Cycles in Random Graphs

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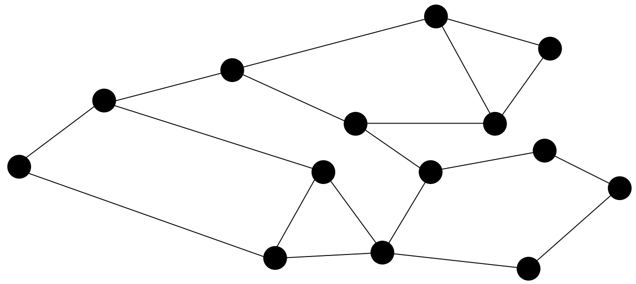
Outline

- Introduction
- Statistical Mechanics Approach
- Application 1: Finding Long Cycles
- Application 2: Vertex and Edge Ranking
- Conclusions and Future Perspectives

Definitions



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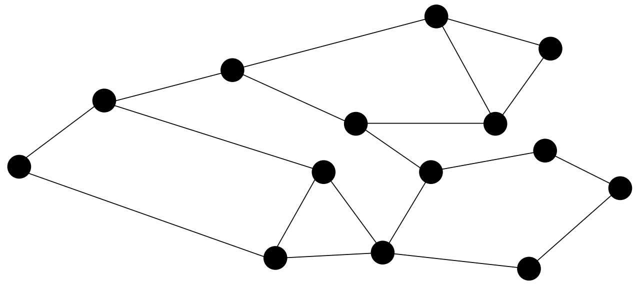

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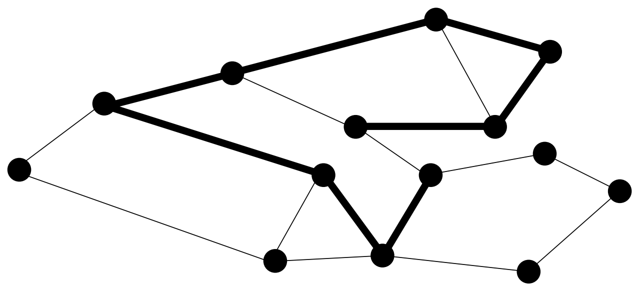

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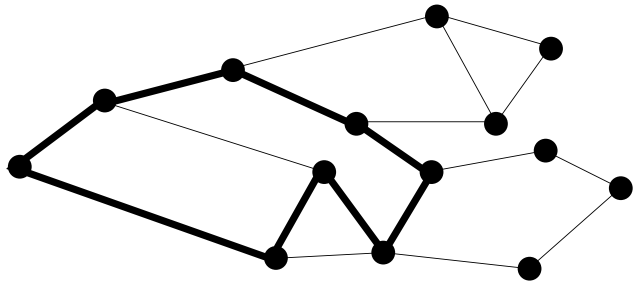

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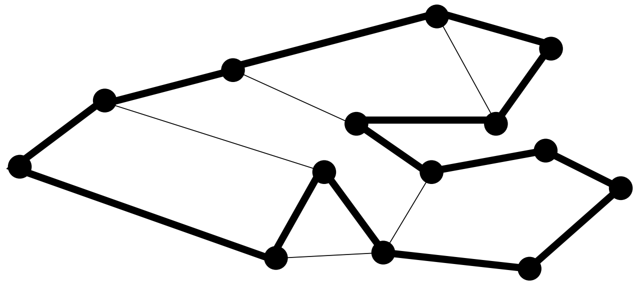

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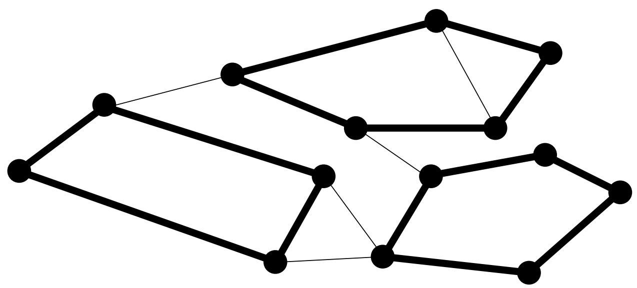

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Hamiltonian cycle = cycle covering all vertices of a graph

cycle cover = union of vertex disjoint cycles covering all vertices of a graph

Interest?

- Graph theory:

  Hamiltonian cycles (= cycles of length N): NP-complete (*cfr.* Traveling Salesman Problem)

  Statistical properties of # cycles on random graph ensembles

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- Understanding Real World Networks (e.g. Internet, WWW, biological networks, social networks):
  - local properties: degree distribution, clustering $\rightarrow$ short cycles
  - global properties: shortest paths, network motives $\rightarrow$ longer cycles
  - dynamics: feedback mechanism
  - vertex ranking

Computational Difficulty

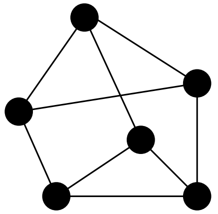
⇒ 3 fundamental questions:

1. Do they exist?
2. If yes, how many?
3. Can we locate them?

Computational Difficulty depends on length L of cycle:

- short cycles ($L = 3, 4, 5$): exhaustive enumeration has time upper bound of $\mathcal{O}(N \times \#\text{cycles})$, where $\#\text{cycles} \propto \exp N$
- intermediate cycles ($\lim_{N\to\infty} \frac{L}{N} = 0$): in limit $N \to \infty$ distribution can be computed for most random graph ensembles
- long extensive cycles ($L \propto N$), e.g., Hamiltonian cycles:

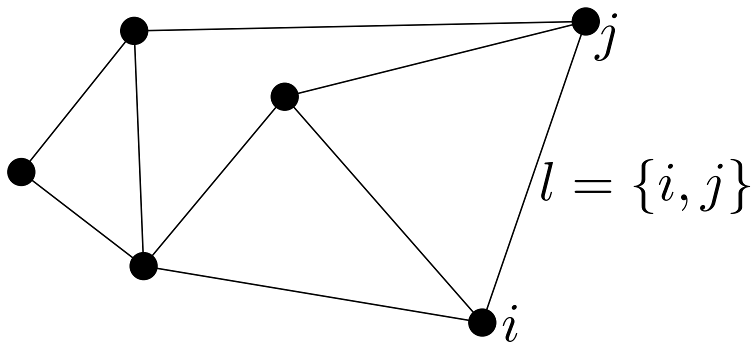
- Regular graphs: Hamiltonian with high probability (Wormald)
- Sparse graphs with minimum degree 3 and bounded maximum degree: conjectured to be Hamiltonian (Wormald)

