#### CS 7535 Markov Chain Monte Carlo Methods

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Topics for the next couple weeks:

- Introduction to Conductance
- Spectral Gap

## 7.1 Coloring

We will continue our discussion of coupling and mixing time from last week, this time using the (slightly more complicated) example of coloring.

Given k different colors and an undirected graph G = (V, E) whose maximum-degree vertex has degree  $\triangle$ , a valid coloring is defined as the assignment of a color to each vertex such that no adjacent vertices have the same colors. Formally, we can define a coloring as:

$$\sigma: V \mapsto \{1, ..., k\}, \text{ where } \forall (v, w) \in E, \sigma(v) \neq \sigma(w).$$

If we define  $\Omega$  as the set of all valid k-colorings, figuring out  $|\Omega|$  is a #P-complete problem. We can, however, design a Markov Chain and a coupling scheme to get a rapid mixing time, thus allowing us to sample u.a.r. from  $\Omega$ . We will show that rapid mixing can be obtained if  $k > 2\Delta$ . We will do this in two stages: (1) use identity coupling to show rapid mixing time when  $k > 3\Delta$ , then (2) use path coupling to accomplish the same when  $k > 2\Delta$ .

# 7.2 Markov Chain

As always, we will start by designing an ergodic Markov Chain whose distribution is uniform over  $\Omega$ . The transition matrix P will adhere to the following scheme:

From any valid state  $X_t \in \Omega$ ,

- 1. Choose  $v \in V$  u.a.r. and a color  $c \in \{1, ..., k\}$  u.a.r.
- 2. For all  $w \in V \setminus v$ , set  $X_{t+1}(w) = X_t(w)$ .

3. 
$$X_{t+1}(v) = \begin{cases} c & \text{if } c \notin X_t(N(v)), \text{ where } N(v) = \text{ set of all neighboring vertices to } v \\ X_t(v) & \text{ otherwise.} \end{cases}$$

The chain is aperiodic (since  $P(\sigma, \sigma) > 0$ , as outlined above) and irreducible when  $k \ge \triangle + 2$ . (To see why we cannot establish irreducibility when  $k = \triangle + 1$ , consider a complete graph such as  $K_3$  with k = 3, and notice that it is impossible to transition from one state to another.) When  $k \ge \triangle + 2$ , we can show irreducibility in the following way. Let  $X, Y \in \Omega$  be any two valid states (i.e. two valid colorings). We can transition (eventually) from X to Y by arbitrarily ordering the vertices  $v_1, ..., v_n$ , and then sequentially re-coloring the vertices in X one by one to match the corresponding vertices in Y. If there is any conflict along the way for a vertex  $v_i$  in X such that coloring  $v_i$  to match the corresponding vertex in Y would cause X's coloring to be invalid, then it must be because  $v_i$  is somehow "blocked" by at least one neighboring vertex  $v_j$  in X where j > i. But since  $k \ge \triangle + 2$ , it is always possible to temporarily re-color  $v_j$  with some other valid color so as to allow  $v_i$  to be colored as needed, and then continue on to  $v_{i+1}$ . (Note that it is never necessary to re-color some other neighboring vertex  $v_l$  where l < i to resolve the conflict for  $v_i$ , because the coloring for  $v_1, ..., v_i$  in X is valid by virtue of the fact that Y is a valid coloring.)

Since the chain is aperiodic and irreducible, it is ergodic. Additionally, for any pair of states  $(i, j) \in \Omega$ ,  $P(i, j) = P(j, i) = \frac{1}{nk}$  if it is possible to transition from *i* to *j* in a single time step, and 0 otherwise. Thus,  $\pi$  is unique and has a uniform distribution. We will now proceed with identity coupling to show that when  $k > 3\Delta$ ,  $T_{mix} = O(n \log n)$ .

