最大次数ΔのC_4フリーグラフの(2Δ-4)彩色数を数え上げるための マルコフ連鎖モンテカルロ法

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概要. 本稿では、C_4フリーグラフのk-彩色数を数え上げるための高速なマルコフ連鎖モンテカルロ法 (MCMC) を提案する。グラフの最大次数をΔとすると、$\Delta \geq 6$のときは$k \geq 2\Delta-4$に対して、また$\Delta = 3, 4, 5$のときはそれぞれ$k \geq 5, 6, 7$に対して、k-彩色数の数え上げが多項式時間で可能である。実行時間は$O(\Delta^2 n \log n)$である。本結果は、特に$\max(2\Delta-4, \Delta+2) \leq k < 11/6\Delta$、$3 \leq \Delta \leq 23$のときに、$C_4$フリーグラフに対する初めての多項式時間$k$-彩色数数え上げアルゴリズムである。

A Markov Chain for $(2\Delta - 4)$-Colorings of C_4-Free Degree-Δ Graphs

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Abstract. In this paper, we present a new rapidly mixing Markov chain for counting the number of proper k-colorings of a C_4-free graph with maximum degree Δ, where $k \geq 2\Delta - 4$ for $\Delta \geq 6$ and $k \geq 5, 6, 7$ for $\Delta = 3, 4, 5$, respectively. This is the first MCMC result for k-coloring C_4-free graphs, where $max(2\Delta-4, \Delta+2) \leq k < \frac{11}{6}\Delta$ and $3 \leq \Delta \leq 23$. The mixing time of our chain is $O(\Delta^2 n \log n)$.

1 Introduction

A proper k-coloring of a graph $G = (V, E)$ is a labeling X of the vertices by colors from the set $C = \{1, 2, \cdots, k\}$, where neighboring vertices must receive different colors. The problem of counting the number of proper k-colorings of a graph has been extensively studied in computer science and statistical physics.

The most successful approach for this problem is the *Markov chain* approach. Rapid convergence of a well-designed Markov chain for a graph corresponds to efficiently counting the number of k-colorings. Jerrum [7] proved that for a graph with maximum degree Δ, a simple Markov chain, known as the *Glauber Dynamics*, achieves rapid mixing in time $O(\frac{k-\Delta}{k-2\Delta} n \log n)$ whenever $k > 2\Delta$ (Note that Jerrum's result can be extended to the case $k = 2\Delta$). Independently, Salas and Sokal proved a closely related result on the phase transition in the Potts model, which have implications for the rapid convergence of the Glauber Dynamics. The chain by Jerrum, Salas, and Sokal is generally called the *JSS chain.*. Their results are the first to relate the convergence property of a Markov chain to the maximum degree of a graph.

By extending the JSS chain, Dyer and Greenhill presented a more rapidly mixing Markov chain for k-colorings. We refer to this chain as the *DG chain.* In the transition of their chain, an edge is chosen uniformly at random and the endpoints of the edges are properly recolored uniformly at random from the permissible pairs of colors. When $k = 2\Delta$, the bound on convergence time is $\Omega^*(n^2)$[1] time faster than that for the JSS chain. Their convergence results are obtained using the method of *path coupling*, introduced by Bubley and Dyer [1]. Furthermore, Bubley, Dyer and Greenhill [2] presented a computer-aided proof that 5 colors are enough for graphs of maximum degree 7, for a new heat-bath Markov chain. Nevertheless, there still existed 2Δ barrier of a given Δ. Vigoda [10] made the first breakthrough beyond the 2Δ barrier by proving that for $k > 11/6\Delta$, the Glauber Dynamics is rapidly mixing in time $O(n^2)$. Their Markov chain is a reminiscent of the Wang-Swendsen-Kotecký (WSK) algorithm [11].

For a restricted class of graphs, Dyer and Frieze [3] gave a rapidly mixing Markov chain in case $k \geq 1.763\Delta$, provided that a graph has some restriction on the degree Δ and girth g, i.e., $\Delta = \Omega(\log n)$ and $g = \Omega(\log \Delta)$. With the same restriction on degree and girth, Molloy [8] improved the lower bound to $k \geq 1.489\Delta$. Hayes [6] improved the condition on girth to $g \geq 5$ for $k \geq 1.763\Delta$, and $g \geq 6$ for $k \geq 1.489\Delta$. Still, the maximum degree needed as $\Delta = \Omega(\log n)$. Recently Dyer et al. [4] showed that Δ can be reduced to a sufficiently (but significantly) large constant.

In this paper, we provide a new Markov chain which also breaks the 2Δ bound for C_4-free graphs. That is, graphs are assumed to contain no cycle of length four. we also assume that the minimum degree of graphs is at least 3. The Markov chain achieves rapid mixing in time $O(\Delta^2 n \log n)$ when $k \geq 2\Delta - 4$ for $\Delta \geq 6$ and $k \geq 5, 6, 7$ for $\Delta = 3, 4, 5$, respectively. Thus, in this paper, we provide the first MCMC results for k-coloring C_4-free graphs, where $max(2\Delta - 4, \Delta + 2) \leq k < \frac{11}{6}\Delta$ and $3 \leq \Delta \leq 23$. Note that our result does not require a large maximum degree.

