# *[AI2613 Lecture 3] FTMC, Coupling, Mixing Time*

*March 11, 2022*

## *1 Fundamental Theorem of Markov Chains*

Recall the fundamental theorem of Markov chains for *finite* chains we introduced in the last lecture.

**Theorem 1 (Fundamental theorem of Markov chains)** *If a finite Markov chain $P \in \mathbb{R}^{n\times n}$ is irreducible and aperiodic, then it has a unique stationary distribution $\pi \in \mathbb{R}^n$. Moreover, for any distribution $\mu \in \mathbb{R}^n$,*

$$\lim_{t\to\infty} \mu^\top P^t = \pi^\top.$$

Today we give a proof of the theorem. To this end, we first study the properties of the transition matrix $P$ of an irreducible and aperiodic chain. Then we introduce the notion of *coupling*, a powerful technique to analyze stochastic processes.

**Claim 2** *Let $P \in \mathbb{R}^{n\times n}$ be an irreducible and aperiodic Markov chain. It holds that*

$$\exists\, t^* : \forall\, i, j \in [n] : \quad P^{t^*}(i,j) > 0\,.$$

We use Lemma 3 to prove Claim 2.

**Lemma 3** *Let $c_1, c_2, \ldots, c_s$ be a group of positive integers satisfying $\gcd(c_1, \ldots, c_s) = 1$. For any sufficiently large integer $b$, there exists $y_1, y_2, \ldots, y_s \in \mathbb{N}$ such that*

$$c_1 y_1 + c_2 y_2 + \cdots c_s y_s = b.$$

That is, there exists some $b_0 > 0$ such that for any $b > b_0$, the diophantine equation $c_1 y_1 + c_2 y_2 + \cdots + c_s y_s = b$ always has non-negative solutions

*Proof.* By Bézout's identity there exists $x_1, x_2, \ldots, x_s \in \mathbb{Z}$ such that

$$c_1 x_1 + c_2 x_2 + \cdots c_s x_s = 1\,.$$

We apply induction on $s$. The case $s = 1$ trivially holds. Assume $s \geq 2$ and the lemma holds for smaller $s$. Let $g = \gcd(c_1, \ldots, c_{s-1})$. By induction hypothesis, we know that

$$\frac{a_1}{g}\cdot x_1 + \frac{a_2}{g}\cdot x_2 + \cdots + \frac{a_{s-1}}{g}\cdot x_{s-1} = b' \iff a_1\cdot x_1 + a_2\cdot x_2 + \cdots + a_{s-1}x_{s-1} = g\cdot b'$$

has non-negative solutions for sufficiently large $b'$. Therefore, we only need to prove that the equation

$$g\cdot b' + a_s \cdot x_s = b \tag{1}$$

has nonegative solution $(b', x_s)$ with sufficiently large $b'$ when $b$ is sufficiently large. In other words, we need to prove for any $b_0 > 0$, eq. (1) has nonegative solution with $b' > b_0$ for any sufficiently large $b$.

Note that $\gcd(g, a_s) = 1$, we can find integers $(y, x)$ such that

$$g \cdot y + a_s \cdot x = 1 \iff g \cdot (by) + a_s \cdot (bx) = b.$$

Noting that for any $k \in \mathbb{Z}_{\geq 0}$, we have $g \cdot (by + ka_s) + a_s \cdot (bx - kg) = b$. We need $by + ka_s > b_0$ and $bx - kg \geq 0$, which are equivalent to

$$\frac{bx}{g} \geq k > \frac{b_0 - by}{a_s}.$$

We can always find such an integer $k$ if $b \geq g(b_0 + a_s)$.