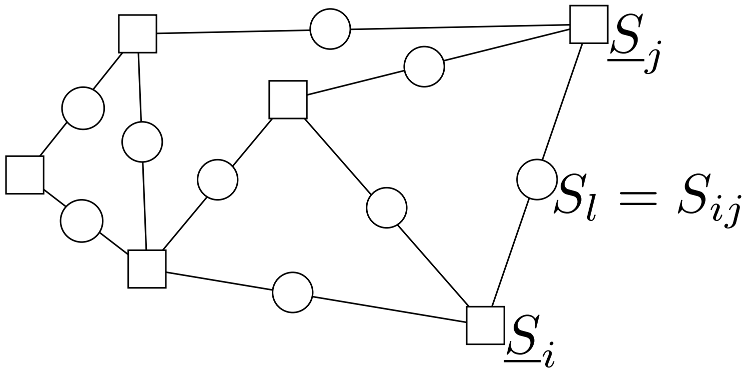


A Constraint Satisfaction Problem for Cycles

- $\forall$ edges l: $S_l = 0/1$ if edge l is absent / present

  $\forall$ vertices i: $\underline{S}_i = \{S_l | l$ is a neighboring edge of vertex $i\}$





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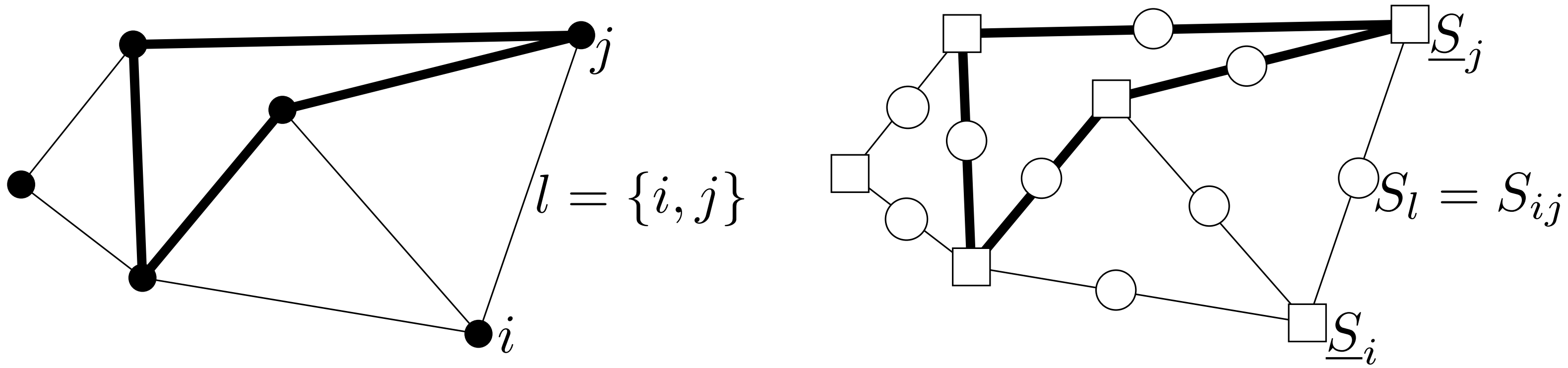

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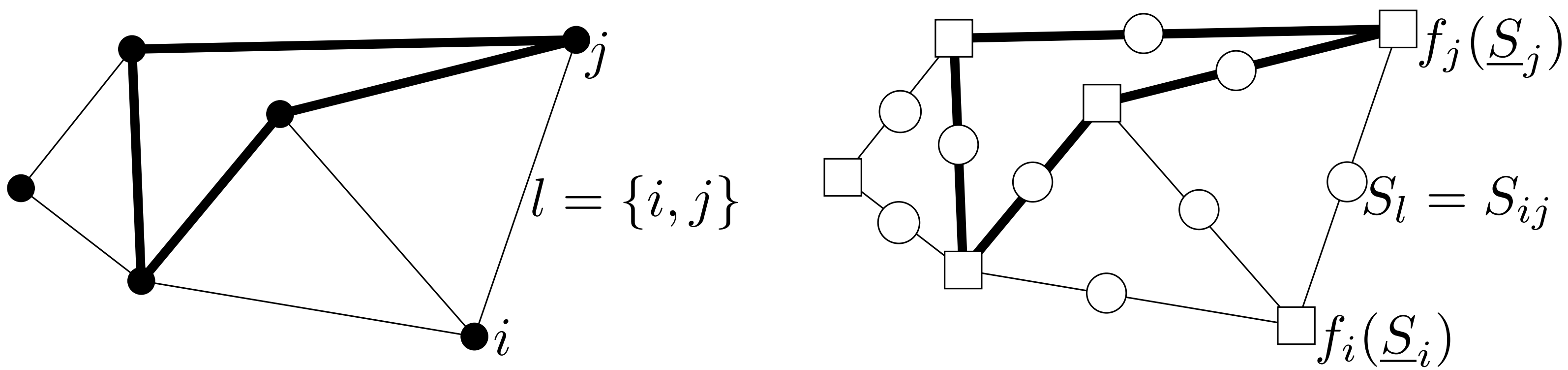

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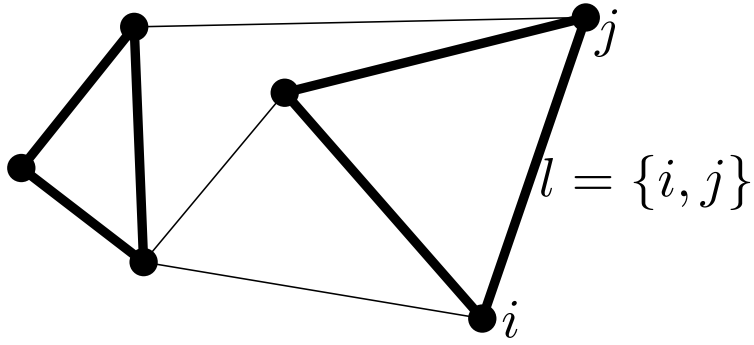