Our chain traverses over the states consisting of a pair of a coloring and a vertex of the input graph, randomly walking over the vertices and recoloring neighbors of the currently visiting vertex, where for recoloring the neighbor vertices it uses the JSS and DG chains. As for analysis we use the path coupling method.

[1] We use the notion Ω^* for hiding a polylogarithmic factor in order, i.e., $\Omega^*(f(n)) = O((\log^k n) f(n))$ for some fixed k.

2 Preliminaries

2.1 Graph Notations

Let $G = (V, E)$ be a connected graph of maximum degree $\Delta \geq 3$. In this paper, we assume that G contains no four-cycle C_4. That is, for any distinct 4 vertices u, v, w, x, at least one of $\{u, v\}, \{v, w\}, \{w, x\}, \{x, u\}$ must be an edge of G. Further, we assume that every vertex of G has degree at least 3 (in other words, the minimum degree of G is at least 3). In fact, this assumption is removable. However, we omit the proof of it due to space limitation.

The set of neighbors of a vertex v is denoted as $\mathcal{N}(v)$. Particularly, $|\mathcal{N}(v)| \leq \Delta$ for every vertex v. Let C be a set of k distinct elements, called *colors*. A mapping X from V to C is a *k-coloring* of G (or simply *coloring* when k is fixed in the context). Let C^V be the set of all k-colorings of G. Thus, $X(v)$ is the color assigned to a vertex v by the coloring X. A vertex v is *properly* colored in the coloring X if $X(v) \neq X(w)$ for all $w \in \mathcal{N}(v)$. A coloring X is called *proper* if every vertex is properly colored in X. Let $\Omega_k(G) \subseteq C^V$ be the set of all proper k-colorings of G.

2.2 The Path Coupling Method

Let $\mathcal{M}$ be an arbitrary ergodic process whose states are in a space Ω. Let π be a distribution over Ω such that, for all $Y \in \Omega$,

$$\sum_{X \in \Omega} \pi(X) \mathbf{P}[\mathcal{M}(X) = Y] = \pi(Y).$$

This distribution π is uniquely determined and called the *stationary* distribution of the chain $\mathcal{M}$. Particularly, π is known as the limit distribution by the outputs of the chain $\mathcal{M}$, let it begin from an arbitrary initial state.

For practical use of the chain $\mathcal{M}$, it must converge quickly to π. In more precise, the mixing time of the chain $\mathcal{M}$ is the least integer $T \geq 0$ such that, for $X \in \Omega, \forall\, t \geq T$,

$$\frac{1}{2} \sum_{Y \in \Omega} |\mathbf{P}[\mathcal{M}^t(X) = X] - \pi(X)| \leq \epsilon,$$

given a parameter $\epsilon > 0$. This value is usually denoted as $\tau(\epsilon)$.

In order to bound the mixing time we use the so-called path-coupling theorem. A coupling of the chain $\mathcal{M}$ is a stochastic process

$$\langle X, Y\rangle \mapsto \langle X', Y'\rangle$$

on $\Omega \times \Omega$ such that each of $X \mapsto X'$, $Y \mapsto Y'$, considered marginally, is a faithful copy of the transaction by $\mathcal{M}$; that is, for all X and Y,

$$\begin{aligned} \sum_{Y'} \mathbf{P}[\langle X, Y\rangle \mapsto \langle X', Y'\rangle] &= \mathbf{P}[\mathcal{M}(X) = X'], \\ \sum_{X'} \mathbf{P}[\langle X, Y\rangle \mapsto \langle X', Y'\rangle] &= \mathbf{P}[\mathcal{M}(X) = Y']. \end{aligned}$$

The *path coupling* theorem involves a subset $\mathcal{S} \subseteq \Omega \times \Omega$. Two states X and Y are *connected* by $\mathcal{S}$ if there is a finite sequence of states $X = X_0, X_1, \ldots, X_r = Y$ such that $\langle X_\ell, X_{\ell+1}\rangle \in \mathcal{S}$ for all $0 \leq \ell \leq r-1$. We say that a graph $(\Omega, \mathcal{S})$ is connected if it is connected as a directed graph with the edges in $\mathcal{S}$, i.e., any two different states in Ω are connected by $\mathcal{S}$.

The path coupling method is first introduced by Bubley and Dyer[1]. Here we refer to a version by Dyer and Greenhill[5].

