely used ...)

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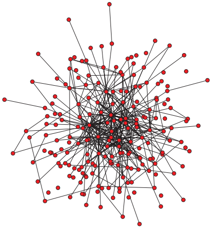

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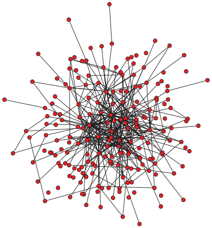

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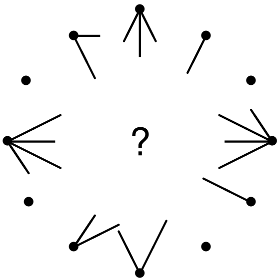

bond creation as elementary moves:
$c_{ij} = 0 \;\rightarrow\; c_{ij} = 1$
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origin of sampling bias:

– process can terminate before $k_i(\mathbf{c}) = k_i$ for all i
(e.g. if remaining 'stubs' require self-loops)

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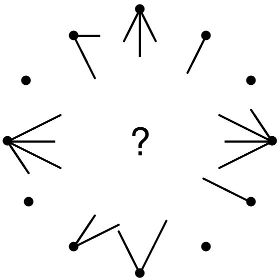

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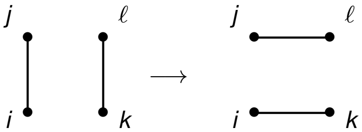

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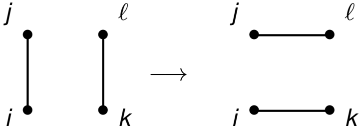

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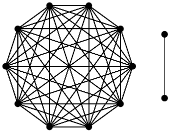

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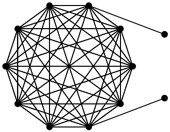

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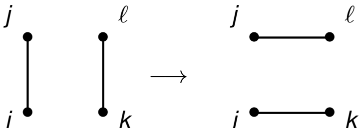

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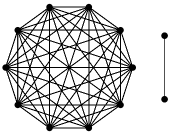

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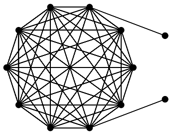

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Constrained Markovian graph dynamics

need to study graph dynamics more systematically ...

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

- stochastic graph dynamics as a Markov chain,
  transition probabilities $W(\mathbf{c}|\mathbf{c}')$

$$\forall \mathbf{c} \in G[\star]: \qquad p_{t+1}(\mathbf{c}) = \sum_{\mathbf{c}' \in G[\star]} W(\mathbf{c}|\mathbf{c}')p_t(\mathbf{c}')$$

- 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: $(\forall F \in \Phi): F^2 = \mathbb{I}$
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construct transition probs $W(\mathbf{c}|\mathbf{c}')$, based on moves $F \in \Phi$, such that process converges to $p_\infty(\mathbf{c}) = Z^{-1} e^{-H(\mathbf{c})}$ on $G[\star]$

- structure:

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

$q(F|\mathbf{c})$: *move proposal probability*

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ergodic auto-invertible moves $F \in \Phi$,
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for acceptance probabilities

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

corollary:

naive edge-swapping, $A(\mathbf{c}|\mathbf{c}') = const$,
corresponds to $H(\mathbf{c}) = -\log n(\mathbf{c})$,
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$$\textit{sampling bias}: \quad p_\infty(\mathbf{c}) = \frac{n(\mathbf{c})}{\sum_{\mathbf{c}' \in G[\star]} n(\mathbf{c}')}$$

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Master equation representation of the process

- soln of Markov chain: $p_n(\mathbf{c})$, $n = 0, 1, 2, \ldots$

  continuous time process, $p_t(\mathbf{c})$, $t \in [0, \infty\rangle$
  via *random durations* of MC steps

  $\pi_m(t) = (t/\tau)^m \mathrm{e}^{-t/\tau}/m!$:
  prob that at time t precisely m MC steps have been made

$$\tau \frac{\mathrm{d}}{\mathrm{d}t} p_t(\mathbf{c}) = \sum_{\mathbf{c}' \in G[\star]} W(\mathbf{c}|\mathbf{c}') p_t(\mathbf{c}') - p_t(\mathbf{c})$$

- work out details,
  using $\Delta_F U(\mathbf{c}) = U(F\mathbf{c}) - U(\mathbf{c})$

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

$$w_F^{\pm}(\mathbf{c}) = \frac{1}{2} \pm \frac{1}{2} \tanh \left[\frac{1}{2} \Delta_F [H(\mathbf{c}) + \log n(\mathbf{c})] \right]$$

- Convergence:

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

$F(t)$ is Lyapunov function $\quad \forall t \geq 0: \quad F(t) \geq 0, \quad \frac{\mathrm{d}}{\mathrm{d}t}F(t) \leq 0$

