

# Randomized Algorithms

## Lecture 16: Total variation distance and coupling

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# Markov chain and mixing times

- ▶ Sampling from a given probability distribution is a fundamental algorithmic tool.
- ▶ We have seen that in some cases one can design a Markov chain that has as stationary distribution our target distribution.
  - ▶ After sufficiently many steps we converge to the target distribution regardless of the initial state.
- ▶ To achieve our goal, we need to have a guarantee of the convergence to the target distribution, this will be the goal of this and next lecture.
  1. This lecture: notion of distance + coupling as a tool to prove mixing times.
  2. Next lecture: path coupling to prove mixing times.

# Total variation distance

## Definition (Definition 12.1)

The total variation distance between two distributions  $D_1$  and  $D_2$  on a countable state space  $S$  is given by

$$\|D_1 - D_2\| = \frac{1}{2} \sum_{x \in S} |D_1(x) - D_2(x)|.$$

Properties:

1. Triangle inequality:  $\|D_1 - D_3\| \leq \|D_1 - D_2\| + \|D_2 - D_3\|$
  2.  $\|D_1 - D_2\| = 0$  only if  $D_1 = D_2$ .
  3.  $0 \leq \|D_1 - D_2\| \leq 1$
- ▶  $\pi$  being the stationary distribution of a Markov chain  $M$ . We want to bound the distance between the distribution of the chain after  $t$  steps when starting at state  $x$ , i.e., bound  $\|p_x^t - \pi\|$ .
  - ▶ We want to show that it becomes  $\epsilon$  small in number of steps  $t$  polynomial on the size of the problem.

# Examples

▶ Two biased coins:

1.  $\{p(0) = p, p(1) = 1 - p\}$ ,
2.  $\{q(0) = 1 - p, q(1) = p\}$  (where  $0 \leq p \leq 1/2$ ),

$$\|p - q\| = \frac{1}{2}(|p - (1 - p)| + |1 - p - p|) = 1 - 2p.$$

▶ Non-overlapping supports:

1. For all  $W \subseteq A$ ,  $D_1(W) > 0$  and  $D_2(W) = 0$ ,
2. where for all  $W \subseteq \bar{A}$ ,  $D_1(W) = 0$  and  $D_2(W) \geq 0$ .

$$\begin{aligned}\|D_1 - D_2\| &= \frac{1}{2} \sum_{x \in S} |D_1(x) - D_2(x)| \\ &= \frac{1}{2} \sum_{x \in A} D_1(x) + \frac{1}{2} \sum_{x \in \bar{A}} D_2(x) = 1\end{aligned}$$

# Operational interpretation

## Definition (Lemma 12.1)

$$\|D_1 - D_2\| = \frac{1}{2} \sum_{x \in S} |D_1(x) - D_2(x)|.$$

For any  $A \subseteq S$  let  $D_i(A) = \sum_{x \in A} D_i(x)$ , i.e., the weight of subspace  $A$ .  
Then

$$\|D_1 - D_2\| = \max_{A \subseteq S} |D_1(A) - D_2(A)|. \quad (1)$$

1. For any  $B \subseteq S$  we have  $\|D_1 - D_2\| \geq |D_1(B) - D_2(B)|$ .
  - ▶ It can also be used to prove non-convergence: if  $\exists B$ , s.t.  $|D_1(B) - D_2(B)| > c$  then also  $\|D_1 - D_2\| > c$ .
2. If  $\|D_1 - D_2\| \leq \epsilon$ :  $D_1$  and  $D_2$  can not be distinguished up to error  $\epsilon$ , i.e., whether you sample from one or the other is indistinguishable on any subset  $B \subseteq S$ !
  - ▶ Probability of guessing distribution 1 or 2 right:  
 $P_{\text{guess}}^{\max} = \frac{1}{2} (1 + \|D_1 - D_2\|)$

## Proof of Lemma 12.1

- ▶  $\|D_1 - D_2\| = \frac{1}{2} \sum_{x \in S} |D_1(x) - D_2(x)|.$
- ▶  $A \subseteq S : \|D_1 - D_2\| = \max_{A \subseteq S} |D_1(A) - D_2(A)|.$

### Proof.

1. Let  $S^+ \subseteq S$  s.t.  $D_1(x) \geq D_2(x)$  and  $S^-$  complement
2.  $\max_{A \subseteq S} D_1(A) - D_2(A) = D_1(S^+) - D_2(S^+)$
3.  $\max_{A \subseteq S} D_2(A) - D_1(A) = D_2(S^-) - D_1(S^-)$
4.  $D_1(S^+) + D_1(S^-) = 1 = D_2(S^+) + D_2(S^-)$ 
  - ▶  $D_1(S^+) - D_2(S^+) = D_2(S^-) - D_1(S^-)$
5.  $\max_{S \subseteq S} |D_1(A) - D_2(A)| = |D_1(S^+) - D_2(S^+)| = |D_1(S^-) - D_2(S^-)|$
6.  $|D_1(S^+) - D_2(S^+)| + |D_1(S^-) - D_2(S^-)| = 2\|D_1 - D_2\|$  (Def. TV)

□

# Mixing time

## Definition (Definition 12.2)

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

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

We also define

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

1.  $\tau(\epsilon)$  is called mixing time.
2. A chain is rapidly mixing if  $\tau(\epsilon)$  is polynomial in  $\log(1/\epsilon)$  and the size of the problem.
3. There are two main techniques for upper-bounding mixing time:
  - ▶ Coupling: nice tight bounds when it works.
  - ▶ Conductance: worse bounds, works on a larger pool.