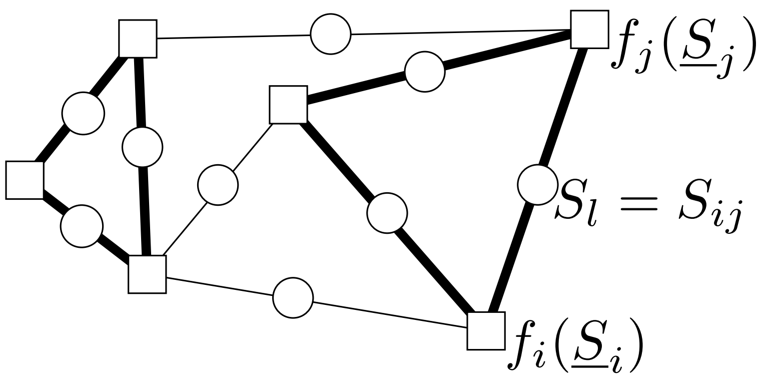

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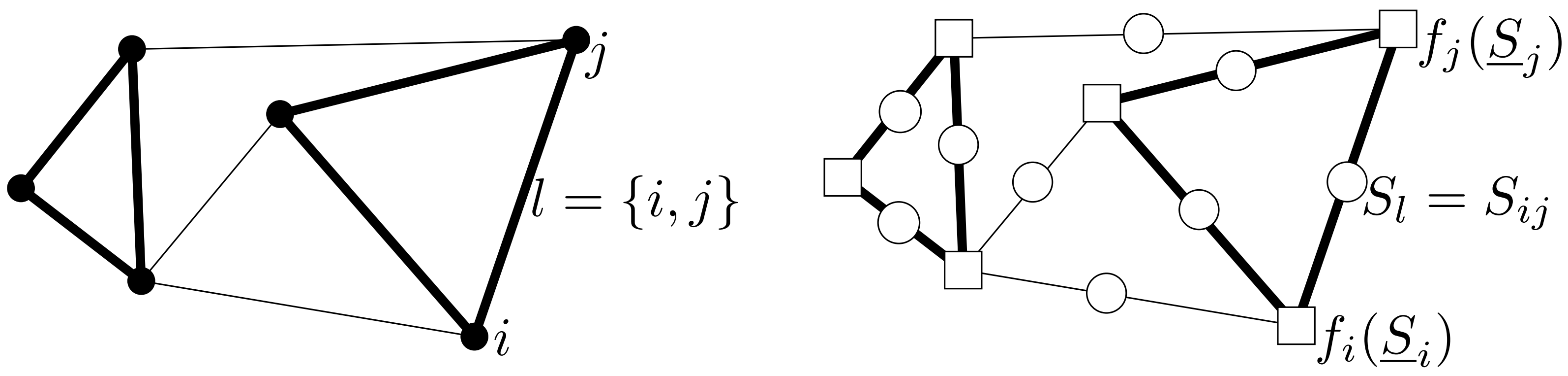

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$u = 1$ uniform sampling

$u \to \infty$ cycles of longest length (e.g. Hamiltonian cycles)

I.1 Decimation $\Rightarrow$ Hamiltonian Cycles

for $n = 1$ **to** M

- choose l_n: S_{l_n} is undefined
- draw S_{l_n} according to $\mathrm{Prob}[S_{l_n}|S_{l_1},\ldots,S_{l_{n-1}}]$

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$$\text{for } u \to \infty \Rightarrow \begin{cases} \text{cycle cover} & \text{if } \underline{S} \text{ consists of more than one cycle} \\ \text{hamiltonian cycle} & \text{if } \underline{S} \text{ consists of just one cycle} \end{cases}$$

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Problem 1: $\mathrm{Prob}[S_{l_n}|S_{l_1}, \dots, S_{l_{n-1}}]$

$\rightarrow$ approximate by means of Belief Propagation $\Leftrightarrow \mathrm{Prob}[\underline{S}] = \prod g(\underline{S}_x)$

Problem 2: probability law selecting set of cycles of total length L

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Belief Propagation

Compute partition function $Z = \sum_{\underline{x}} w(\underline{x})$

$\Leftrightarrow$ Minimizing the corresponding Gibbs free energy functional

$$F_{\text{Gibbs}}[p_{\text{var}}] = \sum_{\underline{x}} p_{\text{var}}(\underline{x}) \ln \left(\frac{p_{\text{var}}(\underline{x})}{w(\underline{x})} \right)$$

since $\min_{p_{\text{var}}} F_{\text{Gibbs}}[p_{\text{var}}] = F_{\text{Gibbs}}[P_{\text{Gibbs}}] = -\ln Z.$

Mean Field approximation: factorizable trial distributions

$p_{\text{MF}}(\underline{x}) = \prod_i p_i(x_i)$

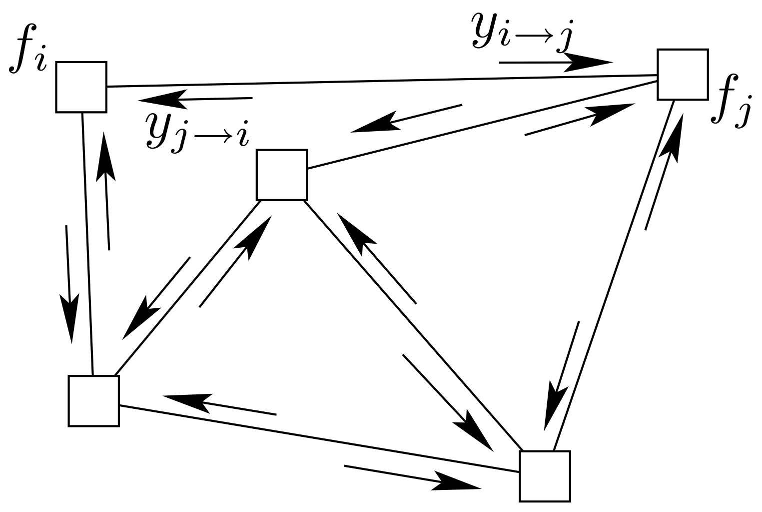
Bethe approximation: take first order correlations into account

e.g. $p_{\text{Bethe}}(\underline{x}) = \frac{\prod_{\{i,j\}} p_{ij}(x_i, x_j)}{\prod_i p_i(x_i)}$ demanding normalized distributions p_i, p_{ij} and consistency

$\Rightarrow$ Introduce Lagrange Multipliers

$\Leftrightarrow$ Finding fixed point of the corresponding distributed Belief Propagation (BP) algorithm.

Belief Propagation



- Initialize messages $y_{i\to j}$ randomly.
- Iterate BP until convergence, where each update takes up a time $\mathcal{O}(M)$:

$$y_{i\to j} = f_1\left(u, \{y_{k\to i}\}_{k\in\partial i\setminus j}\right)$$

$$\Rightarrow \quad p_l(S_l = 1) = \frac{u y_{i\to j} y_{j\to i}}{1+u y_{i\to j} y_{j\to i}}$$

On a tree-like graph:

- BP converges fast!
- F_{Bethe}, and thus BP, is exact!

On a general graph with cycles:

- In theory, BP does not necessarily converge, but in practice it often does after a reasonable amount of iterations.
  $\Rightarrow$ Allows to investigate larger graphs $\sim \mathcal{O}(10^6)$.