Theorem 1 *Let $\langle X, Y\rangle \mapsto \langle X', Y'\rangle$ be a coupling of the Markov chain $\mathcal{M}$ and let δ be any integer valued metric defined on $\Omega \times \Omega$. Let $D = \max_{X,Y\in\Omega} \delta(X, Y)$. Let $\mathcal{S} \subseteq \Omega \times \Omega$ such that the graph $(\Omega, \mathcal{S})$ is connected. Suppose that there exists $\beta < 1$ such that*

$$\mathbf{E}[\delta(X', Y')] \leq \beta\delta(X, Y), \ \forall (X, Y) \in \mathcal{S}.$$

Then, the mixing time is bounded as follows. [2]

$$\tau(\epsilon) \leq \frac{\log(D\epsilon^{-1})}{1-\beta}.$$

3 A New Markov Chain

3.1 Definitions

Let $s \leq 2n$ and

$$[s] = \{0, \ldots, s-1\}.$$

We refer to elements in $[s]$ as *orders*. We introduce a mapping σ from $[s]$ to V such that $\sigma([s]) = V$ (i.e. σ is an onto-mapping), and for every $i \in [s]$, $\{\sigma(i), \sigma(i+1)\} \in E$ and $\sigma(i-1) \neq \sigma(i+1)$, where we identify $\sigma(-1)$ with $\sigma(s-1)$ and $\sigma(s)$ with $\sigma(0)$. Notice that such a mapping σ exists because the minimum degree of G is at least 3. We fix the mapping σ throughout the paper, and define a new Markov chain $\mathcal{M}(\Omega_k(G) \times [s])$ over state space $\Omega_k(G) \times [s]$. Note that the first component of a sate (X, i) is a coloring and the second component i is an order.

[2] All logarithms are based on the natural number.

Before defining the state transitions of $\mathcal{M}(\Omega_k(G) \times [s])$, let us make a brief intuitional description. For an order $i \in [s]$ let

$$\begin{aligned} \mathcal{E}(i) = \{\{v, w\} : \{v, w\} \in E, \\ v, w \in \mathcal{N}(\sigma(i)) - \{\sigma(i-1), \sigma(i+1)\}\ \} \\ \cup \{\{v, v\} : v \in \mathcal{N}(u) - \{\sigma(i-1), \sigma(i+1)\}\ \} \end{aligned}$$

A transition from a state (X, i) consists of three stages. First, move the order i to $i' \in \{i, i+1, i-1\}$. Secondly, choose an edge from $\mathcal{E}(i')$, uniformly at random. Finally, choose colors $c(v)$ and $c(w)$, uniformly at random, such that both v and w are properly colored in X; if a selflooping edge $\{v, v\}$ is chosen then let $c(v)$ be a random proper color of v in X.

To be more precise, we make some preparation. Let $nibble(i)$ be a random variable of values in $\{-1, 0, 1\} \times \{same, recol\}$ such that,

$$nibble(i) = \begin{cases} (0, same) & \text{with prob. } \frac{2}{3s} \\ (0, recol) & \text{with prob. } \frac{1}{3s} \\ (1, same) & \text{with prob. } \frac{3s-3i-4}{3s} \\ (1, recol) & \text{with prob. } \frac{1}{3s} \\ (-1, same) & \text{with prob. } \frac{3i-1}{3s} \\ (-1, recol) & \text{with prob. } \frac{1}{3s}. \end{cases}$$

For $e \in E \cup \{\{v, v\} : v \in V\}$ and $X \in C^V$, let C_X^e be the set of all proper colors to the ends of e for X; that is,

$$C_X^{\{v,w\}} = \{\ (c, c') \in C^V \times C^V : c(v) \neq X(u) \text{ for all } u \in \mathcal{N}(v) - \{w\}, c(u') \neq X(w) \text{ for all } u' \in \mathcal{N}(w) - \{v\} \text{ and } c = c' \text{ iff } v = w\ \}$$

where we may abbreviate (c, c) as c. Notice that if $e = \{v, v\}$, then C_X^e is the set of all proper colors of v in X. Denote by $X_{e\to c}$ the coloring obtained from X by recoloring v by $c(v)$ and w by $c(w)$. Then both v and

w are properly colored in $X_{e \to c}$ if and only if $c \in C_X^{\{v,w\}}$, for a given coloring $c \in C^V$.

Now we are ready to define the transitions of Markov chain $\mathcal{M}(\Omega_k(G) \times [s])$. Given a sate (X_t, i_t) at time t, (X_{t+1}, i_{t+1}) is defined as follows.

(i) Let $(a, \alpha) = \mathit{nibble}(i_t)$. Let $i_{t+1} = i_t + a$. If $\alpha = \mathit{same}$ then let $X_{t+1} = X_t$.

(ii) If $\alpha = \mathit{recol}$, then let $i_{t+1} = i_t + a$, choose a pair (e, c) of $e \in \mathcal{E}(i_{t+1})$, and $c \in C_X^e$ uniformly at random, and let $X_{t+1} = (X_t)_{e \to c}$.

