Randomized Algorithms Lecture 17: Path Coupling

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Recap: TV and Coupling

Our goal: We want to sample from a MC with stationary distribution π in time poly(*n*) and $\log(1/\epsilon)$.

- ► TV distance: $||D_1 D_2|| = \frac{1}{2} \sum_{x \in \Omega} |D_1(x) D_2(x)|$
- Lower bound mixing time: $|D_1(A) - D_2(A)| \le \max_{A \subseteq \Omega} |D_1(A) - D_2(A)| = ||D_1 - D_2||$
- ▶ Upper-bounds on mixing time (Coupling): $||D_1 - D_2|| \le \inf \Pr(X \ne Y)$ for a coupling (X, Y) of D_1 and D_2 .
- We want to prove that $\|P^t(x, \cdot) \pi\| \le \varepsilon$ fast enough
- ► Coupling lemma: $\Pr(X_T \neq Y_T | X_0 = x, Y_0 = y) \le \epsilon \Rightarrow \tau(\epsilon) \le T$

Mixing time

Definition (Definition 12.2)

Let *M* be a finite, irreducible and aperiodic Markov chain over the state space Ω and let π be its stationary distribution. We define $\Delta_x(t), \Delta(t)$ as

$$\Delta_{\mathbf{X}}(t) = \|\mathbf{M}^{t}[\mathbf{X}, \cdot] - \pi\|, \quad \Delta(t) = \max_{\mathbf{X} \in \Omega} \Delta_{\mathbf{X}}(t).$$

We also define

$$\tau_x(\epsilon) = \min\{t : \Delta_x(t) \le \epsilon\}, \quad \tau(\epsilon) = \max_{x \in \Omega} \tau_x(\epsilon).$$

1. $\tau(\varepsilon)$ is called mixing time.

2. A chain is rapidly mixing if $\tau(\varepsilon)$ is polynomial in $\log(1/\varepsilon)$ and the size of the problem.

Coupling as upper-bound of TV distance

Definition (Definition 12.2)

A coupling of two probability distributions μ and ν is a pair of random variables (*X*, *Y*) defined on a single probability space, i.e., a joint probability distribution *q* on $\Omega \times \Omega$ such that

$$\sum_{\mathbf{y}\in\Omega} q(\mathbf{x},\mathbf{y}) = \mu(\mathbf{x}) \text{ and } \sum_{\mathbf{x}\in\Omega} q(\mathbf{x},\mathbf{y}) = \mathbf{v}(\mathbf{x}) \tag{1}$$

Definition (Lemma 12.3)

Given distributions $\mu(x)$ and $\nu(x)$ on state space Ω . All couplings (X, Y) satisfy the condition

$$\inf \Pr(X \neq Y) \ge \|\mu - \nu\|.$$
(2)

This will allow us to upper-bound distances between two Markov chains at step t, and also with respect to the stationary distribution, which leads to upper-bounds on mixing times.

Path coupling: the big picture (Book section 12.6)

Neighborhood: states $y \in \Omega$ reachable from x in a single step.

► Distance d(X, Y): the amount of steps to reach y from x. Neighbors if d(X, Y) = 1. Many times d(X, Y) ≤ |V|.

• Distance at step *t* of MC: $d_t = d(X_t, Y_t)$

 $\blacktriangleright \operatorname{Pr}(X_T \neq Y_T | X_0 = x, Y_0 = y) \le \max_{x,y} \operatorname{Pr}(d_T \ge 1) \le \max_{x,y} E[d_T]$

- Our goal is to bound $\max_{x,y} \mathbf{E}[d_T] \leq \epsilon$.
- After some work... (see next slides) E[d_{t+1}] =≤ βE[d_t], with β < 1 (Contraction of expect. distance)</p>

• Iterate
$$\mathbf{E}[d_T] = \leq \beta^T d_0 \leq \beta^T |V|$$

Therefore the chain is guaranteed to have mixed for all times, such that $\beta^T |V| \le \varepsilon$, leading to

$$\tau(\epsilon) = \frac{1}{\log(1/\beta)} \left(\log |V| + \log(1/\epsilon) \right).$$

Many times we can write $\beta = e^{-\alpha/|V|}$, leading to $\tau(\epsilon) = \frac{|V|}{\alpha} (\log |V| + \log(1/\epsilon))$, where α can itself depend on parameters of the problem.

Path Coupling in a nutshell II

- We define a distance d(X, Y). Neighbors if d(X, Y) = 1.
- Our goal is to prove concentration of expect. of distance: $E[d_{t+1}] \le \beta E[d_t]$, with $\beta < 1$.
- ▶ Path: $X_t = Z_0, Z_1, ..., Z_{d_t} = Y_t$ where $d(Z_{i+1}, Z_i) = 1$ ▶ $d_t = \sum_{i=1}^{d_t} d(Z_{i+1}, Z_i)$ (by construction)
- Updated path: $X_{t+1} = Z'_0, Z'_1, ..., Z'_{d_t} = Y_{t+1}$.

