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Title: Approximation schemes for randomly sampling colorings

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Abstract

Graph colouring is arguably one of the most important issues in Graph Theory. However, many of the questions that arise in the area such as the chromatic number problem or counting the number of proper colorings of a graph are known to be hard. This is the reason why approximation schemes are considered.

In this thesis we consider the problem of approximate sampling a proper coloring at random. Among others, approximate samplers yield approximation schemes for the number of colourings of a graph. These samplers are based in Markov chains, and the main requirement of these chains is to mix rapidly, namely in time polynomial in the number of vertices.

Two main examples are the Glauber and the flip dynamics. In the project we study under which conditions these chains mix rapidly and hence under which conditions there exist efficient samplers. The previous result proved rapid mixing of the chains provided $k > (11/6-\varepsilon_0)\Delta$ for some $\varepsilon_0 > 0$. The aim of this project is to study how much can this value ε_0 be increased, and hence prove rapid mixing of the chains under weaker conditions. Our result states that the flip and the Glauber dynamic mixes rapidly provided $k > (11/6-\varepsilon_0)\Delta$ for $\varepsilon_0 = \frac{1}{1320}$.

Keywords: Graph coloring, approximate samplers, Markov chains, randomized algorithms.

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Chapter 1

Introduction

Coloring of graphs is one of the major problems in Graph theory and has always triggered a lot of interest not only among mathematicians but also due to its many applications in other fields.

One of the most studied problems in this area is the chromatic number problem. Given a finite simple graph $G = (V, E)$, and a positive integer k, the goal is to determine whether there exists a proper vertex coloring of G with k colors. Moreover, the minimum value k for which there exists such coloring is called the chromatic number of G, and is denoted by $\chi(G)$. For $k \leq 2$ the existence of a k-coloring can be answered in polynomial time. However, Karp [16] proved that determining the chromatic number of a graph is NP-complete for $k \geq 3$. There is little that we can say about the chromatic number of an arbitrary graph and the existing results in the area require some additional information. For instance, if Δ is the largest vertex degree of the graph, a simple greedy algorithm gives that the graph is $(\Delta+1)$-colourable. Basically the algorithm fixes an ordering of the vertices and colours each of them with a colour not used among its neighbours. This algorithm gives that $\chi(G) \leq \Delta + 1$ and Brook's theorem determines when the bound is tight. In particular, it asserts that for $\Delta \geq 3$, the chromatic number satisfies $\chi(G) = \Delta + 1$ if G contains a clique of order $\Delta + 1$.

A related problem is counting the number of proper k-colorings of a graph. Notice that this problem is harder than determining the chromatic number, and belongs to a class of problems called #P which is the analogous of NP for counting problems. There is a special interest in the problem of counting the number of proper colorings in statistical physics, where it corresponds to approximating the partition function of the zero temperature anti-ferromagnetic Potts model [20].

While counting colorings exactly is #P-complete, which is the analogous of NP-complete for counting, there are efficient algorithms for approximate counting in some cases. Some of them are deterministic and are known as *fully polynomial-time approximation scheme* or FPTAS while others are randomized and are known as *fully polynomial-time randomized approximation scheme* or FPRAS.

It is known that when $k < \Delta$, even approximate counting is NP-hard [10]. As the existence of a k-coloring is ensured for $k \geq \Delta + 1$ due to the greedy algorithm, we restrict the question to these values. Hence the conjecture is whether there exist algorithms for approximate counting for $k \geq \Delta + 1$. This question has repeatedly challenged existing algorithmic techniques and stimulated the development of new ones.

One of the approaches is to use Markov chain Monte Carlo methods (MCMC), given the

strong relation that exists between the problem of counting the number of colorings of a graph and sampling a proper coloring at random. More precisely, finding an approximating scheme for counting can be reduced to finding an (almost) uniform random sampler, known as FPAUS (*fully polynomial almost uniform sampler*). In this case the approximate scheme for counting is randomized.

Another approach is to use deterministic algorithms. These algorithms make use of two main techniques: the correlation decay, i.e. the decreasing influence of colors on distant vertices; and the polynomial interpolation or Barvinok method [1], which uses the absence of zeros of the partition function in a suitable region of the complex plane. However, the results obtained with FPTAS have never improved the bounds given by the randomized schemes [18]. Hence, let us focus on MCMC methods.

MCMC are methods that use a Markov chain whose stationary distribution is the one we are interested in sampling from. In particular, the algorithm runs such chain until the probability distribution is unlikely to be far from the stationary one and selects the current state as the sample. One requirement for this chain is to converge fast to the stationary distribution. Namely to converge in time polynomial in n, the number of vertices, so that the algorithm is also polynomial. In this case the chain is said to mix rapidly and the time to equilibrium is usually bounded using couplings of Markov chains.

The first chain that was studied is called the Glauber dynamics, and it is widely believed to work for $k \geq \Delta + 2$. Glauber runs as follows: at each step, choose a random node and recolor it with a random color not appearing among its neighbours.

The first result in this area was due to Jerrum [13].

Theorem 1.1 ([13]) The Glauber dynamics is rapidly mixing, with mixing time $O(n \log n)$, provided $k > 2\Delta$.

Jerrum's proof presented a bottleneck that was difficult to avoid. Therefore, the effort was put on getting better bounds for restricted families of graphs. Dyer et al. [8] showed rapid mixing for roughly $k \geq 1.489\Delta$ provided the girth is at least 6 and the degree Δ is a sufficiently large constant, while Hayes and Vigoda [12] improved this to $k \geq (1 + \varepsilon)\Delta$ for girth at least 11 and degree Δ logarithmic in the number of vertices. Other results concern random graphs, trees or planar graphs. Dyer et al. [9] proved that one can construct a Markov chain algorithm that with high probability mixes in $O(n \log n)$ time with $k = o(\log \log n)$. In the case of trees, Martinelli, Sinclair and Weitz [19] showed $O(n \log n)$ mixing time for the Glauber dynamics on complete trees when $k > \Delta + 2$ and Δ is constant. And Hayes [11] showed that the Glauber dynamics mixes rapidly for $k > \Delta + c\sqrt{\Delta}$ on planar graphs, which was lately improved to $k = \Omega(\frac{\Delta}{\log \Delta})$.

In a breakthrough work, Vigoda avoided the bottleneck that presented Jerrum's proof and broke the 2Δ barrier. The chain he used to obtain this result was different from the Glauber dynamics. Instead of flipping single vertices, Vigoda proposed to flip 2-colored clusters or Kempe components. This chain, called flip dynamics, is a variant of the Wang-Swendsen-Kotecký (WSK) algorithm [24] and one can prove rapid mixing of the Glauber dynamics from rapid mixing of the flip dynamics, see [6]. Vigoda [23] described a more sophisticated coupling for the flip dynamics and obtained the following result:

Theorem 1.2 ([23]) The flip dynamics is rapidly mixing, with mixing time $O(n \log n)$, provided $k > \frac{11}{6}\Delta$.

In particular, Vigoda devised a one-step coupling using the Hamming metric, which is the distance that counts the number of vertices in which two colorings differ.

However, it is known that any one-step coupling with the Hamming metric can not prove rapid mixing for $k < 11/6\Delta$. There are two natural ways to overcome this issue. On the one hand, Chen and Moitra [4] presented a multi-step coupling using the Hamming metric. And on the other, Delcourt, Perarnau and Postle [5] described an alternative metric for the one-step Vigoda's coupling. By means of these two different strategies, they obtained two independent proofs of Theorem 1.3.

Theorem 1.3 ([4],[5]) There exists $\varepsilon_0 > 0$ such that the flip dynamics is rapidly mixing, with mixing time $O(n \log n)$, provided $k > (\frac{11}{6} - \varepsilon_0)\Delta$.

In their paper, Perarnau et al. [5] obtained $\varepsilon_0 = \frac{1}{84000} \approx 1.19 \cdot 10^{-5}$ while Chen and Moitra obtained $\varepsilon_0 \approx 9.4 \cdot 10^{-5}$. This value ε_0 was thought to be possibly increased, obtaining weaker conditions on rapid mixing on the chains.

The aim of this master thesis is to study how much can this value ε_0 be increased.
We follow the idea described by Delcourt, Perarnau and Postle [5] and we describe an alternative metric different than the Hamming metric and different from the one used in [5]. Through a tighter analysis in the expected variation distance in each step of the coupling we obtain the following result

Theorem 1.4 Theorem 1.3 holds with $\varepsilon_0 = \frac{1}{1320}$.

Taking into account the relation between the mixing time of the flip and the Glauber dynamics, the improvement in Theorem 1.4 also applies in the case of Glauber and we get:

Theorem 1.5 The Glauber dynamics is rapidly mixing, with mixing time $O(n^2 \log n)$, provided $k > (\frac{11}{6} - \varepsilon_0)\Delta$, with $\varepsilon_0 = \frac{1}{1320}$.

Structure of the thesis

We start introducing the main concepts of Markov chains and couplings. Then, we present Monte Carlo Markov Chain methods and we describe the first chain used, the Glauber dynamics. After that, in chapter 4, we study a useful technique in Markov chains, the Path coupling method, which allows to bound the mixing time of a chain, and we apply it to the Glauber dynamics. Then, in chapter 5 we present the flip dynamics and we give the proof of Vigoda's $\frac{11}{6}$ bound (Theorem 1.2). In the following chapter we describe an alternative metric for Vigoda's coupling, different than the one used by Delcourt, Perarnau and Postle. Chapter 8 is devoted to our main result, which improves upon the previous result. Finally in chapter 9 we study the result of Diaconis and Saloff-Coste [6] and we prove rapid mixing of the Glauber dynamics from the flip dynamics and in chapter 10 we relate the problem of counting to the problem of randomly sampling.

Chapter 2

Markov chains

Definition 2.1 A *discrete-time discrete-space stochastic process* $(X_t) = (X_t)_{t\geq 0}$ is a sequence of random variables, where X_t has support on a finite set Ω. Moreover, a stochastic process is a *Markov chain* if it satisfies:

$$Pr(X_{t+1} = y \mid X_0 = x_0 \cap ... \cap X_{t-1} = x_{t-1} \cap X_t = x) = Pr(X_{t+1} = y \mid X_t = x)$$

This property is usually called *Markovian* or *Memoryless property* and refers to the fact that the conditional probability of a transition from state x to state y is the same, no matter what sequence $x_0, x_1, ..., x_{t-1}$ of states preceded the current state x.

Definition 2.2 A Markov chain is *time-homogeneous* if $Pr(X_{t+1} = y \mid X_t = x)$ does not depend on t. Hence we can define $P(x, y) = Pr(X_{t+1} = y \mid X_t = x)$, and we call $P = (P(x, y))_{x,y\in\Omega}$ the *transition matrix* of (X_t).

The Markov chain is fully characterized by the matrix P and the x-th row of P is the distribution $P(x, \cdot)$. Thus P is *stochastic*, that is, for all $x \in \Omega$

$$\sum_{y\in\Omega} P(x, y) = 1$$

.

Given the transition matrix, the probability that $X_{t+1} = y$ can be written as follows:

$$Pr(X_{t+1} = y) = \sum_{x\in\Omega} Pr(X_{t+1} = y \mid X_t = x) \cdot Pr(X_t = x) = \sum_{x\in\Omega} P(x, y) \cdot Pr(X_t = x)$$

From this equation, if μ_t is the distribution at time t (i.e. $\mu_t(x) = Pr(X_t = x)$) we have that:

$$\mu_t = \mu_{t-1}P \tag{1}$$

So, given an initial distribution μ_0 :

$$\mu_t = \mu_0 P^t$$

Now we can study how does the distribution μ_t behave in the long term. From (1) if μ_t has a limit π as $t \to \infty$ any such limit distribution must satisfy $\pi = \pi P$. Namely, π must be a left eigenvector of matrix P.

Definition 2.3 Let (X_t) be a Markov chain with transition matrix P. A probability distribution π is a *stationary distribution* of (X_t) if $\pi = \pi P$.

Clearly if the probability distribution of the Markov chain at t is $\mu_t = \pi$, then $\mu_{t'} = \pi, \forall t' \geq t$. So, if the chain converges, the limiting distribution is stationary.

The following result gives a useful tool to find a stationary distribution of a chain:

Proposition 2.1 Let (X_t) be a Markov chain with transition matrix P. If π is a probability distribution on Ω such that for every $x, y \in \Omega$

$$\pi(x)P(x,y) = \pi(y)P(y,x)$$

then π is a stationary distribution of P.

Proof. The y-th entry of πP is

$$\sum_{x\in\Omega} \pi(x)P(x,y) = \sum_{x\in\Omega} \pi(y)P(y,x) = \pi(y)\sum_{x\in\Omega} P(y,x) = \pi(y)$$

where we have used that P is a stochastic matrix. Hence $\pi P = \pi$.

□

2.1 Properties of Markov chains

Let us define two important properties of Markov chains that are fundamental for the convergence of the Markov chain to a stationary distribution.

Definition 2.4 A Markov chain with transition matrix P is *irreducible* if for any two states $x, y \in \Omega$ there exists an integer t such that $P^t(x,y) > 0$.

Definition 2.5 A Markov chain with transition matrix P is *aperiodic* if for all $x \in \Omega$, $\gcd\{t : P^t(x,x) > 0\} = 1$.

If P is irreducible and aperiodic, the Markov chain converges to a stationary distribution. This result is known as the Fundamental Theorem of Markov Chains.

Moreover, we can ensure that the stationary distribution is the uniform distribution in some chains.

Definition 2.6 A Markov chain with transition matrix P is *symmetric* if for all $x, y \in \Omega$, $P(x,y) = P(y,x)$

If the Markov chain is symmetric, due to Proposition 2.1 the chain converges to the uniform distribution.

2.2 Fundamental Theorem of Markov chains

Theorem 2.2 (Fundamental Theorem of Markov chains) Let (X_t) be an aperiodic and irreducible Markov chain. Then there exists a unique stationary distribution π and for every $x, y \in \Omega$, $\lim_{t\to\infty} Pr(X_t = x \mid X_0 = y) = \pi(x)$.

We refer to Levin-Peres, [17], for the proof of the Fundamental Theorem.

2.3 Mixing time

Once the convergence to a stationary distribution is ensured, we would like to know how fast the Markov chain converges to it.

Definition 2.7 Let μ and ν be probability distributions in Ω. The *total variation distance* between μ and ν is defined as

$$d_{TV}(\mu, \nu) = \sup_{A \subset \Omega} |\mu(A) - \nu(A)|$$

Definition 2.8 Let (X_t) be an aperiodic and irreducible Markov Chain with transition matrix P and let π be its stationary distribution. The *mixing time* is defined as

$$\tau_{mix}(\epsilon) = \min\{t : \max_{x \in \Omega} d_{TV}(P^t(x, \cdot), \pi) \leq \epsilon\}$$

and we denote $\tau_{mix} = \tau_{mix}(1/4)$.

Hence the mixing time measures the time required by a Markov chain to have a small total variation distance with respect to the stationary distribution.

2.4 Coupling

Definition 2.9 Given $(X_t), (Y_t)$ Markov chains, a *coupling* is a joint stochastic process (X_t, Y_t) such that the marginal distributions are the same as the ones of (X_t) and (Y_t) and if $X_t = Y_t$ then $X_{t+1} = Y_{t+1}$.

In general, couplings are useful because a comparison between distributions is reduced to a comparison between random variables. For instance, in the following proposition, $d_{TV}(\mu, \nu)$ is upper bounded by the probability that the random variables X and Y are different, with probability distribution μ, ν respectively, for any (X, Y) coupling.

Proposition 2.3 Let X, Y be random variables with probability distributions μ and ν respectively. Then:

$$d_{TV}(\mu, \nu) \leq \min\{P(X \neq Y : (X, Y) \text{ coupling})\}$$

Proof. Let $A \subset \Omega$. Without loss of generality suppose $\mu(A) \geq \nu(A)$. Then

$$\mu(A) - \nu(A) = P(X \in A) - P(Y \in A) \leq P(X \in A, Y \notin A) \leq P(X \neq Y)$$

Maximizing over $A \subset \Omega$ we obtain the inequality of the statement. □

If fact, it can be shown that $d_{TV}(\mu, \nu) = \min\{P(X \neq Y : (X, Y) \text{ coupling})\}$ and such couplings are called *optimal*, see [17].

Finally, we can think of couplings as Markov chains in Ω^2. We will study further properties of couplings in the following chapters.

Chapter 3

MCMC and first examples

Many of the FPAUS are based on establishing convergence of a Markov chain defined on the set Ω under consideration. The idea is to define a Markov chain (X_t) with state space the one from which we want to sample, and whose stationary distribution is uniform on Ω. If the hypothesis of the Fundamental Theorem of Markov Chains hold (see Theorem 2.2) and the chain is symmetric (see Theorem 2.1), the convergence of (X_t) to the uniform distribution is ensured. Hence, the distribution of (X_t) is arbitrarily close to the uniform for t large enough. For such t, taking X_t as the sample point gives a sample from an almost uniform distribution. Such algorithms are known as Markov Chain Monte Carlo methods (MCMC).

3.1 MCMC for randomly sampling colorings

Markov Chain Monte Carlo Method can be applied to the problem of random sampling a coloring of a graph.

Although it is NP-complete to compute the chromatic number of a graph, there are some conditions that imply that G is k-colorable. For instance, if $k \geq \Delta + 1$, G is k-colorable.

Moreover, for the chains we will study, we will prove that irreducibility and aperiodicity is given when $k \geq \Delta + 2$. So the still opened problem is whether fast mixing can be proven for this value.

Hence, the goal is to find which are the sufficient conditions, on k and Δ, for the Markov chain to converge fast. More precisely, we will say that the Markov chain mixes rapidly if the mixing time is polynomial on the number of vertices n. This is much less than the number of k-colorings of a graph which is exponential in n. Namely, the number of k-colorings of a graph on n vertices is greater than $(k - \Delta)^n$ due to the fact that there are at least $k - \Delta$ available colors at each vertex. Hence, constructing all k-colorings and picking one at random would take time $O(c^n)$, for some constant c, which is exponential in n.

Our first approach is given by the Glauber dynamics.

3.2 Glauber dynamics (I)

Let $G = (V, E)$ and Ω the set of k-colorings of G. The Glauber dynamics is a Markov chain on the set Ω defined by the following transitions:

- Select $w \in V$ uniformly at random
- Select $c \in [k]$ uniformly at random
- If no neighbours of w have color c, recolour w with colour c.

Equivalently, the chain can be defined by the probability of going from any pair of states $\sigma, \tau \in \Omega$, $\sigma \neq \tau$, which is:

$$P(\sigma, \tau) = \begin{cases} \frac{1}{nk} & \text{if } \sigma, \tau \text{ differ at exactly one vertex } v \text{ and } \tau(v) = c' \text{ with } c' \in A_v(\sigma) \\ 0 & \text{otherwise.} \end{cases}$$

where $A_v(\sigma)$ is the set of available colors of v in coloring σ. And we define $P(\sigma, \sigma)$ so that $P(\sigma, \cdot)$ is a probability distribution.

3.2.1 Properties of the chain; stationary distribution

First of all notice that every improper coloring has a positive probability to reach a proper one, but a proper coloring can not move to any improper coloring. Hence, the chain eventually reaches a proper coloring, so the support of the stationary distribution is the set of proper colorings of the graph. In particular, it is enough to consider Ω the set of proper k-colorings of G.

Now, we argue that the stationary distribution is the uniform distribution in this support.

Proposition 3.1 The Glauber dynamics is irreducible and aperiodic for $k \geq \Delta + 2$ and its stationary distribution is the uniform distribution.

Proof. First, the chain is aperiodic because for every state $\sigma \in \Omega$, $P(\sigma, \sigma) > 0$. Moreover, for $k \geq \Delta + 2$, and for any pair $\sigma, \tau \in \Omega$ there exists a positive probability to move between them. For instance the chain could move from σ to τ taking the following movements: Consider an ordering of the vertices of G and try to recolour them in this order. When attempting to recolour vertex v to colour $c = \tau(v)$, some of the neighbours of v might be already coloured with c. Then recolour all these neighbours with an arbitrary available colour different from c and we can do this as the number of colours $k \geq \Delta + 2$.

Hence, for $k \geq \Delta + 2$ the hypothesis of the Fundamental Theorem of Markov Chains (Theorem 2.2) hold, and there exists a stationary distribution of this chain.

Moreover this stationary distribution is the uniform distribution in the set of proper colorings. Let π be such distribution and let us see that Proposition 2.1 holds. Let $\sigma, \tau \in \Omega$. If σ, τ are not proper, then $\pi(\sigma), \pi(\tau) = 0$ and the hypothesis hold. Now suppose one of them is proper and the other not; without loss of generality assume σ is not proper and τ is proper. Then $\pi(\sigma) = 0$ and $P(\tau, \sigma) = 0$ and again the equality of the proposition is fulfilled. And lastly, if σ, τ are proper colorings, then $\pi(\sigma) = \pi(\tau)$ and $P(\sigma, \tau) = P(\tau, \sigma)$. It follows from Proposition 2.1 that the stationary distribution π is uniform in the set of proper colorings.

□

To sum up, the Glauber dynamics converges to the uniform distribution on the set of k-proper colorings of G for $k \geq \Delta + 2$.

Notice that the bound $k \geq \Delta+2$ is tight for irreducibility. For $G = K_n$ and $k = n = \Delta+1$, let σ be a proper k-coloring. Then $P(\sigma, \tau) = 0$ for any $\tau \neq \sigma$ and $P(\sigma, \sigma) = 1$. Hence, for any number of steps, there is not a positive probability to move from one state to a different one.

Chapter 4

Path coupling

The main issue about MCMC is determining how large t must be until the distribution at time t is close enough to the stationary one. To do that recall the definition of the total variation distance between two distributions and impose that μ_t, the distribution at time t, is within ϵ distance from the stationary one. This is in particular the mixing time. So the main problem is to bound the mixing time of the chain.

The method of coupling is a useful tool to obtain bounds on the mixing time of a chain. More precisely, we have results that relate the total variation distance of two probability distributions with the probability that a coupling of two Markov chains with such probability distributions, are not coupled (recall Theorem 2.3).

First, let us define the couplings we will be interested in, those whose expected total variation distance decreases in any step of the chain.

Definition 4.1 Let d denote a metric in Ω and $d_{\max}$ the diameter of Ω under this metric. For an initial pair $(x, y) \in \Omega^2$, a coupling $(x, y) \to (x', y')$ γ-*contracts* for (x, y) for some $\gamma \in (0, 1)$ if

$$\mathbb{E}[d(x', y')] \leq \gamma d(x, y)$$

The following theorem proves that if there exists $\alpha > 0$ and a coupling that $(1 - \alpha)$-contracts for all (x, y), then the Markov chain mixes rapidly.