In the succeeding sections, we will show that the Markov chain outputs the uniform sampling of a proper k-coloring, by taking projection on the coloring component, and also show that the stationary distribution is rapidly mixing for $k \geq 2\Delta - 4$.

3.2 Ergodicity of $\mathcal{M}(\Omega_k(G) \times [s])$

We first show the ergodicity of the chain.

Theorem 2 *If $k \geq \Delta + 2$ then the Markov chain $\mathcal{M}(\Omega_k(G) \times [s])$ is ergodic.*

Proof. is aperiodic, since choosing the same state is given a positive probability. We prove below that it is irreducible for $k \geq \Delta + 2$. Therefore, $\mathcal{M}(\Omega_k(G) \times [s])$ is ergodic when $k \geq \Delta + 2$.

The Hamming distance $H(X, Y)$ between X and Y in C^V is the number of vertices colored differently in X and Y. Let $\mathcal{S}$ be a subset of $\Omega \times \Omega$ such that,

$\langle (X, i), (Y, j) \rangle \in \mathcal{S}$ iff either

1. $|i - j| = 1$ and $X = Y$, or,
2. $i = j$, $H(X, Y) = 1$ and $X(v) \neq Y(v)$ at $v \in \mathcal{N}(\sigma(i)) - \{\sigma(i+1), \sigma(i-1)\}$.

Lemma 1 *If $k \geq \Delta + 2$ then a graph $(\Omega_k(G) \times [s], \mathcal{S})$ is connected.*

Proof. Let $(X, i), (Y, j)$ be states in $\Omega_k(G) \times [s]$. If $H(X, Y) = 0$, then $X = Y$. So (X, i) and (Y, j) are connected by $\mathcal{S}$ as follows: move order from i to j without changing the coloring at all.

Suppose that $H(X, Y) \geq 1$. It is enough to show that: there is a state (Z, ℓ) in $\Omega_k(G) \times [s]$ such that (X, i) and (Z, ℓ) are connected by $\mathcal{S}$ and $H(Z, Y) < H(X, Y)$.

Suppose that colorings X, Y disagree at a vertex v. Let ℓ be an order such that $v = \sigma(\ell)$. Let $U = \{u \in \mathcal{N}(v) : X(u) = Y(v)\}$. Consider the following connection by $\mathcal{S}$, beginning from (X, i):

1. Move order to ℓ and recolor every vertex in $U - \{\sigma(\ell - 1), \sigma(\ell + 1)\}$ by a proper color that is not $Y(v)$.

2. For each $a \in \{-1, 1\}$, move order to m such that $m \notin \{\ell + a - 1, \ell + a + 1\}$ and $\{\sigma(m), \sigma(\ell + a)\} \in E$, and recolor $\sigma(\ell + a)$ by a proper color that is not $Y(v)$.

3. Move order to $\ell + 1$ or $\ell - 1$ and recolor v by $Y(v)$.

4. Move order to ℓ.

Justification of the first step follows. If U is empty, then the second step is passed over. Assume that $U \neq \emptyset$. Let $u \in U$. There are at most Δ colors surrounding u, hence at least $|C| - \Delta \geq 2$ colors can be used for properly recoloring u, one of which is different from $Y(v)$. That color is used for recoloring each $u \in U$ in the second step.

Similarly, the recoloring of the second step is justified. Moreover, since the degree of $\sigma(\ell + a)$ is at least 3, there exist an order m such that $\{\sigma(\ell + a), \sigma(m)\} \in E$ and $m \notin \{\ell + a - 1, \ell + a + 1\}$. Note that $m \notin \{\ell + a - 1, \ell + a + 1\}$ iff $\ell + a \notin \{m - 1, m + 1\}$.

Next, we show that the obtained state (Z, ℓ) witnesses the claim. Clearly, all steps of the procedure are in $\mathcal{S}$, so (X, i) and (Z, ℓ) are connected by $\mathcal{S}$. Furthermore, $H(Z, Y) < H(X, Y)$. In fact, the second step does not increase the Hamming distance from Y, because X and Y disagree on all the vertices in U. In addition, the fourth step decreases the distance by 1. So, $H(Z, Y) < H(X, Y)$. The claim holds. □

Consequently, Theorem 2 is proved. □

3.3 Uniformity of the Stationary Distribution

Since the chain $\mathcal{M}(\Omega_k(G) \times [s])$ is ergodic for $k \geq \Delta + 2$, it converges to the unique distribution after infinite times of excursions. This is the so-called stationary distribution and is denoted by π. To show that the Markov chain achieves the uniform distribution over proper k-colorings, we prove the following.