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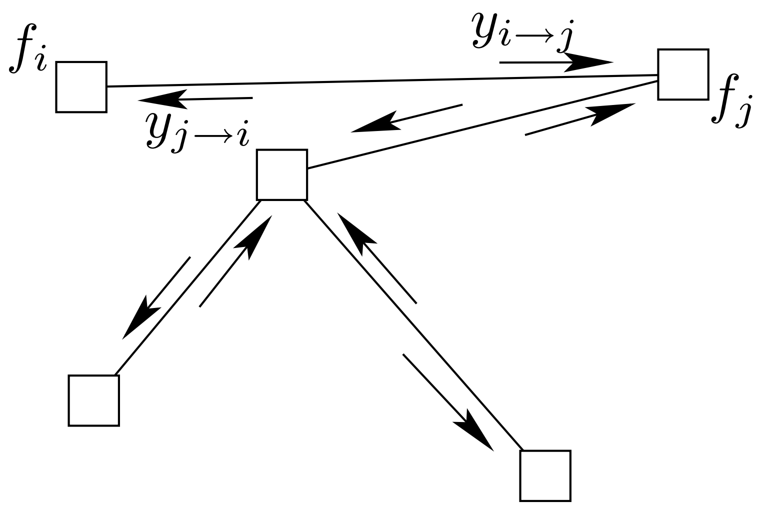

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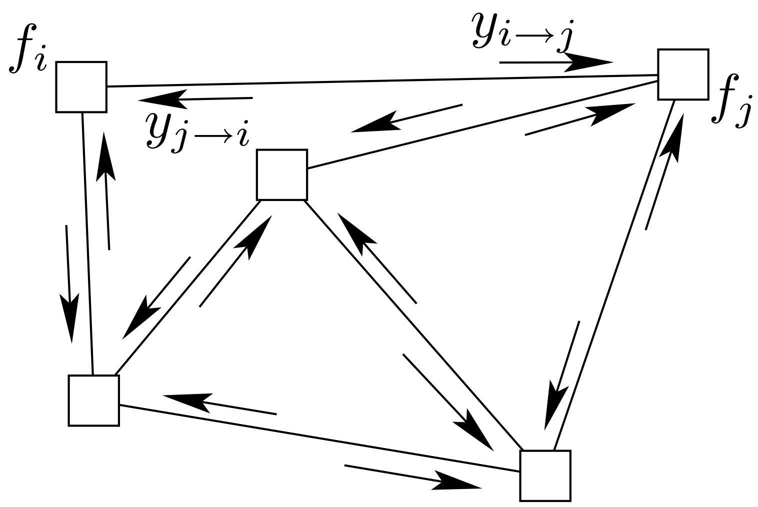

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I.1 Decimation $\Rightarrow$ Hamiltonian Cycles

- Performance on sparse graphs with $N = 100, 200, \ldots, 1600$
  - Regular graphs ($c = 3, 4, 5$): $\forall$ $\mathbf{HC}$
  - Bimodal graphs ($q_{3,4}^{0.5}$,$q_{3,5}^{0.5}$,$q_{4,5}^{0.5}$): $94 - 99\%$ $\mathbf{HC}$ ($\pm 99\%$ $\mathbf{CC}$)

	$q_{3,4}^{0.5}$		$q_{3,5}^{0.5}$		$q_{4,5}^{0.5}$	
	CC	HC	CC	HC	CC	HC
N	DEC		DEC		DEC	
100	99.9	96.0	98.9	69.9	98.7	56.9
200	99.6	96.2	99.7	71.1	98.9	50.0
400	99.7	96.4	99.9	67.7	98.9	50.7
800	99.8	96.7	99.6	68.9	99.6	46.8
1600	99.7	97.8	99.9	68.6	99.9	52.3

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N	$q^{0.5}_{3,4}$ CC	$q^{0.5}_{3,4}$ HC DEC	$q^{0.5}_{3,4}$ HC LR	$q^{0.5}_{3,5}$ CC	$q^{0.5}_{3,5}$ HC DEC	$q^{0.5}_{3,5}$ HC LR	$q^{0.5}_{4,5}$ CC	$q^{0.5}_{4,5}$ HC DEC	$q^{0.5}_{4,5}$ HC LR
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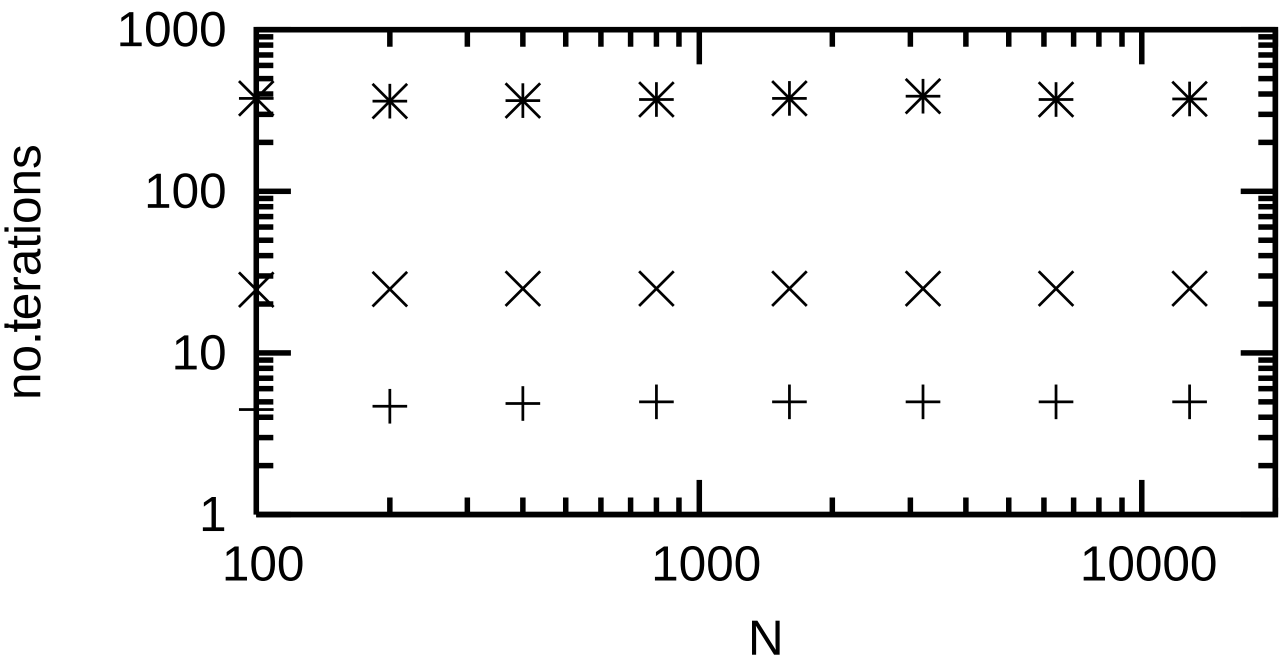
- Time complexity
  - decimation procedure $\sim \mathcal{O}(M^2)$
    e.g. $q_c(k) = \delta_{k,c}$: $c = 3(+), 4(\times), 5(*)$