Theorem 4.1 Let $\alpha > 0$ and suppose the coupling $(1-\alpha)$-contracts for every $(x, y) \in \Omega^2$, then

$$\tau_{mix} = O(\alpha^{-1} \log(d_{\max}))$$

Proof. In order to bound τ_{mix}, we need to bound the total variation distance by $\frac{1}{4}$. Due to Proposition 2.3 we have:

$$\|X_t - Y_t\|_{TV} \leq Pr(X_t \neq Y_t | X_0, Y_0) \leq Pr(d(X_t, Y_t) \geq 1 | X_0, Y_0) \leq \mathbb{E}(d(X_t, Y_t) | X_0, Y_0)$$

where we have applied Markov inequality. It suffices to bound this expectation. As the coupling is contractive by hypothesis, we have:

$$\mathbb{E}(d(X_t, Y_t) | X_0, Y_0) \leq (1 - \alpha) d(X_{t-1}, Y_{t-1} | X_0, Y_0) \leq (1 - \alpha)^t d(X_0, Y_0) \leq e^{-\alpha t} d_{max}$$

because $1 - x \leq e^{-x}$. Then for a given ε

$$\|X_t - Y_t\|_{TV} \leq e^{-\alpha t} d_{\max} \leq \varepsilon$$

is satisfied if

$$t \geq \frac{-\ln \varepsilon + \ln d_{\max}}{\alpha}$$

So, in particular, $\tau_{mix} = O(\alpha^{-1} \log d_{\max})$. □

One of the most usual metrics considered for couplings on graph colorings is the Hamming distance, which counts the number of vertices in the graph whose color differ in the two colorings. More precisely the *Hamming distance* between colorings X and Y is defined as

$$d(X, Y) = |\{v \in V : X(v) \neq Y(v)\}|$$

We can now state the first result concerning mixing time for the Glauber dynamics.

Theorem 4.2 The Glauber dynamics is rapidly mixing, with mixing time $O(n \log n)$, provided $k > 4\Delta$.

Proof. Let (X_t) and (Y_t) be two Glauber dynamics in Ω. We will consider the identity coupling for these chains: we choose the same vertex w and color c in both chains. Now, let $D_t = \{v : X_t(v) \neq Y_t(v)\}$ be the set of disagreeing vertices at time t and $d_t = |D_t|$, the Hamming distance between X_t, Y_t. Then, applying Markov inequality:

$$\mathbb{P}[X_t \neq Y_t] = \mathbb{P}[d_t \geq 1 | X_0, Y_0] \leq \mathbb{E}[d_t | X_0, Y_0]$$

so it is enough to bound this last expectation.

Suppose we are given X_t and Y_t that determine D_t, and we want to find the expectation of d_{t+1} conditioning to d_t

There are 3 cases, which we will denote by good move, bad move or neutral move depending on whether the value of d_{t+1} is smaller, greater or equal to the value of d_t.

- Good move ($d_{t+1} < d_t$): In this case, $D_{t+1} = D_t \setminus \{w\}$. So $w \in D_t$ and color c does not appear in the neighbourhood of w in X_t and Y_t. There are at least $(k - 2\Delta)d_t$ choices for the pair (c, w).

- Bad move ($d_{t+1} > d_t$): In this case, w is recolored in just one chain. Hence w does not belong to D_t but has a neighbour $u \in D_t$ such that the color chosen c is either $X_t(u)$ or $Y_t(u)$. Such choices lead to $D_{t+1} = D_t \cup \{w\}$, and there are at most $2\Delta d_t$.

- Neutral move ($d_{t+1} = d_t$): All the other moves keep $D_{t+1} = D_t$.

As every move happens with probability $\frac{1}{kn}$ we obtain

$$\mathbb{E}[d_{t+1} | d_t] \leq d_t + \frac{1}{kn}(-(k - 2\Delta)d_t + 2\Delta d_t) \leq \left(1 - \frac{1}{kn}\right) d_t$$

where in the last inequality we have used the hypothesis that $k > 4\Delta$.

The coupling is $(1 - \frac{1}{kn})$-contracting, so applying Theorem 4.1 we get that $\tau_{mix} = O(n \log n)$

□

4.1 Path coupling

In some state spaces it may be difficult to bound the distance between a pair of arbitrary states. The path coupling lemma claims that it suffices to define the coupling for a small subset of initial pairs in Ω^2. This subset will be specified by a pre-metric.

Definition 4.2 A *pre-metric* on Ω is a pair (Γ, ω) where Γ is a connected, undirected graph with vertex set Ω, and ω is a positive real-valued function that assigns weights to edges $\sigma\eta$ of Γ such that for every edge $\sigma\tau$, $\omega(\sigma\tau)$ is the minimum weight among all paths between σ and τ. We will refer to adjacent vertices in Γ as *neighboring pairs*.

From this pre-metric, we can define a metric for the whole space Ω. For any $\sigma, \eta \in \Omega$, let $P_{\sigma,\eta}$ be the set of simple paths $\phi = (\phi_0, ..., \phi_s)$ where $\phi_0 = \sigma$ and $\phi_s = \eta$. The metric d induced by the pre-metric is defined as $d(\sigma, \tau) := \min_{\phi \in P_{\sigma,\eta}} \sum_{i=1}^{s} \omega(\phi_{i-1}\phi_i)$, the minimum weighted path between states σ and τ.

Lemma 4.3 (Path coupling) Let (Γ, ω) be a pre-metric in Ω, and let d be the metric induced. If a coupling defined in the edges of Γ $(1-\alpha)$-contracts for some $\alpha > 0$, then there exists a coupling in Ω satisfying

$$\tau_{mix} = O(\alpha^{-1} \log(d_{\max}))$$

Proof. We construct a coupling that $(1-\alpha)$-contracts for all Ω^2 and apply Theorem 4.1. We construct the coupling for an arbitrary pair of states X_t, Y_t by composing couplings along a shortest path between X_t and Y_t in Γ. Let $Z_t^0 = X_t, Z_t^1, ..., Z_t^j = Y_t$ be a shortest path between X_t, Y_t. By hypothesis:

$$\mathbb{E}(d(Z_{t+1}^i, Z_{t+1}^{i+1}) | Z_t^i, Z_t^{i+1}) \leq (1-\alpha) d(Z_t^i, Z_t^{i+1})$$

We obtain that:

$$\begin{aligned} \mathbb{E}(d(X_{t+1}, Y_{t+1}) | X_t, Y_t) &\leq \sum_{1 \leq i < j} \mathbb{E}(d(Z_{t+1}^i, Z_{t+1}^{i+1}) | Z_t^i, Z_t^{i+1}) \\ &\leq (1-\alpha) \sum_{1 \leq i < j} d(Z_t^i, Z_t^{i+1}) = (1-\alpha) d(X_t, Y_t) \end{aligned}$$

The result now follows from Theorem 4.1. □

The strength of the path coupling method is that it requires only comparisons between adjacent states, rather than arbitrary states, and this results in much simpler analyses and better bounds.

4.2 Glauber dynamics (II)

Path coupling can be applied to Glauber dynamics and it yields to a stronger result than the one obtained in section 3.2.

Theorem 4.4 The Glauber dynamics is rapidly mixing, with mixing time $O(n \log n)$, provided $k > 3\Delta$.

Proof. Recall the setting of the Glauber dynamics. Let $\Omega = [k]^V$ the set of all k-colorings of graph G and d the Hamming distance.

Let Γ be the graph with vertex set Ω and adjacencies given by

$$E(\Gamma) = \{X, Y \in \Omega \times \Omega : d(X, Y) = 1\}$$

i.e, pairs of colorings that differ in a single vertex. As $\Omega = [k]^V$, the length of the shortest path between any two states X and Y is $d(X, Y)$. So in particular, the Hamming distance is the distance induced by the pre-metric $(\Gamma, 1)$.

We apply the Path coupling lemma (Lemma 4.3) for Γ and d.

Let $X_t, Y_t \in \Gamma$ be neighboring coloring pairs ($X_tY_t \in \mathrm{E}(\Gamma)$), such that $X_t(v) \neq Y_t(v)$. In order to apply path coupling we consider the identity coupling; both chains attempt to update the same vertex w to the same color c.

Only updates with $w \in N(v)$ and $c \in \{X_t(v), Y_t(v)\}$ will succeed or fail in exactly one chain. So these are the only attempts that might increase the distance by 1. There are at most 2Δ cases in which the distance might increase.

On the other hand, the only updates that decrease the distance are successful recolorings of v. Since the colorings are equal for all vertices different from v, $X_t(N(v)) = Y_t(N(v))$. So there are at most Δ colors in the neighborhood of v, and there are at least $k - \Delta$ available colors for v.

As each update occurs with probability $1/kn$, we get

$$\mathbb{E}(d(X_{t+1}, Y_{t+1})|X_t, Y_t) \leq d(X_t, Y_t) + \frac{1}{kn}(2\Delta - (k - \Delta)) \leq 1 - \frac{1}{kn}$$

for $k > 3\Delta$. Applying the path coupling lemma for $\alpha = \frac{1}{kn}$, the theorem follows.

□

Moreover, modifying the coupling considered, the result can be improved and we obtain the following theorem:

Theorem 4.5 The Glauber dynamics is rapidly mixing, with mixing time $O(n \log n)$, provided $k > 2\Delta$.

Proof. The graph Γ and distance d remain the same as in the previous proof. We simply modify the coupling slightly.

Let X_t and Y_t differing at vertex v. If X_t attempts to recolor $w \in N(v)$ to $X_t(v)$ then Y_t attempts to recolor w to $Y_t(v)$. Similarly, if X_t attempts to recolor $w \in N(v)$ to $Y_t(v)$ then Y_t attempts to recolor w to $X_t(v)$. In all other cases, use the identity coupling.

In the first case, the update fails in both chains. There is no recoloring so the distance does not change. And in the second, the distance is increased by 1. So, with this coupling there are at most Δ recolorings that might increase the distance, attempting to recolor w in X_t to $Y_t(v)$ and to $X_t(v)$ in Y_t.

We now have

$$\mathbb{E}(d(X_{t+1}, Y_{t+1})|X_t, Y_t) \leq 1 + \frac{1}{kn}(\Delta - (k - \Delta)) \leq 1 - \frac{1}{kn}$$

for $k > 2\Delta$.

□

Chapter 5

Flip dynamics: First results

In the previous chapters we have studied MCMC with one particular Markov chain, the Glauber dynamics. The chain chooses a vertex at random and tries to recolor it with a random color not appearing in the neighborhood. As seen in Theorem 4.5, Jerrum [13] devised a coupling for this chain that is rapidly mixing for $k > 2\Delta$.

Vigoda, in his paper [23], presents another Markov chain which has weaker conditions that ensure rapid mixing. This new Markov chain is known as Flip dynamics and it is a variant of the Wang–Swendsen–Kotecký (WSK) algorithm, presented in [24]. In this case, the transitions are given by flips of 2-colored clusters and the bottleneck that appeared in Jerrum's approach, the one in which v has Δ neighbours, can be now avoided. More precisely, when a neighbour of v is recoloured in a chain in a way that would have increased the distance, we can couple it with a flip of size 2 on the other chain in such a way that the distance remains equal. But now, flips of larger clusters must also be described. In this chapter, we describe the Flip dynamics as well as the coupling that gives a lower bound on k for rapid mixing. In particular, the result obtained is that the flip dynamics is rapidly mixing for $k > \frac{11}{6}\Delta$.

5.1 Definition of the chain: Flip dynamics

Recall that $G = (V, E)$ and the state space Ω is the set of k-colorings of G including non-proper ones.

Before specifying the transitions, let us define the concept of alternating path. For a coloring σ, a path $v = x_0, x_1, ..., x_t = w$ is an *alternating path* between vertices v and w using colors c and $\sigma(v)$ if $(x_i, x_{i+1}) \in E$, $\sigma(x_i) \in \{c, \sigma(v)\}$ and $\sigma(x_i) \neq \sigma(x_{i+1})$ for all $i \in [0, t-1]$. Then, the *Kempe component* $S_\sigma(v, c)$ is the following cluster of vertices

$$S_\sigma(v, c) := \{w \in V : \text{there exists an alternating path between } v \text{ and } w \text{ using colors } \sigma(v), c\}$$

Note that for every vertex v the flip of cluster $S_\sigma(v, \sigma(v))$ does not change σ. For convenience, redefine $S_\sigma(v, \sigma(v)) = \emptyset$ for any $v \in V$. Moreover for every vertex $y \in S_\sigma(v, c)$, $S_\sigma(v, c) = S_\sigma(y, c)$ if $\sigma(v) = \sigma(y)$ and $S_\sigma(v, c) = S_\sigma(y, \sigma(v))$ otherwise. So every Kempe component S can be relabelled in $|S|$ ways.

In each transition, the Flip dynamics exchanges the colors in a Kempe component. One convenience of this definition is that flipping a Kempe component in a proper coloring yields to another proper coloring. More precisely, given weights $\{p_i\}_{i\geq 0}$, the transitions are defined as follows:

- Choose v and c uniformly at random in V and $[k]$.
- Let $\alpha = |S_\sigma(v,c)|$. With probability $p = \frac{p_\alpha}{\alpha}$, flip cluster $S_\sigma(v,c)$ by interchanging colors c and $\sigma(v)$ in the cluster.

For every $y \in S_\sigma(v,c)$ there is an equivalent cluster indexed by y. Hence each cluster can be chosen in α different ways, so the probability that a cluster is flipped is actually p_α. If $\mathcal{S}_\sigma$ is the set of all Kempe components in σ, the transitions can be restated as follows:

- Choose a Kempe component $S \in \mathcal{S}_\sigma$ each one with probability $1/nk$.
- Let $\alpha = |S|$ and flip S with probability p_α.

The values of the p_i's will be specified later.

5.1.1 Properties of the chain; stationary distribution

The flip dynamics embeds the transitions of the Glauber dynamics if $p_1 > 0$. Hence the chain is aperiodic and irreducible on the space of colorings for $k > \Delta + 2$. Moreover, as in the Glauber dynamics, the flip dynamics satisfies that every improper coloring has a positive probability to reach a proper one, but a proper coloring can not move to an improper one. Hence, the support of the stationary distribution is again the set of proper k-colorings of G. Using that the chain is symmetric in the set of proper colorings and theorems 2.1, 2.2; the steady state distribution is uniform on the set of proper colorings of G.

5.2 Coupling of the flip dynamics

Now that it is clear that the chain converges to the uniform distribution, we would like to prove that it converges in time $O(n \log n)$ provided k large enough. The first step will be to define a contractive coupling for every pair of neighbouring states in order to use the Path coupling lemma with the Hamming distance.

Let G be a graph and (σ, τ) a neighbouring coloring pair of G differing in vertex v. Then consider when clusters $S_\sigma(x,c), S_\tau(x,c)$ might be different in the sense that $S_\sigma(x,c) \neq S_\tau(x,c)$ or $S_\sigma(x,c) = S_\tau(x,c)$ but there is a vertex y in this set such that $\sigma(y) \neq \tau(y)$.

As v is the only vertex in which the colorings differ, the clusters must involve v. So $v \in S_\sigma(x,c)$ and/or $v \in S_\tau(x,c)$. For that reason, the set of clusters D that might be different in the two chains are $S_\sigma(v,c), S_\tau(v,c)$ for any color c and $S_\sigma(w,\tau(v)), S_\tau(w,\sigma(v))$ for w a neighbour of vertex v.

For $S \notin D$, S is shared in σ and τ so the flip of S in both colorings does not change the distance between them. It is enough to use the identity coupling for moves that flip clusters not in D.

In order to couple the flips of components in D, we decompose D in sets D_c where D_c is the set of Kempe components consisting of $S_\sigma(v,c), S_\tau(v,c)$ and $S_\sigma(w,\tau(v)), S_\tau(w,\sigma(v))$ for w any neighbour of vertex v colored c (basically D_c are the elements in D that involve color c).

For any $\sigma \in \Omega$ and $S \in D$, let σ_S be the coloring obtained from σ after flipping Kempe component S. The expected variation in the Hamming distance satisfies:

$$\begin{aligned}\mathbb{E}[\nabla d_H] &= \mathbb{E}[\nabla d_H | S \notin D] P[S \notin D] + \sum_c \mathbb{E}[\nabla d_H | S \in D_c] P[S \in D_c] = \\ &= \frac{1}{nk} \sum_c \sum_{S \in D_c} [d_H(\sigma_S, \tau_S) - d_H(\sigma, \tau)]\end{aligned} \tag{2}$$

where we have used that sets $S \notin D$ do not modify the Hamming distance, that each Kempe component is selected with equal probability $\frac{1}{nk}$ and that ∇d_H is determined when the Kempe component flipped is given.

Let U_c be the set of neighbours of v that are colored c, and let $\delta_c = |U_c|$. We will denote the elements of U_c by $\{u_1^c, ..., u_{\delta_c}^c\}$, or simply by $\{u_1, ..., u_{\delta_c}\}$ when color c is clear from the context. More precisely

$$D_c = \{S_\sigma(v,c), S_\tau(v,c), \{S_\sigma(w, \tau(v)), S_\tau(w, \sigma(v))\}_{w \in U_c}\}$$

Sets in D_c are disjoint except possibly $D_{\sigma(v)}$ and $D_{\tau(v)}$.

Moreover if $c \notin \{\sigma(v), \tau(v)\}$:

$$S_\sigma(v,c) = \left(\bigcup_{i=1}^{\delta_c} S_\tau(u_i^c, \sigma(v)) \right) \cup \{v\} \qquad S_\tau(v,c) = \left(\bigcup_{i=1}^{\delta_c} S_\sigma(u_i^c, \tau(v)) \right) \cup \{v\} \tag{3}$$

For $c = \sigma(v)$, we have $S_\sigma(v,c) = S_\tau(u, \sigma(v)) = \emptyset$ for all $u \in U_c$. Similarly for $c = \tau(v)$, $S_\tau(v,c) = S_\tau(u, \sigma(v)) = \emptyset$ for $u \in U_c$.

Observation 5.1 One remark that has to be done is that v can have some neighbours $u'_1, ..., u'_m \in N(v)$ colored c that belong to the same Kempe component $S_\tau(u'_1, \sigma(v)) = ... = S_\tau(u'_m, \sigma(v))$. In order to consider the flip with the right probability, redefine $S_\tau(u'_i, \sigma(v)) = \emptyset$ for $1 < i \leq m$. Do the same modifications for $S_\sigma(u'_i, \tau(v))$.

For c such that $\delta_c > 0$, let us define $A_c := |S_\sigma(v,c)|$, $B_c := |S_\tau(v,c)|$, $a_i^c := |S_\tau(u_i, \sigma(v))|$ and $b_i^c := |S_\sigma(u_i, \tau(v))|$. Also, define the vectors $\mathbf{a}^c := (a_i^c : i \in [\delta_c])$ and $\mathbf{b}^c := (b_i^c : i \in [\delta_c])$. We say that (σ, τ) has *configuration* $(A_c, B_c; \mathbf{a}^c, \mathbf{b}^c)$. Also define $a_{max}^c := \max_i a_i^c$ and i_{max}^c a maximizing argument. Analogously, define $b_{max}^c = \max_j b_j^c$ and j_{max}^c a maximizing argument. If the color is known by context, we will just refer to $A, B, a_i, b_j, \mathbf{a}, \mathbf{b}, a_{max}, i_{max}, b_{max}$ and j_{max}. In particular, the following inequalities are satisfied:

$$A \leq 1 + \sum_i a_i, \qquad B \leq 1 + \sum_i b_i \tag{4}$$

with equality if $c \neq \sigma(v), \tau(v)$.

Flips of clusters in the set D_c for σ will be coupled with flips of clusters in the same set D_c for τ. The idea is to couple the big flips, $S_\sigma(v,c)$ and $S_\tau(v,c)$, with the largest of the other flips $S_\tau(u_i, \sigma(v)), S_\sigma(u_j, \tau(v))$. And then, couple the remaining weights of $S_\tau(u_i, \sigma(v))$ and $S_\sigma(u_i, \tau(v))$ as much as possible. Notice that $S_\tau(u_i, \sigma(v)) \subset S_\sigma(v,c)$ and

$S_\sigma(u_j, \tau(v)) \subset S_\tau(v, c)$. In particular, this coupling flips the maximum number of equal elements together, so that the Hamming distance increases as little as possible. It can be understood as a greedy coupling.

More precisely the coupling is defined as follows:

1. Flip $S_\sigma(v, c)$ and $S_\tau(u_{i_{max}}, \sigma(v))$ together with probability p_A
2. Flip $S_\tau(v, c)$ and $S_\sigma(u_{j_{max}}, \tau(v))$ together with probability p_B
3. For all $i \in [\delta_c]$ let $q_i = p_{a_i} - p_A \cdot \mathbb{1}_{i=i_{max}}$ and $q'_i = p_{b_i} - p_B \cdot \mathbb{1}_{i=j_{max}}$.
   (a) Flip $S_\tau(u_i, \sigma(v))$ and $S_\sigma(u_i, \tau(v))$ together with probability $\min(q_i, q'_i)$
   (b) Flip $S_\tau(u_i, \sigma(v))$ with probability $q_i - \min(q_i, q'_i)$
   (c) Flip $S_\sigma(u_i, \tau(v))$ with probability $q'_i - \min(q_i, q'_i)$

Proposition 5.2 The above dynamics is a coupling.

Proof. Notice that each Kempe component S is flipped with probability $p_{|S|}$. So, the marginal distributions are equal to the distribution defined by the flip dynamics.

Moreover if $X_t = Y_t$ for some t, then the flip corresponds to the identity coupling and hence $X_{t+1} = Y_{t+1}$.

The definition of coupling holds.

□

Given a configuration $(A, B; \mathbf{a}, \mathbf{b})$, define $H(A, B; \mathbf{a}, \mathbf{b}) := (A - a_{max} - 1)p_A + (B - b_{max} - 1)p_B + \sum_i (a_i \cdot q_i + b_i \cdot q'_i - \min(q_i, q'_i))$. The previous coupling gives us the following bound:

Proposition 5.3

$$\mathbb{E}[\nabla d_H] \leq \frac{1}{nk}\Big(- |\{c : \delta_c = 0\}| + \sum_{c:\ \delta_c > 0} H(A_c, B_c, \mathbf{a}^c, \mathbf{b}^c)\Big) \tag{5}$$

Proof. From equation (2) we need to bound $\mathbb{E}[\nabla d_H | S \in D_c]$. Let us analyze the variation of the Hamming distance for each coupled move in D_c. Let c fixed and $(A, B; \mathbf{a}, \mathbf{b})$ the configuration in a neighboring coloring pair (σ, τ) before the flip.

First, consider the case in which $\delta_c = 0$. Here, $D_c = \{S_\sigma(v, c), S_\tau(v, c)\}$ and $S_\sigma(v, c) = S_\tau(v, c) = \{v\}$. The coupling in this situation corresponds to the identity coupling and yields to colorings σ', τ' with $\sigma'(v) = \tau'(v) = c$. So, in this case, $\nabla d_H = -1$.

Now let us analyse the case in which $\delta_c > 0$ and $c \neq \sigma(v), \tau(v)$.

Move 1) increases d_H by at most $(A - a_{max} - 1)$ because the colorings are still identical in the set of vertices that corresponded to $S_\tau(u_{i_{max}}, \sigma(v))$ before the flip and we substract 1 due to the fact that vertex v was already colored different before the flip. Equivalently move 2) increases the Hamming distance by at most $(B - b_{max} - 1)$.

For move 3a) the Hamming distance increases by $a_i + b_i - 1$, the sum of sizes of both components minus 1 for u_i which is the vertex that have in common.

Moves 3b) and 3c) increase the distance by a_i and b_i respectively.