Theorem 3 *π is a production of the uniform distribution over proper k-colorings and the binomial distribution over the orders.*

Proof. Notice that this is not so trivial, because the Markov chain $\mathcal{M}(\Omega_k(G) \times [s])$ is neither symmetric nor time-reversible. For example, let $(X, i) \in \Omega_k(G) \times [s]$, $1 \leq i \leq s-2$, $e \in \mathcal{E}(i+1) - \mathcal{E}(i)$, and $c \in C^e_X$. Suppose that $c \neq X(e)$. Then, state (X, i) transforms to $(X_{e\to c}, i+1)$ with a positive probability, but there is no chance that $(X_{e\to c}, i+1)$ transforms to (X, i).

Now, a precise proof follows. Let U be the uniform distribution over $\Omega_k(G)$. Let B_s be the distribution over $[s]$ such that

$$B_s(i) = \binom{s-1}{i} / 2^{s-1}.$$

Then, it is enough to show the following lemma.

Lemma 2 *For all $X \in \Omega_k(G)$ and $i \in [s]$, $\pi((X, i)) = U(X)B_s(i)$.*

Proof. Let (X, i) and (Y, j) be states in $\Omega_k(G) \times [s]$. Let $P((X, i), (Y, j))$ be the probability that (X, i) transforms to (Y, j) by one step of the chain $\mathcal{M}(\Omega_k(G) \times [s])$.

Then, it is enough to show the following

$$\sum_{X,i} U(X)B_s(i)P((X, i), (Y, j)) = U(Y)B_s(j),$$

for every $(Y, j) \in \Omega_k(G) \times [s]$, because these equations uniquely fix the stationary distribution π as claimed in the lemma.

By symmetry of transition of $\mathcal{M}(\Omega_k(G) \times [s])$, we have

$$P((X, i), (Y, j)) = P((Y, i), (X, j))$$

for every states (X, i) and (Y, j) in Ω. Therefore,

$$U(X)B_s(i)P((X, i), (Y, j)) = U(Y)B_s(i)P((Y, i), (X, j)).$$

Summing it over all $X \in \Omega_k(X)$ and $i \in [s]$ gives that

$$\sum_{X,i} U(X)B_s(i)P((X, i), (Y, j)) = \sum_{X,i} U(Y)B_s(i)P((Y, i), (X, j)).$$

Now, we show that the left hand side is equal to $U(Y)B_s(i)$. In the left hand side, term $P((Y, i), (X, j))$ is nonzero if and only if $i \in \{j-1, j, j+1\} \cap [s]$. Therefore, it is written as

$$U(Y) \sum_X \sum_{i\in\{j-1,j,j+1\}\cap[s]} B_s(i)P((Y, i), (X, j)).$$

Let $\mathcal{M}(\Omega_k(G) \times [s])(Y, i) = (Z, k)$. If $X \neq Y$ then the transition probability $P((Y, i), (X, j))$ is

$$\mathbf{P}[k = j \wedge \alpha = \mathit{recol}] \cdot \mathbf{P}[Z = X | k = j \wedge \alpha = \mathit{recol}],$$

while if $X = Y$ then it is

$$\mathbf{P}[k = j \wedge \alpha = \mathit{recol}] \cdot \mathbf{P}[Z = X | k = j \wedge \alpha = \mathit{recol}] + \mathbf{P}[k = j \wedge \alpha = \mathit{same}],$$

where the two events $Z = X$ and $k = j \wedge \alpha = \mathit{recol}$ are mutually independent, and

$$\sum_{X\neq Y} \mathbf{P}[Z = X | k = j \wedge \alpha = \mathit{recol}] = 1 - \mathbf{P}[Z = Y | k = j \wedge \alpha = \mathit{recol}],$$

so

$$U(Y) \sum_X \sum_{i\in\{j-1,j,j+1\}\cap[s]} B_s(i)P((Y, i), (X, j)) = U(Y) \sum_{i\in\{j-1,j,j+1\}\cap[s]} B_s(i)\mathbf{P}[k = j]$$

where by definition of *nibble*,

$$\mathbf{P}[k = j] = \begin{cases} \frac{s-j}{s} & \text{if } i = j-1 \\ \frac{1}{s} & \text{if } i = j \\ \frac{j+1}{s} & \text{if } i = j+1, \end{cases}$$

So the right hand side is

$$U(Y) \sum_{i\in\{j-1,j,j+1\}\cap[s]} B_s(i)\mathbf{P}[k = j] = U(Y)B_s(j).$$

Hence, Lemma 2 and Theorem 3 are proved. □

3.4 Path Coupling and Rapid Mixing of $\mathcal{M}(\Omega_k(G) \times [s])$

We define the distance between states (X, i) and (Y, j) as

$$\delta((X,i),(Y,j)) = H(X,Y) + |i-j|.$$

We now prove that the chain $\mathcal{M}(\Omega_k(G) \times [s])$ is rapidly mixing when $k \geq \max(2\Delta - 4, \Delta + 2)$, by applying Theorem 1.

