Canonical Paths for Markov Chain Monte Carlo: from Art to Science

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Joint work with Lingxiao Huang and Pinyan Lu

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Simons Institute for the Theory of Computing

Matchings

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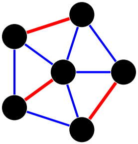

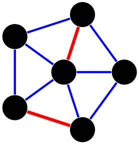

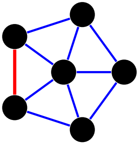

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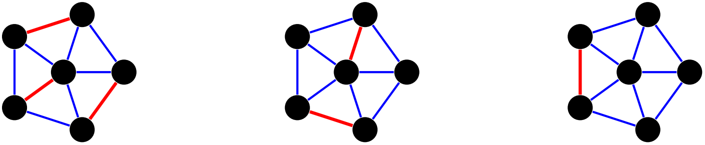

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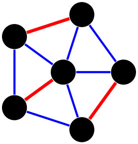

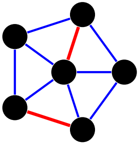

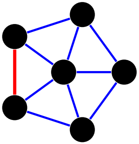

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The problem admits FPRAS via the Markov chain Monte-Carlo technique.

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A fully polynomial-time randomized approximation scheme (FPRAS) outputs a number M^* satisfying

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Jerrum and Sinclair defined a Markov chain to uniformly sample matchings in a graph $G = (V, E)$.

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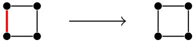

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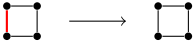
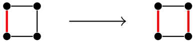


(ADD) if both u and v are not matched, $M' = M + e$;



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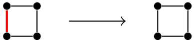

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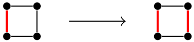
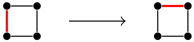


(REPLACE) if exactly one of u and v is matched by an edge e', $M' = M - e + e'$;



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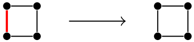

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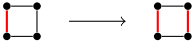

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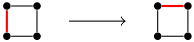

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The chain is rapidly mixing if for every distribution σ on Ω, $\|P^t\sigma - \pi\|_{TV} \leq \varepsilon$ for $t = \text{poly}(n, \varepsilon^{-1})$.

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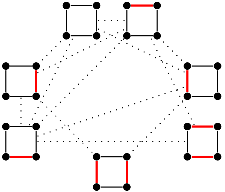

We want to route $\pi(x)\pi(y)$ units between every pair (x, y) of distinct configurations in Ω^2 via a set of weighted paths $\Gamma_{x,y}$.

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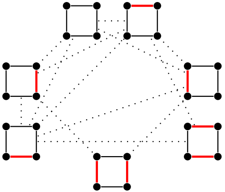

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The family of paths $\Gamma := \bigcup_{x,y \in \Omega^2}$ is called the canonical paths.

The congestion of canonical paths Γ is

$$\rho(\Gamma) = \max_{e=(u,v)} \frac{1}{Q(e)} \sum_{\gamma \in \Gamma \text{ with } e \in \gamma} w(\gamma),$$

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Theorem (Sinclair)

A lazy reversible Markov chain is rapidly mixing if for some canonical paths Γ, it holds that $\rho(\Gamma) \leq \text{poly}(n)$.

Canonical Paths for Jerrum-Sinclair's Chain

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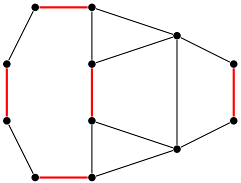
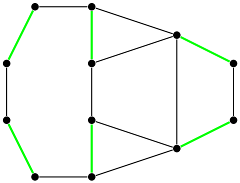
Consider two matchings M and M' in a graph G.



M



M'

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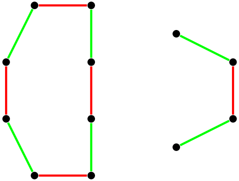

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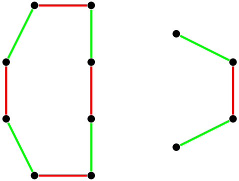

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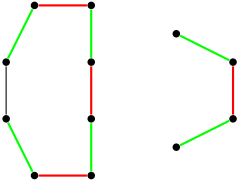

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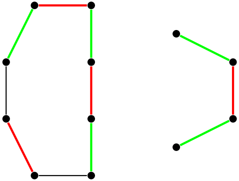

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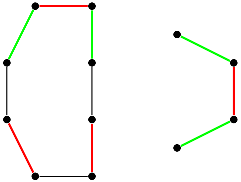

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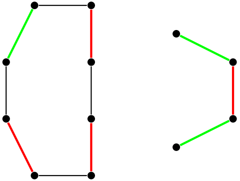

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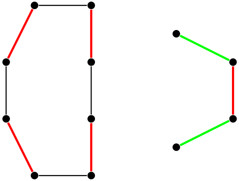

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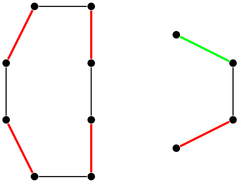

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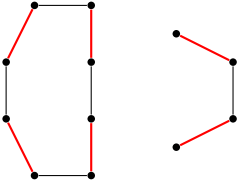

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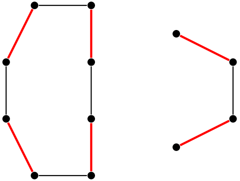

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This family of canonical paths admits $\text{poly}(n)$ congestion, and thus the Markov chain is rapidly mixing.