Taking into account the probabilities for which every flip is made, we get:

$$\mathbb{E}[\nabla d_H | S \in D_c, c \neq \sigma(v), \tau(v)] \leq (A - a_{max} - 1) \cdot p_A + (B - b_{max} - 1) \cdot p_B + \sum_i \Big((a_i + b_i - 1) \cdot \min(q_i, q_i') + a_i \cdot [q_i - \min(q_i, q_i')] + b_i \cdot [q_i' - \min(q_i, q_i')] \Big) = H(A, B, \mathbf{a}, \mathbf{b}) \tag{6}$$

Lastly, we refer to [3] for the case $c = \sigma(v), \tau(v)$. Using technical details it can be seen that the above inequality

$$\mathbb{E}[\nabla d_H | S \in D_c, c \in \{\sigma(v), \tau(v)\}] \leq H(A, B, \mathbf{a}, \mathbf{b}) \tag{7}$$

also holds.

So, considering all possible values of c we get that:

$$\mathbb{E}[\nabla d_H] \leq \frac{1}{nk} \Big(- |\{c : \delta_c = 0\}| + \sum_{c:\ \delta_c > 0} H(A_c, B_c, \mathbf{a}^c, \mathbf{b}^c) \Big)$$

□

5.3 Linear programming and choice of flip weights

In order to apply path coupling lemma, and so to prove rapid mixing of the flip dynamics, we need the coupling to be contractive. Hence the aim is to find weights that make the expected variation in distance negative.

This variation will depend on the configurations that have the graph with both colorings and the number of moves that can increase and decrease the Hamming distance.

Definition 5.1 A configuration $(A, B; \mathbf{a}, \mathbf{b})$ is *realizable* if there exists a graph G, a neighboring coloring pair (σ, τ) defined in G and a color c such that $(A, B; \mathbf{a}, \mathbf{b}) = (A_c, B_c; \mathbf{a}^c, \mathbf{b}^c)$.

Namely, a configuration is realizable if some neighboring coloring pair (σ, τ) has it. In particular a configuration is realizable if and only if it satisfies the inequality (4). We will refer to δ_c as the *size* of the realizable configuration.

An example of a realizable configuration is shown in Figure 5.1.

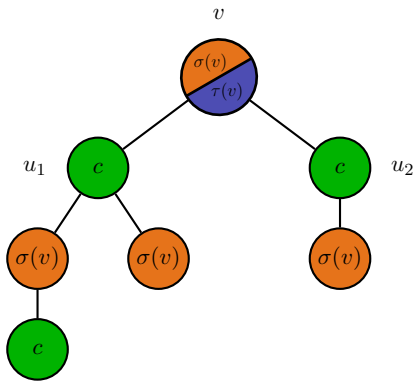

Figure 5.1: Configuration $(7,3;(4,2),(1,1))$, which is a realizable configuration. Here we represent both colorings σ, τ, which only differ in v.

Observation 5.4 Values of $(A, B; \mathbf{a}, \mathbf{b})$ do not identify uniquely the subgraph associated to those vertices. In particular, one configuration $(A, B; \mathbf{a}, \mathbf{b})$ admits many representations in the graph. Figure 5.2 gives an example of colorings in two different subgraphs that correspond to the same configuration, in this case configuration $(4,2;(3),(1))$.

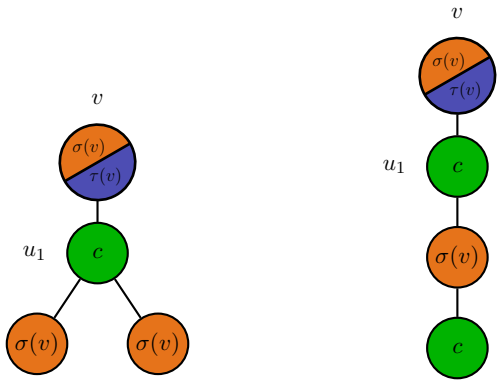

Figure 5.2: Two representations of the configuration $(4,2;(3),(1))$

Proposition 5.5 Suppose that there exists $\lambda > 0$ such that $H(A, B; \mathbf{a}, \mathbf{b}) \leq -1 + \lambda m$ for all realizable configurations $(A, B; \mathbf{a}, \mathbf{b})$, where m is the size of the configuration. Then the coupling is contractive for $k > \lambda\Delta$.

Proof. From Proposition 5.3 we have that

$$\mathbb{E}[\nabla d_H] = \frac{1}{nk}\Big(-|\{c : \delta_c = 0\}| + \sum_{c:\ \delta_c>0} H(A_c, B_c, \mathbf{a}^c, \mathbf{b}^c)\Big) \leq \frac{1}{nk}\Big(-|\{c : \delta_c = 0\}| +$$

$$\sum_{c:\ \delta_c>0} (-1 + \lambda\delta_c)\Big) = \frac{1}{nk}\Big(-k + \lambda \sum_{c:\ \delta_c>0} \delta_c\Big) \leq \frac{1}{nk}\Big(-k + \lambda\Delta\Big) < 0$$

where in the last inequality we have used the hypothesis that $k > \lambda\Delta$.

More precisely, if $(\{X_t\}, \{Y_t\})$ is a coupling of the flip dynamics and (X_t, Y_t) is a neighboring coloring pair, we have:

$$\mathbb{E}[d_H(X_{t+1}, Y_{t+1})] \leq d_H(X_t, Y_t) + \frac{1}{nk}\Big(- k + \lambda\Delta\Big) \leq 1 - \frac{c}{nk},$$

for some $c > 0$. □

So, our goal will be to find weights p_i such that $H(A, B, \mathbf{a},\mathbf{b}) \leq -1 + \lambda m$ for all realizable configurations $(A, B; \mathbf{a},\mathbf{b})$. The path coupling lemma then gives us that the mixing time is $O(n \log n)$.

In particular, we want to find the minimum λ such that the previous inequalities hold. We obtain the following linear programming problem.

$$\begin{array}{lll} \text{minimize} & \lambda & \\ \lambda, \{p_i\}_{i\in\mathbb{N}} & & \\ \text{subject to} & H(A, B; \mathbf{a},\mathbf{b}) \leq -1 + \lambda m, & \text{for all realizable (A,B;}\mathbf{a},\mathbf{b}\text{) of size } m, \\ & p_0 = 0 \leq p_i \leq p_{i-1} \leq p_1 = 1, & \text{for all } i \geq 2 \end{array} \tag{8}$$

There are some issues that must be considered in this linear program. The first one is that there are infinitely many variables. The second one is that there is an infinite number of constraints. And the third is that it might be difficult to enumerate all possible realizable configurations.

Vigoda handles the first problem by restricting to flips of components of size at most 7. Or equivalently by imposing $p_\alpha = 0$ for $\alpha \geq 7$. We can argue this in terms of two inequalities that give us this value for p_7. Consider the configurations $(3, 2; (1), (1))$ and $(7, 3; (3, 3), (1, 1))$. For these configurations, inequality $H(A, B; \mathbf{a},\mathbf{b}) \leq -1 + \lambda m$ in (8) corresponds to:

$$\begin{array}{rcl} p_1 + p_2 - 2p_3 - \min(p_1 - p_2, p_2 - p_3) & \leq & -1 + \lambda \\ 2p_1 + 5p_3 - \min(p_1 - p_3, p_3 - p_7) & \leq & -1 + 2\lambda \end{array} \tag{9}$$

These inequalities already give us that $\lambda \geq \frac{11}{6}$, with equality only possible if $p_7 = 0$. The linear program will give us this value $\lambda = 11/6$ and we will claim that no other coupling could give a better bound.

The second issue can be solved by the following 2 observations:

Lemma 5.6 $H(A, B; \mathbf{a},\mathbf{b}) \leq (A - 2a_{max})p_A + (B - 2b_{max})p_B + \sum_i (a_i p_{a_i} + b_i p_{b_i} - \min(p_{a_i}, p_{b_i}))$

Proof. Let $g(w_i) = a_i p_{a_i} + b_i p_{b_i} - \min\{p_{a_i}, p_{b_i}\}$ and $f(w_i) = (a_i \cdot q_i + b_i \cdot q_i' - \min(q_i, q_i'))$ Then:

- If $i \neq i_{max}, j_{max}$ then $f(w_i) = g(w_i)$.

- If $i = i_{max} = j_{max}$ then $f(w_i) = a_i(p_{a_i} - p_A) + b_i(p_{b_i} - p_B) - \min\{p_{a_i} - p_A, p_{b_i} - p_B\} \leq a_i p_{a_i} + b_i p_{b_i} - \min\{p_{a_i}, p_{b_i}\} - p_A(a_i - 1) - p_B(b_i - 1) = g(w_i) - p_A(a_i - 1) - p_B(b_i - 1)$
- If $i = i_{max} \neq j_{max}$ then $f(w_i) = a_i(p_{a_i} - p_A) + b_i p_{b_i} - \min\{p_{a_i} - p_A, p_{b_i}\} \leq a_i p_{a_i} + b_i p_{b_i} - \min\{p_{a_i}, p_{b_i}\} - p_A(a_i - 1) = g(w_i) - p_A(a_i - 1)$.

  Analogously if $i = j_{max} \neq i_{max}$ then $f(w_i) \leq g(w_i) - p_B(b_i - 1)$

So adding for all i we have that

$$\sum_i f(w_i) \leq p_A + p_B - p_A a_{max} - p_B b_{max} + \sum_i g(w_i)$$

And for $H(A, B; \mathbf{a}, \mathbf{b})$ we get

$$H(A, B; \mathbf{a}, \mathbf{b}) = (A - a_{max} - 1)p_A + (B - b_{max} - 1)p_B + \sum_i f(w_i) \leq (A - 2a_{max})p_A + (B - 2b_{max})p_B + \sum_i g(w_i)$$

□

Lemma 5.7 Consider for all i the additional constraints $ip_i \leq 1, (i-1)p_i \leq \frac{1}{3}$ and $(i-2)p_i \leq 2/9$.
Let $(A, B; \mathbf{a}, \mathbf{b})$ be a realizable configuration of size m greater or equal than 3.
If $\{p_i\}_{i \in \mathbb{N}}$ satisfy the additional constraints, then for $\lambda \geq \frac{49}{27}$ (and in particular for $\lambda \geq \frac{11}{6}$):

$$H(A, B; \mathbf{a}, \mathbf{b}) \leq -1 + \lambda m.$$

Proof. Consider the bound given for $H(A, B; \mathbf{a}, \mathbf{b})$ in the previous lemma. Hypothesis give that $(A - 2a_{max})p_A, (B - 2b_{max})p_B \leq 2/9$ and without loss of generality assume $a_i \geq b_i$ for all i, and so $p_{a_i} \leq p_{b_i}$. Then, by lemma 5.6:

$$H(A, B; \mathbf{a}, \mathbf{b}) \leq \frac{4}{9} + \sum_i ((a_i - 1)p_{a_i} + b_i p_{b_i})$$

Using that $ip_i \leq 1$ and that $(i-1)p_i \leq \frac{1}{3}$, we have:

$$H(A, B; \mathbf{a}, \mathbf{b}) \leq \frac{4}{9} + m\left(\frac{1}{3} + 1\right) \leq -1 + \frac{49}{27}m \leq -1 + \lambda m \quad \text{for } m > 2.$$

□

In particular any configuration that satisfies $m \geq 3$, satisfies the contractive condition for $k > \frac{11}{6}\Delta$ given that the weights satisfy the additional properties.

This already makes the linear program finite in the number of variables and constraints.
Finally, we can enumerate all possible realizable configurations as follows. For $c \neq \sigma(v), \tau(v)$ we can enumerate them by considering all possible $(A, B; \mathbf{a}, \mathbf{b})$ such that $A = 1 + \sum_i a_i$ and $B = 1 + \sum_i b_i$ and the size of A and B are less than 7 (see condition (4)).
For $c = \sigma(v), \tau(v)$, we refer to [3] and it is enough to include constraints:

- $ip_i \leq 1 \quad \forall i,$
- $(B-b_2)p_B + b_1 p_{b_1} \leq -1+2\lambda \quad$ for $B = b_1+b_2,\ 1 \leq b_1 \leq b_2 \leq 6, B \leq 6.$

This linear program, which we will denote by linear program 1 or LP1, is now finite and can be described as follows:

$$
\begin{array}{lrll}
\underset{\lambda,\{p_i\}_{i\in\{0,1,\ldots,7\}}}{\text{minimize}} & \lambda & & \\
\text{subject to} & H(A,B;\mathbf{a},\mathbf{b}) & \leq -1+\lambda m, & \forall a,b \in \{0,7\}^m \setminus \{(0,\ldots 0)\}, m \in \{1,2\} \\
 & & & A = 1+\sum_{i=1}^{m} a_i, \quad B = 1+\sum_{i=1}^{m} b_i, \\
 & & & A,B \leq 7, \quad A \geq B \\
 & (B-b_2)p_B + b_1 p_{b_1} & \leq -1+2\lambda & B = b_1+b_2, 1 \leq b_1 \leq b_2 \leq 6, B \leq 6. \\
 & p_0 = 0 \leq p_i \leq p_{i-1} & \leq p_1 = 1, & \text{for all } i \geq 2 \\
 & p_7 & = 0, & \\
 & ip_i & \leq 1, & \text{for all } i \\
 & (i-1)p_i & \leq \tfrac{1}{3}, & \text{for all } i \\
 & (i-2)p_i & \leq \tfrac{2}{9}, & \text{for all } i
\end{array}
$$

where in the first inequality we have added $A \geq B$ in order to consider each configuration up to symmetry only once.

Notice that the first constraint corresponds to realizable configurations of size strictly less than 3 and color $c \neq \sigma(v), \tau(v)$.

The second one corresponds to the case $c = \sigma(v), \tau(v)$. And the last 3 constraints imply inequality $H(A,B;\mathbf{a},\mathbf{b}) \leq -1+\lambda m$ for realizable configurations of size $m \geq 3$ and colors $c \neq \sigma(v), \tau(v)$.

LP1 is solved using the Matlab code in the appendix "Matlab code for solving LP1 and LP2". The feasible region of this linear program is not empty and we consider the solution that minimizes λ.

More precisely, we obtain that the optimal λ is $\lambda^* = 11/6$ and the values of the p_i's are:

$$p_1 = 1, p_2 = \frac{13}{42}, p_3 = \frac{1}{6}, p_4 = \frac{2}{21}, p_5 = \frac{1}{21}, p_6 = \frac{1}{84}, p_\alpha = 0 \quad \forall \alpha \geq 7 \tag{10}$$

which are also the values that Vigoda obtained in his paper (see [23]).

In particular and to summarize, the flip dynamics with these parameters is $\frac{1}{kn}$-contractive and, applying the Path coupling lemma (Lemma 4.3) we have the following result.

Theorem 5.8 The flip dynamics is rapidly mixing, with mixing time $O(n \log n)$, provided $k > \frac{11}{6}\Delta$.

Finally, we claim that this is the best result that can be obtained using the Hamming distance. More precisely:

Theorem 5.9 If $k < \frac{11}{6}\Delta$ there exists no choice of flip parameters $\{p_\alpha\}_{\alpha\in\mathbb{N}}$ and one-step coupling such that it is contractive under the Hamming metric.

The proof can be found in [3]. Basically, it shows 2 counterexamples of neighbouring coloring pairs for which any one-step coupling can't do better.

Chapter 6

Flip dynamics: use of an Alternative metric

Theorem 5.9 states that it is not possible to cross the $\frac{11}{6}$ barrier with one-step coupling for the flip dynamics with the Hamming metric. This can be circumvented in two different ways: Considering multi-step couplings with the same metric or considering a one step coupling using an alternative metric. We will discuss the second approach.

The new metric considered will be based in the fact that not many configurations attain equality in $H(A, B; \mathbf{a}, \mathbf{b}) \leq -1 + \lambda m$ with $\lambda = \frac{11}{6}$. The ones pushing λ to be $\frac{11}{6}$ will be called extremal configurations.

6.1 Extremal configurations

Let $\mathbf{p}$ be the solution given by LP 1 described in (10). In order to define the alternative metric, we need to distinguish those configurations that reach equality for the constraint $H(A, B; \mathbf{a}, \mathbf{b}) \leq -1 + \lambda m$.

Using the code for LP1 given in the appendix "Matlab code for solving LP1 and LP2", we see that there are only 6 configurations for the choice of flip parameters $\mathbf{p}$ that attain equality $H(A, B; \mathbf{a}, \mathbf{b}) = -1 + \lambda m$ (this number is given by the variable *tight_ineq*). However, among those, two of them already force the objective value to be $\frac{11}{6}$, which are $(3, 2; (2), (1))$ and $(7, 3; (3, 3), (1, 1))$ up to symmetries. We will focus on these configurations and we will refer to them as the *extremal configurations*. In particular let $\Pi = \{(3, 2; (2), (1)), (2, 3; (1), (2)), (7, 3; (3, 3), (1, 1)), (3, 7; (1, 1), (3, 3))\}$ be the set of extremal configurations. We also define Π^i to be the set of extremal configurations of size i for $i \in \{1, 2\}$, in particular $\Pi^1 = \{(3, 2; (2), (1)), (2, 3; (1), (2))\}$ and $\Pi^2 = \{(7, 3; (3, 3), (1, 1)), (3, 7; (1, 1), (3, 3))\}$.

Recall that we are considering (σ, τ) a neighbouring colouring pair, so (σ, τ) only differ in one vertex v. In particular, $(3, 2; (2), (1))$ corresponds to the configuration of size 1 in which the Kempe component in σ, $S_\sigma(v, c)$ has size 3 and the Kempe component $S_\tau(v, c)$ has size 2. Moreover, let u be the neighbour of v colored c. Values (2), (1) indicate that there is one neighbour of u (different than v) colored $\sigma(v)$ and none colored $\tau(v)$. Equivalently, the configuration $(7, 3; (3, 3), (1, 1))$ is the one that has $|S_\sigma(v, c)| = 7$ and $|S_\tau(v, c)| = 3$. The extremal configurations are represented in Figure 6.1.

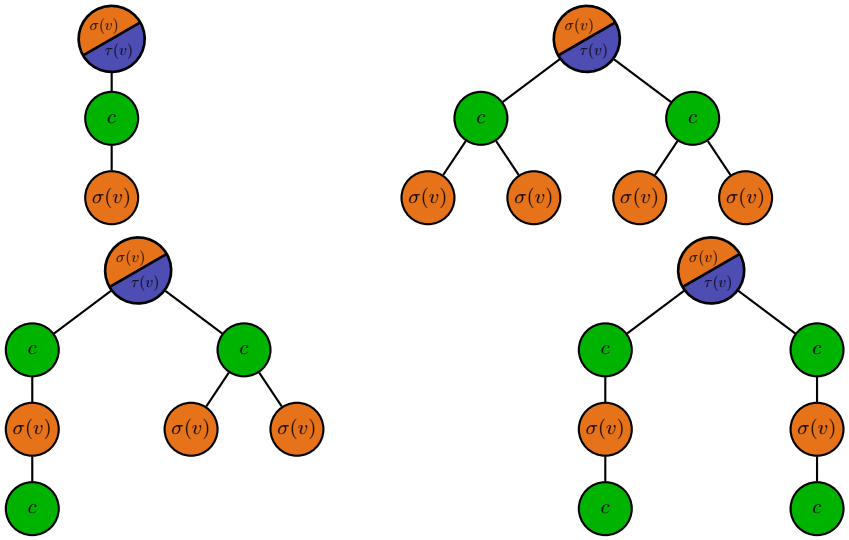

Figure 6.1: These are the extremal configurations (up to symmetry) that push λ to be 11/6. Although there is only one extremal configuration up to symmetry of size 2, $(7,3;(3,3),(1,1))$, it can arise from 3 different subgraphs.

The constraints that correspond to these 2 extremal configurations are given in the system of equations (9) and the objective value for these 2 constraints is minimized to 11/6 only if $p_3 = 1/6$ and $p_7 = 0$. Fixing these values for p_3 and p_7, we study the new objective value for the rest of realizable configurations. In particular, we define LP2 a new linear program as follows:

$$
\begin{array}{lrll}
\underset{\lambda,\{p_i\}_{i\in\{0,1,\ldots,7\}}}{\text{minimize}} & \lambda & & \\
\text{subject to} & H(A,B;\mathbf{a},\mathbf{b}) & \leq -1+\lambda m, & \forall a,b\in\{0,7\}^m\setminus\{(0,\ldots 0)\}, m\in\{1,2\} \\
 & & & A=1+\sum_{i=1}^{m} a_i, \quad B=1+\sum_{i=1}^{m} b_i \\
 & & & A,B\leq 7, \quad A\geq B \\
 & & & \mathbf{(A,B;a,b)\neq(3,2;(2),(1))}, \\
 & & & \mathbf{(A,B;a,b)\neq(7,3;(3,3),(1,1))} \\
 & (B-b_2)p_B+b_1p_{b_1} & \leq -1+2\lambda & B=b_1+b_2, 0\leq b_1\leq b_2\leq 6, b_2>0. \\
 & p_0=0\leq p_i\leq p_{i-1} & \leq p_1=1, & \text{for all } i\geq 2 \\
 & p_7=0 & \mathbf{p_3=1/6}, & \\
 & ip_i & \leq 1, & \text{for all } i \\
 & (i-1)p_i & \leq \tfrac{1}{3}, & \text{for all } i \\
 & (i-2)p_i & \leq \tfrac{2}{9}, & \text{for all } i
\end{array}
$$

Notice that this is the problem obtained from LP1 erasing the constraints for the 2 extremal configurations and adding constraint $p_3 = 1/6$. The differences between LP1 and LP2 are written in blue.

Observation 6.1 LP2 is solved in the appendix "Matlab code for solving LP1 and LP2" and the optimal solution is $\lambda = 161/88$ for the flip parameters:

$$p_1 = 1; p_2 = 185/616; p_3 = 1/6; p_4 = 47/462; p_5 = 9/154; p_6 = 2/77; p_7 = 0;$$

Moreover the constraints in LP1 that are not contained in LP2 are implied by $p_3 = 1/6$ and $p_7 = 0$. Hence the assignment $\mathbf{p} = \{p_\alpha\}_{\alpha \in N_0}$ given by Observation 6.1 for $\alpha \in [6]$ and $p_0 = 0$ is a feasible solution of LP1 with the same objective value $11/6$.

All together gives the following proposition.

Proposition 6.2 Given $(A, B; \mathbf{a}, \mathbf{b})$ a realizable configuration of size m,

$$H(A, B; \mathbf{a}, \mathbf{b}) \leq \begin{cases} -1 + \frac{11}{6} \cdot m, & \text{if } (A, B; \mathbf{a}, \mathbf{b}) \text{ is a extremal configuration for } \mathbf{p}, \\ -1 + \frac{161}{88} \cdot m, & \text{otherwise.} \end{cases}$$

given the parameters

$$p_1 = 1; p_2 = 185/616; p_3 = 1/6; p_4 = 47/462; p_5 = 9/154; p_6 = 2/77; p_7 = 0.$$

This proposition tells us that the term $11/6$ is only tight for a few configurations. And this will be the key point for defining an alternative metric.

6.2 Definition of the alternative metric

The aim is to construct a contractive coupling for $k > (11/6 - \varepsilon_0)\Delta$ using a metric different than the Hamming one.

The metric for Ω will be defined from a pre-metric (Γ, ω). Let Γ be the graph having Ω as vertex set and adjacencies between colorings that differ in a single vertex.