Theorem 4 *Let G be a graph with maximum degree $\Delta \geq 3$ and having no C_4. The Markov chain $\mathcal{M}(\Omega_k(G) \times [s])$ is rapidly mixing for $k \geq \max(2\Delta - 4, \Delta + 2)$. The mixing time of $\mathcal{M}(\Omega_k(G) \times [s])$ is bounded as follows.*

$$\tau(\epsilon) = O((\Delta-2)(\Delta-1)\, n \log(n/\epsilon)).$$

Proof. Let $\langle (X,i),(Y,j) \rangle$ be an arbitrary pair in $\mathcal{S}$. We define a coupling

$$\langle (X,i),(Y,j) \rangle \mapsto \langle (X',i'),(Y',j') \rangle$$

of chain $\mathcal{M}(\Omega_k(G) \times [s])$ in following cases.

Case I. $i \neq j$. By definition of $\mathcal{S}$, $X = Y$. Without loss of generality, $j = i + 1$.

Let

$$nibble_2(i) = \begin{cases} (1,0,same,same) & \text{w.p. } \frac{2}{3s} \\ (1,0,recol,recol) & \text{w.p. } \frac{1}{3s} \\ (0,-1,same,same) & \text{w.p. } \frac{2}{3s} \\ (0,-1,recol,recol) & \text{w.p. } \frac{1}{3s} \\ (1,1,same,same) & \text{w.p. } \frac{3s-3i-7}{3s} \\ (1,1,same,recol) & \text{w.p. } \frac{1}{3s} \\ (-1,-1,same,same) & \text{w.p. } \frac{3i-1}{3s} \\ (-1,-1,recol,same) & \text{w.p. } \frac{1}{3s}, \end{cases}$$

where w.p. stands for with probability. We define $\langle (X',i'),(Y',n') \rangle$ by the following procedure:

1. Let $(a, b, \alpha, \beta) = nibble_2(i)$.
2. Let $i' = i + a$ and $j' = j + b$.
3. If $i' = j'$ and $\alpha = recol$ then choose a pair (e, c) of $e \in \mathcal{E}(j')$ and $c \in C_X^e$ uniformly at random, and let $X' = Y' = X_{e \to c}$.
4. If $i' \neq j'$ and $(\alpha, \beta) = (recol, same)$ then choose a pair (e, c) of $e \in \mathcal{E}(i')$ and $c \in C_X^e$ uniformly at random, and let $X' = X_{e \to c}$ and $Y' = Y$.
5. If $i' \neq j'$ and $(\alpha, \beta) = (same, recol)$ then choose a pair (e, c) of $e \in \mathcal{E}(j')$ and $c \in C_X^e$ uniformly at random, and let $X' = X$ and $Y' = Y_{e \to c}$.
6. Otherwise, let $X' = X$ and $Y' = Y$.

It is immediate to examine that this is a coupling of $\mathcal{M}(\Omega_k(G) \times [s])$.

To apply the coupling theorem, we now compute the upper bound of expectation

$$E[\delta((X',i'),(Y',j')) - 1].$$

If $i' = j'$ then $\delta((X',i'),(Y',j')) = 0$, else if $i' \neq j'$ and either $\alpha = recol$ or $\beta = recol$ then $\delta((X',i'),(Y',j')) \leq 3$, else $\delta((X',i'),(Y',j')) = 1$. The consequent upper bound of E_I is

$$-\mathbf{P}[|a+b| = 1] + 2\mathbf{P}[\,|a+b| = 2 \text{ and}$$
$$(\alpha,\beta) \in \{(recol, same),(same,recol)\}\,]$$
$$\leq -\frac{2}{s} + \frac{4}{3s} = -\frac{2}{3s} := E_I.$$

Case II. $i = j$. By definition of $\mathcal{S}$, $H(X,Y) = 1$, and X, Y differs at a vertex v in $\mathcal{N}(\sigma(i)) - \{\sigma(i-1), \sigma(i+1)\}$.

We define $\langle (X',i'),(Y',j') \rangle$ by the following procedure.

1. Let $(a, \alpha) = nibble(i)$.
2. Let $i' = j' = i + a$.
3. If $\alpha = same$ then let $X' = Y' = X$.
4. If $\alpha = recol$ and $v \notin \mathcal{N}(\sigma(i')) - \{\sigma(i'-1), \sigma(i'+1)\}$ then choose an edge $e = \{u, w\} \in \mathcal{E}(i')$ uniformly at random and a proper color $c \in C_X^e$ to the edge e uniformly at random. Then, let $X' = X_{e \to c}$ and $Y' = Y_{e \to c}$.
5. If $\alpha = recol$ and $v \in \mathcal{N}(\sigma(i')) - \{\sigma(i'-1), \sigma(i'+1)\}$ then choose an edge $e = \{u, w\} \in \mathcal{E}(i')$ uniformly at random.
   (a) If $u \neq w$ and $v \in \mathcal{N}(\sigma(i')) - \{\sigma(i'-1), \sigma(i'+1)\}$ then define $\langle (X',i'),(Y',j') \rangle$ as in the DC chain. That is,

i. $v \notin \{u,w\}$, $\{v,w\} \in E$ and $\{u,w\} \notin E$. This case divides into 8 subcases and defines $\langle X', Y' \rangle$ for each. See Dyer and Greenhill (2000).