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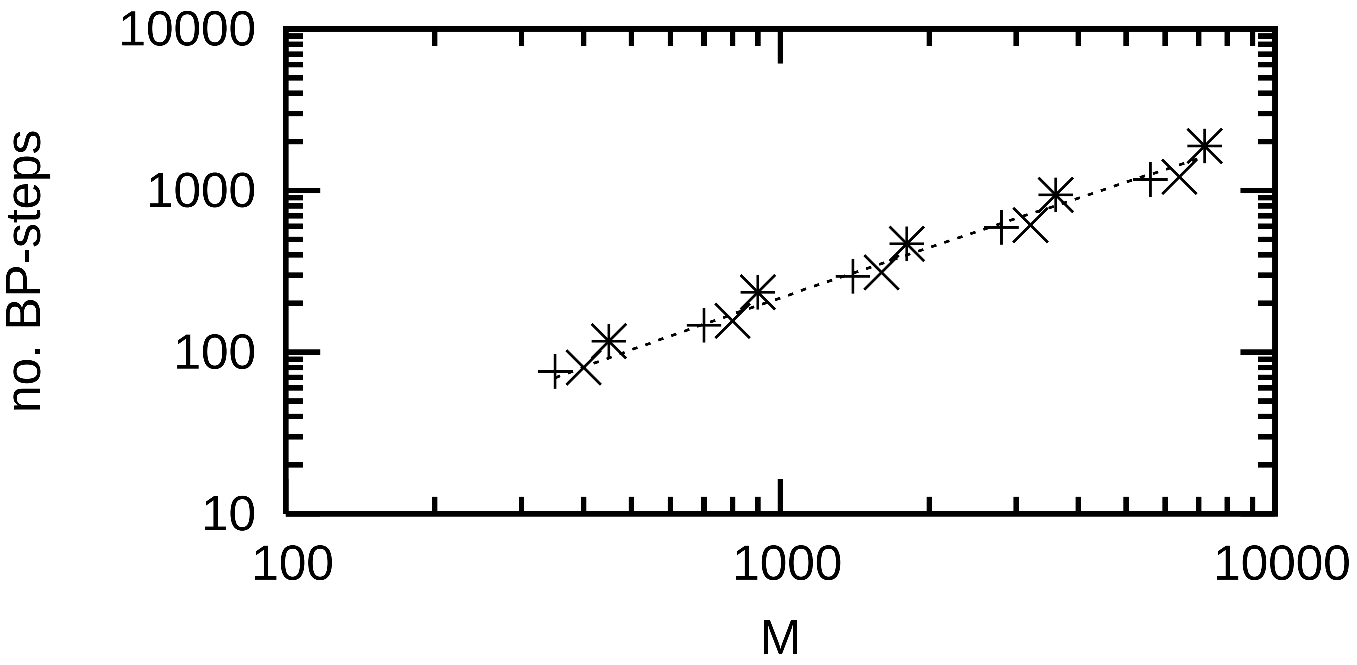

slope $\simeq 0.23$

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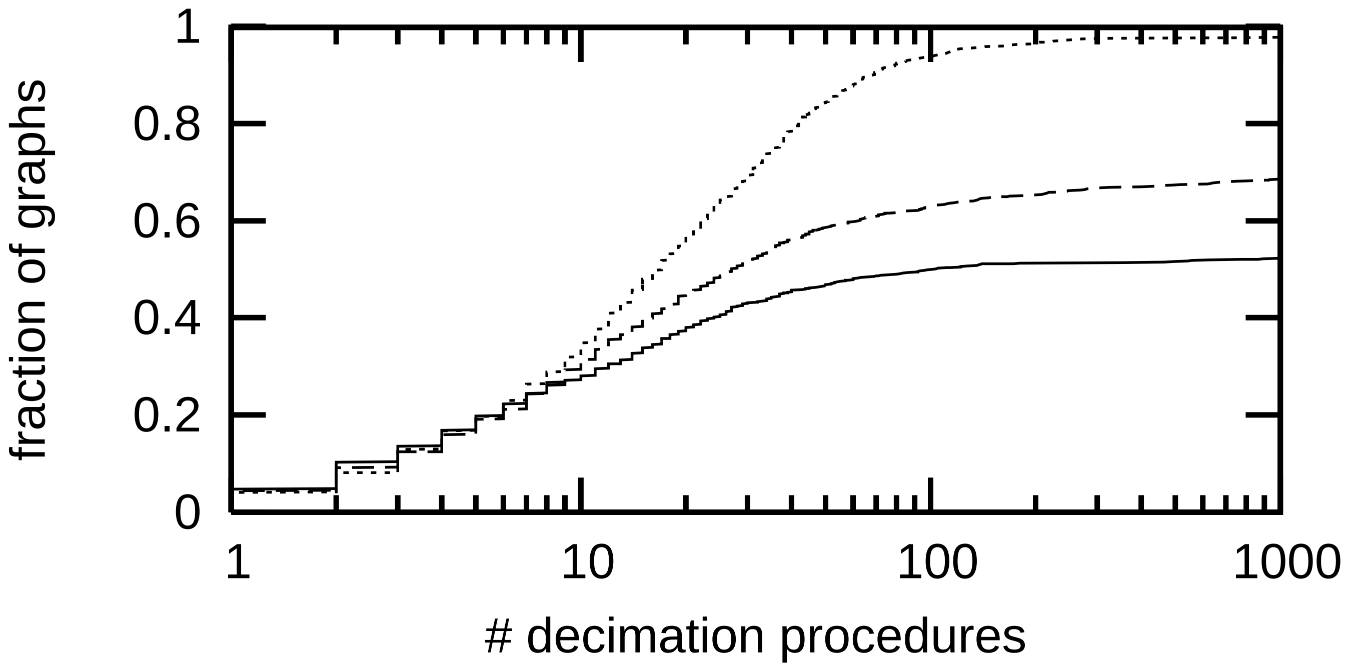
    e.g. $q_{3,4}^{0.5}$ (dotted curve), $q_{3,5}^{0.5}$ (dashed curve), $q_{4,5}^{0.5}$ (full line)