For σ, τ a neighbouring coloring pair, we define:

$$C^1_{\sigma,\tau}(v) = \{c \in [k] : (A_c, B_c; \mathbf{a}^c, \mathbf{b}^c) \text{ is an extremal configuration for } (\sigma, \tau) \text{ of size } 1\}$$

$$C^2_{\sigma,\tau}(v) = \{c \in [k] : (A_c, B_c; \mathbf{a}^c, \mathbf{b}^c) \text{ is an extremal configuration for } (\sigma, \tau) \text{ of size } 2\}$$

and let $C_{\sigma,\tau}(v) = C^1_{\sigma,\tau}(v) \cup C^2_{\sigma,\tau}(v)$.

Notice that $C^1_{\sigma,\tau}(v)$, $C^2_{\sigma,\tau}(v)$ are the sets of colors that appear in extremal configurations of size 1 or 2 respectively and that for each color in $C^2_{\sigma,\tau}(v)$ there are 2 neighbours of v that participate in a extremal configuration.

We also define $\gamma^1_{\sigma,\tau}(v) := |C^1_{\sigma,\tau}(v)|/\Delta$ and $\gamma^2_{\sigma,\tau}(v) := 2|C^2_{\sigma,\tau}(v)|/\Delta$ which are the number of neighbours of v that appear in 1-extremal configurations and 2-extremal configurations respectively normalised by a factor Δ. And let $\gamma_{\sigma,\tau}(v) := \gamma^1_{\sigma,\tau}(v) + \gamma^2_{\sigma,\tau}(v)$, which is the number of neighbours of v that appear in some extremal configuration normalised by a factor Δ. In particular $\gamma_{\sigma,\tau}(v) \leq 1$.

Let $\eta_1, \eta_2 \in (0, \frac{1}{4})$, that will be defined later. We define the weight function as follows:

$$\omega(\sigma, \tau) := 1 - \eta_1(1 - \gamma^1_{\sigma,\tau}(v)) - \eta_2(1 - \gamma^2_{\sigma,\tau}(v)))$$

Notice that $\omega(\sigma, \tau) \in [1 - \eta_1 - \eta_2, 1 - \min(\eta_1, \eta_2)]$, in particular smaller than 1. As $\eta_1, \eta_2 < \frac{1}{4}$, every edge has weight greater than $\frac{1}{2}$, so every edge is a minimum weighted path. Hence (Γ, ω) is a pre-metric.

Basically, this new pre-metric takes into account the proportion of extremal configurations in each state. As the 11/6 bottleneck is due to them, the new pre-metric puts more weight in neighbouring coloring pairs that have those extremal configurations.

Now, let d be the metric induced by (Γ, ω). The weight function w satisfies that $w(\sigma, \tau) \leq 1$ for $(\sigma, \tau) \in \Gamma$ and using minimum weighted paths, $d(\tilde{\sigma}, \tilde{\tau}) \leq d_H(\tilde{\sigma}, \tilde{\tau})$ for any $(\tilde{\sigma}, \tilde{\tau}) \in \Omega^2$. So we can define

$$d_B(\tilde{\sigma}, \tilde{\tau}) := d_H(\tilde{\sigma}, \tilde{\tau}) - d(\tilde{\sigma}, \tilde{\tau}) \tag{11}$$

Although d_B might not be a metric, we will use the fact that it is non-negative.

As done with the Hamming metric, we have to study the expected variation in distance d in one step of the greedy coupling. This analysis is done in the next chapter.

Chapter 7

Analysis of the Alternative metric: Expected variation distance

In this chapter we want to study under which conditions the coupling is contractive using the alternative metric. Our goal will be to prove contractness for colorings satisfying $k > (11/6 - \varepsilon_0)\Delta$, a weaker condition that the one obtained for the 1-step coupling using the Hamming distance. The coupling is defined in section 5.2 and we take the assignment of flip parameters given in Observation 6.1. As rapid mixing of the flip dynamics is already known for $k > 11/6\Delta$, we will focus on $k \leq 11/6\Delta$. Moreover, due to LP2, we know that $k \geq 161/88\Delta$. Hence, we will consider that $k \in [\frac{161}{88}\Delta, \frac{11}{6}\Delta]$.

We begin with some definitions. For any neighbouring coloring pair (σ, τ) and a step of the greedy coupling $(\sigma, \tau) \longrightarrow (\sigma', \tau')$ we define:

$$\nabla(\sigma, \tau) := nk\mathbb{E}[d(\sigma', \tau') - d(\sigma, \tau)] \tag{12}$$

Due to (11) and linearity of expectation, $\nabla(\sigma, \tau)$ can be decomposed into the sum of two terms $\nabla(\sigma, \tau) = \nabla_H(\sigma, \tau) + \nabla_B(\sigma, \tau)$ defined as:

$$\nabla_H(\sigma, \tau) := nk\mathbb{E}[d_H(\sigma', \tau') - 1] \tag{13}$$
$$\nabla_B(\sigma, \tau) := -nk\mathbb{E}[d_B(\sigma', \tau') - d_B(\sigma, \tau)] \tag{14}$$

In order to bound $\nabla(\sigma, \tau)$ we will bound the terms ∇_H and ∇_B separately.

First we bound the contribution of $\nabla_H(\sigma, \tau)$, the Hamming part.

Proposition 7.1 Let $\delta = \frac{11}{6} - \frac{161}{88}$. For any (σ, τ) neighbouring coloring pair we have

$$\nabla_H(\sigma, \tau) \leq \left(\frac{11}{6} - \delta(1 - \gamma_{\sigma,\tau})\right)\Delta - k$$

Proof.

$$\nabla_H(\sigma, \tau) = nk \cdot \mathbb{E}(d_H(\sigma', \tau') - 1) \leq \left(- |\{c : \delta_c = 0\}| + \sum_{c:\ \delta_c > 0} H(A_c, B_c, \mathbf{a}^c, \mathbf{b}^c)\right)$$

where we have used Proposition 5.3. Now, due to Proposition 6.2 we get

$$\nabla_H(\sigma,\tau) \leq \frac{11}{6}\cdot\Delta\cdot\gamma_{\sigma,\tau} + \frac{161}{88}\Delta(1-\gamma_{\sigma,\tau}) - k = \left(\frac{11}{6} - \delta(1-\gamma_{\sigma,\tau})\right)\Delta - k \tag{15}$$

□

Once the contribution of ∇_H is bounded, we proceed to bound ∇_B in the next section.

7.1 Study of ∇_B

First recall that D_c is the set of Kempe components that involve color c and vertex v. Now we define the event $X_c = \{S \in D_c\}$ as the event that the Kempe component flipped S belongs to D_c. This event is well defined as in the greedy coupling $S \in D_c$ in one chain if it also does in the other. And let $\overline{X}$ be the complementary event of the union of X_c; $\overline{X} = \overline{\bigcup_{c\in[k]} X_c}$. In particular $\overline{X}$ is the event that the component flipped does not involve v. In order to bound ∇_B we split its analysis conditioning on the events X_c and $\overline{X}$. We define

$$\nabla_B(\sigma,\tau,c) := -nk\mathbb{E}[\mathbb{1}_{X_c}\cdot(d_B(\sigma',\tau') - d_B(\sigma,\tau))] \tag{16}$$

$$\overline{\nabla_B}(\sigma,\tau) := -nk\mathbb{E}[\mathbb{1}_{\overline{X}}\cdot(d_B(\sigma',\tau') - d_B(\sigma,\tau))] \tag{17}$$

With these definitions $\nabla_B(\sigma,\tau)$ can be bounded as follows $\nabla_B(\sigma,\tau) = \overline{\nabla_B}(\sigma,\tau) + \sum_{c\in[k]}\nabla_B(\sigma,\tau,c)$.

Proposition 7.2

$$\sum_{c\in[k]}\nabla_B(\sigma,\tau,c) = O(1)$$

Proof. In order to bound $\nabla_B(\sigma,\tau,c)$ we study the term $d_B(\sigma,\tau) - d_B(\sigma',\tau')$.

First, notice that either $\sigma' = \tau'$ or $\sigma'(v) \neq \tau'(v)$ by the definition of the coupling.

In the first case, $d_B(\sigma,\tau) - d_B(\sigma',\tau') = 0$ and we are done.

In the second case, $d_B(\sigma',\tau')$ can be computed using a minimum weighted path. More precisely, σ' and τ' differ in at most 6 vertices, due to the fact that the Kempe component flipped has size at most 6 ($p_j = 0$ for $j \geq 7$) and if $S \in D_c$ then $v \in S$.

Hence there exist colorings $\sigma' = \zeta_0, ..., \zeta_s = \tau'$ with $s \leq 6$ such that $d_H(\zeta_i, \zeta_{i+1}) = 1$ and

$$d_B(\sigma',\tau') = \sum_{i=0}^{s-1} d_B(\zeta_i,\zeta_{i+1}) \tag{18}$$

As $\sigma'(v) \neq \tau'(v)$, there exist j such that (ζ_j, ζ_{j+1}) differ at vertex v and this is the only vertex in which they differ.

Moreover, due to the fact that (σ,τ) is a neighbouring coloring pair, $d_H(\sigma,\tau) = 1$ and

$$d_B(\sigma,\tau) = d_H(\sigma,\tau) - d(\sigma,\tau) = 1 - \omega(\sigma,\tau) = \eta_1(1-\gamma^1_{\sigma,\tau}(v)) + \eta_2(1-\gamma^2_{\sigma,\tau}(v))$$

In the same way, $d_B(\zeta_j,\zeta_{j+1}) = \eta_1(1-\gamma^1_{\zeta_j,\zeta_{j+1}}(v)) + \eta_2(1-\gamma^2_{\zeta_j,\zeta_{j+1}}(v))$.

We will now argue that the difference between these two values is $O(\frac{1}{\Delta})$. Notice that for each pair (ζ_i,ζ_{i+1}), at most the color of one neighbour of v is changed. Hence at most j neighbours of v in ζ_j differ with respect to σ and each of the different neighbours contributes

with at most $\frac{l}{\Delta}$ to $(\gamma^l_{\zeta_j,\zeta_{j+1}}(v) - \gamma^l_{\sigma,\tau}(v))$ for $l \in \{1,2\}$. This implies that substracting both values we get:

$$d_B(\sigma,\tau) - d_B(\zeta_j,\zeta_{j+1}) = \eta_1(\gamma^1_{\zeta_j,\zeta_{j+1}}(v) - \gamma^1_{\sigma,\tau}(v)) + \eta_2(\gamma^2_{\zeta_j,\zeta_{j+1}}(v) - \gamma^2_{\sigma,\tau}(v)) \leq \max\{\eta_1,\eta_2\}\frac{2j}{\Delta} \leq$$
$$\leq \max\{\eta_1,\eta_2\}\frac{2s}{\Delta} \leq \frac{3}{\Delta}$$

using that $\eta_1, \eta_2 \leq 1/4$. Now, as d_B is non-negative and due to equality (18):

$$d_B(\sigma,\tau) - d_B(\sigma',\tau') \leq d_B(\sigma,\tau) - d_B(\zeta_j,\zeta_{j+1}) = O\left(\frac{1}{\Delta}\right)$$

Taking into account that $P(X_c = 1) = \frac{\delta_c+1}{nk}$ and that $k \leq \frac{11}{6}\Delta$, we get

$$\sum_{c\in[k]} \nabla_B(\sigma,\tau,c) \leq 3 \cdot \frac{\Delta + k}{\Delta} = O(1)$$

□

Now it remains to bound $\overline{\nabla_B}(\sigma,\tau)$.

Let $\overline{\mathcal{D}} = (S_\sigma \cup S_\tau) \setminus \mathcal{D}$ be the set of Kempe components of σ and τ that do not involve vertex v. In particular $\overline{X} = \{S \in \overline{\mathcal{D}}\}$.

For a coloring σ and $S \in S_\sigma$, let σ_S be the coloring obtained from σ after flipping Kempe component S. Since $d_H(\sigma,\tau) = 1$, $d_B(\sigma,\tau) = \eta_1(1 - \gamma^1_{\sigma,\tau}(v)) + \eta_2(1 - \gamma^2_{\sigma,\tau}(v))$. Moreover as we are considering flips in $S \in \overline{\mathcal{D}}$, the Hamming distance remains equal, so $d_H(\sigma_S,\tau_S) = 1$ and $d_B(\sigma_S,\tau_S) = \eta_1(1 - \gamma^1_{\sigma_S,\tau_S}(v)) + \eta_2(1 - \gamma^2_{\sigma_S,\tau_S}(v))$.

It follows that

$$\overline{\nabla_B}(\sigma,\tau) = -nk \sum_{S\in\overline{\mathcal{D}}} P(S \text{ flipped})[d_B(\sigma_S,\tau_S) - d_B(\sigma,\tau)] = -nk \sum_{S\in\overline{\mathcal{D}}} \frac{p_{|S|}}{nk}[\eta_1(\gamma^1_{\sigma,\tau}(v) - \gamma^1_{\sigma_S,\tau_S}(v))$$
$$+ \eta_2(\gamma^2_{\sigma,\tau}(v) - \gamma^2_{\sigma_S,\tau_S}(v))] = \sum_{S\in\overline{\mathcal{D}}} p_{|S|}[\eta_1(\gamma^1_{\sigma_S,\tau_S}(v) - \gamma^1_{\sigma,\tau}(v)) + \eta_2(\gamma^2_{\sigma_S,\tau_S}(v) - \gamma^2_{\sigma,\tau}(v))] \tag{19}$$

For each $c \in [k]$ and $i \in \{1,2\}$ we define:

$$\xi^1_{\sigma,\tau}(v,c,S) := \begin{cases} -1, & \text{if } c \in C^1_{\sigma,\tau}(v) \text{ and } c \notin C^1_{\sigma_S,\tau_S}(v) \\ 1, & \text{if } c \notin C^1_{\sigma,\tau}(v) \text{ and } c \in C^1_{\sigma_S,\tau_S}(v) \\ 0, & \text{otherwise.} \end{cases}$$

$$\xi^2_{\sigma,\tau}(v,c,S) := \begin{cases} -2, & \text{if } c \in C^2_{\sigma,\tau}(v) \text{ and } c \notin C^2_{\sigma_S,\tau_S}(v) \\ 2, & \text{if } c \notin C^2_{\sigma,\tau}(v) \text{ and } c \in C^2_{\sigma_S,\tau_S}(v) \\ 0, & \text{otherwise.} \end{cases}$$

and

$$\overline{\nabla_B}(\sigma,\tau,c,\mathcal{S}') := \frac{1}{\Delta} \sum_{S\in\mathcal{S}'} p_{|S|}[\xi^1_{\sigma,\tau}(v,c,S)\eta_1 + \xi^2_{\sigma,\tau}(v,c,S)\eta_2] \tag{20}$$

Basically, $\frac{\xi^i_{\sigma,\tau}(v,c,S)}{\Delta}$ is the contribution of color c to $(\gamma^i_{\sigma_S,\tau_S}(v) - \gamma^i_{\sigma,\tau}(v))$ for $i = 1, 2$. With these definitions note that

$$\overline{\nabla_B}(\sigma,\tau) = \sum_{c\in[k]} \overline{\nabla_B}(\sigma,\tau,c,\overline{\mathcal{D}})$$

.

Observation 7.3 As seen in Observation 5.4, values of $(A, B; \mathbf{a},\mathbf{b})$ do not identify uniquely the subgraph associated to those vertices. Hence the value of $\mathcal{A}_i(A, B; \mathbf{a},\mathbf{b})$ may depend on this representation. We will consider the greatest value for any possible representation of $(A, B; \mathbf{a},\mathbf{b})$.

7.1.1 $\overline{\nabla_B}$ for extremal configurations

The following lemma bounds the contribution of $\overline{\nabla_B}(\sigma,\tau,c,\overline{\mathcal{D}})$ for each color c appearing in one extremal configuration. Recall that as $S \in \overline{\mathcal{D}}$, vertex v is not included in the Kempe component flipped and S is the same in both colorings (in this case the coupling is the identity).

Lemma 7.4 For every neighboring coloring pair (σ,τ) and color c we have:
A) If $c \in C^1_{\sigma,\tau}(v)$, then $\overline{\nabla_B}(\sigma,\tau,c,\overline{\mathcal{D}}) \le -\frac{2\eta_1(k-\Delta-2)}{\Delta} + (-\eta_1 + 2\eta_2)\cdot \mathbb{1}_{\{2\eta_2>\eta_1\}}$
B) If $c \in C^2_{\sigma,\tau}(v)$, then $\overline{\nabla_B}(\sigma,\tau,c,\overline{\mathcal{D}}) \le -\frac{12\eta_2(k-\Delta-2)}{\Delta} + k\cdot\frac{\eta_1-2\eta_2}{3\Delta}\cdot \mathbb{1}_{\{2\eta_2<\eta_1\}}$

Proof. Recall that the extremal configurations are (3,2;(2),(1)) and (7,3;(3,3),(1,1)) up to symmetries. Let $c \in C^i_{\sigma,\tau}(v)$ for $i \in \{1, 2\}$, namely (σ,τ) has an extremal configuration for such color. We define the following set of components:

$$\mathcal{S}_0 = \{S \in \overline{\mathcal{D}} : c \notin C_{\sigma_S,\tau_S}(v)\}$$
$$\mathcal{S}_1 = \{S \in \overline{\mathcal{D}} : c \in C^1_{\sigma_S,\tau_S}(v)\}$$
$$\mathcal{S}_2 = \{S \in \overline{\mathcal{D}} : c \in C^2_{\sigma_S,\tau_S}(v)\}$$

which are the set of Kempe components in $\overline{\mathcal{D}}$ whose flip yields to a non-extremal configuration, to a 1-extremal and to a 2-extremal configuration for color c respectively. Note that $\overline{\mathcal{D}} = \mathcal{S}_0 \cup \mathcal{S}_1 \cup \mathcal{S}_2$.

Now if $i = 1$, then for every $S \in \mathcal{S}_1$ we have $\xi^1_{\sigma,\tau}(v,c,S), \xi^2_{\sigma,\tau}(v,c,S) = 0$ so

$$\overline{\nabla_B}(\sigma,\tau,c,\overline{\mathcal{D}}) = \overline{\nabla_B}(\sigma,\tau,c,\mathcal{S}_0) + \overline{\nabla_B}(\sigma,\tau,c,\mathcal{S}_2)$$

And when $i = 2$, then for every $S \in \mathcal{S}_2$ we have $\xi^1_{\sigma,\tau}(v,c,S), \xi^2_{\sigma,\tau}(v,c,S) = 0$ so

$$\overline{\nabla_B}(\sigma,\tau,c,\overline{\mathcal{D}}) = \overline{\nabla_B}(\sigma,\tau,c,\mathcal{S}_0) + \overline{\nabla_B}(\sigma,\tau,c,\mathcal{S}_1)$$

We will distinguish the cases $i = 1$ and $i = 2$. Let us begin with the case $i = 1$.
For $c \in C^1_{\sigma,\tau}(v)$ and $S \in \mathcal{S}_2$, we have that $\xi^1_{\sigma,\tau}(v,c,S) = -1$ and $\xi^2_{\sigma,\tau}(v,c,S) = 2$. It remains to see in how many ways we can move from a 1-extremal configuration to a 2-extremal configuration. Let $u \in U_c$ be the neighbour of v colored with c. Then in order to obtain a 2-extremal configuration, one of the neighbours of v different than u, call it u',

must change its color to c. There are Δ ways to choose such neighbour u', and as it has to change its color to c, the Kempe component is uniquely determined.

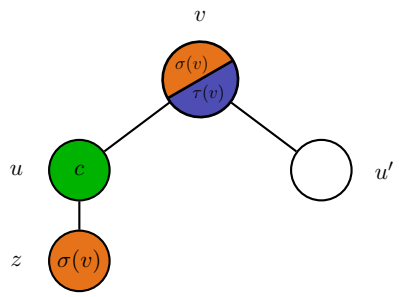

Figure 7.1: In order to get a 2-extremal configuration from a 1-extremal configuration one neighbour of v different than u must change its color to c. Ther are at most Δ ways to choose u' and then the Kempe component that has to be flipped is $S_\sigma(u', c)$.

Hence, for $c \in C^1_{\sigma,\tau}(v)$ and recalling (20) we get:

$$\overline{\nabla_B}(\sigma, \tau, c, \mathcal{S}_2) \leq (-\eta_1 + 2\eta_2) \cdot \mathbb{1}_{\{2\eta_2 > \eta_1\}}$$

where we have added the indicator function due to the fact that this is only a positive and tight contribution to the expected variation distance if $2\eta_2 > \eta_1$.

For $c \in C^2_{\sigma,\tau}(v)$ and $S \in \mathcal{S}_1$, we have that $\xi^1_{\sigma,\tau}(v, c, S) = 1$ and $\xi^2_{\sigma,\tau}(v, c, S) = -2$. We now count how many sets $S \in \overline{\mathcal{D}}$ can convert one 2-extremal configuration into a 1-extremal configuration. Let U_c be the set of neighbours of v colored with c. The only way to convert this extremal configuration into a 1-extremal configuration is changing the color of at least one of the vertices in U_c. There are 2 choices for the vertex in U_c and less than k options for the new color c'. Therefore, there are less than $2k$ Kempe components. Now we argue that each Kempe component must have size greater or equal than 3. Suppose, without loss of generality, that $(A, B; \mathbf{a}, \mathbf{b}) = (7, 3; (3, 3), (1, 1))$. If $S = S_\sigma(u_1, c')$, then S has to modify $S_\tau(u_2, \sigma(v))$ in order to obtain 1-extremality (as $|S_\tau(u_2, \sigma(v))| = 3$ and in the 1-extremal configuration has size at most 2). This implies that the Kempe component has to be larger or equal than 2. Moreover it can not be 2 as $S_\tau(u_1, \sigma(v)), S_\tau(u_2, \sigma(v))$ would be equal (see Figure 7.2) which contradicts Observation 5.1. Analogously for $S = S_\sigma(u_2, c')$.

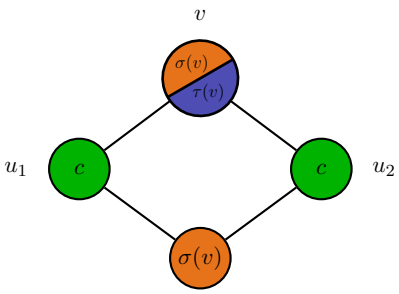

Figure 7.2: If $|S_\sigma(u_1, c')| = 2$ and $S_\sigma(u_1, c')$ intersects $S_\tau(u_2, \sigma(v))$ then $S_\tau(u_1, \sigma(v)) = S_\tau(u_2, \sigma(v))$.

Hence each of the $2k$ Kempe components has size greater than 3 and we get:

$$\overline{\nabla_B}(\sigma,\tau,c,\mathcal{S}_1) \leq 2k \cdot \frac{p_3}{\Delta} \cdot (\eta_1 - 2\eta_2) \cdot \mathbb{1}_{\{2\eta_2<\eta_1\}} = 2k \cdot \frac{\eta_1 - 2\eta_2}{6\Delta} \cdot \mathbb{1}_{\{2\eta_2<\eta_1\}}$$

where again we impose with the indicator function that this is only considered when it is positive.