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The problem of counting matchings corresponds to the Holant problem with every $f_v = [1, 1, 0, 0, \ldots, 0]$.

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Example

Let $x = (1,0,1,1,1,1) \in \{0,1\}^{[5]}$, then

$$\begin{aligned}\mathcal{M}_x = \{&\{\{1,3\},\{4,5\},\{6\}\},\{\{1,4\},\{3,5\},\{6\}\},\{\{1,5\},\{3,4\},\{6\}\},\\ &\{\{1,3\},\{4,6\},\{5\}\},\{\{1,4\},\{3,6\},\{5\}\},\{\{1,6\},\{3,4\},\{5\}\},\\ &\{\{1,3\},\{5,6\},\{4\}\},\{\{1,5\},\{3,6\},\{4\}\},\{\{1,6\},\{3,5\},\{4\}\},\\ &\{\{1,4\},\{5,6\},\{3\}\},\{\{1,5\},\{4,6\},\{3\}\},\{\{1,6\},\{4,5\},\{3\}\}\\ &\{\{3,4\},\{5,6\},\{1\}\},\{\{3,5\},\{4,6\},\{1\}\},\{\{3,6\},\{4,5\},\{1\}\}\}\end{aligned}$$

Definition

Let J be a finite set. A function $f : \{0,1\}^J \to \mathbb{R}^+$ is windable, if there exists values $B(x, y, M) \geq 0$ for all $x, y \in \{0,1\}^J$ and all $M \in \mathcal{M}_{x \oplus y}$ satisfying:

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Intuitively, every $M \in \mathcal{M}_{x \oplus y}$ corresponds to a canonical path in Γ_{xy}, with weight proportional to $B(x,y,M)$.

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Let J be a finite set. A function $f : \{0,1\}^J \to \mathbb{R}^+$ is windable, if there exists values $B(x,y,M) \geq 0$ for all $x, y \in \{0,1\}^J$ and all $M \in \mathcal{M}_{x \oplus y}$ satisfying:

1. $f(x)f(y) = \sum_{M \in \mathcal{M}_{x \oplus y}} B(x,y,M)$ for all $x, y \in \{0,1\}^J$, and
2. $B(x,y,M) = B(x \oplus S, y \oplus S, M)$ for all $x, y \in \{0,1\}^J$ and all $S \in M \in \mathcal{M}_{x \oplus y}$.

The definition, essentially captures the way one route flows in the canonical paths arguments.

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Condition 2 allows us to apply flow-encoding argument to bound the congestion.

Half Edges

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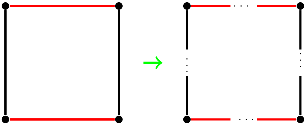

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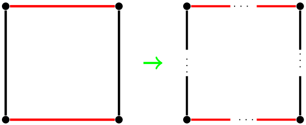
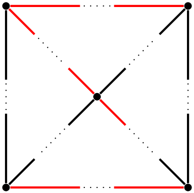
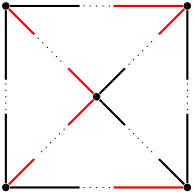


We use Ω_k to denote the set of configurations with k inconsistent (full) edges.



An assignment in Ω_1



An assignment in Ω_3

Markov Chain for Windable Functions

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For every two configurations $\sigma, \pi \in \Omega$, define the transition probability:

$$P'(\sigma,\pi) = \begin{cases} \frac{2}{n^2}\min\left(1, \frac{w_\Lambda(\pi)}{w_\Lambda(\sigma)}\right), & \text{if } d(\sigma,\pi) = 2; \\ 1 - \frac{2}{n^2}\sum_{\rho:d(\sigma,\rho)=2}\min\left(1, \frac{w_\Lambda(\rho)}{w_\Lambda(\sigma)}\right), & \text{if } \sigma = \pi; \\ 0, & \text{otherwise.} \end{cases}$$

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We then make the chain lazy by setting

$$P(\sigma,\pi) = \begin{cases} \frac{1+P'(\sigma,\pi)}{2}, & \text{if } \sigma = \pi; \\ \frac{P'(\sigma,\pi)}{2}, & \text{if } \sigma \neq \pi. \end{cases}$$

Approximation via Windability

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Corollary

There exists an FPRAS for Holant($\mathcal{F}$) if

1. Every function in $\mathcal{F}$ is windable;
2. For every instance Λ, it holds that $\frac{w_\Lambda(\Omega_2)}{w_\Lambda(\Omega_0)} \leq \text{poly}(n)$.