□

*Proof.* [Proof of Claim 2]

The property of irreducibility implies that

$$\forall\, i, j : \exists\, t : \quad P^t(i, j) > 0\,.$$

Suppose that there are $s$ loops of length $c_1, c_2, \ldots, c_s$ starting from and ending at state $i$. Then by aperiodicity we have

$$\gcd(c_1, c_2, \ldots, c_s) = 1\,.$$

For any sufficiently large $m$ and any pair of states $(i, j)$, by Lemma 3 and irreducibility, there exists a path from $i$ to $j$ with exactly $m$ steps. Thus, there exist $t^* > 0$ such that for any state pair $(i, j)$, $P^{t^*}(i, j) > 0$. Furthermore, for any $t > t^*$, $P^t(i, j) > 0$ for any $i, j \in \Omega$.

□

### 1.1 Coupling

To measure how close the two distributions are, we need to define the distance between them.

**Definition 4 (Total Variation Distance)** . *The total variation distance between two distributions $\mu$ and $\nu$ on a countable state space $\Omega$ is given by*

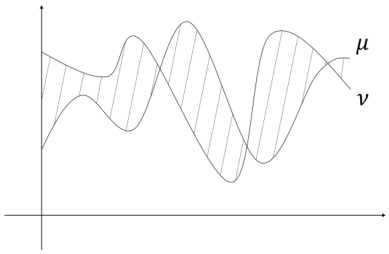
$$D_{\mathrm{TV}}(\mu, \nu) = \frac{1}{2} \sum_{x \in \Omega} |\mu(x) - \nu(x)|.$$

We can look at the following figure of two distributions on the sample space. The total variation distance is half the area enclosed by the two curves.

This figure gives us the intuition of the following proposition which states that the total variation distance can be equivalently viewed in another way.

**Proposition 5** *We define $\mu(A) = \sum\limits_{x \in A} \mu(x)$, $\nu(A) = \sum_{x \in A} \nu(x)$, then we have*

$$D_{\mathrm{TV}}(\mu, \nu) = \max_{A \subseteq \Omega} |\mu(A) - \nu(A)|.$$




The coupling of two distributions is simply a joint distribution of them.

**Definition 6 (Coupling)** . *Let $\mu$ and $\nu$ be two distributions on the same space $\Omega$. Let $\omega$ be a distribution on the space $\Omega \times \Omega$. If $(X, Y) \sim \omega$ satisfies $X \sim \mu$ and $Y \sim \nu$, then $\omega$ is called a coupling of $\mu$ and $\nu$.*

In other words, the marginal probabilities of the disjoint distribution $\omega$ are $\mu$ and $\nu$ respectively. A special case is when $x$ and $y$ are independently. However, in many applications, we want $x$ and $y$ to be correlated while keeping their respect marginal probabilities correct.

We now give a toy example about how to construct different couplings on two fixed distributions. There are two coins: the first coin has probability $\frac{1}{2}$ for head in a toss and $\frac{1}{2}$ for tail, and the second coin has probability $\frac{1}{3}$ and $\frac{2}{3}$ respectively. We now construct two couplings as follows.

| prob $x$ \ $y$ | HEAD | TAIL |
|---|---|---|
| HEAD | 1/3 | 1/6 |
| TAIL | 0 | 1/2 |

| prob $x$ \ $y$ | HEAD | TAIL |
|---|---|---|
| HEAD | 1/6 | 1/3 |
| TAIL | 1/6 | 1/3 |

The table defines a joint distribition and the sum of a certain row/column equal to the corresponding marginal probability. It is clear that both table are couplings of the two coins. Among all the possible couplings, sometimes we are interested in the one who is "mostly coupled".

**Lemma 7 (Coupling Lemma)** . *Let $\mu$ and $\nu$ be two distributions on a sample space $\Omega$. Then for any coupling $\omega$ of $\mu$ and $\nu$ it holds that,*

$$\mathbf{Pr}_{(X,Y)\sim\omega}[X \neq Y] \geq D_{\mathrm{TV}}(\mu, \nu).$$

*And furthermore, there exists a coupling $\omega^*$ of $\mu$ and $\nu$ such that*

$$\mathbf{Pr}_{(X,Y)\sim\omega^*}[X \neq Y] = D_{\mathrm{TV}}(\mu, \nu).$$

*Proof.* For finite $\Omega$, designing a coupling is equivalent to filling a $\Omega \times \Omega$ matrix in the way that the marginals are correct.