# Coupling as upper-bound of TV distance

## Definition (Definition 12.2)

A coupling of two probability distributions  $\mu$  and  $\nu$  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

$$\sum_{y \in \Omega} q(x, y) = \mu(x) \text{ and } \sum_{x \in \Omega} q(x, y) = \nu(y) \quad (2)$$

## Definition (Lemma 12.3)

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

$$\inf \Pr(X \neq Y) \geq \|\mu - \nu\|. \quad (3)$$

- ▶ 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.



## Coupling example I

$$\text{Coupling: } \sum_{y \in \Omega} q(x, y) = \mu(x) \text{ and } \sum_{x \in \Omega} q(x, y) = \nu(y)$$

$$\text{Bound on TV: } \inf \Pr(X \neq Y) \geq \|\mu - \nu\|$$

Consider two fair coins:  $\mu(x) = \nu(x) = c(x) = 1/2$ .

It is trivial to see that  $\|\mu - \nu\| = \|c - c\| = 0$  as both are equal.

A trivial coupling consist of two independent coins

- ▶ Because  $q(x, y) = c(x)c(y) \Rightarrow \sum_{y \in \Omega} q(x, y) = c(x) = 1/2$ .
- ▶ Remark that  $\Pr(X \neq Y) = 1/2 > 0 = \|\mu - \nu\|$

## Coupling example II

$$\text{Coupling: } \sum_{y \in \Omega} q(x, y) = \mu(x) \text{ and } \sum_{x \in \Omega} q(x, y) = \nu(y)$$

$$\text{Bound on TV: } \inf \Pr(X \neq Y) \geq \|\mu - \nu\|$$

Consider two fair coins:  $\mu(x) = \nu(x) = c(x) = 1/2$ .

It is trivial to see that  $\|\mu - \nu\| = \|c - c\| = 0$  as both are equal.

Consider now a perfectly correlated coin:

- ▶ Because  $q(0,0) = q(1,1) = 1/2 \Rightarrow \sum_{y \in \Omega} q(x,y) = c(x) = 1/2$ .
- ▶ Remark that  $\Pr(X \neq Y) = 0 = \|\mu - \nu\|$
- ▶ Can we saturate the lower-bound building correlated joint distribution!

## Coupling example III

Consider the distributions

1.  $\{\mu(0) = 3/4, \mu(1) = 1/4\}$

2.  $\{\nu(0) = 1/4, \nu(1) = 3/4\}$

▶ Remark that  $\|\mu - \nu\| = 1/2$ .

▶ The following algorithm generates a coupling.

### Algorithm COUPLING COINS()

1. Generate a random bit with  $p(b_1 = 0) = 1/2$ .

2. **if**  $b_1 = 0$  **then**

    Generate perfect random bit  $b_2$  and fix  $X = Y = b_2$ .

3. **else**

    Fix  $X = 0$  and  $Y = 1$

▶ Always  $\exists$  a coupling saturating  $|D_1 - D_2|$

## Proof Lemma 12.3 (upper-bound)

- ▶  $A \subseteq S : \|\mu - \nu\| = \max_{A \subseteq S} |\mu(A) - \nu(A)|$ .
- ▶ Bound on TV:  $\inf \Pr(X \neq Y) \geq \|\mu - \nu\|$

### Proof.

1.  $\mu(A) - \nu(A) = \Pr\{X \in A\} - \Pr\{Y \in A\}$
- 2.

$$\begin{aligned}\mu(A) - \nu(A) &= (\Pr\{X \in A, Y \in A\} + \Pr\{X \in A, Y \notin A\}) - \\ &\quad (\Pr\{X \in A, Y \in A\} + \Pr\{X \notin A, Y \in A\}) \\ &= \Pr\{X \in A, Y \notin A\} - \Pr\{X \notin A, Y \in A\} \\ &\leq \Pr\{X \notin A, Y \in A\} \\ &\leq \Pr\{X \neq Y\}\end{aligned}$$



It has to hold for all coupling  $(X, Y)$ , including the one that provides the minimum of  $\Pr(X \neq Y)$ .