Now we bound $\overline{\nabla_B}(\sigma,\tau,c,S_0)$, so our aim is to count in how many ways an extremal configuration can be converted into a non-extremal configuration in a step of the flip dynamics. Flips of components $S \in S_0$ imply that for $i=1$, $\xi^1_{\sigma,\tau}(v,c,S) = -1$ and $\xi^2_{\sigma,\tau}(v,c,S) = 0$ and for $i=2$, $\xi^1_{\sigma,\tau}(v,c,S) = 0, \xi^2_{\sigma,\tau}(v,c,S) = -2$. As the contribution is negative, we will only focus on Kempe components of size 1, and we will obtain an upper bound of the term $\overline{\nabla_B}(\sigma,\tau,c,S_0)$.

Consider $S \in S_0$ of size 1, so $p_{|S|} = p_1 = 1$. Basically, S will remove an extremal configuration if it selects a vertex w different from v of the extremal configuration and changes its color to c' with $c' \notin \sigma(N(w)) \cup \{\sigma(v), \tau(v), c\}$. So there are at least $(k - \Delta - 2)$ choices for c' taking into account that either $\sigma(v), \tau(v)$ or c belong to $N(w)$. Moreover, for $i=1$, there are 2 possible choices for vertex w while for $i=2$, there are 6 choices (see Figure 7.3).

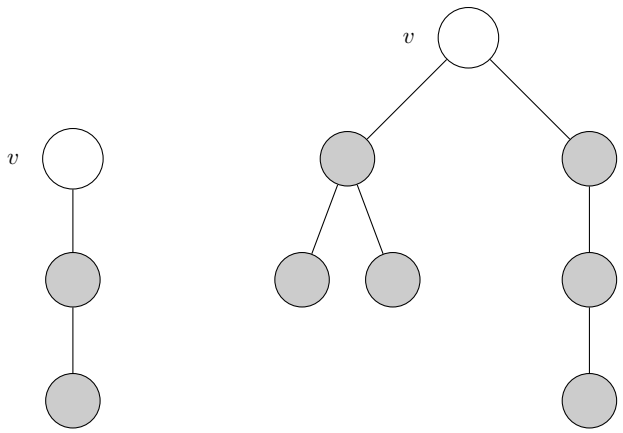

Figure 7.3: Recall extremal configurations of size 1 and 2. There are either 2 or 6 vertices different than v respectively, which are represented in grey. Grey vertices are the ones that can be recolored in order to break extremality.

Hence:

- For $i=1$: $\overline{\nabla_B}(\sigma,\tau,c,S_0) \leq \frac{\eta_1}{\Delta} 2(k-\Delta-2) \cdot \xi^1_{\sigma,\tau}(v,c,S) = -\frac{2\eta_1}{\Delta}(k-\Delta-2)$
- For $i=2$: $\overline{\nabla_B}(\sigma,\tau,c,S_0) \leq \frac{\eta_2}{\Delta} 6(k-\Delta-2) \cdot \xi^2_{\sigma,\tau}(v,c,S) = -\frac{12\eta_2}{\Delta}(k-\Delta-2)$

Finally, from the bounds of $\overline{\nabla_B}(\sigma,\tau,c,S_0)$, $\overline{\nabla_B}(\sigma,\tau,c,S_1)$ and $\overline{\nabla_B}(\sigma,\tau,c,S_2)$ we have that
For $i=1$

$$\overline{\nabla_B}(\sigma,\tau,c,\overline{D}) \leq -\frac{2\eta_1(k-\Delta-2)}{\Delta} + (-\eta_1 + 2\eta_2) \cdot \mathbb{1}_{\{2\eta_2>\eta_1\}}$$

For $i = 2$

$$\overline{\nabla_B}(\sigma, \tau, c, \overline{D}) \leq -\frac{12\eta_2(k - \Delta - 2)}{\Delta} + k \cdot \frac{\eta_1 - 2\eta_2}{3\Delta} \cdot \mathbb{1}_{\{2\eta_2 < \eta_1\}}$$

□

7.1.2 $\overline{\nabla_B}$ for non-extremal configurations; case $c \in C^1_{\sigma_S,\tau_S}(v)$

Now we want to study the case in which $c \notin C_{\sigma,\tau}(v)$ and $c \in C_{\sigma_S,\tau_S}(v)$, after the flip of a Kempe component $S \in \overline{\mathcal{D}}$. Let $(A, B; \mathbf{a}, \mathbf{b}) \notin \Pi$ be the non-extremal configuration and define $\mathcal{R}_i(A, B; \mathbf{a}, \mathbf{b}) := \{S \in \overline{\mathcal{D}} : c \in C^i_{\sigma_S,\tau_S}(v)\}$, the set of Kempe components $S \in \overline{\mathcal{D}}$ whose flip yields to an i-extremal configuration from configuration $(A, B; \mathbf{a}, \mathbf{b})$ for $i \in \{1, 2\}$. Also define $\mathcal{A}_i(A, B; \mathbf{a}, \mathbf{b}) := \sum_{S \in \mathcal{R}_i(A,B;\mathbf{a},\mathbf{b})} p_{|S|}$. Let $U_c = \{u_1, ..., u_{\delta_c}\}$ be the set of neighbours of v colored with c and denote by U_c^S the set of neighbours of v colored c after the flip of the Kempe component S, more precisely $U_c^S := N(v) \cap (\sigma_S)^{-1}(c)$.

For simplicity, let us define the sets

$$\mathcal{H} = \{(4, 2; (3), (1)), (3, 3, (2), (2)), (5, 3; (2, 2), (1, 1), (4, 4; (2, 1), (1, 2)) \text{ up to symmetry}\}$$

and

$$\mathcal{G} = \{(8, 3; (4, 3), (1, 1)), (9, 3; (5, 3), (1, 1)), (10, 4; (3, 3, 3), (1, 1, 1)) \text{ up to symmetry}\}$$

First we bound $\mathcal{A}_1(A, B; \mathbf{a}, \mathbf{b})$.

Lemma 7.5 We have

$$\mathcal{A}_1(A, B; \mathbf{a}, \mathbf{b}) \leq \begin{cases} 2k + \Delta p_2 & \text{if } (A, B; \mathbf{a}, \mathbf{b}) \in \mathcal{H} \\ \frac{4}{3}k & \text{otherwise} \end{cases}$$

Moreover for configurations $(A, B; \mathbf{a}, \mathbf{b}) \in \mathcal{G}$ we have $\mathcal{A}_1(A, B; \mathbf{a}, \mathbf{b}) \leq 2k \cdot p_3$.

Proof. Let S be a Kempe component whose flip yields to a 1-extremal configuration, so we have that $U_c^S = \{u^S\}$, $u^S \in N(v)$. We study the value of $\mathcal{A}_1(A, B; \mathbf{a}, \mathbf{b})$ distinguishing the different values of δ_c before flipping the component:

- $\delta_c = 0$

  In this case, $U_c = \emptyset$ so one neighbour of v, call it u, has to change its color to c. The Kempe component that has to be flipped is uniquely determined by the choice of u and color c, more precisely it is $S_\sigma(u, c)$. The contribution is then $\mathcal{A}_1(A, B; \mathbf{a}, \mathbf{b}) \leq \Delta \leq \frac{4}{3}k$.

- $\delta_c = 1$

  In this case $U_c = \{u\}$. We will distinguish the case where $U_c^S = U_c$ and the case where $U_c^S \neq U_c$. In particular, define

$$\mathcal{B}_1(A, B; \mathbf{a}, \mathbf{b}) := \sum_{\substack{S \in R_1(A,B;\mathbf{a},\mathbf{b}) \\ S: U_c^S \neq U_c}} p_{|S|}, \qquad \mathcal{C}_1(A, B; \mathbf{a}, \mathbf{b}) := \sum_{\substack{S \in R_1(A,B;\mathbf{a},\mathbf{b}) \\ S: U_c^S = U_c}} p_{|S|}$$

so $\mathcal{A}_1(A, B; \mathbf{a}, \mathbf{b}) = \mathcal{B}_1(A, B; \mathbf{a}, \mathbf{b}) + \mathcal{C}_1(A, B; \mathbf{a}, \mathbf{b})$.

If $U_c^S \neq U_c$ and as in the previous analysis of $\delta_c = 0$, there are at most Δ Kempe components leading to a 1-extremal configuration, but each has size at least 2, due to the fact that it has to include vertices u and u^S. The contribution is $\mathcal{B}_1(A, B; \mathbf{a}, \mathbf{b}) \leq \Delta p_2$.

Now, consider the case $U_c^S = U_c = \{u\}$. For our analysis, let us define the set $N := N(u^S) \bigcap [S_\sigma(u^S, \tau(v)) \cup S_\tau(u^S, \sigma(v))]$, which are the neighbours of u^S different than v colored $\sigma(v)$ or $\tau(v)$.

If N is empty, a neighbour of u has to flip its color to either $\sigma(v)$ or $\tau(v)$. There are at most 2Δ options for such S, so $\mathcal{C}_1(A, B; \mathbf{a}, \mathbf{b}) \leq 2\Delta$.

If $|N| = 1$, $N = \{w\}$, there are 2 options; either w belongs to the extremal configuration or it does not, which are represented in Figure 7.4. In the first case, the vertex or vertices that have to change its color are uniquely determined. More precisely, let $z \in N(w) \cap S_\sigma(w, c) \setminus \{u\}$, which is well defined because $(A, B; \mathbf{a}, \mathbf{b})$ is non-extremal. In order to get a 1-extremal configuration, the Kempe component flipped has to be $S = S_\sigma(z, c')$ for $c' \in [k]$, so there are at most k options for such Kempe component S. And in the second case, the Kempe component must include w and another neighbour of u. These 2 vertices already define the Kempe component S so there are at most Δ options for S each of size at least 2. Adding both values we get an upper bound of $\mathcal{C}_1(A, B; \mathbf{a}, \mathbf{b}) \leq k + \Delta p_2$.

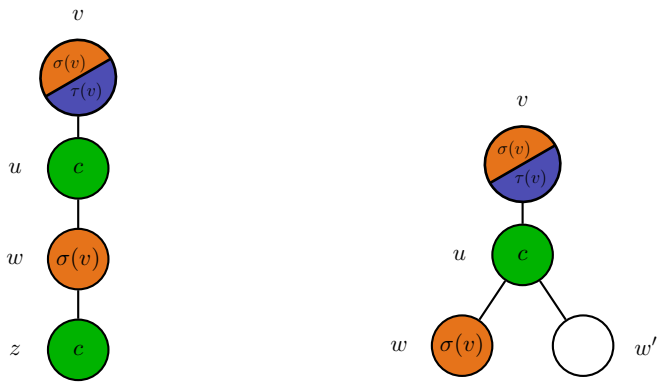

Figure 7.4: Representation of the 2 options for $|N| = 1$.

For the following cases, choose a color c' in $[k]$ and study the Kempe components $S_\sigma(w, c')$ with $w \in N$.

If $|N| > 2$, then only one component $S_\sigma(w, c')$ with $w \in N$ can lead to a 1-extremal configuration with its flip. Basically, the Kempe component must contain all the vertices of N except possibly one. So once the color c' is chosen, the Kempe component that has to be flipped is uniquely determined (see Figure 7.5). Therefore $\mathcal{C}_1(A, B; \mathbf{a}, \mathbf{b}) \leq k$.

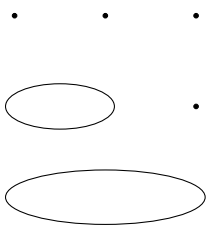

Figure 7.5: Representation of sets $S_\sigma(w_i, c')$ for $|N| = 3$, $N = \{w_1, w_2, w_3\}$ and $w_i \in N$. Either $S_\sigma(w_i, c')$ are all different or $S_\sigma(w_1, c') = S_\sigma(w_2, c') \neq S_\sigma(w_3, c')$ (up to permutation) or $S_\sigma(w_1, c') = S_\sigma(w_2, c') = S_\sigma(w_3, c')$. Only in the last 2 cases, the flip of a Kempe component can yield to 1-extremality, because there is a Kempe component that contains all vertices of N except possibly one.

Otherwise, $|N| = 2$ and the flip of both Kempe components $S_\sigma(w, c')$ with $w \in N$, could lead to a 1-extremal configuration. So, given that there are k options for color c', there are at most $2k$ Kempe components transforming the configuration into an extremal one. Notice that case $2k$ is a very particular case. It is only obtained when $N(w) \cap \sigma^{-1}(c) = \{u\}$ for both $w \in N$, i.e. the only neighbour of w colored c is u (see Figure 7.6). For the other configurations with $|N| = 2$, there exists $w \in N$ such that $N(w) \cap \sigma^{-1}(c) \setminus \{u\} \neq \emptyset$. Let $N = \{w_1, w_2\}$, and suppose without loss of generality that $z \in N(w_1) \cap \sigma^{-1}(c) \setminus \{u\}$. Then there are at most k options for Kempe components $S_\sigma(w_1, c')$, for $c' \in [k]$ but flips of $S_\sigma(w_2, c') \neq S_\sigma(w_1, c')$ do not yield to extremal configurations. In particular, $S_\sigma(w_2, c')$ must contain vertex z in order to reach extremality, namely colors $\{c, \sigma(w_2)\}$ which are $\{c, \sigma(v)\}$ or $\{c, \tau(v)\}$. But then $v \in S$, so $S \notin \overline{\mathcal{D}}$ (see Figure 7.6). So the only positive contribution in $\mathcal{C}_1(A, B; \mathbf{a}, \mathbf{b})$ is given by $S_\sigma(w_1, c')$, hence at most k.

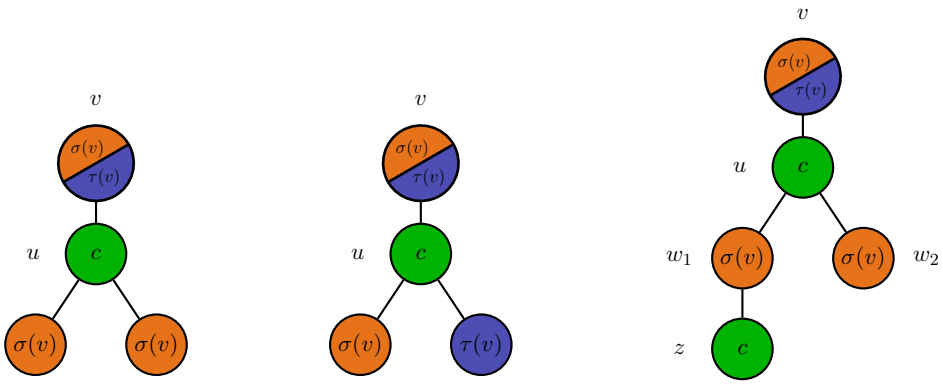

Figure 7.6: The first 2 configurations, $(4, 2, (3), (1))$ or $(3, 3, (2), (2))$ up to symmetries, are the only ones with $\delta_c = 1$ that can move to a 1-extremal configuration in $2k$ different Kempe flips. For the rest of configurations with $|N| = 2$, assume $z \in N(w_1) \cap \sigma^{-1}(c) \setminus \{u\}$. Then only flips of Kempe components $S_\sigma(w_1, c')$ may lead to extremality and the contribution is k.

Hence we have that $\mathcal{C}_1(A, B; \mathbf{a}, \mathbf{b}) \leq k + \Delta p_2$ except for configurations $(4, 2, (3), (1))$, $(3, 3, (2), (2))$ up to symmetries for which $\mathcal{C}_1(A, B; \mathbf{a}, \mathbf{b}) \leq 2k$.

All together gives us a bound of $\mathcal{A}_1(A, B; \mathbf{a},\mathbf{b}) = \mathcal{B}_1(A, B; \mathbf{a},\mathbf{b}) + \mathcal{C}_1(A, B; \mathbf{a},\mathbf{b}) \leq 2k + \Delta p_2$ for configurations $(4, 2; (3), (1)), (3, 3, (2), (2))$ and $\mathcal{A}_1(A, B; \mathbf{a},\mathbf{b}) = \mathcal{B}_1(A, B; \mathbf{a},\mathbf{b}) + \mathcal{C}_1(A, B; \mathbf{a},\mathbf{b}) \leq k + 2\Delta p_2 \leq \frac{4}{3}k$ otherwise.

- $\delta_c = 2$

  As $\delta_c^S = 1$, one vertex of U_c must change its color with the flip. As there are at most 2 choices for the vertex in U_c, $\mathcal{A}_1(A, B; \mathbf{a},\mathbf{b}) \leq 2k$. Again, this bound is tight only for one specific case; when flipping any of the two vertices in U_c lead to a 1-extremal configuration. This case is shown in Figure 7.7.

  For the other configurations, either one of the flips do not yield extremality or one of the 2 Kempe components must have size greater than 3 (the argument is analogous to the case $c \in C^2_{\sigma,\tau}(v) \cap C^1_{\sigma_S,\tau_S}(v)$ from Lemma 7.4). So $\mathcal{A}_1(A, B; \mathbf{a},\mathbf{b}) \leq k(p_1 + p_3)$.

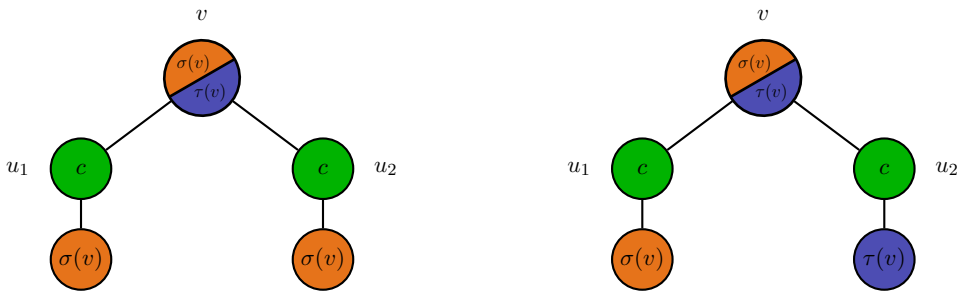

Figure 7.7: These are the only cases with $\delta_c = 2$ in which up to $2k$ Kempe flips could lead to 1-extremal configurations. They are configurations $(5, 3, (2, 2), (1, 1))$ or $(4, 4, (2, 1), (1, 2))$ up to symmetries.

- $\delta_c \geq 3$

  As in the previous case, all but one vertices of U_c must change their color. Take a color $c' \in [k]$ and study the Kempe components $S_\sigma(u, c')$ with $u \in U_c$. Recalling Figure 7.5, only the flip of one Kempe component can yield to a 1-extremal configuration. Hence $\mathcal{C}_1(A, B; \mathbf{a},\mathbf{b}) \leq k$.

Summing up, we get that $\mathcal{A}_1(A, B; \mathbf{a},\mathbf{b}) \leq 2k + \Delta p_2$ for configurations $(4, 2; (3), (1))$, $(3, 3, (2), (2))$, $(5, 3; (2, 2), (1, 1))$ and $(4, 4; (2, 1), (1, 2))$ up to symmetry and $\mathcal{A}_1(A, B; \mathbf{a},\mathbf{b}) \leq \max\{k + 2\Delta p_2, k + kp_3\} \leq \frac{4}{3}k$ otherwise, taking into account the values of the p_i's and the fact that $k > \frac{161}{88}\Delta$.

Finally, we study configurations $(A, B; \mathbf{a},\mathbf{b}) = (8, 3; (4, 3), (1, 1)), (9, 3; (5, 3), (1, 1))$ and $(10, 4; (3, 3, 3), (1, 1, 1))$ up to symmetries, which we will need in the following sections. As in all cases $\delta_c > 1$ one vertex of U_c must change its color. Choose a color c' and study the Kempe components $S_\sigma(u, c')$ with $u \in U_c$. The flip of at most two Kempe components could lead to a 1-extremal configuration, and the structure of the configurations imply that each Kempe component must have size at least 3 in order to reach the 1-extremal configuration (again the argument is analogous to the case $c \in C^2_{\sigma,\tau}(v) \cap C^1_{\sigma_S,\tau_S}(v)$ from Lemma 7.4). Hence we get that for these configurations $\mathcal{A}_1(A, B; \mathbf{a},\mathbf{b}) \leq 2k \cdot p_3$.

□

7.1.3 $\overline{\nabla_B}$ for non-extremal configurations; case $c \in C^2_{\sigma_S,\tau_S}(v)$

For $\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b})$ we proceed in a slightly different way. Recall that $(A, B; \mathbf{a}, \mathbf{b}) = (A, B; (a_1, ...a_{\delta_c}), (b_1, ..., b_{\delta_c}))$ is a non-extremal configuration and $U_c = \{u_1, ..., u_{\delta_c}\}$ is the set of neighbours of v colored with c. Fix the 2-extremal configuration $(A^*, B^*; \mathbf{a}^*, \mathbf{b}^*) = (A^*, B^*; (a_1^*, a_2^*), (b_1^*, b_2^*))$, $(A^*, B^*; \mathbf{a}^*, \mathbf{b}^*) \in \Pi^2$. For any Kempe component S, let $U_c^S = N(v) \cap (\sigma_S)^{-1}(c)$ be the set of neighbours of v colored c after Kempe flip of S.

Now, we define $\mathcal{T} := \{S \in \overline{\mathcal{D}} : (A^S, B^S; \mathbf{a}^S, \mathbf{b}^S) = (A^*, B^*; \mathbf{a}^*, \mathbf{b}^*)\}$, the set of Kempe components whose flip yields to that 2-extremal configuration.

Consider the partition $\mathcal{T} = \mathcal{T}_1 \cup \mathcal{T}_2 \cup \mathcal{T}_3$ with

$$\begin{aligned}
\mathcal{T}_1 &:= \{\mathcal{S} \in \overline{\mathcal{D}} : U_c^S \setminus U_c \neq \emptyset\} \\
\mathcal{T}_2 &:= \{\mathcal{S} \in \overline{\mathcal{D}} : U_c \setminus U_c^S \neq \emptyset\} \setminus \mathcal{T}_1 \\
\mathcal{T}_3 &:= \{\mathcal{S} \in \overline{\mathcal{D}} : U_c = U_c^S\}
\end{aligned}$$

For every $S \in \mathcal{T}_3$, as $(A, B; \mathbf{a}, \mathbf{b})$ is non-extremal, there exists $x \in \{a, b\}$ and $j \in \{1, 2\}$, such that $x_j \neq x_j^S$. So we can consider the following partition of $\mathcal{T}_3$:

$$\begin{aligned}
\mathcal{T}_3^- &= \{\mathcal{S} \in \mathcal{T}_3 : \exists j, \quad x_j < x_j^S\} \\
\mathcal{T}_3^+ &= \{\mathcal{S} \in \mathcal{T}_3 : \exists j, \quad x_j > x_j^S\} \setminus \mathcal{T}_3^-
\end{aligned}$$

From the definition of $\mathcal{T}_j$ we define $\mathcal{B}_j = \mathcal{B}_j(A, B; \mathbf{a}, \mathbf{b}) := \sum_{S \in \mathcal{T}_j(A,B;\mathbf{a},\mathbf{b})} p_{|S|}$. Also define $\mathcal{B}_3^+ = \sum_{S \in \mathcal{T}_3^+(A,B;\mathbf{a},\mathbf{b})} p_{|S|}$ and $\mathcal{B}_3^- = \sum_{S \in \mathcal{T}_3^-(A,B;\mathbf{a},\mathbf{b})} p_{|S|}$. We first bound these quantities.

