Rapid mixing and Markov bases

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Fibers

Let $A \in \mathbb{Z}^{m \times d}$ and $b \in \mathbb{Z}^d$, the $b$-fiber of $A$ is

$$F_{A,b} := \{ u \in \mathbb{N}^d : A \cdot u = b \}.$$ 

Fiber graphs

Let $M \subseteq \ker(A) \cap \mathbb{Z}^d$. The graph $F_{A,b}(M)$ has vertices $F_{A,b}$ and $u, v \in F_{A,b}$ are adjacent if $u - v \in \pm M$.

Markov bases

$M$ is a Markov basis if $F_{A,b}(M)$ is connected for all $b \in \mathbb{Z}^d$.

Theorem (Diaconis, Sturmfels, 1996)

$M \subseteq \mathbb{Z}^d$ is a Markov basis of $A$ if and only if $I_M = I_A$. 

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Walking randomly on fibers

Algorithm (Simple Walk)

**Input:** \( b \in \mathbb{N}_A, \ u_0 \in \mathcal{F}_{A,b}, \ r \in \mathbb{N} \)

**Output:** Uniform sample of \( \in \mathcal{F}_{A,b} \)

\[
\text{FOR } i = 1..r \\
\quad \text{Sample } m \in \pm \mathcal{M} \text{ uniformly} \\
\quad \text{IF } u_i + m \in \mathbb{N}^d \\
\quad \quad \text{THEN } u_i = u_{i-1} + m \\
\quad \quad \text{ELSE } u_i = u_{i-1} \\
\text{RETURN } u_r
\]

→ This gives an irreducible and aperiodic Markov chain.

**Convergence Theorem of Markov chains**

\[
\text{After } r = \mathcal{O} \left( \frac{-1}{\log(|\lambda|)} \right) \text{ steps, } u_r \text{ can be regarded as an uniform sample of } \mathcal{F}_{A,b} \\
\text{−1} < \lambda < 1: \text{ SLEM of transition matrix of the random walk.}
\]
Analysing the speed

What is fast?

$(G_n)_{n \in \mathbb{N}}$ sequence of graphs with simple walk

- **Expanders**: number of steps needed is independent of $n$
- **Rapid mixing**: number of steps needed is polynomial in $\log |V(G_n)|$

→ Consider $(n \cdot b)_{n \in \mathbb{N}} \subseteq \mathbb{N} A$

Expander and rapid mixing

For any $n \in \mathbb{N}$, let $\lambda_n$ be the SLEM of the simple walk on $\mathcal{F}_{A,n \cdot b}(\mathcal{M}_n)$

- $(\mathcal{F}_{A,n \cdot b}(\mathcal{M}_n))_{n \in \mathbb{N}}$ is an expander if $\lambda_n \leq 1 - \epsilon$ for all $n \in \mathbb{N}$
- $(\mathcal{F}_{A,n \cdot b}(\mathcal{M}_n))_{n \in \mathbb{N}}$ is rapidly mixing if $\lambda_n \leq 1 - \frac{1}{p(\log n)}$ for all $n \in \mathbb{N}$

Algebraic statistics

Use the same moves for every right-hand side: $\mathcal{M}_n := \mathcal{M}$
Fiber walks can be slow!

No expander

- \( H := \begin{pmatrix} I_3 & I_3 & 0 & 0 & -1_3 & 0 \\ 0 & 0 & I_3 & I_3 & 0 & -1_3 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix} \)

- Hemmecke-Ray \( \{ n \cdot e_7 : n \in \mathbb{N} \} \)

- \( \lim_{n \to \infty} \lambda(\text{Gröbner}) = 1 \)

- \( \lim_{n \to \infty} \lambda(\text{Graver}) = 1 \)

Not rapidly mixing

- \( A := (1, 1) \in \mathbb{Z}^{1 \times 2}, \mathcal{M} := \{ (1, -1)^t \}, b = 1 \)

- \( \mathcal{F}_{A,n}(\mathcal{M}) \cong \cdots \)

\( \Rightarrow \) SLEM of \( \mathcal{F}_{A,n}(\mathcal{M}) \geq 1 - \frac{1}{n+1} \)

- Is this (asymptotic) behaviour typical for fiber walks?
Edge-expansion

Edge-expansion, Cheeger constant

\[ h(G) := \min_{|U| \leq \frac{1}{2}|V|} \frac{\#(\text{edges leaving } U)}{|U|} \]

Expander Mixing Lemma

Simple walk on \(d\)-regular graph \(G\): \(1 - \frac{h(G)}{d} \leq |\lambda| \leq 1 - \frac{h(G)^2}{d^2}\)

Why is this convenient for fibers?

