

DTMC and Applications

Def: $(X_n)_{n \in \mathbb{Z}_{\geq 0}}$ is DTMC if it satisfies Markovian property: $P(X_{n+1} = i_{n+1} \mid X_k = i_k, 1 \leq k \leq n) = P(X_{n+1} = i_{n+1} \mid X_n = i_n)$

Remark: i) The equation can be extended:

$$P(X_{n+1} \in A_{n+1} \mid X_k \in A_k, 1 \leq k \leq n) =$$

$$P(X_{n+1} \in A_{n+1} \mid X_n \in A_n), \text{ for } A_k \subset S, 1 \leq k \leq n+1.$$

ii) A : past. B : present. C : future.

$$\Rightarrow P(C \mid DA) = P(C \mid B), \text{ depend on present.}$$

$$P(A \mid C \mid B) = P(A \mid B) P(C \mid B). A, C \text{ have}$$

the same role.

A DTMC is specified by:

i) State space S (discrete), at most countable.

ii) Initial dist. π_0 : $X_0 \sim \pi_0$.

iii) Prob. transition rules: $P = (P_{ij})$.

(1) Metropolis Method:

To simulate a dist. π on finite states space

S . One way is using Limit Thm to approxi.

On a connected graph. Define N_{ij} is set

of neighbour points of j . $\lambda(i)$ is $\# N(i)$

① Run a random Walk on the graph:

$$P_{rw}(i, j) = \begin{cases} 1/\lambda(i) & j \in N(i) \\ 0 & j \notin N(i) \end{cases}$$

$\pi_{rw}(i) = \lambda(i) / \sum_j \lambda(j)$, is stationary dist.

② Modification:

Note $\pi_{rw}(i) \propto \lambda(i)$. if we want: $\pi(i) \propto f(i) \lambda(i)$

$$\text{Set: } p(i, j) = \begin{cases} \min\{1, f(j)/f(i)\} / \lambda(i) & j \in N(i) \\ 1 - \sum_{j \in N(i)} p(i, j) & j = i \\ 0 & \text{otherwise} \end{cases}$$

Pf: $\pi(i) p(i, j) \propto \min\{f(i), f(j)\}$. By symmetry:

$$\pi(i) p(i, j) = \pi(j) p(j, i) \Rightarrow \pi p = \pi, \text{ stationary.}$$

Interpret: 1) Choose a neighbour of i w.p. $1/\lambda(i)$

2) If $f(j) \geq f(i)$, then accept j .

3) If $f(j) < f(i)$, then reject w.p. $1 - \frac{f(j)}{f(i)}$

Imp: We don't need to know $\pi(i)$, exactly.

Avoid Normalization.

(2) Simulated Annealing:

Target: Find $i \in S$ s.t. $c(i) = \min_S c(k)$. where $c(i)$ is the cost function. def on set of nodes S in a graph. $|S| < \infty$.

Def: prob. dist. $q_T = \{q_T(i) | i \in S\}$ on S is:

$$q_T(i) = c(i) e^{-c(i)/T} / G(T). \quad G(T) = \sum_S c(i) e^{-c(i)/T}$$

Prmk: i) Choose $f(i) = e^{-c(i)/T}$ in Metropolis Method

$$z(i) \propto c(i) f(i) \Rightarrow z(i) = q_T(i).$$

ii) T stands for temperature.

Denote: $S^* = \{i^* \in S | c(i^*) = \min_S c(k)\}$. With a dist.

$$q^* \text{ on } S^* \text{ is } q^*(i) = c(i) / \sum_{S^*} c(i). \text{ if } i \in S^*.$$

$$q^*(i) = 0 \text{ if } i \notin S^*.$$

Prmk: We only put positive prob. on optimal.

Prop, $q_T \xrightarrow{T \downarrow 0} q^*$ as $T \downarrow 0$.