## 7.3 Identity Coupling

Let  $X_t, Y_t$  be a pair of colorings at time t. Choose, u.a.r, the same vertex v and same color c for both  $X_t$ and  $Y_t$ , and for each state re-color v with c only if doing so would be legal. It should be clear that this coupling scheme will sometimes result in a "bad" outcome, i.e. one in which the number of disagreeing vertices increases after a time step. Let's make this more concrete by defining the concept of "agreeing" and "disagreeing" vertices at time t:

$$A_{t} = \{v : X_{t}(v) = Y_{t}(v)\}\$$
$$D_{t} = \{v : X_{t}(v) \neq Y_{t}(v)\}\$$

Let us now compute the probability of such a "bad" outcome. The only way this outcome can occur is if  $X_t(v) = Y_t(v)$  and the color c is legal for exactly one of the two states. There are a total of  $|A_t|$  vertices that agree at time t, and assuming that  $v \in A_t$ , there are at most  $2\delta_t(v)$  colors that would cause the "bad" outcome, where  $\delta_t(v) = |D_t \cap N(v)|$ . In other words, the number of "bad" colors is bounded from above by twice the number of disagreeing neighbors of v at time t. As an illustrative example, Fig. 7.1 below shows that there are a total of 4 disagreeing neighbors of vertex v between the two states, and 2(4) = 8 bad colors to choose from. It should be clear that in this example, the number of bad colors cannot exceed 8 no matter how the neighboring vertices were colored.

Therefore, in general the total number of "bad" outcomes from one time step to the next is  $\sum_{v \in A_t} 2\delta_t(v)$ , and thus

$$Pr(|D_{t+1}| = |D_t| + 1) = \frac{1}{nk} \sum_{v \in A_t} 2\delta_t(v)$$

where the normalizing factor  $\frac{1}{nk}$  reflects the fact that we have a total of n vertices and k colors to choose from.

Let us now compute the probability of a "good" outcome, where  $|D_{t+1}| = |D_t| - 1$ . A good outcome occurs when  $v \in D_t$  and c is legal for both states (i.e. no neighboring vertex in either  $X_t$  or  $Y_t$  contains color c). The number of such good outcomes given  $v \in D_t$  is bounded from below by:  $\sum_{v \in D_t} (k - 2\Delta + a_t(v))$ , where  $a_t(v) = |A_t \cap N(v)|$ . To convince yourself this lower bound is correct, consider Fig. 7.2 and note that there are a total of k - 2(4) + 2 valid colors to choose from (as Y, B, M, R, O, and C are the only "bad" colors),



Figure 7.1: An example of  $X_t$  and  $Y_t$ , with vertex v as shown and the capital letters indicating the color associated with each vertex.

and that this lower bound would remain the same if we were to change the color of a neighboring vertex from its current color M to R, such that in each state two neighboring vertices now have R as their color, and the number of "bad" colors has shrunk from 6 to 5 (Y, B, R, O, and C).



Figure 7.2: Another example of  $X_t$  and  $Y_t$ , with slightly different coloring.

Hence, we can compute the probability of a "good" outcome:

$$Pr(|D_{t+1}| = |D_t| - 1) \ge \frac{1}{nk} \sum_{v \in D_t} k - 2\triangle + a_t(v)$$

We are now ready to compute an upper bound on the expected value of  $|D_{t+1}|$ :

$$\begin{split} E[|D_{t+1}] &\leq |D_t| + \frac{1}{nk} \sum_{v \in A_t} 2\delta_t(v) - \frac{1}{nk} \sum_{v \in D_t} (k - 2\triangle + a_t(v)) \\ &\leq |D_t| + \frac{1}{nk} \left[ \sum_{v \in A_t} 2\delta_t(v) - \sum_{v \in D_t} 2a_t(v) - \sum_{v \in D_t} (k - 3\triangle) \right] & \text{since } 2\triangle - a_t(v) \leq 3\triangle - 2a_t(v) \\ &\leq |D_t| + \frac{1}{nk} (0 - |D_t|) & \text{since } \sum_{v \in A_t} 2\delta_t(v) = \sum_{v \in D_t} 2a_t(v), \text{ and } k - 3\triangle \geq 1 \\ &= |D_t| \left(1 - \frac{1}{nk}\right). \end{split}$$