ii. $v \notin \{u,w\}$, $\{v,w\} \in E$ and $\{u,w\} \in E$. See Dyer and Greenhill (2000), too.

iii. $v \notin \{u,w\}$, $\{v,w\} \notin E$ and $\{u,w\} \notin E$. Choose $c \in C_X^e$ uniformly at random and let $X' = X_{e\to c}, Y' = Y_{e \to c}$.

iv. $v \in \{u,w\}$. Choose $c \in C_X^e$ uniformly at random and let $X' = Y' = X_{e\to c}$.

(b) If $u = w$ then define $\langle X', Y' \rangle$ as in the JSS chain. That is,

i. $v \neq w$ and $\{v,w\} \in E$. This case divides into 4 subcases and define $\langle X', Y' \rangle$ for each. See Jerrum (1995).

ii. $v \neq w$ and $\{v,w\} \notin E$. Choose $c \in C_X^e$ uniformly at random and let $X' = X_{e\to c}, Y' = Y_{e\to c}$.

iii. $v = w$. Choose $c \in C_X^e$ uniformly at random and let $X' = Y' = X_{e\to c}$.

We need to justify step 4 of Case II, claiming that v is adjacent to none of the vertices in $\mathcal{N}(\sigma(i')) - \{\sigma(i'-1), \sigma(i'+1)\}$, so that X' and Y' in the step are proper colors of G in spite of $X'(v) \neq Y'(v)$. In fact, for an arbitrary w in the set, if $\{v,w\} \in E$ then four vertices $\sigma(i), \sigma(i'), w$ and v form a square with possibly diagonals in G, i.e. all of $\{\sigma(i), \sigma(i')\}, \{\sigma(i'), w\}, \{w, v\}$ and $\{v, \sigma(i)\}$ are edges of G, a contradiction.

Theorem 5 (Dyer and Greenhill [5]) *Let $E_{DG,\iota}$ be the expectation of $H(X',Y') - 1$ under the condition that $\alpha = recol$ and an edge e are chosen as in ι of 4-(a), $\iota \in \{\mathrm{i}, \mathrm{ii}\}$. Then, for every $\Delta \geq 3$ and $k \geq \Delta + 2$,*

$$E_{DG,\mathrm{i}} \leq \begin{cases} \frac{19}{36} & k = \Delta + 2 \\ \frac{(k-\Delta+1)(k-\Delta)+2(k-\Delta)+1}{((k-\Delta+1)(k-\Delta)+1))(k-\Delta+1)} & \text{o.w.} \end{cases}$$

$$E_{DG,\mathrm{ii}} \leq \frac{2(k-\Delta+1)}{(k-\Delta)^2}.$$

Theorem 6 (Jerrum [7]) *Let E_{JSS} be the expectation of $H(X',Y')$ under the condition that $\alpha = recol$ and an edge e are chosen as i of in 4-(b). Then, for every $\Delta \geq 3$ and $k \geq \Delta + 2$,*

$$E_{JSS} \leq \frac{1}{k - \Delta}$$

Lemma 3 *Let*

$$B(t) = (-E_{DG,\mathrm{i}} + E_{DG,\mathrm{ii}}/2)t^2 + ((\Delta-3)E_{DG,\mathrm{i}} - E_{DG,\mathrm{ii}}/2 + E_{JSS} - 1)t - 1$$

and suppose that $\beta := \max_{0 \leq t \leq \Delta - 3} B(t)$ is negative. Then,

$$\tau(\epsilon) \leq -\frac{3s(\Delta-2)(\Delta-1)}{2\beta} \log(n\epsilon^{-1}).$$

Proof. Theorem 1 proves the lemma, if $\beta < 0$ and, in both Cases I and II, the expectation $\mathbf{E}[H(X',Y') - 1]$ is bounded from above by $\frac{2\beta}{3s(\Delta-2)(\Delta-1)}$. By definition, $\Delta \geq 3$ and $-1 \leq \beta$, hence $E_I \leq \frac{2\beta}{3s(\Delta-2)(\Delta-1)}$. For steps 3 and 4 of case II, their contributions to E_{II} are nonpositive.