Pf: Check $q_T(i) \rightarrow q^*(i)$: divide $e^{-\min_S c(i)/T}$. Set $T \downarrow 0$

procedure: 1') Simulate the stationary π_T by Metropolis method. $A_T = (A_T(i,j))_{S \times S}$ is its prob. transition matrix. def by (1) @.

2') When dist. is approaching π_T nearly.

Decrease the temperature to $T_2 < T_1$.

Then approxi. π_{T_2} by A_{T_2} prob. matrix.

3') Repeat these steps. let $T_n \rightarrow 0$ ($n \rightarrow \infty$)

Next. Suppose we have $X_0 \sim \nu_0$. We will cool the temperature at each step. i.e. $P(X_n = i | X_{n-1} = j) = A_{T_{n-1}}(j, i)$

i.e. $X_n \sim \nu_0 A_{T_0} A_{T_1} \dots A_{T_{n-1}}$ $T_n \downarrow 0$.

Denote: $A^{(n)} = \prod_{k=1}^n A_{T_k}$. $\nu^{(n)} = \nu_0 A^{(n)}$.

$r = \min_{i \in S} \max_{j \in S} c(i, j)$, c is distance, and finite :

$S_c = \{i \mid c(i, j) > c(i, i), \text{ exist some } j \in N(i)\}$.

$L = \max_{i \in S} \max_{j \in N(i)} |c(i, j) - c(i, i)|$. max local fluctuation.

Rank: S_c is set of points which is not local max. Then r is min radius of $i \in S_c$ st. contain all $j \in S$

\Rightarrow Our goal is simulating π^* :

Thm. (Main Thm)

For cooling schedule $(T_n)_{n \geq 0}$ satisfies:

i) $T_{n+1} < T_n$, $\forall n \geq 0$. ii) $T_n \rightarrow 0$ ($n \rightarrow \infty$)

iii) $\sum_k e^{-rL/T_{k-1}} = \infty$. Then, we have:

$$\|A^{(n)}(i, \cdot) - \pi^*\| = \sup_{S \subset S} |A^{(n)}(i, S) - \pi^*(S)| \xrightarrow{n \rightarrow \infty} 0, \forall i$$

Pf: It's application of theory of time-inhomogeneous Markov chain. will be proven later.

Rmk: We can schedule proper temperatures

$$(T_n) = (Y/\log n) \cdot Y \geq rL.$$

(3) Ergodicity of

Time-inhomogeneous MC:

Consider a time-inhomogeneous Markov Chain (X_n) .

From X_n to X_{n+1} , it has different prob. transition matrix P_n . Denote: $P^{(m,n)} = \prod_{k=m}^n P_k$.

Def: i) (X_n) is strongly ergodic if \exists dist. π^*

$$\text{s.t. } \lim_{n \rightarrow \infty} \sup_{i \in S} \|P^{(m,n)}(i, \cdot) - \pi^*\| = 0, \forall m$$

ii) (X_n) is weakly ergodic if:

$$\lim_{n \rightarrow \infty} \sup_{i,j} \|P^{(m,n)}(i, \cdot) - P^{(m,n)}(j, \cdot)\| = 0, \forall m$$

Rmk: i) "Weak ergodic" is kind of "loss of memory" after a long time. But: it's unnecessary to converge to some dist.

ii) " $\forall m$ " is because we don't want some prob. matrix P_i to determine the whole convergence. (like seq. conv.)

① Ergodic Coefficient:

Define: $\delta(P) = \sup_{i,j} \|P(i, \cdot) - P(j, \cdot)\|$, for prob matrix P .

Rmk: $\delta(p) = 0 \Rightarrow$ Next move doesn't depend on current state. i.e. lose memory totally.

Lemma $\delta(pa) \leq \delta(p) \delta(a)$. $\forall p, a$ prob. matrix.