Now recall that  $Pr(X_t \neq Y_t) \leq E[|D_t|]$ , and that by induction  $E[|D_t|] \leq |D_0| \left(1 - \frac{1}{nk}\right)^t$ . Therefore,

$$Pr(X_t \neq Y_t) \le E[|D_t|] \le |D_0| \left(1 - \frac{1}{nk}\right)^t \le ne^{\frac{-t}{nk}} \le \frac{1}{4} \text{ for } t \ge nk \log (4n).$$

We have thus achieved a coupling time  $T_{couple}$  with high confidence  $\geq \frac{3}{4}$ , and by extension shown that  $T_{mix}$  is bounded asymptotically by  $O(nk \log n)$  in the event where  $k > 3\Delta$ . As a reminder, what we have shown is related to mixing time simply by assuming that  $Y_0$  is sampled from the stationary distribution  $\pi$  (which is allowed since  $Y_0$  can be any arbitrary starting state), and we are assured with a high probability that  $X_t = Y_t$ , meaning the total variation distance between  $X_t, Y_t$  is  $\leq \frac{1}{4}$ .

Next, we will improve upon our result by letting  $k > 2\Delta$  and showing via a different coupling scheme the same upper bound for  $T_{mix}$ .

# 7.4 Path Coupling

We will assume the same Markov Chain as before. Recall that  $|D_t|$ =the total number of disagreeing vertices between states  $X_t, Y_t$  at time t. We can equivalently think of this as the Hamming Distance  $H(X_t, Y_t)$ . It turns out that if we can devise an improved coupling scheme for the situation where  $H(X_t, Y_t) = 1$ , then we can use this to derive a better coupling for any arbitrary pair of states.

Let us consider a pair of states  $X_t, Y_t$  where  $H(X_t, Y_t) = 1$  and z is the sole disagreeing vertex. As before, we stipulate that a vertex v and color c are each chosen uniformly at random. We will analyze three possible cases:

- 1.  $v \notin z \cup N(z)$ . In this case, we know  $v \in A_t$  and that  $v \in A_{t+1}$  since the chosen color c will be either legal for both states or illegal for both states. Therefore,  $H(X_{t+1}, Y_{t+1}) = 1$ . This is neither a "bad" nor a "good" outcome.
- 2. v = z. In this case a "bad" outcome isn't possible, and there are at least  $k \Delta$  "good" color choices which would cause  $X_{t+1} = Y_{t+1}$ .
- 3.  $v \in N(z)$ . In this case a "good" outcome isn't possible, and there are at most 2 "bad" color choices which would cause  $H(X_{t+1}, Y_{t+1}) = H(X_t, Y_t) + 1$ .

In general, then, the probability of "good" and "bad" outcomes provided that  $H(X_t, Y_t) = 1$  is as follows:

$$Pr(|D_{t+1}|=0 \mid H(X_t, Y_t)=1) \ge \frac{k - \Delta}{nk}$$
$$Pr(|D_{t+1}|=2 \mid H(X_t, Y_t)=1) \le \frac{2\Delta}{nk}$$

Thus, if we make no changes to our previous identity coupling scheme and maintain the constraint of  $k > 3\Delta$ , we can verify the conditional expectation  $E[|D_{t+1}| \mid |D_t|=1] \leq |D_t| - \frac{k-\Delta}{nk} + \frac{2\Delta}{nk} = 1 - \frac{1}{nk}(k-3\Delta) \leq 1 - \frac{1}{nk}$ . But now we can let  $k > 2\Delta$  by improving our coupling for case 3 above: Assume that  $v \in N(z)$  and the two "bad" colors are  $\{R, B\}$ . If the randomly chosen color  $c \in \{R, B\}$ , then let  $X_{t+1}(v) = c$  and  $Y_{t+1}(v) \in \{R, B\} \setminus \{c\}$  provided the coloring is legal, otherwise let  $X_{t+1}(v) = X_t(v)$  and  $Y_{t+1}(v) = Y_t(v)$ . Notice that with this new coloring scheme, we still preserve the marginal randomness for the individual states (when looked at isolation,  $X_t$  and  $Y_t$  are each a faithful copy of the original Markov Chain that adheres to

the transition matrix P), but now there is only one "bad" color choice when  $v \in N(z)$ . This means that the conditional expected value is now:

$$E[|D_{t+1}| \mid |D_t| = 1] \le |D_t| - \frac{k - \triangle}{nk} + \frac{\triangle}{nk} = 1 - \frac{1}{nk}(k - 2\triangle) \le 1 - \frac{1}{nk}$$

where  $k > 2\triangle$ .