Lemma 7.6 We have

1. $\mathcal{B}_1 \leq \Delta$. Moreover $\mathcal{B}_1 \leq \Delta p_2$ if $\delta_c \neq 1$.
2. $\mathcal{B}_2 \leq 3k$ and $\mathcal{B}_2 = 0$ if $\delta_c \leq 2$.
3. $\mathcal{B}_3^- \leq 2\Delta$, $\mathcal{B}_3^+ \leq 3k$ and $\mathcal{B}_3 = 0$ if $\delta_c \neq 2$.

Proof. We first bound $|\mathcal{T}_j|$, for $j \in \{1, 2, 3\}$. Recall that for $(A^S, B^S; \mathbf{a}^S, \mathbf{b}^S) = (A^*, B^*; \mathbf{a}^*, \mathbf{b}^*)$ a 2-extremal configuration, $\delta_c^S = 2$ and $x_j^S \in \{1, 3\}$.

To bound the size of $\mathcal{S}' \in \{\mathcal{T}_1, \mathcal{T}_3^-\}$ we do the following. In this case, there exists a vertex z in the neighbourhood of the Kempe component associated to σ or τ that belongs to the corresponding component in σ_S or τ_S. Let $\pi = \sigma$ and $\varphi = \tau$ if this Kempe component is the one associated to σ and $\pi = \tau$, $\varphi = \sigma$ otherwise. If there exists a set $N(\mathcal{S}')$ such that $S \cap N(\mathcal{S}') \neq \emptyset$ for any $S \in \mathcal{S}'$, then any $S \in \mathcal{S}'$ can be described as $S = S_\varphi(w, c')$ with $w \in N(\mathcal{S}')$ and a unique color $c' \in \{c, \pi(v)\}$. Therefore $|\mathcal{S}'| \leq |N(\mathcal{S}')|$.

If $\mathcal{S}' = \mathcal{T}_1$, and $S \in \mathcal{S}'$, take $N(\mathcal{S}') = N_1 = N(v)$. It is straightforward to see that $S \cap N_1 \neq \emptyset$. Hence $|\mathcal{T}_1| \leq \Delta$.

If $\mathcal{S}' = \mathcal{T}_3^-$, and $S \in \mathcal{S}'$ recall that there exists j such that $x_j < x_j^S$. Set $\pi = \sigma$, $\varphi = \tau$ if $x = a$ and $\pi = \tau$, $\varphi = \sigma$ if $x = b$. Then define $N(\mathcal{T}_3^-) = N_3$ the set of neighbours of $S_\varphi(u_j, \pi(v))$. This set satisfies that $S \cap N_3 \neq \emptyset$. So $|\mathcal{T}_3^-| \leq x_j \Delta \leq (x_j^S - 1)\Delta \leq 2\Delta$.

To bound the size of $\mathcal{S}' \in \{\mathcal{T}_2, \mathcal{T}_3^+\}$ we proceed as follows. For $S \in \mathcal{S}'$, there is a vertex in the Kempe component associated to σ or τ that does not belong to the corresponding

Kempe component in σ_S, τ_S. If there exists a set $R(\mathcal{S}')$ such that $S \cap R(\mathcal{S}') \neq \emptyset$ for any $S \in \mathcal{S}'$, then any $S \in \mathcal{S}'$ can be decribed as $S = S_\sigma(w, c)$ for $w \in R(\mathcal{S}')$ and $c \in [k]$. Hence, $|\mathcal{S}'| \leq |R(\mathcal{S}')|k$.

If $\mathcal{S}' = \mathcal{T}_2$, and $S \in \mathcal{S}'$, define $l := \min\{\delta_c, \delta_c^S + 1\} = \min\{\delta_c, 3\}$ and let $R(\mathcal{T}_2) = R_2 = \{u_1, ..., u_l\}$, with $u_i \in U_c$ for $i \in [l]$. We have that $|S \cap U_c| = |U_c \setminus U_c^S| \geq 1$ and $|S \cap R_2| \geq |S \cap U_c| - (\delta_c - l) \geq |S \cap U_c| - (\delta_c - (\delta_c^S + 1)) = |S \cap U_c| - |U_c \setminus U_c^S| + 1 = 1$. Hence as $|R_2| = l \leq 3$ we have $|\mathcal{T}_2| \leq 3k$.

If $\mathcal{S}' = \mathcal{T}_3^+$, and $S \in \mathcal{S}'$, there exists j such that $x_j > x_j^S$ and set $\pi = \sigma, \varphi = \tau$ if $x = a$ and $\pi = \tau, \varphi = \sigma$ if $x = b$. Now, let $R(\mathcal{T}_3^+) = R_3$ be the set of x_j^S vertices in $S_\varphi(u_j, \pi(v)) \setminus \{u_j\}$ that minimize distance to u_j. As $u_j \notin R_3$, we have that $S \cap R_3 \neq \emptyset$ and $|R_3| = x_j^S \leq 3$, so $|\mathcal{T}_3^+| \leq x_j^S k \leq 3k$.

Once we have $|\mathcal{T}_j|$ bounded, $\mathcal{B}_j$ can be trivially bounded by $\mathcal{B}_j \leq |\mathcal{T}_j| \cdot p_1 = |\mathcal{T}_j|$ due to the fact that the p_i's are decreasing and $p_1 = 1$.

Finally, in the case of $\mathcal{B}_1$, $p_{|S|} = 1$ only if $S = \{w\}$, with $w \in N(v)$, so one necessary condition is that $\delta_c = \delta_c^S - 1 = 1$. Otherwise, we have that $|S| \geq 2$. Therefore, we obtain the desired result. □

From the previous lemma we are now able to compute $\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b})\Big|_{(A^*, B^*; \mathbf{a}^*, \mathbf{b}^*)}$, namely the value of $\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b})$ given that the flip of the Kempe component yields the 2-extremal configuration $(A^*, B^*; \mathbf{a}^*, \mathbf{b}^*)$.

Lemma 7.7 Once fixed $(A^*, B^*; \mathbf{a}^*, \mathbf{b}^*) \in \Pi^2$ we have:

$$\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b})\Big|_{(A^*, B^*; \mathbf{a}^*, \mathbf{b}^*)} \leq \begin{cases} 3k + \Delta p_2 & \text{if } (A, B; \mathbf{a}, \mathbf{b}) \in \mathcal{G} \\ \frac{4}{3}k + \Delta p_2 & \text{otherwise} \end{cases}$$

Proof. We want to study for which Kempe components $S \in \overline{\mathcal{D}}$ we get $(A^S, B^S; \mathbf{a}^S, \mathbf{b}^S) = (A^*, B^*; \mathbf{a}^*, \mathbf{b}^*)$ and recall that $\Pi^2 = \{(7, 3; (3, 3), (1, 1)), (3, 7; (1, 1), (3, 3))\}$. We will consider that $(A^*, B^*; \mathbf{a}^*, \mathbf{b}^*) = (7, 3; (3, 3), (1, 1))$ and will consider the results up to symmetry.

Now, recall lemma 7.6. First we argue when $\mathcal{B}_2 = 3k$ or $\mathcal{B}_3^+ = 3k$ are tight.

$\mathcal{B}_2$ is only not null when $\delta_c > 2$. From the proof of the lemma, $\mathcal{B}_2 = 3k$ only if $\min\{\delta_c, 3\} = 3$ and the flip considered has size 1. This implies that $\delta_c = 3$ and the bound is tight when the flip of any of the Kempe components $S_\sigma(u, c')$ for $u \in \{u_1, u_2, u_3\} = U_c$ and $c' \in [k]$, leads to the same 2-extremal configuration. Hence $|S_\sigma(u, c')| = 1$ and the 3 flips yield to $(A^*, B^*; \mathbf{a}^*, \mathbf{b}^*)$ only if $(A, B; \mathbf{a}, \mathbf{b}) = (10, 4; (3, 3, 3), (1, 1, 1))$.

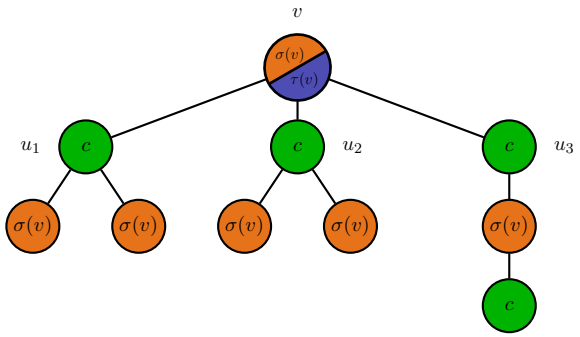

Figure 7.8: Configuration $(10, 3; (3, 3, 3), (1, 1, 1))$ is the only one with $\delta_c = 3$ that can move to $(7, 3; (3, 3), (1, 1))$ in up to $3k$ flips of size 1. Recall that this configuration has $|S_\tau(u_i, \sigma(v))| = 3$ and in the graph each $S_\tau(u_i, \sigma(v))$ can be a tree of height 1 or 2

If $\delta_c = 3$ and $(A, B; \mathbf{a}, \mathbf{b}) \neq (10, 4; (3, 3, 3), (1, 1, 1))$, then there exists $x \in \{a, b\}$, $j \in \{1, 2, 3\}$ such that $x_j \neq x_j^*$. As in the case of $\mathcal{B}_3^-$, if $x_j < x_j^*$ then the bound is simply $2\Delta < \frac{4}{3}k$. Otherwise, if $x_j > x_j^*$, assume without loss of generality that $x_j = a_1$ and $a_1 \geq 4 > a_1^* = 3$. Then, for $c' \in [k]$, the flip of $S_\sigma(u_1, c')$ may lead to the extremal configuration and the contribution is upper bounded by k. But Kempe components $S_\sigma(u_2, c'), S_\sigma(u_3, c')$ have to modify the Kempe component $S_\tau(u_1, \sigma(v))$ in order to obtain extremality. This implies that the size of these Kempe components have to be larger or equal than 2. Moreover, $|S_\sigma(u_2, c')|$ can not be 2, as $S_\tau(u_1, \sigma(v)), S_\tau(u_2, \sigma(v))$ would be equal, see Figure 7.9. Equivalently $|S_\sigma(u_3, c')| \geq 3$. The bound is then $k + 2kp_3$.

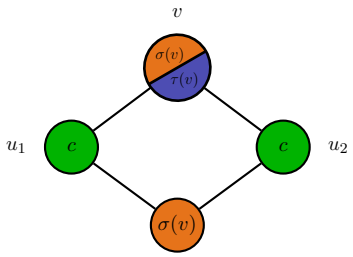

Figure 7.9: If $|S_\sigma(u_2, c')| = 2$ and $S_\sigma(u_2, c')$ intersects $S_\tau(u_1, \sigma(v))$ then $S_\tau(u_1, \sigma(v)) = S_\tau(u_2, \sigma(v))$

For $\delta_c > 3$, two vertices in U_c must be flipped in order to obtain $\delta_c^S = 2$. Hence as both vertices are colored c, the Kempe component must have size greater than 3 (otherwise they would be the same component). We get $|S_\sigma(w, c')| \geq 3$, and $\mathcal{B}_2 \leq 3kp_3 < \frac{4}{3}k$.

To summarise $\mathcal{B}_2 \leq 3k$ for configuration $(10, 4; (3, 3, 3), (1, 1, 1))$ up to symmetry and $\mathcal{B}_2 \leq \frac{4}{3}k$ otherwise.

Again from the proof of lemma 7.6, $\mathcal{B}_3^+ = 3k$ only if $x_j > x_j^S = 3$ and $y \in \{a, b\} \setminus \{x\}$ satisfies $y_1 = y_2 = 1$. As we consider, $(A^*, B^*; \mathbf{a}^*, \mathbf{b}^*) = (7, 3; (3, 3), (1, 1))$ we have $x = a, y = b$. Let $N := N(u_j) \cap S_\tau(u_j, \sigma(v))$, the set of neighbours of u_j different than v colored $\sigma(v)$. We analyse all the possible values of $|N|$:

1. $|N| = 0$: This case is not possible due to the fact that $|N| = 0$ implies that $a_j = 1$ and $a_j = 1 \not> 3 = a_j^*$.

2. $|N| = 1$: Let $N = \{w\}$. Either $w \in S_{\tau_S}(u_j, \sigma(v))$ or $w \notin S_{\tau_S}(u_j, \sigma(v))$, that is w belongs to the extremal configuration after the Kempe flip or not. In the first option, consider the set of 2 vertices in $S_\tau(w, c) \setminus \{u_j, w\}$ that minimize the distance to w. One of them has to change its color in order to obtain extremality, so there are at most $2k$ options of size 1. This is only tight for the configuration $(8, 3; (4, 3), (1, 1))$, see Figure 7.10.

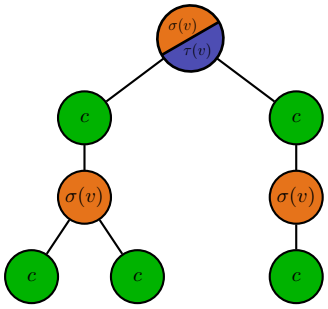

Figure 7.10: Configuration $(8, 3; (4, 3), (1, 1))$ is the only configuration with $|N| = 2$ that can yield to $(A^*, B^*; \mathbf{a}^*, \mathbf{b}^*)$ in $2k$ Kempe flips of size 1.

Otherwise, the bound is $k + \Delta p_2$. Let us argue it with the aid of Figure 7.11. If $|N(w) \cap \sigma^{-1}(c) \setminus \{u_j\}| \geq 2$ (second and third figures), only the flip of one Kempe component $S_\sigma(z_i, c')$, may lead to extremality and hence the contribution is k (recall arguments in Figure 7.5 and Figure 7.6). Only if $|N(w) \cap \sigma^{-1}(c) \setminus \{u_j\}| = 1$ (first figure) either $S_\sigma(t, c')$, with $c' \in [k]$ and $t \in N(z) \cap S_\sigma(w, c) \setminus \{w\}$ or $S_\sigma(z', c)$, with $z' \in N(w) \setminus \{u_j, z\}$ may lead to extremality. Hence there are k options for the first option and Δp_2 for the second due to the fact that $S_\sigma(z', c)$ must also contain vertex z.

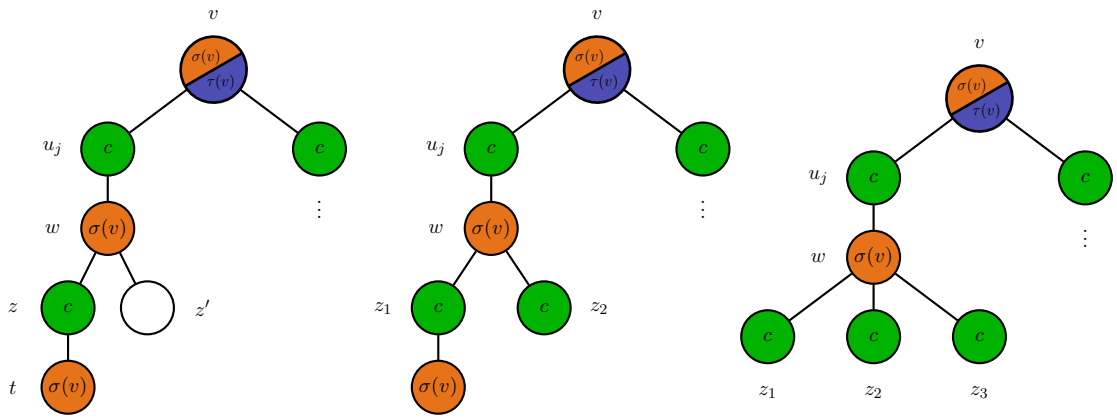

Figure 7.11: If the configuration is different from $(8, 3; (4, 3), (1, 1))$, the contribution is at most $k + \Delta p_2$.

In the second case, if $w \notin S_{\tau_S}(u_j, \sigma(v))$, another vertex $w' \in N(u_j)$, $w' \neq w$, belongs to $S_{\tau_S}(u_j, \sigma(v))$. There are Δ options to choose such vertex w', and the Kempe component is uniquely determined by vertices $\{w, w'\}$ so the bound is Δp_2. Adding both values we get a bound of $2k + \Delta p_2 < 3k$ for configuration $(8, 3; (4, 3), (1, 1))$ or $k + 2\Delta p_2 \leq \frac{4}{3}k$ otherwise.

3. $|N| = 2$: As $|N| = 2$ and the configuration is non-extremal, there exists a neighbour z of N in $S_\tau(u_j, \sigma(v))$ different than u_j. We consider the set of 3 vertices $R_3 = \{N, z\}$ and study the flips of $S_\sigma(t, c')$ for $t \in R_3$ (the argument is similar to the one of $\mathcal{T}_3^+$). Only the flips of the three vertices lead to extremality in a very particular case; see Figure 7.12. In the other cases at most the flip of two of them lead to extremality and the bound $2k$ is tight only for configuration $(9, 3; (5, 3), (1, 1))$. For the rest of configurations the bound is $k + kp_3$ due to the fact that one of the components S must have size greater than 2. Hence, the bound is either $\max\{3k, 2k\} = 3k$ for configurations $(8, 3; (4, 3), (1, 1))$ and $(9, 3; (5, 3), (1, 1))$ or $k + kp_3 < \frac{4}{3}k$ otherwise.

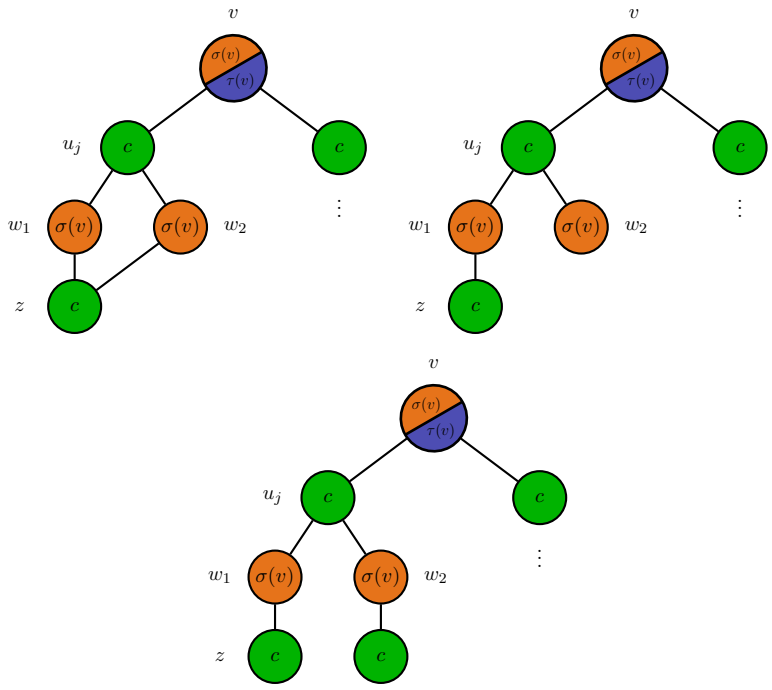

Figure 7.12: The first figure corresponds to the only representation of $(8, 3; (4, 3), (1, 1))$ that admits $3k$ Kempe flips of size 1 moving to $(7, 3; (3, 3), (1, 1))$. The second figure is another representation of $(8, 3; (4, 3), (1, 1))$ that admits $2k$ Kempe flips. Configuration $(9, 3; (5, 3), (1, 1))$ moves to $(7, 3; (3, 3), (1, 1))$ in up to $2k$ different Kempe flips of size 1. For the rest of configurations the upper bound is $k + kp_3$

4. $|N| = 3$: Choose color c' and study flips of Kempe components $S_\sigma(w, c')$ with $w \in N$. At most the 3 of them lead to an extremal configuration and this is only possible if the configuration is $(8, 3; (4, 3), (1, 1))$. Otherwise, the case is analogous to the computation of $\mathcal{B}_2$ for $\delta_c = 3$. We get a bound of $\frac{4}{3}k$.

5. $|N| \geq 4$: Take an arbitrary set $R_3 \subset N$ with $|R_3| = 3$ and study flips of $S_\sigma(w, c')$ with $w \in R_3$ and $c' \in [k]$. At most the 3 Kempe flips lead to extremality and the Kempe components must contain 2 vertices of U_c. The contribution is then upper bounded by $3kp_2 < \frac{4k}{3}$.

To sum up $\mathcal{B}_3^+ \leq 3k$ if the configuration is $(8, 3; (4, 3), (1, 1))$ or $(9, 3; (5, 3), (1, 1))$ up to symmetry and $\mathcal{B}_3^+ \leq \frac{4k}{3}$ otherwise.

Now, notice that $\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b})\Big|_{(A^*,B^*;\mathbf{a}^*,\mathbf{b}^*)} = (\mathcal{B}_1 + \mathcal{B}_2 + \mathcal{B}_3)(A, B; \mathbf{a}, \mathbf{b})$. As the values of $\mathcal{B}_j, j \in [3]$, depend on δ_c, we maximize over the different cases $\delta_c \leq 1$, $\delta_c = 2$ and $\delta_c \geq 3$. We obtain

$$\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b})\Big|_{(A^*,B^*;\mathbf{a}^*,\mathbf{b}^*)} \leq \begin{cases} 3k + \Delta p_2, & \text{if } (A, B; \mathbf{a}, \mathbf{b}) \in \mathcal{G} \\ \frac{4}{3}k + \Delta p_2, & \text{if } (A, B; \mathbf{a}, \mathbf{b}) \notin \mathcal{G} \end{cases}$$

□

In the previous lemma, we fix in advance the extremal configuration to get a bound of $\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b})\Big|_{(A^*,B^*;\mathbf{a}^*,\mathbf{b}^*)}$. From there we could already find a bound for $\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b})$ by just adding $\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b})\Big|_{(A^*,B^*;\mathbf{a}^*,\mathbf{b}^*)}$ twice; that is adding the contributions of the two different 2-extremal configurations $(7, 3; (3, 3), (1, 1))$ and $(3, 7; (1, 1), (3, 3))$. Even so, we are interested in obtaining a tighter bound, and the following lemma gives this bound.

Lemma 7.8 We have

$$\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b}) \leq \begin{cases} 3k + \Delta p_2 & \text{if } (A, B; \mathbf{a}, \mathbf{b}) \in \mathcal{G} \\ 2k & \text{otherwise} \end{cases}$$

Moreover for configurations $(A, B; \mathbf{a}, \mathbf{b}) \in \mathcal{H}$, we have $\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b}) \leq \Delta$.

Proof. The proof is done using 3 claims. The first and second claims give us the value of $\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b})$ for configurations in $\mathcal{G}$ and $\mathcal{H}$ respectively. And the third tells us that the only configuration that can move to both 2-extremal configurations with flips of size 1 is $(5, 5; (3, 1), (1, 3))$ with $\mathcal{A}_2(5, 5; (3, 1), (1, 3)) \leq 2$. As a corollary of the third claim, we have that for $(A, B; \mathbf{a}, \mathbf{b}) \notin \mathcal{G} \cup \mathcal{H} \cup (5, 5; (3, 1), (1, 3))$ the bound is $\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b}) \leq \mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b})\Big|_{(A^*,B^*;\mathbf{a}^*,\mathbf{b}^*)} \cdot (p_1 + p_2)$ due to the fact that at least 2 vertices have to be flipped to obtain one of the 2-extremal configurations. This gives us that $\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b}) \leq (\frac{4}{3}k + \Delta p_2) \cdot (p_1 + p_2)$, so we conclude.