- Proof (standard):

use detailed balance

$$\frac{\mathrm{d}}{\mathrm{d}t}F(t) = -\frac{1}{2\tau} \sum_{\mathbf{c},\mathbf{c}'\in G[\star]} W(\mathbf{c}|\mathbf{c}')\mathrm{e}^{-H(\mathbf{c}')} \Big[[H(\mathbf{c}) + \log p_t(\mathbf{c})] - [H(\mathbf{c}') + \log p_t(\mathbf{c}')]\Big] \times \Big[\mathrm{e}^{H(\mathbf{c}) + \log p_t(\mathbf{c})} - \mathrm{e}^{H(\mathbf{c}') + \log p_t(\mathbf{c}')}\Big] \leq 0$$

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

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$$\frac{\mathrm{d}}{\mathrm{d}t}F(t) = -\frac{1}{2\tau} \sum_{\mathbf{c},\mathbf{c}'\in G[\star]} W(\mathbf{c}|\mathbf{c}')\mathrm{e}^{-H(\mathbf{c}')} \Big[[H(\mathbf{c})+\log p_t(\mathbf{c})] - [H(\mathbf{c}')+\log p_t(\mathbf{c}')]\Big] \times \Big[\mathrm{e}^{H(\mathbf{c})+\log p_t(\mathbf{c})} - \mathrm{e}^{H(\mathbf{c}')+\log p_t(\mathbf{c}')}\Big] \leq 0$$

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

- stationarity: $\frac{\mathrm{d}}{\mathrm{d}t}F(t) = 0$,
write $p(\mathbf{c}) = \chi(\mathbf{c})\mathrm{e}^{-H(\mathbf{c})}$,

$$(\forall \mathbf{c},\mathbf{c}' \in G[\star]): \quad W(\mathbf{c}|\mathbf{c}') = 0 \;\; \text{or} \;\; \chi(\mathbf{c}) = \chi(\mathbf{c}')$$

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

Degree-constrained dynamics of nondirected graphs

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

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

  $Q = \{(i,j,k,\ell) \in \{1,\ldots,N\}^4 |\ i<j<k<\ell\}$, 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 $\alpha \in \{1,2,3\}$

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

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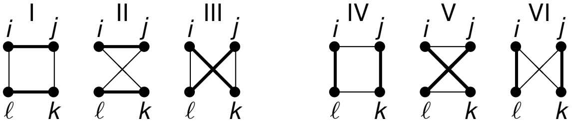

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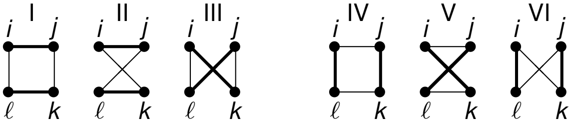

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to implement the Markov chain,
need to calculate graph mobility **analytically**

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

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– state-dependent part can be ignored if $\langle k^2\rangle k_{\max}/\langle k\rangle^2 \ll N$
(in which case naive edge swapping is harmless)

– computational feasibility:
calculate change $\Delta_{ijk\ell;\alpha} n(\mathbf{c})$ for each executed move $F_{ijk\ell;\alpha}$

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Example

many possible moves *only <u>one</u> move ...*

$N = 100$

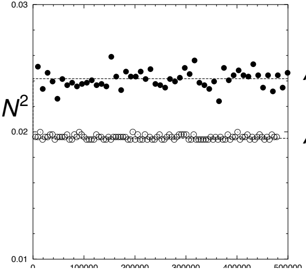
naive versus correct acceptance probabilities

predictions:

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

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

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

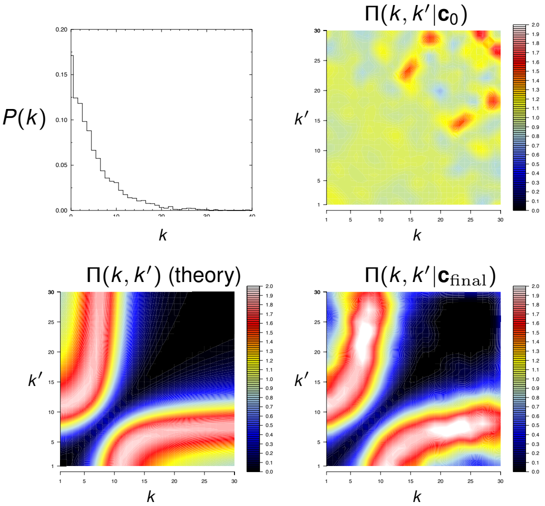


executed moves

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

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

Example



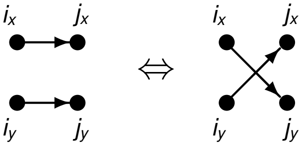
$N = 4000$,
$\overline{k} = 5$

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

Degree-constrained dynamics of directed graphs

- 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 $\quad F: G_F[\mathbf{k}^{\rm in},\mathbf{k}^{\rm out}] \to G[\mathbf{k}^{\rm in},\mathbf{k}^{\rm out}]$