Canonical Paths for Windable Functions

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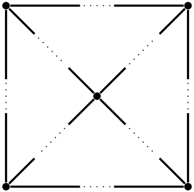
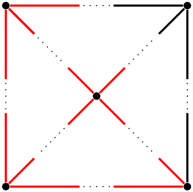
Consider two configurations $x \in \Omega_0$ and $y \in \Omega_2$.



$x \in \Omega_0$



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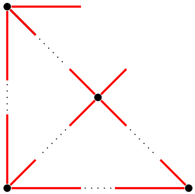
Canonical Paths for Windable Functions

Their symmetric difference is



$z := x \oplus y \in \Omega_2$

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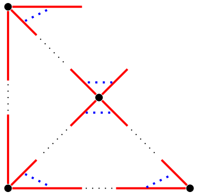

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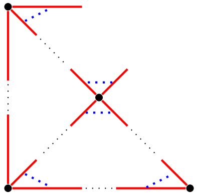

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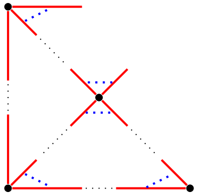

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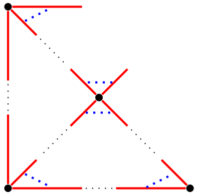

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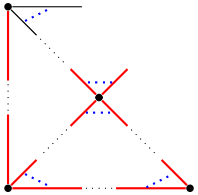

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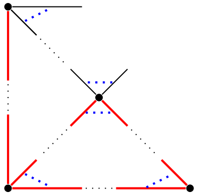

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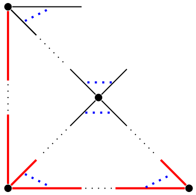

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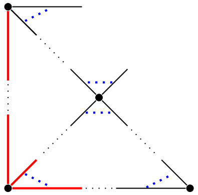

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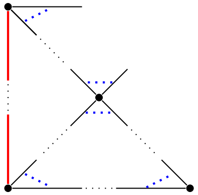

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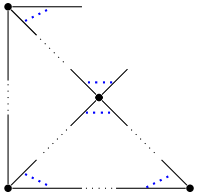

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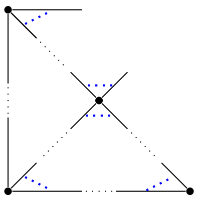

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The weight of this path is proportional to $\prod_{v \in V} B(x|_{E(v)}, y|_{E(v)}, M_v)$.

Windability for Symmetric Functions

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The pinning of a symmetric function $f(x) = [f_0, f_1, \ldots, f_d]$ is a function of the form $[f_i, f_{i+1}, \ldots, f_{i+m}]$.

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Theorem

Given a symmetric function $F : \{0,1\}^d \to \mathbb{R}^+$, F is windable if and only if for every pining G of F with arity m, the function $H(x) = [h_0, h_1, \ldots, h_m] := G(x)G(\bar{x})$ satisfies the following condition: The linear equations $\mathbf{A}_m\mathbf{x} = \mathbf{h}$ has a nonnegative solution $\mathbf{x} \geq 0$, where $\mathbf{h} = [h_0, h_1, \ldots, h_{\lfloor \frac{m}{2} \rfloor}]$.

For every integer $m \geq 1$, the matrix $\mathbf{A}_m$ is defined as follows:

- If $m = 2n$ is even, then $\mathbf{A}_m = (a_{ij})_{\substack{0 \leq i \leq n \\ 0 \leq j \leq n}} \in \mathcal{Q}^{(n+1)\times(n+1)}$ where

$$a_{ij} = \begin{cases} \binom{i}{j}\binom{2n-i}{j} j!(i-j-1)!!(2n-i-j-1)!! & \text{if } i \equiv j \pmod 2; \\ 0 & \text{otherwise.} \end{cases}$$

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The term a_{ij} of A_m has following combinatorial explanation:

- There are m labeled balls, i of them are red and $m-i$ of them are blue;
- The value a_{ij} is the number of ways to partition m balls into pairs (with at most one singleton) such that the number of pairs with different colors is j.

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Then we can reduce the task of finding $B(x, y, M)$s to solving a system of linear equations.

Example: Matchings

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It is also straightforward to see that $\frac{w(\Omega_2)}{w(\Omega_0)} \leq 4n^4$.

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It is easy to check that f_v is windable with our characterization.

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Corollary

For every $b \leq 7$, there exists an FPRAS for counting b-matchings.

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All previous FPRAS can be extended to edge weighted version: subdividing each edge e and introduce a new constraint $[1, 0, w_e]$.

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Is every windable function realizable by a matchgate?