Let $\Delta_0 = |N(\sigma(i')) - \{\sigma(i'+1), \sigma(i'-1)\}|$, and t be the number of edges in $\mathcal{E}(i') - \{v,v\}$ adjacent to v. By definitions, $0 \leq \delta_0 \leq \Delta - 2$ and $0 \leq t \leq \Delta_0 - 1$. Let $k_{DG,\iota}$, $\iota \in \{\mathrm{i}, \mathrm{ii}\}$, be the number of those edges in $\mathcal{E}(i') - \{v,v\}$ falling into configuration ι of (a); Let k_{JSS} be that number for subcase (b). Then, we have

$$\begin{aligned} k_{DG,\mathrm{i}} &= t(\Delta_0 - t - 1) \\ k_{DG,\mathrm{ii}} &= t(t-1)/2 \\ k_{JSS} &= t \end{aligned}$$

We remain analysis for each configuration of step 5. First, $|\mathcal{E}(i')| = \Delta_0(\Delta_0-1)/2 + \Delta_0 = \Delta_0(\Delta_0+1)/2$. Among these edges, $k_{DG,\mathrm{i}}$ edges fall into confuguration (a)-i, so the contribution of confuguration (a)-i to E_{II} is at most $\mathbf{P}[\alpha = recol]\frac{k_{DG,\mathrm{i}}E_{DG,\mathrm{i}}}{\Delta_0(\Delta_0+1)/2}$. Similarly, configuration (a)-ii and (b)-i contributes to E_{II} by $\mathbf{P}[\alpha = recol]\frac{k_{DG,\mathrm{ii}}E_{DG,\mathrm{ii}}}{\Delta_0(\Delta_0+1)/2}$ and $\mathbf{P}[\alpha = recol]\frac{k_{JSS}E_{JSS}}{\Delta_0(\Delta_0+1)/2}$, respectively. On the other hand, the contributions of both (a)-iii and (b)-ii are at most 0. Finally, the contribution of (a)-iv and (b)-iii is $\mathbf{P}[\alpha = recol]\frac{-t}{\Delta_0(\Delta_0+1)/2}$ and $\mathbf{P}[\alpha = recol]\frac{-1}{\Delta_0(\Delta_0+1)/2}$, respectively. In all,

$$E_{II} \leq \mathbf{P}[\alpha = recol]\,(k_{DG,\mathrm{i}}E_{DG,\mathrm{i}} + k_{DG,\mathrm{ii}}E_{DG,\mathrm{ii}}$$

$$+k_{JSS}E_{JSS} - (t+1))/(\Delta_0(\Delta_0+1)/2)$$
$$= (k_{DG,\mathrm{i}}E_{DG,\mathrm{i}} + k_{DG,\mathrm{ii}}E_{DG,\mathrm{ii}} + k_{JSS}E_{JSS}$$
$$-(t+1))/(3s\Delta_0(\Delta_0+1)/2)$$

To this upperbound of E_{II}, we substitute the above numbers of $k_{DG,\mathrm{i}}, k_{DG,\mathrm{ii}}, k_{JSS}$ and the expectations in Theorem 5 and 6, then taking maximum over $0 \leq \Delta_0 \leq \Delta - 2$ and $0 \leq t \leq \Delta_0 - 1$, deriving an upperbound $\frac{2\beta}{3s(\Delta-2)(\Delta-1)}$ of E_{II}. □

By definition of β and Theorems 5 and 6, the following upper bound of β is obtained, where $\beta = -\frac{7}{36}$ is achieved when $\Delta = 6$ and $k = 8$.

Lemma 4 *If* $\Delta \geq 3$ *and* $k \geq \max(2\Delta - 4, \Delta + 2)$ *then* $\beta \leq -\frac{7}{36}$.

Sketch of Proof. We first note that for $k \geq 2\Delta - 5$, the upper bounds of β can be positive occasionally. Namely, the right hand side of the equation in Lemma 3 is evaluated as 3/2, 1, 67/84 for $\Delta = 7, 8, 9$, respectively. (For larger Δ, $\max_t B(t)$is also positive.)

Differentiating $B(t)$ by Δ, we can prove that it is monotonically decreasing on Δ for $\Delta \geq 6$. (The analysis is essentially done for the upper bound of $E_{DG,\mathrm{i}}$ in Theorem 5.) Furthermore, it is shown to be monotonically decreasing on k for $k \geq 2\Delta - 4$. Finally, we evaluate β of the end case $(\Delta, k) = (6, 8)$, obtaining $\beta = -\frac{7}{36}$, Hence, β is negative when $\Delta \geq 6$ and $k \geq 2\Delta - 4$. Similar analysis holds for $\Delta \in \{3, 4\}$ and $k \geq \max(2\Delta - 4, \Delta + 2)$, too. □

Finally, Lemmas 3 and 4 immediately derive Theorem 4.

4 Concluding Remarks

We have presented a new rapid mixing Markov chain for k-colorings of C_4-free graphs with minimum degree 3 and maximum degree Δ, where $k \geq \max(2\Delta - 4, \Delta + 2)$. The detailed analysis on the upper bounds in Theorem 5 and Lemma 3, and the removal of the minimum degree assumption will be included in the full version of the paper. We conjecture that C_4-free condition of the input graph could be removed by allowing to use two more colors.

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