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

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

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

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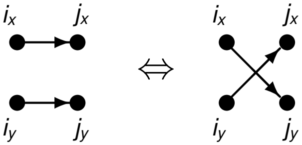

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difference with nondirected graphs:

edge swaps *no longer ergodic* (Rao, 1996)
(unless self-interactions are allowed)

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

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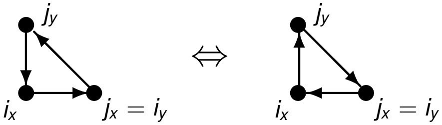

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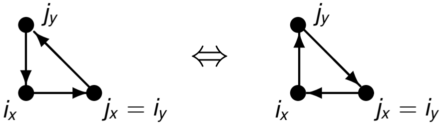

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Example

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

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

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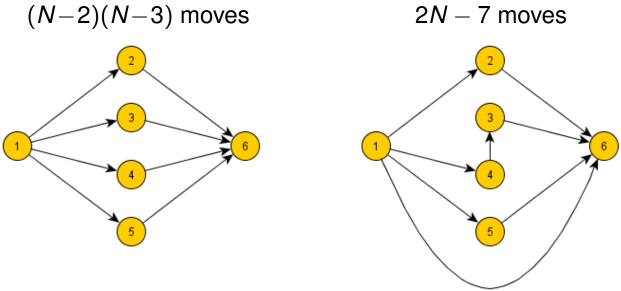

predicted values versus
equilibrated dynamics for $\langle n(\mathbf{c})\rangle / N^2$:

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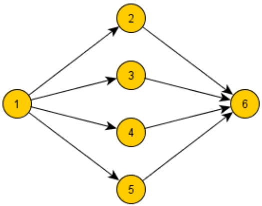
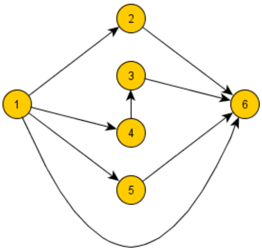


$2N-7$ moves



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Summary

- standard 'matching' end 'edge swapping' algorithms,
  for generating graphs **c** with prescribed degrees, are *both biased*
- need exact method for generating random graphs **c**
  with prescribed degrees and prescribed sampling probabilities $p(\mathbf{c})$
- exact degree constrained Markovian graph dynamics can be defined,
  guaranteed to evolve to any prescribed measure $p(\mathbf{c})$
- process requires nontrivial state acceptance probabilities,
  that involve the mobilities $n(\mathbf{c})$ of states
- nondirected graph: edge swaps only
  directed graphs: edge swaps and 3-cycle reversals
- mobilities can be calculated exactly
- theory worked out, implemented and tested
  for nondirected and directed graphs

Summary

- standard 'matching' end 'edge swapping' algorithms, for generating graphs **c** with prescribed degrees, are *both biased*
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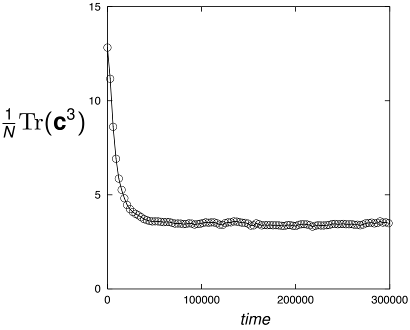
Current and future work

Development of theory for tailored graph ensembles characterised by statistics of **loops** ...

(in addition to degrees and degree correlations)

- calculate Shannon entropies
- dynamics (constrained by degrees and loops)
- graph ensembles defined by eigenvalue spectrum
- loops versus closed paths (see talk by Clara Gracio)



protein interaction networks

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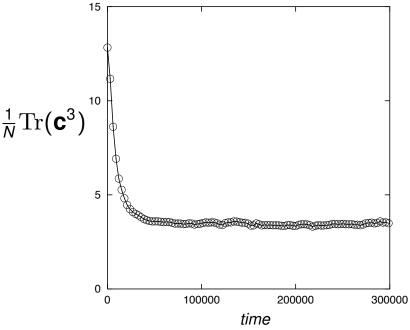

protein interaction networks

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- Clara Gracio

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- Jens Kleinjung
- Thomas Schlitt

grants:

BBSRC bioscience for the future

EPSRC Engineering and Physical Sciences Research Council

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