Clearly we have

$$\begin{aligned}\mathbf{Pr}[X = Y] &= \sum_{t\in\Omega} \mathbf{Pr}[X = Y = t] \\ &\leq \sum_{t\in\Omega} \min\{\mu(t), \nu(t)\}.\end{aligned}$$

Thus,

$$\begin{aligned}\mathbf{Pr}\left[X \neq Y\right] &\geq 1 - \sum_{t\in\Omega} \min\left(\mu(t), \nu(t)\right) \\ &= \sum_{t\in\Omega} \left(\mu(t) - \min\left\{\mu(t), \nu(t)\right\}\right) \\ &= \max_{A\subseteq\Omega} \left\{\mu(A) - \nu(A)\right\} \\ &= D_{\mathrm{TV}}(\mu, \nu).\end{aligned}$$

To construct $\omega^*$ achieving the equality, for every $t \in \Omega$, we let $\mathbf{Pr}_{(X,Y)\sim\omega^*}\left[X = Y = t\right] = \min\left\{\mu(t), \nu(t)\right\}$. □

The coupling lemma provides a way to upper bound the distance between two distributions: For any two distributions $\mu$ and $\nu$ and any coupling $\omega$ of $\mu$ and $\nu$, an upper bound for $\mathbf{Pr}_{(X,Y)\sim\omega}\left[X \neq Y\right]$ is an upper bound for $D_{TV}(\mu, \nu)$. This is a quite useful approach to bound the total variation distance.

### 1.2 Proof of FTMC

*Proof.* We already know that $P$ has a stationary distribution $\pi$. What we would like to show is that for all starting distribution $\mu_0$, it holds that

$$\lim_{t\to\infty} D_{\mathrm{TV}}(\mu_t, \pi) = 0\,,$$

where $\mu_t^\intercal = \mu_0^\intercal P^t$.

Suppose that $\{X_t\}$ and $\{Y_t\}$ are two identical Markov chains starting from different distribution, where $Y_0 \sim \pi$ while $X_0$ is generated from an arbitrary distribution $\mu_0$.

Now we have two sequence of random variables:

$$\begin{array}{ccccccccccccc}
\mu_0 & & \mu_1 & & & & & & \mu_t & & & & \\
\wr & & \wr & & & & & & \wr & & & & \\
X_0 & \to & X_1 & \to & X_2 & \to & \cdots & \to & X_t & \to & X_{t+1} & \to & \cdots \\
\\
Y_0 & \to & Y_1 & \to & Y_2 & \to & \cdots & \to & Y_t & \to & Y_{t+1} & \to & \cdots \\
\wr & & \wr & & & & & & \wr & & & & \\
\pi & & \pi & & & & & & \pi & & & &
\end{array}$$

The coupling lemma establishes the connection between the distance of distributions and the discrepancy of random variables. To show that $D_{\mathrm{TV}}(\mu_t, \pi) \to 0$, it is sufficient to construct a coupling $\omega_t$ of $\mu_t$ and $\pi$ and then compute $\mathbf{Pr}_{(X_t,Y_t)\sim\omega_t}\left[X_t \neq Y_t\right]$.

Here we give a simple coupling. Let $(X_t, Y_t) \sim \omega_t$ and we construct $\omega_{t+1}$. If $X_t = Y_t$ for some $t \geq 0$, then let $X_{t'} = Y_{t'}$ for all $t' > t$, otherwise $X_{t+1}$ and $Y_{t+1}$ are independent. Namely, $\{X_t\}$ and $\{Y_t\}$ are two independent Markov chains until $X_t$ and $Y_t$ reach the same state for some $t \geq 0$, and once they meet together then they move together forever. The coupling lemma tells us that $D_{\mathrm{TV}}(\mu_t, \pi) \leq \mathbf{Pr}_{(X_t,Y_t)\sim\omega_t}\left[X_t \neq Y_t\right]$.