More precisely we have the following claims and proofs:

Claim 1: Configurations in $\mathcal{G}$ satisfy $\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b}) \leq 3k + \Delta p_2$.

Proof of claim 1: Recall that $\mathcal{G} = \{(8, 3; (4, 3), (1, 1)), (9, 3; (5, 3), (1, 1)), (10, 4; (3, 3, 3), (1, 1, 1))\}$ up to symmetry.

For configuration $(10, 4; (3, 3, 3), (1, 1, 1))$ up to symmetry, as $\delta_c = 3 > 2 = \delta_c^S$ one vertex of U_c must be flipped. The choice of such a vertex and color already determine the extremal configuration. Hence $\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b}) \leq 3k$ holds.

For the other configurations, $\delta_c = 2$ so the only non-zero contributions are the ones related to $\mathcal{B}_1$ and $\mathcal{B}_3$. Sets in $\mathcal{T}_1$ do not depend on the extremal configuration we are moving to. More precisely, once fixed the vertex $w \in U_c^S \setminus U_c$, the Kempe component $S_\sigma(w, c)$ already determine the extremal configuration which the flip yields. Hence the contribution Δp_2 is tight without conditioning on the extremal configuration.

For the contribution of $\mathcal{B}_3$ we have the following. Without loss of generality assume we have configurations $(8, 3; (4, 3), (1, 1)), (9, 3; (5, 3), (1, 1))$. Then $|S_\tau(u_1, \sigma(v))| \geq 4$. Let $N_1 = N(u_1) \cap S_\tau(u_1, \sigma(v))$. Notice that for $|N_1| \geq 2$ the extremal configuration $(3, 7; (1, 1), (3, 3))$ can not be achieved (see Figure 7.13). This is due to the fact that the Kempe component should flip vertices in N_1 colored $\sigma(v)$ to $\tau(v)$, and the resulting coloring would have $|S_{\sigma_S}(u_1, \tau(v))| \geq 4$, which is not possible for a extremal configuration.

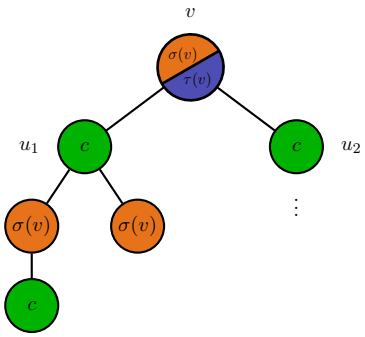

Figure 7.13: Case $|N_1| \geq 2$: Flipping neighbours of u_1 and u_2 different than v to color $\tau(v)$ do not yield to extremality

Now, let $|N| = 1$, $N = \{w\}$, and consider $M = N(w) \cap S_\tau(u_1, \sigma(v)) \setminus \{u_1\}$. If $|M| \geq 2$ it is not possible to move to extremal configuration $(3, 7; (1, 1), (3, 3))$ because we should flip vertices colored $c, \sigma(v), \tau(v)$, as shown in Figure 7.14.

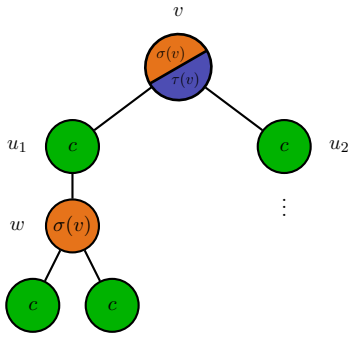

Figure 7.14: Case $|N| = 1, |M| > 2$ can not yield to the extremal configuration $(3, 7; (1, 1), (3, 3))$, because we should flip vertex w, colored $\sigma(v)$ to color $\tau(v)$ and this flip do not yield to extremality as $|S_{\sigma_S}(u_1, \tau(v))| \geq 4$.

Case $|M| = 1$, $M = \{m\}$, is the only case in which we can get to both extremal configurations. In order to get configuration $(7, 3; (3, 3), (1, 1))$, fix $z \in N(m) \cap S_\sigma(v, c) \setminus \{w\}$. The Kempe component flipped must be $S_\sigma(z, c')$ for $c' \in [k]$. Hence there are k options. And in order to reach configuration $(3, 7; (1, 1), (3, 3))$ the Kempe component is unique, in particular it is $S_\sigma(w, \tau(v))$. Hence the contribution is at most p_1. Adding both values we get a bound of $k + p_1$ and taking into account the contribution of $\mathcal{B}_1, \mathcal{B}_3$, we get that $\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b}) \leq k + p_1 + \Delta p_2 < 3k + \Delta p_2$.

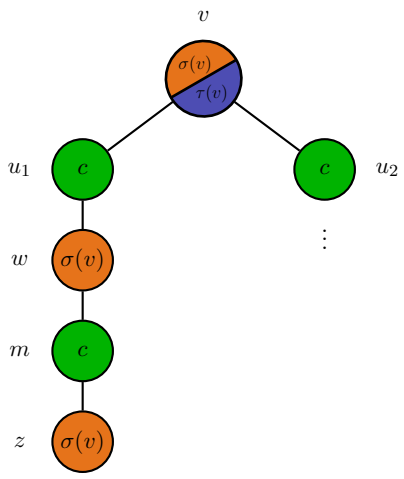

Figure 7.15: Only if $|N| = 1, |M| = 1$, we can move to both extremal configurations

Claim 2: Configurations in $\mathcal{H}$ satisfy $\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b}) \leq \Delta$.

Proof of claim 2: Configurations $(4, 2; (3), (1)), (3, 3, (2), (2))$ satisfy $\delta_c = 1$, so the only non-zero $\mathcal{B}_j$ for $j \in \{1, 2, 3\}$ is $\mathcal{B}_1$. Moreover only one extremal configuration can be achieved, otherwise the Kempe component should flip colors $\sigma(v), \tau(v)$ and c. So $\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b}) \leq \Delta$. For the other 2 configurations, $(5, 3; (2, 2), (1, 1))$ and $(4, 4; (2, 1), (1, 2))$ satisfy $\delta_c = 2$ so $\mathcal{B}_2 = 0$ and $\mathcal{B}_1 = \Delta p_2$. Moreover $\mathcal{B}_3^+ = 0$ due to the fact that these two configurations satisfy $x_i \leq 2$ for any i. Hence for any Kempe component S there exists x_j such that $x_j < x_j^S = x_j^* = 3$ so $\mathcal{T}_3^+ = \emptyset$. Finally $\mathcal{B}_3^- = 2\Delta p_2$, where the last term is multiplied by p_2 due to the fact that at least 2 vertices have to be flipped. Again and due to the same reason it is only possible to move to one 2-extremal configuration. Therefore the bound is $\mathcal{A}_2(A, B; \mathbf{a}, \mathbf{b}) \leq 3\Delta p_2 \leq \Delta$ as $p_2 < 1/3$.

Claim 3: The only configuration that can move to both 2-extremal configurations with flips of size 1 is $(5, 5; (3, 1), (1, 3))$.

Proof of claim 3: If the configuration can move to both 2-extremal configurations with flips of size 1, it must only differ in one vertex with respect to each 2-extremal configuration. Hence $(5, 5; (3, 1), (1, 3))$, shown in Figure 7.16, is the only possibility.

Moreover, once fixed the extremal configuration, configuration $(5, 5; (3, 1), (1, 3))$ can only move to that extremal configuration with a unique Kempe flip. Hence the contribution is $\mathcal{A}_2(5, 5; (3, 1), (1, 3)) \leq p_1 + p_1 = 2$.

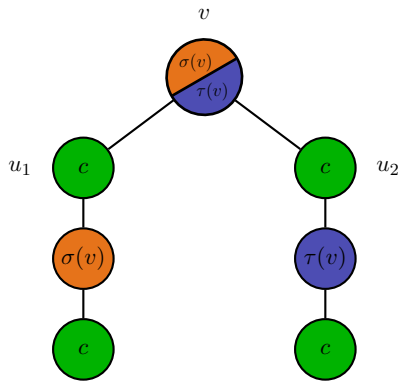

Figure 7.16: Configuration $(5,5;(3,1),(1,3))$ is the unique configuration that can move to both 2-extremal configurations with flips of size 1. Moreover the representation that admits it, is unique (only as a rooted tree with 2 leaves)

Finally, Claims 1, 2 and 3 imply that for $(A,B;\mathbf{a},\mathbf{b}) \notin \mathcal{G}\cup\mathcal{H}\cup(5,5;(3,1),(1,3))$, the bound $\mathcal{A}_2(A,B;\mathbf{a},\mathbf{b})\Big|_{(A^S,B^S;\mathbf{a}^S,\mathbf{b}^S)} \leq (\frac{4}{3}k+\Delta p_2)$ is only tight for one of the two extremal configurations. For the other, the Kempe component flipped S has size $|S|\geq 2$ so we can multiply its contribution by p_2.

We get that for $(A,B;\mathbf{a},\mathbf{b}) \notin \mathcal{G}\cup\mathcal{H}\cup(5,5;(3,1),(1,3))$ the bound is $\mathcal{A}_2(A,B;\mathbf{a},\mathbf{b}) \leq \mathcal{A}_2(A,B;\mathbf{a},\mathbf{b})\Big|_{(A^S,B^S;\mathbf{a}^S,\mathbf{b}^S)} \cdot(p_1+p_2) \leq (\frac{4}{3}k+\Delta p_2)\cdot(1+p_2) < 2k$, where we have used that $p_2 = 185/616$. □

Corollary 7.9 If $c \notin C_{\sigma,\tau}(v)$, then

$$\overline{\nabla_B}(\sigma,\tau,c,\overline{\mathcal{D}}) \leq \max\left\{\left(\frac{2k}{\Delta}+p_2\right)\eta 1+2\eta_2,\left(\frac{2k}{\Delta}p_3\right)\eta_1+2\left(\frac{3k}{\Delta}+p_2\right)\eta_2,\left(\frac{4/3k}{\Delta}\right)\eta_1+2\left(\frac{2k}{\Delta}\right)\eta_2\right\}$$

Proof. Recall definition of $\overline{\nabla_B}(\sigma,\tau,c,\overline{\mathcal{D}})$ in (20) and let $(A,B;\mathbf{a},\mathbf{b}) \notin \Pi$, hence the color associated to this configuration c, satisfies $c \notin C_{\sigma,\tau}(v)$. Notice that for $i\in\{1,2\}$, $\xi^i_{\sigma,\tau}(v,c,S)\neq 0$ if and only if $S\in\mathcal{R}_i(A,B;\mathbf{a},\mathbf{b})$, the set of Kempe components whose flips yields to an i-extremal configuration. In particular:

$$\overline{\nabla_B}(\sigma,\tau,c,\overline{\mathcal{D}}) = \max_{(A,B;\mathbf{a},\mathbf{b})\notin\Pi}\frac{\mathcal{A}_1(A,B;\mathbf{a},\mathbf{b})\cdot\xi^1\cdot\eta_1}{\Delta}+\frac{\mathcal{A}_2(A,B;\mathbf{a},\mathbf{b})\cdot\xi^2\cdot\eta_2}{\Delta}$$

Moreover in this case $\xi^i_{\sigma,\tau}(v,c,S)=i$, so:

$$\overline{\nabla_B}(\sigma,\tau,c,\overline{\mathcal{D}}) = \max_{(A,B;\mathbf{a},\mathbf{b})\notin\Pi}\frac{\mathcal{A}_1(A,B;\mathbf{a},\mathbf{b})\cdot\eta_1}{\Delta}+2\cdot\frac{\mathcal{A}_2(A,B;\mathbf{a},\mathbf{b})\cdot\eta_2}{\Delta}$$

Considering the values of $\mathcal{A}_1(A,B;\mathbf{a},\mathbf{b}),\mathcal{A}_2(A,B;\mathbf{a},\mathbf{b})$ we obtain the desired bound. □

Chapter 8

Main result

We now show that the coupling with the metric d defined in section 6.2 contracts in expectation and the proof of the main result of our work. Again, we assume that $k \geq \frac{161}{88}\Delta$.

Theorem 8.1 For the flip parameters $\mathbf{p}$ given in Observation 6.1 there exists $\mu > 0$ such that for every $k > (\frac{11}{6} - \varepsilon_0)\Delta$, with $\varepsilon_0 = \frac{1}{1320}$, and every neighboring coloring pair (σ, τ), the greedy coupling satisfies $\nabla(\sigma, \tau) \leq -\mu k$ for sufficiently large Δ.

Proof. Recall that $\delta = \frac{11}{6} - \frac{161}{88} = \frac{1}{264}$ and set $\eta_1 = 2.85\eta_2$ and $\eta_2 = \frac{\delta\Delta}{13.5k - 5.7\Delta}$.

Notice that from Corollary 7.9, fixing $\eta_1 = 2.85\eta_2$, we obtain that for $c \notin C_{\sigma,\tau}(v)$, then

$$\overline{\nabla_B}(\sigma, \tau, c, \overline{\mathcal{D}}) \leq \frac{4k}{\Delta}\left(\frac{\eta_1}{3} + \eta_2\right) = \frac{7.8k \cdot \eta_2}{\Delta}$$

Using this result together with (12), Theorem 7.1 and Lemma 7.4 we get

$$\nabla(\sigma, \tau) \leq \left[\frac{11}{6} - \left(\frac{2\eta_1(k - \Delta - 2)}{\Delta}\right)\gamma^1_{\sigma,\tau}(v) - \left(\frac{12\eta_2(k - \Delta - 2)}{\Delta} + k\frac{(\eta_1 - 2\eta_2)}{3\Delta}\right)\frac{\gamma^2_{\sigma,\tau}(v)}{2} - \right.$$
$$\left. - \left(\delta - \frac{7.8k\eta_2}{\Delta}\right)(1 - \gamma_{\sigma,\tau}(v))\right]\Delta - k$$

We would like to bound the above expression for any possible value of $\gamma^i_{\sigma,\tau}(v)$. The above bound is maximized when the following expression is minimized:

$$\left(\frac{2\eta_1(k - \Delta - 2)}{\Delta}\right)\gamma^1_{\sigma,\tau}(v) + \left(\frac{12\eta_2(k - \Delta - 2)}{\Delta} + k\frac{(\eta_1 - 2\eta_2)}{3\Delta}\right)\frac{\gamma^2_{\sigma,\tau}(v)}{2} + \left(\delta - \frac{7.8k\eta_2}{\Delta}\right)(1 - \gamma_{\sigma,\tau}(v))$$

Recall that $\gamma_{\sigma,\tau}(v), \gamma^i_{\sigma,\tau}(v) \in [0, 1]$, for $i = 1, 2$, and that $\gamma_{\sigma,\tau}(v) = \gamma^1_{\sigma,\tau}(v) + \gamma^2_{\sigma,\tau}(v)$. Hence, the above expression is a linear convex combination of the function evaluated in $\gamma^i_{\sigma,\tau}(v)$ in the extremal points. Due to convexity the minimum corresponds to some extremal point $(\gamma^1_{\sigma,\tau}(v), \gamma^2_{\sigma,\tau}(v)) \in \{(0, 0), (0, 1), (1, 0)\}$.

Also note that $\varepsilon_0 = \frac{\delta}{5}$ and as $k > (\frac{11}{6} - \varepsilon_0)\Delta = (\frac{11}{6} - \frac{\delta}{5})\Delta$, there exists some small constant $\mu > 0$ such that $(\frac{11}{6} - \frac{\delta}{5})\Delta \leq k - \mu k$. It follows from straightforward computations that for sufficiently large Δ:

$$\nabla(\sigma, \tau) \leq \left(\frac{11}{6} - \frac{\delta}{5}\right)\Delta - k \leq -\mu k$$

□

We proceed with the proof of our main result:

Proof of Theorem 1.4. By Theorem 8.1, for the flip probabilities $\mathbf{p}$ there exist $\varepsilon_0 = \frac{1}{1320}, \mu > 0$ such that if $k \geq (11/6 - \varepsilon_0)\Delta$, then the greedy coupling $(\sigma, \tau) \longrightarrow (\sigma', \tau')$ defined on neighbouring coloring pairs (σ, τ) satisfies

$$\nabla(\sigma, \tau) = nk\mathbb{E}[d(\sigma', \tau') - d(\sigma, \tau)] \leq -\mu k$$

In particular, as $d(\sigma, \tau) \leq 1$ for (σ, τ) a neighbouring coloring pair:

$$\mathbb{E}[d(\sigma', \tau')] \leq d(\sigma, \tau) - \frac{\mu}{n} \leq \left(1 - \frac{\mu}{n}\right) d(\sigma, \tau)$$

The coupling defined in the set of neighbouring coloring pairs is then contractive with respect to the metric d, where $\mu > 0$ is a constant. Due to the Path Coupling Lemma (Lemma 4.3), the flip dynamics mixes in time

$$\tau_{mix} = O\left(\frac{n}{\mu} \log n\right) = O(n \log n)$$

□

Chapter 9

Relation between flip and Glauber dynamics

In the previous chapters we have studied different arguments to prove rapid mixing of the flip dynamics. In this chapter, we prove that, once proved rapid mixing of the flip dynamics under some conditions on k and Δ, the Glauber dynamics mixes under the same conditions in time $O(n \cdot \tau_{flip})$. We prove it using the comparison technique described by Diaconis and Saloff-Coste [6], which relates the eigenvalues of the transition matrices of two Markov chains. Moreover, the second eigenvalue is related to the mixing time of the Markov chains (see [7], [14]). These two results allow to derive an inequality relating the mixing time of both chains, which is the proposition we will use, see [21].

The result is strongly connected to the study of the underlying graph of both chains. Recall the setting of the two Markov Chains. Glauber and flip dynamics have the same state space Ω, the space of proper k-colorings, and the same stationary distribution π, which is uniform on Ω. If P is the transition matrix of a Markov Chain then the underlying graph associated to the dynamic is $G = (\Omega, E(P))$ where $E(P) = \{(\sigma, \tau) : P(\sigma, \tau) > 0\}$. As the chains are symmetric, the underlying graphs of the flip and the Glauber dynamics, G_{flip} and G_{GD} respectively, are undirected.

We begin with some definitions. For each move $(\sigma, \tau) \in E(P_{\text{flip}})$ we define associated paths of moves in $E(P_{GD})$. Instead of defining a single one, we define a set of fractional paths called a flow. More precisely let γ denote a path $(\eta_0, \eta_2, ..., \eta_k)$ where each $(\eta_i, \eta_{i+1}) \in E(P_{GD})$ and with length $|\gamma| = k$. For each $(\sigma, \tau) \in E(P_{\text{flip}})$ let $\Gamma_{\sigma,\tau} = \{\gamma : \eta_0 = \sigma, \eta_k = \tau\}$ be the set of paths from σ to τ.

A flow is a set of functions $f = f_{\sigma,\tau} : \Gamma_{\sigma,\tau} \longrightarrow \mathbb{R}^+$ satisfying that $\sum_{\gamma \in \Gamma_{\sigma,\tau}} f(\gamma) = 1$.

The idea is to simulate a transition of the flip dynamics using several Glauber transitions, in such a way that the number of paths traversing any particular Glauber edge is minimized. In particular, the goal is to define flows minimizing $A_{\eta,\xi}$ defined as

$$A_{\eta,\xi} := \frac{1}{P_{GD}(\eta, \xi)} \sum_{\gamma \in \Gamma_{\sigma,\tau} : (\eta,\xi) \in \gamma} |\gamma| f(\gamma) P_{\text{flip}}(\sigma, \tau)$$

Observe that $P_{GD}(\eta, \xi) \geq 1/nk$ while $P_{\text{flip}}(\sigma, \tau) \leq 1/nk$. In addition we will define flows such that $f(\gamma) = 0$ for $|\gamma| \geq 7$ which follows from the fact that the flip dynamics do not flip

Kempe components of size greater than 6. Hence, the quantity $A_{\eta,\xi}$ is simplified to

$$A_{\eta,\xi} \leq 6 \sum_{\gamma \in \Gamma_{\sigma,\tau}:(\eta,\xi)\in\gamma} f(\gamma) \tag{21}$$

And we will be interested in the maximum of $A_{\eta,\xi}$ over all edges that we will denote by A^*:

$$A^* = \max_{(\eta,\xi)\in E(P_{GD})} A_{\eta,\xi}$$

In particular we will use Diaconis and Saloff-Coste result to bound the mixing time of the Glauber dynamics in terms of this quantity A^* and the mixing time of the flip dynamics. We use the version described in [21].

Theorem 9.1

$$\tau_{GD} = O(A^* \tau_{flip} \log |\Omega|)$$

Now we apply Theorem 9.1 to proof Theorem 1.5.

Proof of Theorem 1.5. Since $|\Omega| \leq k^n$, $\log(|\Omega|) \leq n \log k$ and it suffices to define a flow such that $A^* = O(1)$ in order to proof Theorem 1.5 from Theorem 9.1.
From (21) we want to upper bound $\sum_{\gamma \in \Gamma_{\sigma,\tau}:(\eta,\xi)\in\gamma} f(\gamma)$ for any possible edge (η, ξ).
Let (σ, τ) be an edge of P_{flip}. The move from σ to τ interchanges colors c, c' on a cluster $S = T \cup T'$ with $\sigma(v) = c$ for all $v \in T$ and $\sigma(v) = c'$ for all $v' \in T'$. A natural way to simulate this flip using several Glauber flips is the following: first recolor each vertex in T to an arbitrary color, then recolor each vertex in T' to color c and finally recolor each vertex in T to color c'.

The arbitrary color used in the first step to recolor $v \in T$ can be chosen among the set of available colors of v, namely from the set $A_v = A_v(\sigma) = [k] \setminus \{\sigma(v) \bigcup_{w\in N(v)} \sigma(w)\}$.

Now let

$$\psi = \{\psi_1, ..., \psi_{|T|}\}$$

be such that $\psi_i(v_i) \in A_{v_i}$ for each $v_i \in T$. And denote the set of all ψ to be $\Psi_{\sigma,\tau}$. If we fix an ordering of the vertices of G, then each set ψ defines a canonical path γ_ψ as follows:

Stage 1: In order, consider each $v \in T$ and recolor it to $\psi(v)$.
Stage 2: In order, recolor each vertex $v \in T'$ to color c.
Stage 3: In order, recolor each vertex $v \in T$ to color c'.