► $d_{t+1} \leq \sum_{i=1}^{d_t} d(Z'_{i+1}, Z'_i)$ (by triangle inequality)

- 1. For our problem of interest prove $\mathbf{E}[d(Z'_{i+1}, Z'_i)] \leq \beta d(Z_{i+1}, Z_i) = \beta.$
- 2. Leads to $\mathbf{E}[d_{t+1}|d_t] \le \sum_{i=1}^{d_t} \mathbf{E}[d(Z'_{i+1}, Z'_i)] \le \beta d_t.$
- 3. Then $\mathbf{E}[d_{t+1}] \leq \mathbf{E}[\mathbf{E}[d_{t+1}|d_t]] \leq \beta \mathbf{E}[d_t]$.

Left to do: prove $\mathbf{E}[d(Z'_{i+1}, Z'_i)] \leq \beta$ for our problem of interest.

Glauber dynamics for independent sets

Consider Glauber dynamics to sample from the Gibbs distribution of independent sets of a graph G = (V, E).

• Let $\pi(x)$ the Gibbs distribution on independent sets:

$$\pi(x) = \begin{cases} \frac{\lambda^{|x|}}{Z(\lambda)} & \text{if } x(v)x(w) = 0 \quad \forall \{v, w\} \in E \\ 0 & \text{Otherwise.} \end{cases}$$
(3)

where $|x| = \sum_{v \in V} x(v)$ and $Z(\lambda) = \sum_{x \in \chi} \lambda^{|x|}$ normalizes π .

Algorithm GLAUBERIS(G = (V, E))

- 1. Start with an arbitrary IS X_0
- 2. for $i \leftarrow 0$ to "whenever"

7.

3. Choose *v* uniformly at random from *V*.

4. Set
$$X_{t+1}(w) = X_t(w) \forall w \neq v$$
.

- 5. **if** $\exists w' \in N(v)$, s.t. $X_t(w') = 1$ set $X_t(v) = 0$ (M1)
- 6. else $X_{t+1}(v) = 1$ with probability $\lambda/(1 + \lambda)$ (M2)

or
$$X_{t+1}(v) = 0$$
 with probability $1/(1+\lambda)$

Proof Strategy

- 1. Construct a coupling (X_t, Y_t) : chose same *v* for both chains.
- 2. We define a distance $d_t = d(X_t, Y_t) = |Y_t \setminus X_t| + |X_t \setminus Y_t|$
- 3. We will construct a path coupling by having a path $X_t = Z_0, Z_1, ..., Z_{d_t} = Y_t$ where Z_{i+1} and Z_i are neighbors.
- 4. We will prove $\mathbf{E}[d_{t+1}|d_t = 1] \le 1 c(\lambda)/n \le e^{-c(\lambda)/n}$
- 5. This will lead to $\mathbf{E}[d_{t+1}] \leq e^{-c(\lambda)/n} \mathbf{E}[d_t]$

Therefore the chain is guaranteed to have mixed for all times

$$\tau(\epsilon) = \frac{n}{c(\lambda)} \left(\log n + \log(1/\epsilon) \right).$$

where $c(\lambda) = 1 - \lambda(\Delta - 1)/(1 + \lambda)$, which lead to rapid mixing sufficient condition $\lambda < (\Delta - 1)^{-1}$.

Key aspects of the proof

We will now prove $\mathbf{E}[d_{t+1}|d_t = 1] \leq 1 - \frac{c(\lambda)}{n}$.

- Without loss of generality, let $X_t = I$ and $Y_t = I \cup \{x\}$
- We do not care about how X_t or Y_t change but on when they have different updates that lead to d_{t+1} ≠ d_t.
- The discussion needs to consider three scenarios:
 - 1. Case I: when v = x ($d_{t+1}d_t = d_t 1$).
 - 2. Case II: when $v \notin N(x) \cup \{x\} (d_{t+1} = d_t + 1)$.
 - 3. Case III: when $v \in N(x)$ ($d_{t+1} = d_t + 1$).

Case I: when $v = x (d_{t+1} - d_t = 0)$



- If we select the vertex v where X_t and Y_t differ, all neighbors are the same in both chains, which implies the chain applies same move to both.
- ► Because either $X_t(v) = 1$ ($Y_t(v) = 0$) or $Y_t(v) = 1$ ($X_t(v) = 0$), all its neighbors have to be 0.
- Therefore the MC will chose move M2.
- ▶ Whatever is the update, now we have $X_t(v) = Y_t(v)$ where before we had $X_t(v) \neq Y_t(v)$, which means that $(X_{t+1}, Y_{t+1}) = 0$.