Let $t^*$ be the same $t^*$ with Claim 2. Let $\alpha$ be a positive constant such that $P^{t^*}(i, j) \geq \alpha > 0$ for any state pair $(i, j)$. Define event $B$ as $\{\exists t < t^*, X_t = Y_t\}$.

We have that

$$\begin{aligned}\mathbf{Pr}\left[X_{t^*} = Y_{t^*}\right] &= \mathbf{Pr}\left[X_{t^*} = Y_{t^*}|B\right]\mathbf{Pr}\left[B\right] + \mathbf{Pr}\left[X_{t^*} = Y_{t^*}|\bar{B}\right]\mathbf{Pr}\left[\bar{B}\right]\\ &\geq 1\cdot\mathbf{Pr}\left[B\right] + \mathbf{Pr}\left[X_{t^*} = Y_{t^*} = 1|\bar{B}\right]\mathbf{Pr}\left[\bar{B}\right]\\ &\geq \mathbf{Pr}\left[B\right] + \alpha^2\mathbf{Pr}\left[\bar{B}\right]\\ &\geq \alpha^2.\end{aligned}$$

By the coupling and the Markov property, we have

$$\begin{aligned}\mathbf{Pr}\left[X_{2t^*} \neq Y_{2t^*}\right] &= \mathbf{Pr}\left[X_{2t^*} \neq Y_{2t^*}|X_{t^*} = Y_{t^*}\right]\mathbf{Pr}\left[X_{t^*} = Y_{t^*}\right]\\ &\quad + \mathbf{Pr}\left[X_{2t^*} \neq Y_{2t^*}|X_{t^*} \neq Y_{t^*}\right]\mathbf{Pr}\left[X_{t^*} \neq Y_{t^*}\right]\\ &\leq \mathbf{Pr}\left[X_{2t^*} \neq Y_{2t^*}|X_{t^*} \neq Y_{t^*}\right]\mathbf{Pr}\left[X_{t^*} \neq Y_{t^*}\right]\\ &\leq (1-\alpha^2)^2.\end{aligned}$$

Then we have $\mathbf{Pr}\left[X_{kt^*} \neq Y_{kt^*}\right] \leq (1-\alpha^2)^k$ by recursion. It yields that

$$\mathbf{Pr}\left[X_t \neq Y_t\right] = \sum_{x_0, y_0 \in [n]} \mu_0(x_0)\cdot\pi(y_0)\cdot\mathbf{Pr}\left[X_t \neq Y_t|X_0 = x_0, Y_0 = y_0\right] \to 0$$

as $t \to \infty$. □

## 2 Mixing Time

We are ready to study the convergence rate of Markov chains. We start with the notion of mixing time. For any $\varepsilon > 0$, the mixing time of a Markov chain $P$ up to error $\varepsilon$ is the minimum step $t$ such that if we run the Markov chain from any initial distribution, its total variation distance to the stationary distribution is at most $\varepsilon$. Formally,

$$\tau_{\text{mix}}(\varepsilon) := \max_{\mu_0}\min_{t} D_{\text{TV}}(\mu_t, \pi) \leq \varepsilon.$$

Recalling in our proof of FTMC using the coupling argument, we obtain the following inequality

$$D_{\text{TV}}(\mu_t, \pi) \leq \mathbf{Pr}_{(X_t, Y_t)\sim\omega_t}\left[X_t \neq Y_t\right].$$

Therefore, if we can construct a coupling $\omega_t$ such that for two arbitrary initial distributions, $\mathbf{Pr}_{(X_t, Y_t)\sim\omega_t}\left[X_t \neq Y_t\right] \leq \varepsilon$, then $\tau_{\text{mix}}(\varepsilon) \leq t$.