Pf: Set $A = \{k \mid (pa)_{i,k} > (pa)_{j,k}\}$.

$$\begin{aligned} \forall i, j \in S: \sum_{k \in S} ((pa)_{i,k} - (pa)_{j,k})^+ &= \sum_{k \in A} (\square - \square) \\ &= \sum_{k \in A} \sum_{l \in S} p_{il} a_{lk} - p_{jl} a_{lk} \\ &= \sum_{l \in S} (p_{il} - p_{jl}) \sum_{k \in A} a_{lk} \\ &\leq \sum_S (p_{il} - p_{jl})^+ \sup_l \sum_{k \in A} a_{lk} - (p_{il} - p_{jl}) \inf_l \sum_{k \in A} a_{lk} \\ &\stackrel{\sum p_{il} - p_{jl} = 0}{=} \sum_{l \in S} (p_{il} - p_{jl})^+ \left(\sup_l \sum_{k \in A} a_{lk} - \inf_l \sum_{k \in A} a_{lk} \right) \\ &\leq \sum_S (p_{il} - p_{jl})^+ \delta(a) \leq \delta(p) \delta(a). \end{aligned}$$

Lemma For dist. π, m and prob matrix P . We have:

$$\|(\pi - m)P\| \leq \|\pi - m\| \delta(P).$$

$$\begin{aligned} \text{pf: } \forall m \leq S. \left| \sum_m (\pi - m)P(i) \right| &= \left| \sum_{i \in M} \sum_{t \in S} (\pi - m)_t P_{ti} \right| \\ &= \left| \sum_S (\pi - m)_t \sum_{i \in M} P_{ti} \right| \quad (\text{By } \sum (\pi - m)_t = 0) \\ &\leq \sum_{t \in S} (\pi - m)_t^+ \left(\sup_t \sum_{i \in M} P_{ti} - \inf_t \sum_{i \in M} P_{ti} \right) \\ &\leq \sum_S (\pi - m)_t^+ \delta(P) = \|\pi - m\| \delta(P). \end{aligned}$$

Lemma If \exists column of a prob. matrix whose entries $\geq \alpha$.

Then: $\delta(a) \leq 1-n$.

Pf: $\delta(a) = \sup_{i,j} \sum_S (a_{ik} - a_{jk})^+ = \sup_{i,j} \sum_A (a_{ik} - a_{jk})$
 $\leq \sup_{i,j} \sum_A a_{i,k} - a \leq 1-n$

where suppose that column has index i_0 .

WLOG. $i_0 \in A = \{a_{i,k} > a_{j,k}\}$. Other-

wise: consider A^c . since $\sum a_{ik} - a_{jk} = 0$.

prop. If $\exists (n_k) \uparrow \infty$. $\sum (1 - \delta(p^{(n_k, n_{k+1})})) = \infty$. Then:
 (X_n) is weakly ergodic.

Pf: By $1-x \leq e^{-x}$. We have: $\prod_n \delta(p^{(n_k, n_{k+1})}) = 0$. $\forall m$.

$$\Rightarrow \delta(p^{(n_k, n_{k+1})}) \leq \prod_{i=k}^{L-1} \delta(p^{(n_i, n_{i+1})}) \rightarrow 0 \text{ as } L \rightarrow \infty$$

$$So: \delta(p^{(n, n')}) \lesssim \delta(p^{(n_k, n_{k+1})}) \prod_{i=k}^{L(n)} \delta(p^{(n_i, n_{i+1})}) \xrightarrow{n \rightarrow \infty} 0$$

prop. If (X_n) is weakly ergodic. $\exists (z_k)_{k \geq 0}$ stationary
 list. for $(p_k)_{k \geq 0}$. st. $\sum \|z_k - z_{k+1}\| < \infty$. Then:
 (X_n) is strongly ergodic. $z^* = \lim_n z_n$.