# Coupling of Markov chains

1. We have two chains  $X_t$  and  $Y_t$  that independently behave like the original one, governed by the transition rule  $P$ .
2. We couple the chains  $X$  and  $Y$ , on a joint chain  $Z = (X, Y)$ .
3. We design a Markov process  $M$  acting on  $Z$  (both  $X$  and  $Y$ ), such that locally on each chain it still behaves as  $P$ , but globally the process is correlated.
  - ▶  $\Pr(X_{t+1} = x' | Z_t = (x, y)) = P(x, x')$ ,
  - ▶  $\Pr(Y_{t+1} = y' | Z_t = (x, y)) = P(x, x')$ .
4. We are interested in chains that:
  - ▶ Bring the two copies of the chain to the same state
  - ▶ Once in same state they will make exactly the same move and remain equal

# Coupling Lemma

## Lemma (Lemma 12.2|Coupling lemma)

Let  $Z_t = (X_t, Y_t)$  be a coupling for a Markov chain  $M$  on a state space  $S$ . Suppose there is a  $T$  such that, for every  $x, y \in S$ ,

$$\Pr(X_T \neq Y_T | X_0 = x, Y_0 = y) \leq \epsilon$$

Then

$$\tau(\epsilon) \leq T.$$

# Shuffling cards

- ▶ We want to couple two chains: think of having two decks of card arranged in different configurations  $X_0$  and  $Y_0$ .
- ▶ Each configuration is a given arrangement of the cards of a deck.
- ▶ Coupling:
  1. Choose a position  $j$  uniformly at random from deck 1 and then generate  $X_{t+1}$  from  $X_t$  by moving the  $j$ -th card to the top. Let's call that card  $C$ .
  2. Search for card  $C$  on the second deck and move it to the top to obtain  $Y_{t+1}$  from  $Y_t$ .
- ▶ The movements of card when looking at the deck independently is a standard reshuffling of card with probability  $1/n$ .
- ▶ Once a card is moved to the top it follows the same trajectory on both decks.
- ▶ Mixing when all cards have been moved to the top.
- ▶ We have mapped the problem to coupon collector:  
 $\tau(\epsilon) = n \log(n/\epsilon)$ .

# Lazy random Walk on Hypercube

- ▶ Lazy random walk on the hypercube  $\bar{x} = (x_1, x_2, \dots, x_n)$ .
  1. Select a coordinate uniformly at random from 1 to  $n$ .
  2. Set the value to 0 or 1 with equal probability  $1/2$ .
- ▶ Remark that with probability  $1/2$  you remain in the same configuration  $\Rightarrow$  aperiodicity.
- ▶ Coupling between  $X_t$  and  $Y_t$  via implementing the same move on both chains.
- ▶ Once the  $i$ -th coordinate chosen both chain will agree on  $i$  in future moves.
- ▶ The problem is again mapped to a coupon collector:  
 $\tau(\epsilon) = n \log(n/\epsilon)$ .



## 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  $d(X, Y) \leq |V|$ .
  - ▶ Distance at step  $t$  of MC:  $d_t = d(X_t, Y_t)$
- ▶  $\Pr(X_T \neq Y_T | X_0 = x, Y_0 = y) \leq \max_{x,y} \Pr(d_T \geq 1) \leq \max_{x,y} \mathbf{E}[d_T]$
- ▶ Our goal is to bound  $\max_{x,y} \mathbf{E}[d_T] \leq \epsilon$ .
- ▶ After some work...
- ▶  $\mathbf{E}[d_{t+1}] \leq \beta \mathbf{E}[d_t]$ , with  $\beta < 1$  (Contraction of expect. distance)
- ▶ 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  $\beta^T |V| \leq \epsilon$ , leading to

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

Many times we can write  $\beta = e^{-\alpha/|V|}$ , leading to

$\tau(\epsilon) = \frac{|V|}{\alpha} (\log |V| + \log(1/\epsilon))$ , where  $\alpha$  can itself depend on parameters of the problem.

# Coupling Lemma

## Lemma (Lemma 12.2|Coupling lemma)

Let  $Z_t = (X_t, Y_t)$  be a coupling for a Markov chain  $M$  on a state space  $S$ . Suppose there is a  $T$  such that, for every  $x, y \in S$ ,

$$\Pr(X_T \neq Y_T | X_0 = x, Y_0 = y) \leq \epsilon$$

Then

$$\tau(\epsilon) \leq T.$$

## Proof of Lemma 12.2: Coupling lemma

- ▶  $\Pr(X_T \neq Y_T | X_0 = x, Y_0 = y) \leq \epsilon \Rightarrow \tau(\epsilon) \leq T$
- ▶ Choose  $Y_0$  according to the uniform distribution and  $X_0$  takes an arbitrary value. For  $T, \epsilon$  such that lemma is satisfied and for any  $A \subseteq S$ :

$$\begin{aligned}\Pr(X_T \in A) &\geq \Pr((X_T = Y_T) \cap (Y_T \in A)) \\ &= 1 - \Pr((X_T \neq Y_T) \cup Y_T \notin A) \\ &\geq (1 - \Pr(Y_T \notin A)) - \Pr(X_T \neq Y_T) \\ &\geq \Pr(Y_T \in A) - \epsilon \\ &= \pi(A) - \epsilon\end{aligned}$$

- ▶ The same argument for  $S - A$  shows:  $\Pr(X_T \notin A) \geq \pi(S - A) - \epsilon$  or equivalently  $\Pr(X_T \in A) \leq \pi(A) + \epsilon$ .
- ▶ It follows:

$$\|\rho_x^T - \pi\| = \max_{x, A} |\rho_x^T(A) - \pi(A)| \leq \epsilon.$$