**Example 1 (Random walk on hypercube)** . *Consider the random walk on the n-cube. The state space $\Omega = \{0,1\}^n$, and there is an edge between two state $x$ and $y$ iff $\|x-y\|_1 = 1$. We start from a point $X_0 \in \Omega$. In each step,*

- *With probability $\frac{1}{2}$ do nothing.*
- *Otherwise, pick $i \in [n]$ uniformly at random and flip $X(i)$.*

*It's equivalent to the following process:*

- *Pick $i \in [n], b \in \{0,1\}$ uniformly at random.*
- *Change $X(i)$ to $b$.*

*Now we analyze the mixing time of the process using coupling. The apply the following simple coupling rule:*

- *We couple two walks $X_t$ and $Y_t$ by choosing the same $i, b$ in every step.*

*Once a position $i \in [n]$ has been picked, $X_t(i)$ and $Y_t(i)$ will be the same forever. Therefore, the problem again reduces to the coupon collector problem.*

*For $t \geq n \log n + cn$, the probability that the $i^{th}$ dimention is not chosen is*

$$\left(1 - \frac{1}{n}\right)^{n \log n + cn} \leq \frac{e^{-c}}{n}.$$

*Then the probability that there exists at least one dimention which is not chosen is no larger than $e^{-c}$. We want this value to be less than $\epsilon$. Then we choose $c > \log \frac{1}{\epsilon}$. Thus,*

$$\tau_{\text{mix}}(\varepsilon) \leq n \log \frac{n}{\varepsilon}.$$

*Let's modify the process a bit by changing $\frac{1}{2}$ into $\frac{1}{n+1}$, i.e. w.p. $\frac{1}{n+1}$ do nothing, to make the lazy walk more active. Note that we add the lazy move in order to make the chain aperiodic.*

*Now in this case, we describe another coupling of $X_t, Y_t$. Without loss of generality, we can reorder the entries of two vectors so that all disagreeing entries come first. Namely there exists an index $k$ such that $X_t(i) \neq Y_t(i)$ if $1 \leq i \leq k$, and $X_t(i) = Y_t(i)$ for $i > k$. Our coupling is as follows:*

- *If $k = 0$, $Y$ acts the same as $X$.*
- *If $k = 1$, $Y$ acts the same as $X$ except when $X$ flips the first entry, $Y$ does nothing and vice versa.*
- *For $k > 2$, we distinguish between whether $X$ flip indices in $[k]$:*
  - *If $X$ did nothing or flipped one of $i > k$: $Y$ acts the same.*
  - *If $X$ flipped $1 \leq i \leq k$: $Y$ flips $(i \bmod k) + 1$, i.e. $1 \mapsto 2, 2 \mapsto 3, \cdots, k-1 \mapsto k, k \mapsto 1$.*

*It's clear that the above is indeed a coupling. In fact, this coupling acts like a doubled speed coupon collector, since in the case $k > 2$ we can always collect two coupons at a time when lady luck is smiling. It is therefore conceivable that*

$$\tau_{mix} \leq \frac{1}{2} n \log n + O(n).$$

**Example 2 (Shuffling cards)** *. Given a deck of $n$ cards, consider the following rule of shuffling*

- *pick a card uniformly at random;*

- *put the card on the top.*

*The shuffling rule can be viewed as a random walk on all $n!$ permutations of the $n$ cards and it is easy to verify that the uniform distribution is the stationary distribution. Let us design a coupling for this Markov chain. That is, let $X_t$ and $Y_t$ be decks of cards, and we construct $X_{t+1}$ and $Y_{t+1}$ by*

- *picking the same random card and put it on the top.*

Note that we are picking the "same card", not the card at the same location. That is, we draw a random card from $X_t$, say $\heartsuit K$, and then we pick $\heartsuit K$ in $Y_t$ as well.

*This is clearly a coupling, and once some card, say $\heartsuit K$ has been picked, then $\heartsuit K$ in two decks will be always at the same location. Therefore, if we ask in how many rounds $T$, $X_T = Y_T$, then the question is equivalent to the coupon collector problem again. So we have,*

$$\tau_{\mathrm{mix}}(\varepsilon) \leq n \log \frac{n}{\varepsilon}.$$