Pf: 1) $\sum \|z_k - z_{k+1}\| < \infty \Rightarrow \lim z_n = z^*$ exist.

$$\|p^{(k,m)}(i, \cdot) - z^*(\cdot)\| \leq \|p^{(k,m)}(i, \cdot) - z_k p^{(k,m)}\|$$

$$+ \|z_k p^{(k,m)} - z_m\| + \|z_m - z^*\| =: A_1 + A_2 + A_3$$

$$2) A_1 \leq \|p^{(k,l)}(i, \cdot) - z_l(\cdot)\| \delta(p^{(l,m)}),$$

$$\rightarrow 0 \text{ as } m \rightarrow \infty. \forall l.$$

$$3') A_2 = \lambda_l p^{(l,m)} - \lambda_m = \lambda_l p_l \cdot p^{(l+1,m)} - \lambda_m$$

$$= \lambda_l \cdot p^{(l+1,m)} - \lambda_m$$

$$= \lambda_{l+1} p^{(l+1,m)} - \lambda_m + (\lambda_l - \lambda_{l+1}) p^{(l+1,m)}$$

$$= \dots = \sum_{k=l}^{m-1} (\lambda_k - \lambda_{k+1}) p^{(k+1,m)}$$

$$\Rightarrow A_2 \leq \sum_{k=l}^{m-1} \|\lambda_k - \lambda_{k+1}\| \rightarrow 0 \text{ (} m \rightarrow \infty \text{)}. \text{ (} \delta < p \leq 2 \text{)}.$$

$$4') A_3 \rightarrow 0 \text{ (} m \rightarrow \infty \text{)} \text{ by 1'). Directly.}$$

② Proof of Main Thm:

Define: Node i_0 is called center. if $i_0 = \arg \max_{j \in S} \ell(i_0, j)$

$$= r = \min_{S_0} \max_S \ell(i, j) \quad , \quad D = \max_i \lambda(i).$$

$$1') \text{ Show: } \sum_{k \geq 1} (1 - \delta \cdot p^{(kr-r, kr)}) = \infty \quad , \quad P_n = A_{T_n}.$$

Pf: For $i \neq j$: $P_{ij}(n) = \min \{1, e^{-\ell(i,j)/T_n}\} / \lambda(i) \geq e^{-L/T_n} / D.$

$$P_{i_0, i_0}(n) = 1 - \sum_{j \in N(i_0)} P_{ij}(n) \xrightarrow{n \rightarrow \infty} 1 - \sum_{\substack{j \in N(i_0) \\ \ell(j) \leq \ell(i_0)}} 1/\lambda(i)$$

$$= \sum_{\substack{j \in N(i_0) \\ \ell(j) > \ell(i_0)}} 1/\lambda(i) > 0 \text{ by } i_0 \in S_0.$$

$$\Rightarrow P_{i_0, i_0}(n) \geq e^{-L/T_n} / D \text{ for } \forall \text{ large } n.$$

$$S_0 = p^{(m-r, m)} \ell(i, i_0) \geq e^{-rL/T_n} / D^{-r} \quad \forall i \in S. \quad \forall m.$$

$$\text{By Lemma: } (1 - \delta \cdot p^{(m-r, m)}) \geq n.$$

$$2') \text{ Show: } \sum \|\lambda_n - \lambda_{n+1}\| < \infty \text{ where } \lambda_n(i) = \frac{\lambda(i) e^{-\ell(i)/T_n}}{G(T_n)}$$

for strongly ergodic.

Lemma: i) $i \in S^* \Rightarrow z_n(i) < z_{n+1}(i) \cdot \forall n$.

ii) $i \notin S^* \Rightarrow \exists \tilde{n}_i$ st. $z_{n+1}(i) < z_n(i) \cdot \forall n \geq \tilde{n}_i$.

Pf: i) is directly check.

ii) $f_i(T) =: e^{-c(i)/T} / h(T)$.