Therefore: $\mathbf{E}[d_{t+1} - d_t | d_t = 1] = -1/n$ *RA* (2023/24) – *Lecture* 17 – *slide* 10 Case II: when $v \notin N(x) \cup \{x\} (d_{t+1} = d_t + 1)$



- ▶ All neighbors of $w \notin N(v) \cup \{v\}$ are equal on both chains
- MC implements the same update (M1 or M2 with same output) on both chains.
- ► Because initially $X_t(w) = Y_t(w)$ and also $X_{t+1}(w) = Y_{t+1}(w)$ we have $d_{t+1} = d_t$.

We obtain: $E[d_{t+1} - d_t | d_t = 1] = 0$

Case III: when $v \in N(x)$ ($d_{t+1} = d_t + 1$)



- ► If $v \in N(x)$ and assume without lost of generality that $X_t(x) = 1(Y_t(x) = 0)$.
- ▶ What may happen is that the MC implements move M1 to X_t and M2 to Y_t potentially leading to $Y_{t+1}(v) = 1 \neq X_{t+1}(v)$ and $d_{t+1} = d_t + 1$.
- This can only happen if all neighbors of *v* in *Y_t* are 0 and the move M2 select output 1 for *v*, which has probability ≤ λ/(1 + λ).

We obtain:

$$\mathbf{E}[d_{t+1} - d_t | d_t = 1] \le \frac{\Delta}{n} \left(\frac{\lambda}{1+\lambda}\right). \tag{4}$$

An equivalent argument works for the case $X_t(v) = 0$ ($Y_t(v) = 1$). RA(2023/24) - Lecture 17 - slide 12

Final step

We will now prove $\mathbf{E}[d_{t+1}|d_t = 1] \leq 1 - \frac{c(\lambda)}{n}$.

- Without loss of generality, let $X_t = I$ and $Y_t = I \cup \{x\}$
- We do not care about how X_t or Y_t change but on when they have different updates that lead to d_{t+1} ≠ d_t.
- The discussion depends on what is the neighborhood of y. Because Δ = 4, there exist three cases:

1. Case I: (when
$$v = x$$
) $\mathbb{E}[d_{t+1} - d_t|d_t = 1] = -1/n$.

- 2. Case II ($v \notin N(x) \cup \{x\}$: $\mathbf{E}[d_{t+1} d_t|d_t = 1] = 0$.
- 3. Case III ($v \in N(x)$): $\mathbb{E}[d_{t+1} d_t|d_t = 1] \leq \frac{\Delta}{n} \left(\frac{\lambda}{1+\lambda}\right)$.

We obtain:

$$\mathbf{E}[d_{t+1}|d_t=1] \le 1 - \frac{1}{n} + \frac{\Delta}{n} \left(\frac{\lambda}{1+\lambda}\right) = 1 - \frac{1}{n} \left(\frac{1-\lambda(\Delta-1)}{1+\lambda}\right).$$
(5)

If $\lambda < (\Delta - 1)^{-1}$ we obtain: $\mathbf{E}[d_{t+1}|d_t = 1] \leq 1 - \frac{c(\lambda)}{n} \leq e^{-c(\lambda)/n}$ with $c(\lambda) = 1 - \lambda(\Delta - 1)/(1 + \lambda) \geq 0$.

Recap of proof strategy of this example

- 1. We designed a coupling (X_t, Y_t) : chose same *v* for both chains.
- 2. We defined a distance $d_t = d(X_t, Y_t) = |Y_t \setminus X_t| + |X_t \setminus Y_t|$
- 3. We construct a path coupling by having a path $X_t = Z_0, Z_1, ..., Z_{d_t} = Y_t$ where Z_{i+1} and Z_i are neighbors.
- 4. We proved $\mathbf{E}[d_{t+1}|d_t = 1] \le (1 c(\lambda)/n \le e^{-c(\lambda)/n}$
- 5. This will lead to $\mathbf{E}[d_{t+1}] \leq e^{-c(\lambda)/n} \mathbf{E}[d_t]$

Therefore the chain is guaranteed to have mixed for all times

$$\tau(\epsilon) = \frac{n}{c(\lambda)} \left(\log n + \log(1/\epsilon) \right).$$

where $c(\lambda) = 1 - \lambda(\Delta - 1)/(1 + \lambda)$, which lead to rapid mixing sufficient condition $\lambda < (\Delta - 1)^{-1}$.

What if $E[d(Z'_{i+1}, Z'_i)] = 1$?

Lemma (Bubley and Dyer 1997 (cont'd)) If $\mathbb{E}[d_{t+1}|d_t] \leq d_t$ an there is some $\alpha > 0$ such that $\Pr[d(X', Y') \neq d(X, Y)] \geq \alpha$ for all $(X, Y) \in \Omega \times \Omega$, then

$$\tau(\varepsilon) \leq \left\lceil \frac{\textit{e}|\textit{V}|^2}{\alpha} \right\rceil \lceil \ln(\varepsilon^{-1}) \rceil.$$