\(\mathcal{F}_{A,n_1} \cdot b(\mathcal{M})\) \hspace{1cm} \(\mathcal{F}_{A,n_2} \cdot b(\mathcal{M})\)
How fast are fiber walks?

Theorem (W.; 2015)

Let $\mathcal{M}$ be a Markov basis of $A$ and let $b \in \mathbb{N}A$ with $\dim(\mathcal{F}_{A,b}) > 0$. Then:

- $\lim_{n \to \infty} h(\mathcal{F}_{A,n \cdot b}(\mathcal{M})) = 0$ (no expander)
- $h(\mathcal{F}_{A,n \cdot b}(\mathcal{M})) \in O\left(\frac{1}{n}\right)$ (not rapidly mixing)

Graver vs. Gröbner vs. Markov

Using more structural moves does not improve mixing asymptotically.

A way out?

Use an “adapted” Markov basis $\mathcal{M}_n^b$ for every $\mathcal{F}_{A,n \cdot b}$ and control

$$\frac{h(\mathcal{F}_{A,n \cdot b})}{|\mathcal{M}_n^b|}.$$

- In general, $|\mathcal{M}_n^b| = O(\log n)$ does not suffice to obtain rapid mixing.
Can we construct expanders on fibers?

Adaption

Let $\mathcal{M} = \{m_1, \ldots, m_r\} \subseteq \mathbb{Z}^d$ be a Markov basis, $n \in \mathbb{N}$, and $b \in \mathbb{NA}$.

$$\mathcal{M}_n^b := \left\{ \sum_{j=1}^r \lambda_j m_j : \lambda_1, \ldots, \lambda_r \in \mathbb{Z}, \sum_{j=1}^r |\lambda_j| \leq \text{Diam}(\mathcal{F}_{A,n \cdot b}(\mathcal{M})) \right\}.$$

SLEM: $1 - \frac{|\mathcal{F}_{A,n \cdot b}|}{|\mathcal{M}_n^b|}$

Theorem (W.; 2015)

$\text{Diam}(\mathcal{F}_{A,nb}(\mathcal{M})) \in \mathcal{O}(n) \Rightarrow (\mathcal{F}_{A,nj b}(\mathcal{M}_{nj}^b))_{j \in \mathbb{N}}$ is an expander.
Computational results

Sampling from $\mathcal{M}_i^b$
- Sample coefficients $\lambda_i \in [l_i, u_i]$ and use the move $\sum_{i=1}^{r} \lambda_i m_i$.

Hemmecke-Ray

$\mathcal{F}_{H_3, n \cdot e_7}(\text{Gröbner}_n^{e_7})$
- $n = 10^3$: 3.551.720
- $n = 10^6$: 4.058.733
- $n = 10^{50}$: 4.059.281

$3 \times 3$ independence model

$\mathcal{F}_{A_{33}, n \cdot 1_6}(\mathcal{M}_i^{16})$
- $n = 10^{10}$: 21.062.343
- $n = 10^{100}$: 37.255.074
- $n = 10^{1000}$: 37.255.074

Adapted vs. conventional
- $A = (1, 1, 1)$
- $\mathcal{M} = \{e_1 - e_2, e_1 - e_3\}$
- $b_n = n \cdot 1$
This talk was about

- Fiber walks are (asymptotically) slow.
- Adaption of Markov basis can lead to expanders.

How?

Analyse sequences of fiber graphs in varying dimension (parametric Markov bases)? Which right-hand sides should be considered?

\[(\mathcal{F}_{A_n, ?}(M_n))_{n \in \mathbb{N}}\]

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Thanks!