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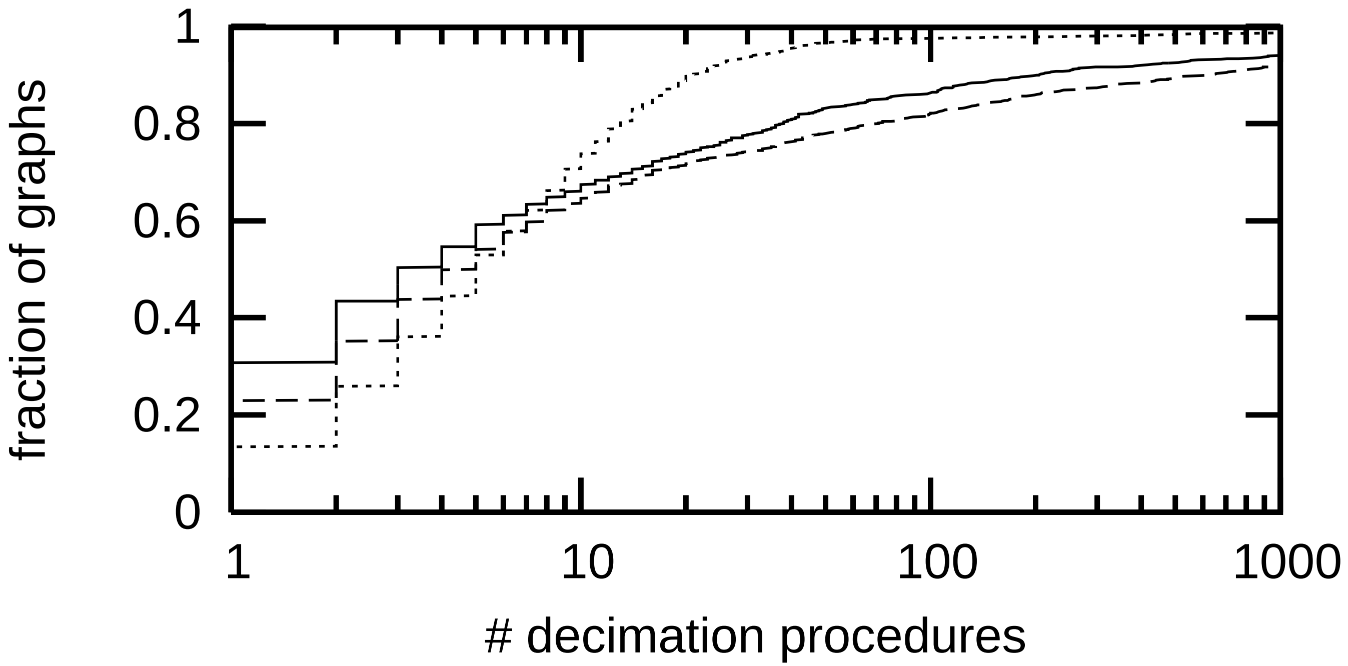

Optimization: Local rewiring $\Rightarrow$ CC $\rightarrow$ HC

I.2 Markov Chain Monte Carlo Sampling

Ergodic, fast mixing Markov Chain $\underline{S}, \underline{S}', \underline{S}'', \ldots$, which admits $\mathrm{Prob}[\underline{S}]$ as unique stationary distribution.

$\rightarrow$ Ergodic? Convergence time?

$\rightarrow$ Determine appropriate transitions $\underline{S} \rightarrow \underline{S}'$, and transition rates $W(\underline{S} \rightarrow \underline{S}')$: e.g. by means of detailed balance:

$$W(\underline{S} \rightarrow \underline{S}')\mathrm{Prob}[\underline{S}] = W(\underline{S}' \rightarrow \underline{S})\mathrm{Prob}[\underline{S}']$$

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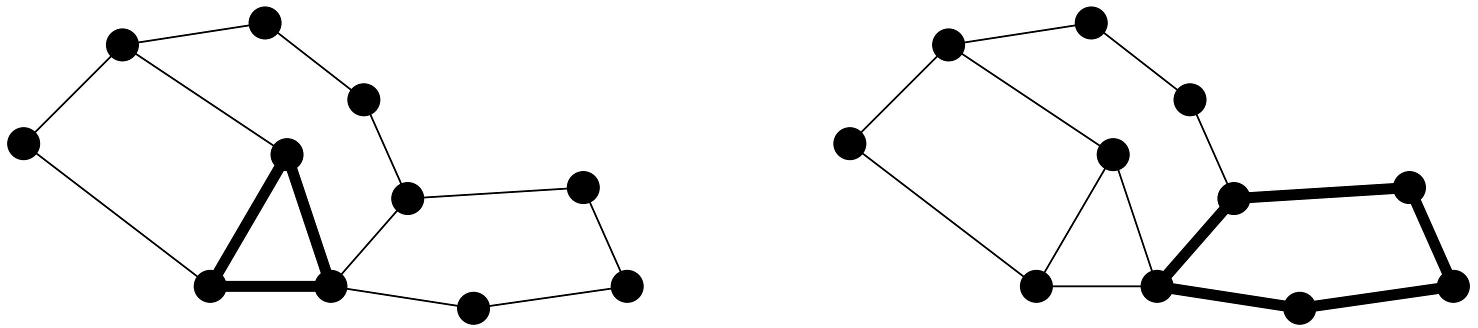

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$n_{\underline{S}} =$ number of disjoint paths of configuration S

$\eta \in [0,1)$

$$\tilde{f}_i(\underline{S}_i) = \begin{cases} 1 & \text{if } \sum_{l\in\partial i} S_l \in \{0,2\} \\ \epsilon \in [0,1] & \text{if } \sum_{l\in\partial i} S_l = 1 \\ 0 & \text{otherwise} \end{cases}$$

I.2 Monte Carlo $\Rightarrow$ Hamiltonian Cycles

- Succes rate:
  - Regular graphs of size $N = 100, 200, 400, 800 : 100\%$
  - Bimodal graphs ($q^{0.5}_{3,4}$,$q^{0.5}_{3,5}$,$q^{0.5}_{4,5}$) of size $N = 100, 200, 400, 800 : 100\% \rightarrow$ Comfirmation of Wormald's conjecture on non-regular graphs