The good news is that we can use the above result to devise a coupling for other pairs of states with Hamming Distances greater than 1. Suppose we have a pair of states  $(X, Y) \in \Omega^2$  where H(X, Y) = l, l > 1. We can define a sequence  $W_0, W_1, ..., W_l \in \Omega$  where:

- (a)  $\forall i, H(W_{i-1}, W_i) = 1.$
- (b)  $W_0 = X, W_l = Y.$

Essentially, we have constructed a "shortest path" from X to Y where all of the intermediate states  $W_i$  are such that adjacent states are apart by one Hamming Distance. Recall the coupling scheme we previously devised and notice that it can simply be thought of as a function: given a set of colors to be assigned to state  $X_t$ , we can figure out the set of colors to be assigned to state  $Y_t$ . Now it is clear that for every  $i \leq l$ , there is a coupling for  $(W_{i-1}, W_i)$ . We can thus compose couplings (similar to how we can compose functions) along the path  $W_0, W_1, ..., W_l$ , as follows:

- Map  $(W_0 = X, W_1)$  to  $(W'_0 = X', W'_1)$  according to the coupling, where  $W_0 \to W'_0$  is a random transition, and the same is true for  $W_1 \to W'_1$ .
- For each  $i \ge 1$ , map  $(W_i, W_{i+1})$  to  $(W'_i, W'_{i+1})$  in accordance to the coupling, conditional on  $W'_i$  already having been chosen.

Continue this process all the way to  $W_l = Y$  and  $W'_l = Y'$ . Then we have constructed a coupling for  $(X, Y) \rightarrow (X', Y')$  via composition. It remains to be proven how good this coupling is in terms of the expected change in Hamming Distance:

$$E[H(X',Y')] \leq E\left[\sum_{i=1}^{l} H(W'_{i-1},W'_{i})\right]$$
$$= \sum_{i=1}^{l} E[H(W'_{i-1},W'_{i})]$$
$$\leq \sum_{i=1}^{l} \left(1 - \frac{1}{nk}\right)$$
for  $k > 2 \triangle$ 
$$= l\left(1 - \frac{1}{nk}\right)$$
$$= H(X,Y)\left(1 - \frac{1}{nk}\right)$$

In other words, we have just shown that with the above path coupling,  $E[|D_{t+1}|] = |D_t|(1 - \frac{1}{nk})$ , and by extension  $E[|D_t|] \le n(1 - \frac{1}{nk})^t$ , meaning that once again we have

$$Pr(X_t \neq Y_t) \le n\left(1 - \frac{1}{nk}\right)^t \le \frac{1}{4} \text{ for } t \ge nk \ln(4n), k > 2\triangle$$

We finish by stating the Path Coupling Theorem (Bubley, Dyer '97):

**Theorem 7.1** For a finite ergodic Markov chain  $\in \Omega$ , let  $S \subseteq \Omega \times \Omega$  such that  $(\Omega, S)$  is connected. For  $(X, Y) \in \Omega \times \Omega$ , let dist(X, Y) = length of shortest path between X and Y in  $(\Omega, S)$ . If there exists  $\beta < 1$  such that  $\forall (X_t, Y_t) \in S$ , there exists a coupling  $(X_t, Y_t) \to (X_{t+1}, Y_{t+1})$  where  $E[dist(X_{t+1}, Y_{t+1})] \leq \beta dist(X_t, Y_t)$ , then  $T_{mix}(\epsilon) \leq \frac{log(D_{max}/\epsilon)}{1-\beta}$ , where  $D_{max} = \max_{(X,Y)\in\Omega^2} (dist(X,Y))$ .