As we do not want to increase the flow in any particular edge we define the flow such that it is distributed evenly among all possible paths γ_ψ:

$$f(\gamma_\psi) := \frac{1}{|\Psi_{\sigma\tau}|}$$

First we upper bound $f(\gamma_\psi)$. Notice that $A_v \geq k - \Delta$ which is $\Omega(k)$ due to the fact that $k > (\frac{11}{6} - \varepsilon_0)\Delta$. Therefore $|\Psi_{\sigma\tau}| = \Omega(k^{|T|})$ and

$$f(\gamma_\psi) = O(k^{-|T|})$$

Then we upper bound the number of paths that traverse any particular edge. We partition such paths in terms of the size of the associated set T. Let

$$R_i(\eta,\xi) := \{\gamma_\psi : (\eta,\xi) \in \gamma_\psi, \psi \in \Psi_{\sigma,\tau}, |T| = i\}$$

With this definition,

$$A_{\eta,\xi} \leq K_2 \sum_i \frac{|R_i(\eta,\xi)|}{k^i} \tag{22}$$

So our aim is to compute $|R_i(\eta,\xi)|$ and hence to count the number of paths traversing any particular edge (η,ξ), and having $|T| = i$. Notice that a specific path γ is uniquely determined by the sets of vertices T, T', colors c, c', set of colors ψ as well as the colors $\sigma(x)$ for any $x \notin S$. From the coloring η, the values of $\sigma(x)$ for all $x \notin S$ are already known. Now, suppose that move $\eta \longrightarrow \xi$ recolors vertex $v \in V$. We divide our analysis of $|R_i(\eta,\xi)|$ considering the stage in which we traverse edge (η,ξ):

Stage 2: In this case notice that $c = \xi(v)$ and $c' = \eta(v)$. We also know that $v \in T'$. Cluster $S = T \cup T'$ satisfies that $|S| \leq 6$ so the number of such clusters containing v is at most Δ^5. Since all vertices of T' have color c or c' in η, given a candidate set T the corresponding set T' is fixed (T' is the set of vertices colored c, c' adjacent to some vertex of T). Hence the set T is the only variable and as $|T| = i$, there are at most $O(\Delta^i)$ choices for T. Moreover, once T is chosen, colors ψ are fixed; more precisely $\psi(v) = \eta(v)$ for $v \in T$. Therefore, assuming edge (η,ξ) is traversed during stage 2 of the path, then $|R_i(\eta,\xi)| = O(k^i)$.

Stage 1: In this case $v \in T$, $c = \eta(v)$ and $\psi(v) = \xi(v)$. We do not know the value of c', hence there are at most k possible choices for it. Now, consider the sets T_1, T_2 in $T \setminus \{v\}$ with T_1 the vertices in T that have already been colored and T_2 the vertices in T that have not been recolored. Again, and due to the same argument as before, there are at most $O(\Delta^{|T_1|})$ choices for the vertices in T_1 and for each $w \in T_1$ we know $\psi(w) = \eta(w)$. Moreover, for a specific T_1 vertices in T_2 and T' are uniquely determined: neighbours of vertices in T_1 colored c and c' respectively. The only thing that remains is the choice of colors ψ for the vertices of T_2. And for T_2 there are $O(k^{|T_2|})$ choices for the associated colors ψ. Combining the choices for color c' and sets T_1 and ψ we get $|R_i(\eta,\xi)| = O(k^{1+|T_2|}\Delta^{|T_1|}) = O(k^i)$.

Stage 3: Symmetrical to stage 1.

So, adding all the contributions we have that the total number of paths traversing edge (η,ξ) and satisfying $|T| = i$ is $|R_i(\eta,\xi)| = O(k^i)$. Combining with (22) we get that $A^* = O(1)$ and this ends the proof of Theorem 1.5.

□

Chapter 10

Random sampling and approximate counting

In the previous chapters we studied Markov chains in order to obtain efficient random samplers, namely fully polynomial almost uniform samplers (FPAUS). We have studied two dynamics; Glauber and flip, and the relation between them.

Random sampling is closely related to approximate counting. In 1986, Jerrum, Valiant, and Vazirani [15] proved the equivalence between approximate counting and approximate sampling for self-reducible problems. Although we won't define the concept of self-reducibility, we will follow the proof in Levin-Peres book [17] to prove the reduction from approximate counting to approximate sampling in the case of colorings.

In this way, one efficient algorithm for sampling a coloring at random (FPAUS) yields an efficient approximation algorithm for counting the number of colorings of a graph (FPRAS).

Theorem 10.1 Let G be a graph on n vertices and $k \in \mathbb{N}$.

If the Glauber dynamics mixes rapidly on the set of k-colorings of G, then there exists an FPRAS for estimating the number of k-colorings of G.

More precisely, let τ_{mix} be the mixing time of the Glauber dynamics, which is polynomial in n. Given parameters η, ε, there exists a random variable W which can be simulated in time $C_{\eta,\varepsilon} \cdot n \cdot \tau_{mix}$ such that

$$P\left\{\frac{(1-\varepsilon)}{|\Omega|} \leq W \leq \frac{(1+\varepsilon)}{|\Omega|}\right\} \geq 1-\eta$$

where $C_{\eta,\varepsilon}$ is a constant that depends on η, ε.

In particular, $\frac{1}{W}$ approximates $|\Omega|$, the number of colorings of G.

Proof. Let σ_0 be a k-proper coloring of G. Enumerate the vertices of G as $\{v_1, v_2, ..., v_n\}$ and define for $j = 0, ..., n$

$$\Omega_j := \{\sigma \in \Omega : \sigma(v_i) = \sigma_0(v_i) \text{ for } i > j\}$$

The elements of Ω_j have j free vertices, and $n-j$ vertices colored as in σ_0. A random element of Ω_j can be generated using a slight modification of the Glauber dynamics. Basically, only the colors of vertices $\{v_1, ..., v_j\}$ can be updated so the bound on the mixing time still holds

with j replacing n. Moreover the stationary distribution is the uniform distribution in Ω_j, and we will denote it by π_j.

We run the Glauber dynamics in Ω_j and we have that it converges to the uniform distribution π_j in polynomial time in the number of vertices. Therefore for $T := \tau_{mix}(\frac{\varepsilon}{6nke})$ we have that

$$d_{TV}(P^T(\sigma_0), \pi_j) = \|P^T(\sigma_0, \cdot) - \pi_j(\cdot)\|_{TV} \leq \frac{\varepsilon}{6kn} \tag{23}$$

We will approximate the ratio $\frac{|\Omega_{j-1}|}{|\Omega_j|}$. A random element of Ω_j can be generated by running the Markov chain for T steps. We compute $a_n := \lceil \frac{27kn}{\eta\varepsilon^2} \rceil$ elements of Ω_j. Denote by S_j the sample obtained.

Let σ_j^i be the i-th sample of S_j and let Z_j^i be the indicator random variable that the i-th sample of S_j is also an element of Ω_{j-1}, i.e., if $\sigma_j^i(v_j) = \sigma_0(v_j)$. Due to (23):

$$\left|\mathbb{E}(Z_j^i) - \pi_j(\Omega_{j-1})\right| = \left|P^T(\sigma_0, \Omega_{j-1}) - \pi_j(\Omega_{j-1})\right| \leq \frac{\varepsilon}{6kn}$$

Define $W_j := \frac{1}{a_n}\sum_{i=1}^{a_n} Z_j^i$, which corresponds to the proportion of elements in S_j that belong to Ω_{j-1}. We see that W_j approximates $\frac{|\Omega_{j-1}|}{|\Omega_j|}$:

$$\left|\mathbb{E}(W_j) - \frac{|\Omega_{j-1}|}{|\Omega_j|}\right| = \left|\frac{1}{a_n}\cdot\sum_{i=1}^{a_n}\mathbb{E}(Z_j^i) - \pi_j(\Omega_{j-1})\right| \leq \frac{1}{a_n}\cdot\sum_{i=1}^{a_n}|\mathbb{E}(Z_j^i) - \pi_j(\Omega_{j-1})| \leq \frac{\varepsilon}{6kn} \tag{24}$$

Hence,

$$\frac{|\Omega_{j-1}|}{|\Omega_j|} - \frac{\varepsilon}{6kn} \leq \mathbb{E}(W_j) \leq \frac{|\Omega_{j-1}|}{|\Omega_j|} + \frac{\varepsilon}{6kn}$$

Dividing by $\frac{|\Omega_{j-1}|}{|\Omega_j|}$ and taking into account that $\frac{|\Omega_{j-1}|}{|\Omega_j|} \geq \frac{1}{k}$ we get:

$$1 - \frac{\varepsilon}{6n} \leq \mathbb{E}(W_j)\cdot\frac{|\Omega_j|}{|\Omega_{j-1}|} \leq 1 + \frac{\varepsilon}{6n}$$

Let $W := \prod_{i=1}^n W_i$. Notice that the $\{W_j\}$ are independent and that $|\Omega| = |\Omega_n| = \frac{|\Omega_n|}{|\Omega_0|}$ because $\Omega_0 = \{\sigma_0\}$. Then, multiplying the above inequality for all terms W_i, $i \in [n]$, we get:

$$1 - \frac{\varepsilon}{6} \leq \left(1 - \frac{\varepsilon}{6n}\right)^n \leq \mathbb{E}(W)\cdot\frac{|\Omega_n|}{|\Omega_0|} \leq \left(1 + \frac{\varepsilon}{6n}\right)^n \leq e^{\frac{\varepsilon}{6}} \leq 1 + \frac{\varepsilon}{3} \tag{25}$$

where we have applied that $e^x \leq 1 + 2x$ for $x \in [0, 1]$ and $(1-x)^n \geq 1 - nx$. In particular

$$\left|\mathbb{E}(W) - \frac{1}{|\Omega|}\right| \leq \frac{\varepsilon}{3|\Omega|} \tag{26}$$

We now show that W is concentrated around this value.

First, we compute $\mathrm{Var}(W_j)$. Notice that Z_j^i is a indicator random variable so it is non-negative, $\mathbb{E}((Z_j^i)^2) = \mathbb{E}(Z_j^i)$ and $\mathbb{E}(Z_j^i)$ is equal for all i, which gives that $\mathbb{E}(W_j) = \mathbb{E}(Z_j^i)$. Moreover they are independent. Taking into account these properties we have

$$\mathrm{Var}(W_j) = \frac{1}{a_n^2}\sum_{i=1}^{a_n}(\mathbb{E}(Z_j^i) - (\mathbb{E}(Z_j^i))^2) \leq \frac{1}{a_n^2}\sum_{i=1}^{a_n}\mathbb{E}(Z_j^i) = \frac{\mathbb{E}(Z_j^i)}{a_n} = \frac{\mathbb{E}(W_j)}{a_n}$$

Dividing both sides of the inequality by $\mathbb{E}(W_j)^2$ we get

$$\frac{\mathrm{Var}(W_j)}{\mathbb{E}(W_j)^2} \leq \frac{1}{a_n \mathbb{E}(W_j)}$$

Since $\frac{|\Omega_{j-1}|}{|\Omega_j|} \geq \frac{1}{k}$, and from equation (24) we get that:

$$\mathbb{E}(W_j) \geq \frac{1}{k} - \frac{\varepsilon}{6kn} \geq \frac{1}{3k}$$

So the two previous inequalities give:

$$\frac{\mathrm{Var}(W_j)}{\mathbb{E}(W_j)^2} \leq \frac{1}{a_n \mathbb{E}(W_j)} \leq \frac{3k}{a_n} \tag{27}$$

Also due to the independence of the random variables W_i:

$$\mathbb{E}\left(\frac{W}{\mathbb{E}(W)}\right)^2 = \mathbb{E}\left[\prod_{i=1}^{n}\left(\frac{W_i}{\mathbb{E}(W_i)}\right)^2\right] = \prod_{i=1}^{n}\frac{\mathbb{E}(W_i^2)}{\mathbb{E}(W_i)^2}$$

Substracting 1 from both sides shows that:

$$\frac{\mathrm{Var}\ W}{\mathbb{E}(W)^2} = \prod_{i=1}^{n}\left[1 + \frac{\mathrm{Var}\ (W_i)}{\mathbb{E}(W_i)^2}\right] - 1$$

Then

$$\frac{\mathrm{Var}(W)}{\mathbb{E}(W)^2} \leq \prod_{i=1}^{n}\left[1 + \frac{3k}{a_n}\right] - 1 = \prod_{i=1}^{n}\left[1 + \frac{\eta\varepsilon^2}{9n}\right] - 1 \leq e^{\frac{\eta\varepsilon^2}{9}} - 1 \leq \frac{2\eta\varepsilon^2}{9} \tag{28}$$

where we have applied the same inequalities as in (25).

Applying Chebyshev's inequality to the random variable W and inequality (28)

$$P\left\{|W - \mathbb{E}(W)| \geq \mathbb{E}(W) \cdot \frac{\varepsilon}{2}\right\} \leq \eta$$

If the event $|W - \mathbb{E}(W)| < \mathbb{E}(W) \cdot \frac{\varepsilon}{2}$ is satisfied, then using (26) and the triangle inequality

$$\left|W - \frac{1}{|\Omega|}\right| \leq |W - \mathbb{E}(W)| + \left|\mathbb{E}(W) - \frac{1}{|\Omega|}\right| \leq \mathbb{E}(W) \cdot \frac{\varepsilon}{2} + \frac{\varepsilon}{3|\Omega|} \leq \frac{\varepsilon}{|\Omega|} \tag{29}$$

Hence

$$P\left\{\left|W - \frac{1}{|\Omega|}\right| \leq \frac{\varepsilon}{|\Omega|}\right\} \geq 1 - \eta$$

Finally, for each of the n variables W_i, $i = 1, ..., n$ we need to simulate each of the a_n chains for T steps. The total time needed is

$$T \cdot a_n = C_{\eta,\varepsilon} \cdot n \cdot \tau_{mix}$$

which is polynomial in n due to the fact that the Glauber dynamics mixes rapidly. □

As Theorem 1.5 states that the Glauber dynamics mixes rapidly for $k > (11/6 - \varepsilon_0)\Delta$ we obtain the following corollary:

Corollary 10.2 Let G be a graph and Δ the maximum vertex degree of G. Then there exists an FPRAS for computing the number of k-colorings of G for $k > (11/6 - \varepsilon_0)\Delta$ with ε_0 given in Theorem 1.4.

Chapter 11

Conclusions

Following the idea introduced by Delcourt, Perarnau and Postle [5], in this thesis we describe an alternative metric for Vigoda's greedy coupling. The motivation is given by Theorem 5.9 which states that for $k < \frac{11}{6}\Delta$ there is not any one-step coupling contractive under the Hamming distance.

The new metric takes into account the presence of extremal configurations in the colorings, which avoid rapid mixing of the chain beyond the value $11/6$. More precisely, the new metric gives more weight to neighboring coloring pairs having extremal configurations. This makes the expected variation distance decrease in these cases and allows to prove rapid mixing under weaker restrictions.

In their paper, Chen, Perarnau et al. [3] defined a metric d that took into account the presence of 1-extremal and 2-extremal configurations together.

The first modification is that our metric d considers the contribution of 1-extremal and 2-extremal configurations separately and with different weights η_1 and η_2.

Moreover, in this thesis we have introduced some improvements in the study of the expected variation in d_B for flips of Kempe components $S \in \overline{\mathcal{D}}$, not involving vertex v. We have taken into account the size of the Kempe components flipped and hence the probability that they are flipped. And we have done a tighter analysis on the number of sets that allow moving within the classes of extremal and non-extremal configurations. As it is harder to destroy a 1-extremal than a 2-extremal configuration and the contribution of movements from 2-extremal configurations to 1-extremal configurations is small, the metric penalises more the presence of 1-extremal configurations. In the definition of the metric this corresponds to a larger value of η_1 than η_2.

The last refinement corresponds to Proposition 7.2. This proposition studies the expected variation in d_B for flips of Kempe components $S \in \mathcal{D}_c$, in particular flips involving vertex v. As the Kempe component flips at most 6 vertices, the proportion of extremal configurations before and after the flip do not differ a lot, and hence the variation in d_B is small. The proposition proves that this variation is constant, while in the previous paper this was upper bounded by $(k + \Delta)$.

Recall that for non-extremal configurations Proposition 6.2 already tell us that using this metric $k \geq \frac{161}{88}\Delta$. Hence using the technique considered in this thesis, the improvement could be at most $\delta\Delta$ for $\delta = \frac{11}{6} - \frac{161}{88}$.

The modifications described above yield Theorem 1.4, 1.5, which say that the flip and the

Glauber dynamics are rapidly mixing for $k > (\frac{11}{6} - \frac{\delta}{5})\Delta = (\frac{11}{6} - \frac{1}{1320})\Delta$ while the previous result gave rapid mixing for $k > (\frac{11}{6} - \frac{\delta}{318})\Delta = (\frac{11}{6} - \frac{1}{84000})\Delta$.

There are several ways in which it is possible to continue the work of this master thesis.

One option would be to increase the optimum value $\frac{11}{6}$ to $\frac{11}{6} + \varepsilon$ and describe the extremal configurations for this new optimum. If the suboptimum value was less than $\frac{161}{88}$, we could get a better bound on rapid mixing.

Another option would be to describe the tight configurations for the value $\frac{161}{88}$, which we will call *pseudo-extremal* configurations, and consider them in the description of the metric. However, the analysis would be quite tough due to the fact that we should study all the transitions, not only between extremal and non-extremal configurations, but also between them and pseudo-extremal configurations.

We could also modify the Markov chain used. For instance we could consider flips of 3-colored-cluster components. In this case the difficulty yields in the description of the coupling.

And finally, we could focus on deterministic algorithms. An open question is whether there exist an FPTAS for counting colorings provided $k > (2 - \varepsilon)\Delta$.

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Appendix: Code

Matlab code for solving LP1

```
%LINEAR PROGRAM, minimizes f(x) st. M*x<=t, Aeq*x=beq, lb<=x<=
    ub

M = [];
k = 7;
%inc=number of variables: k variables p_i and lambda
inc = k+1;
%sol_Vigoda = [1; 13/42; 1/6; 2/21; 1/21; 1/84; 0; 11/6];

%DELTA = 1
for i=1:k
    for j=i:k
        eq = zeros(1,inc);
        eq(1,i) = i;
        eq(1,i+1) = -i;
        eq(1,j) = eq(1,j) + j-1;
        eq(1,j+1) =  eq(1,j+1)-(j-1);
        eq(1,inc) = -1;
        M = [M;eq];
    end
end

%DELTA = 2
for i=1:k
    eq = zeros(1,inc);
    eq(1,1)=2;
    eq(1,i)=2*(i-1);
    if (2*i+1 <= k)
        eq(1,2*i+1)=1;
    end
    eq(1,inc) = -2;
    M = [M;eq];
end
```

```
33
34 %Case c=sigma(v), tau(v)
35 for b2=1:6
36     for b1=1:6-b2
37         B=b1+b2;
38         eq = zeros(1,inc);
39         eq(1,B) = (B-b2);
40         eq(1,b1) = b1;
41         eq(1,inc) = -2;
42         M = [M;eq];
43     end
44 end
45
46 [s1,s2] = size(M);
47 t1 = -1 * ones(s1,1);
48
49 %p_i's are decreasing
50 for i=1:k-1
51     eq = zeros(1,inc);
52     eq(1,i+1) = 1;
53     eq(1,i) = -1;
54     M = [M;eq];
55 end
56
57 %Additional constraints
58 for i=1:k-1
59     eq = zeros(1,inc);
60     eq(1,i) = i;
61     M = [M;eq];
62 end
63
64 for i=1:k-1
65     eq = zeros(1,inc);
66     eq(1,i) = i-1;
67     M = [M;eq];
68 end
69
70 for i=1:k-1
71     eq = zeros(1,inc);
72     eq(1,i) = i-2;
73     M = [M;eq];
74 end
75
76 t = [t1;zeros(k-1,1);ones(k-1,1);1/3*ones(k-1,1);2/9*ones(k
       -1,1)];
77 f = zeros(inc,1);
```

```
78
79 f(inc,1) = 1;
80
81 Aeq = zeros(1,inc);
82 Aeq(1,1)=1;
83 beq = 1;
84 lb = zeros(inc,1);
85 ub = ones(inc,1);
86 ub(inc,1)=100;
87
88 x = linprog(f, M, t,Aeq,beq,lb,ub);
89
90 tight_ineq = 0;
91 indices = [];
92 tol = exp(-15);
93 A = M*x + ones(size(M,1),1);
94 for i=1:size(A,1)
95     if abs(A(i)) < tol
96         tight_ineq = tight_ineq + 1;
97         indices = [indices; i];
98     end
99 end
```

The solution obtained is x = [1, 13/42, 1/6, 2/21, 1/21, 1/84, 0, 11/6] which is the same described by Vigoda in [23].

Matlab code for solving LP2

```
%LINEAR PROGRAM, minimizes f(x) st. M*x<=t, Aeq*x=beq, lb<=x<=ub

M = [];
k=7;
%inc=number of variables; k variables p_i and alpha
inc=k+1;
%sol_Vigoda = [1; 13/42; 1/6; 2/21; 1/21; 1/84; 0; 11/6];
%sol_Perarnau = [1; 185/616; 1/6; 47/462; 9/154; 2/77; 0; 161/88];

%DELTA = 1
for i=1:k
    for j=i:k
        eq = zeros(1,inc);
        eq(1,i) = i;
        eq(1,i+1) = -i;
        eq(1,j) = eq(1,j) + j-1;
        eq(1,j+1) =  eq(1,j+1)-(j-1);
        eq(1,inc) = -1;
        if i ~= 1 || j~=2
            M = [M;eq];
        end
    end
end

%DELTA = 2
for i=1:k
    eq = zeros(1,inc);
    eq(1,1)=2;
    eq(1,i)=2*(i-1);
    if (2*i+1 <= k)
        eq(1,2*i+1)=1;
    end
    eq(1,inc) = -2;
    if i ~= 3
        M = [M;eq];
    end
end

%Case c=sigma(v), tau(v)
for b2=1:6
   for b1=1:6-b2
       B=b1+b2;
```

```
43          eq = zeros(1,inc);
44          eq(1,B) = (B-b2);
45          eq(1,b1) = b1;
46          eq(1,inc) = -2;
47          M = [M;eq];
48      end
49  end
50
51  [s1,s2] = size(M);
52  t1 = -1 * ones(s1,1);
53
54  %p_i's are decreasing
55  for i=1:k-1
56      eq = zeros(1,inc);
57      eq(1,i+1) = 1;
58      eq(1,i) = -1;
59      M = [M;eq];
60  end
61
62  %Additional constraints
63  for i=1:k-1
64      eq = zeros(1,inc);
65      eq(1,i) = i;
66      M = [M;eq];
67  end
68
69  for i=1:k-1
70      eq = zeros(1,inc);
71      eq(1,i) = i-1;
72      M = [M;eq];
73  end
74
75  for i=1:k-1
76      eq = zeros(1,inc);
77      eq(1,i) = i-2;
78      M = [M;eq];
79  end
80
81  t = [t1;zeros(k-1,1);ones(k-1,1);1/3*ones(k-1,1);2/9*ones(k
        -1,1)];
82  f = zeros(inc,1);
83
84  f(inc,1) = 1;
85  Aeq = zeros(3,inc);
86  Aeq(1,1)=1;
87  Aeq(2,3)=1;
```

```
88  Aeq(3,7)=1;
89  beq = [1;1/6;0];
90  lb = zeros(inc,1);
91  ub = ones(inc,1);
92  ub(inc,1)=100;
93
94  x = linprog(f, M, t,Aeq,beq,lb,ub);
95
96  tight_ineq = 0;
97  indices = [];
98  tol = exp(-15);
99  A = M*x + ones(size(M,1),1);
100 for i=1:size(A,1)
101     if abs(A(i)) < tol
102         tight_ineq = tight_ineq + 1;
103         indices = [indices; i];
104     end
105 end
```

The solution obtained is x = [1, 185/616, 1/6, 47/462, 9/154, 2/77, 0, 161/88], which is the same as the one obtained by Delcourt et al. in [5].