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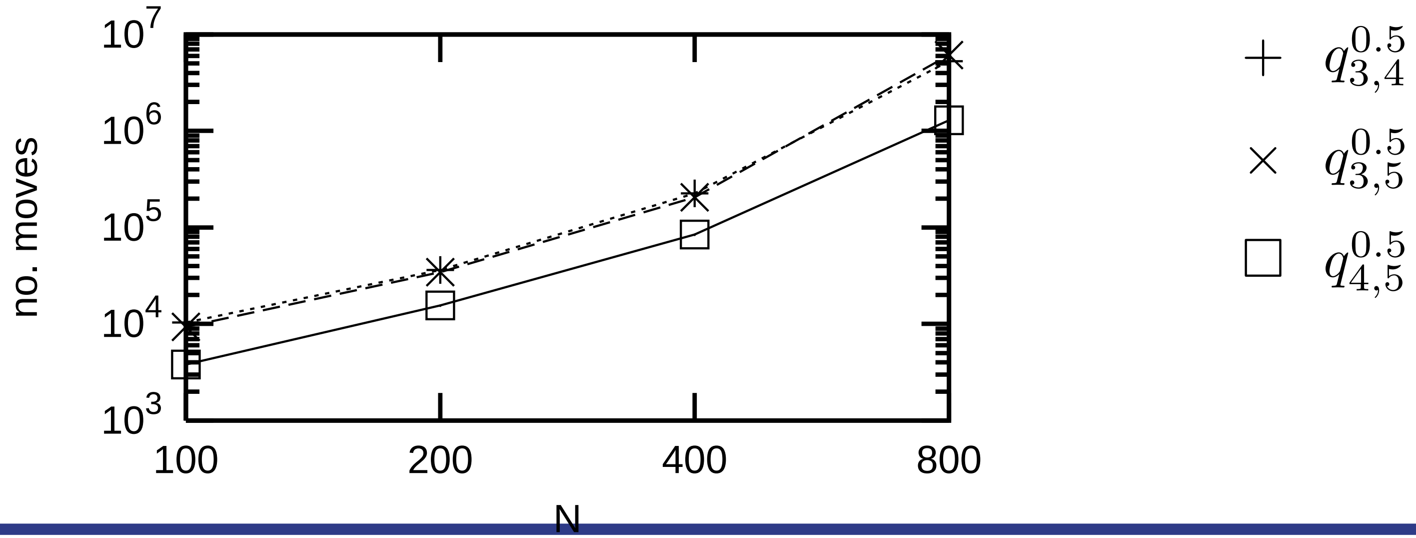
- Time requirements $\rightarrow$ optimized by means of N-fold MC (up to M times faster):
  - Distribution depends on u, ϵ and η
  -



Comparison

We find *Hamiltonian Cycles* for all sparse graphs with $k_{\min} = 3$.

	BP		**MC**
+	versatile	-	very parameter sensitive
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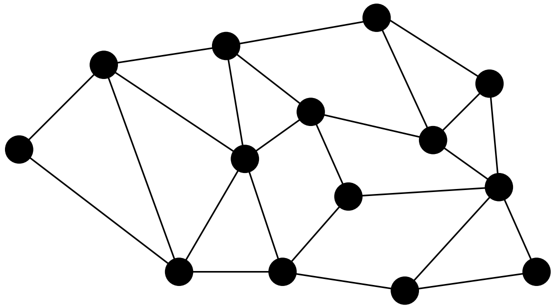
$\rightarrow$ CPU time: e.g. bimodal graph with $q_{3,4}^{0.5}$, $N = 1600$

BP 30’, i.e. 72 trials (70 cycle covers) (with local moves: 5’)

MC 40’ (with optmized parameter values)

II. Vertex (and Edge) Ranking



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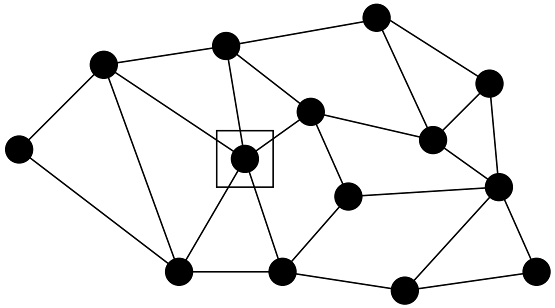

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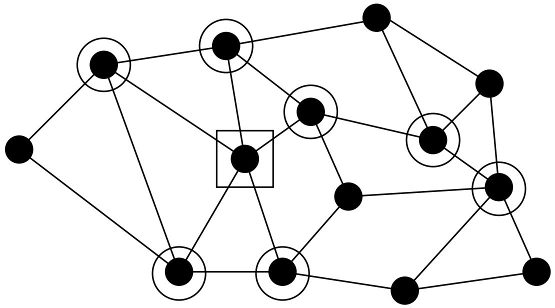

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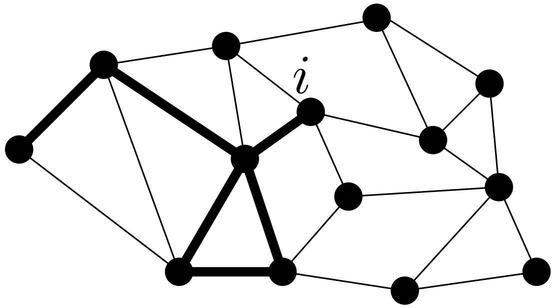

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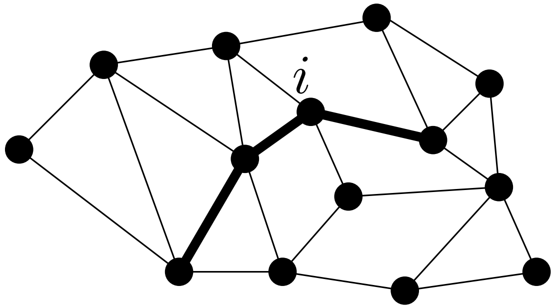

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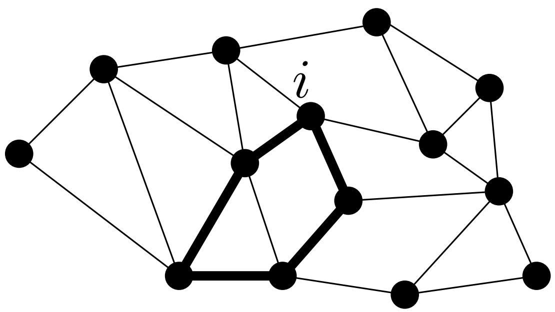

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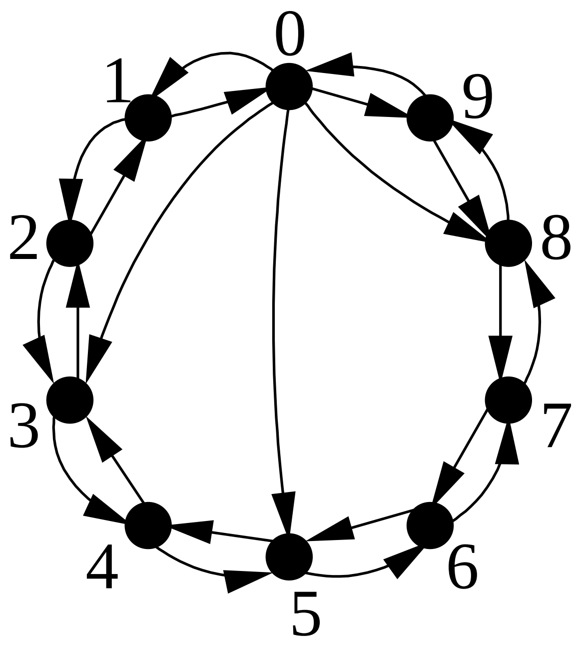
Loop Ranking $\mathcal{L}(i) = \sum_{i \in \mathrm{Cycle}} w(\mathrm{Cycle}) \propto \mathrm{Prob}(i \in \mathrm{Cycle})$

for $\mathrm{Prob}[\underline{S}] = \frac{1}{Z} \prod_l (r_l)^{S_l} \prod_i f_i(\underline{S}_i)$

Directed Small World Network



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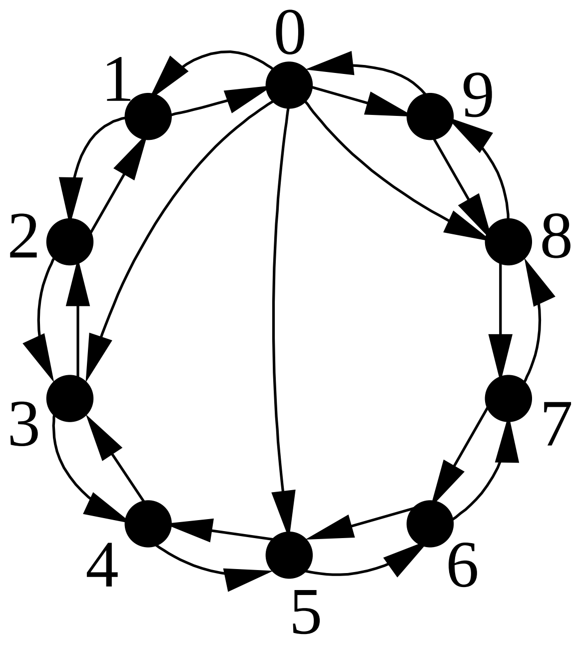
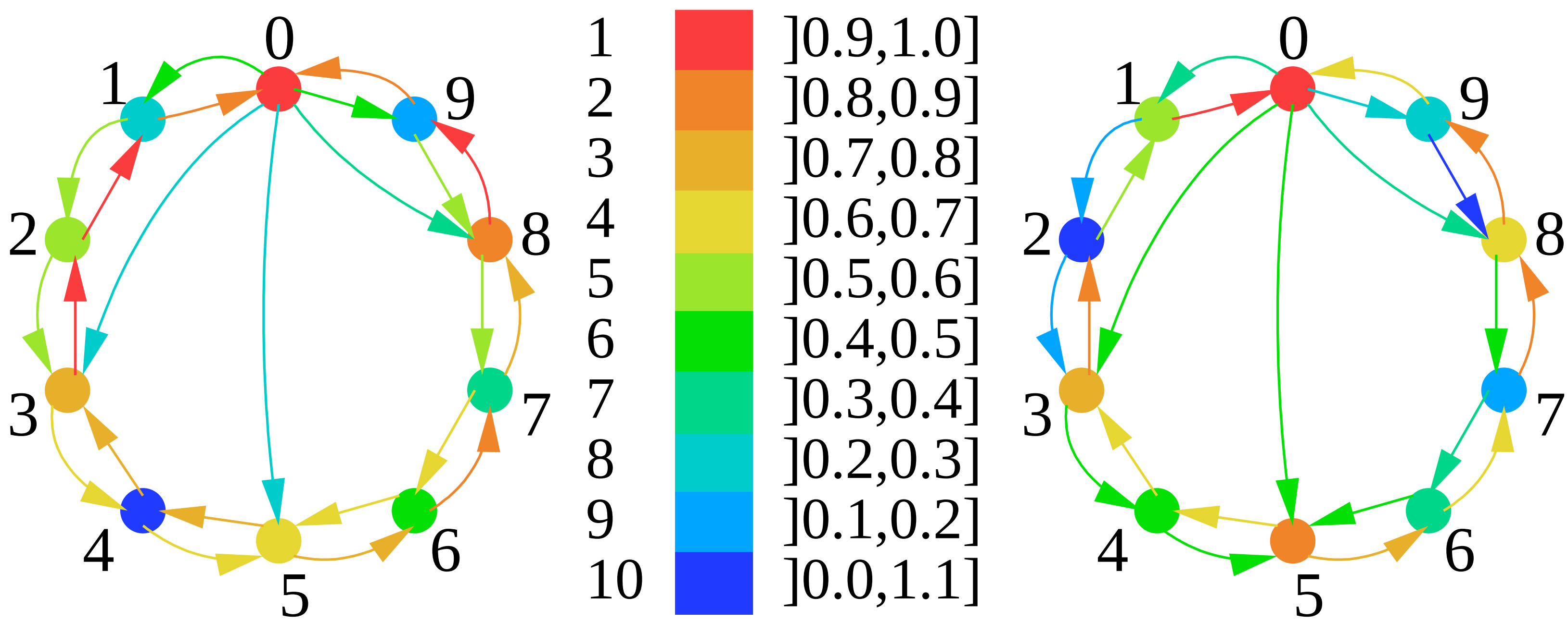


R	i	$\frac{\mathcal{P}(i)}{\mathcal{P}(5)}$	i	$\frac{\mathcal{L}(i)}{\mathcal{L}(0)}$	i	$\frac{\mathcal{B}(i)}{\mathcal{B}(0)}$
1	5	1.00	0	1.00	0	1.00
2	4	0.94	8	0.92	5	0.68
3	3	0.91	3	0.90	3	0.58
4	6	0.90	5	0.89	8	0.55
5	7	0.84	2	0.87	1	0.50
6	8	0.78	6	0.84	4	0.45
7	2	0.71	7	0.83	6	0.45
8	0	0.53	1	0.82	9	0.43
9	9	0.53	9	0.82	7	0.42
10	1	0.49	4	0.81	2	0.39

Directed Small World Network

Loop Ranking

Betweenness Centrality



Path-based Ranking:

- capture importance of vertices on small-world networks
- allow for edge ranking
- lead to similar results for the most important vertices and edges

Conclusions and Future Perspectives

- We find Hamiltonian cycles on regular and non-regular sparse graphs,
  - b.m.o. BP: faster
  - b.m.o. MC: more reliable
- New path-based vertex and edge ranking captures their importance in traffic flow (on directed small world networks).

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$\rightarrow$ Deeper investigation of the level of approximation of BP.

$\rightarrow$ Improve MC by finding optimal parameters in automated way.

$\rightarrow$ Find loops or paths of intermediate length.

$\rightarrow$ Investigate real-world networks (scale free, weighted).

$\rightarrow$ Consider a Potts-like configuration space.