$$f'_i(T) = \lambda(T) \left(\sum_S d_{ik} \right) e^{-c(k)/T} (c(i) - c(k))$$

$$\geq \lambda(T) \left(\lambda_1 e^{-\frac{c(i)}{T}} + \lambda_2 e^{-\frac{c(m)}{T}} \right)$$

where $\lambda(T) \geq 0$, $\lambda_1 = \sum_{c(k) \geq c(i)} d_{ik} (c(i) - c(k))$

and $\lambda_2 = \sum_{c(k) < c(i)} d_{ik} (c(i) - c(k))$, $c(m) = \min_k c(k)$
 $\{c(k) < c(i)\}$

by i) $\notin S^*$, $\{k \mid c(k) < c(i)\} \neq \emptyset$

\Rightarrow for sufficiently small T , $(T_n \downarrow \text{ as } n \uparrow)$

Return to pf:

$$\text{Choose } \tilde{n} = \max_{i \notin S^*} \{\tilde{n}_i\}, \quad \sum_{\tilde{n}} \|z_n - z_{n+1}\| = \sum_{\tilde{n}} \sum_{i \notin S^*} (z_{n+1}(i) - z_n(i))^+$$

$$= \sum_{i \notin S^*} \sum_{\tilde{n}} (z_{n+1}(i) - z_n(i))^+, \text{ by monotone Lemma.}$$

$$\Rightarrow \sum_{\tilde{n}} \|z_n - z_{n+1}\| \leq \sum_{i \notin S^*} \sum_{\tilde{n}} (z_{n+1}(i) - z_n(i))$$

$$= \sum_{S^*} (z^*(i) - z_{\tilde{n}}(i)) \leq z^*(S^*) = 1$$

(4) Card Shuffling:

Q: How close is the deck of cards being random after n shufflings?

i) Rule: Take the top card and insert it into a random position of the deck. equally likely. (May be top again)

ii) Markov Chain:

State space = S_{52} permutation of deck of cards.

so that $|S_{52}| = 52!$

initial dist. = $\pi_0(\beta) = 1$. $\beta = \{ \text{card } k \text{ on position } k \}$

(\downarrow position 1
position 52)

Remark: Stationary π is: $\pi(q) = 1/52!$. $\forall q \in S_{52}$.

and note: (X_n) is irred. aperiodic. MC.

$\Rightarrow \| \pi_n - \pi \| \rightarrow 0$. ($n \rightarrow \infty$)

① Cost of random time:

We will find a random time T . s.t. $X_T \sim \text{Uni}(52!)$.

Def: i) U_n is the position of top card move at the n^{th} shuffling. $U_n \stackrel{i.i.d}{\sim} \text{Unif}(52)$.

ii) $T_1 = \inf \{ n \geq 1 \mid U_n = 52 \}$. $T_k = \inf \{ n > T_k \mid U_n \geq 53-k \}$.

Remark: i) T_k means the time when the top card is inserted below card $52-k$ (so it's in a random position). At time $T = T_1 + 1$. We insert card 52 to a random position. Then we have a deck shuffled randomly!

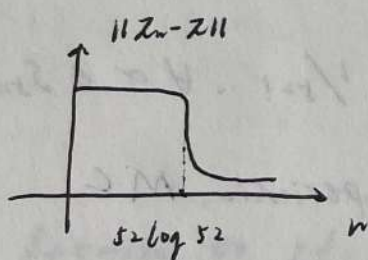
ii) We don't know T_k exactly happen, but know $T = T_{s1} + 1$. since the top card is s_2 at time T_{s1} .

For finding $E(T)$:

$$T_1 \sim \text{Geo}(\frac{1}{s_2}), T_2 - T_1 \sim \text{Geo}(\frac{2}{s_2}) \dots T_k - T_{k-1} \sim \text{Geo}(\frac{k}{s_2})$$

$$T = \sum_{k=1}^{s_2} (T_k - T_{k-1}) + T_1 \Rightarrow E(T) = s_2 \left(\sum_{k=1}^{s_2} \frac{1}{k} \right) \sim s_2 \log s_2.$$

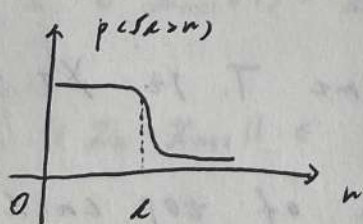
② Threshold Phenomenon:



at T , $\|Z_n - z\|$ will have a abrupt decrease from nearly 1 to nearly 0 at $n = \lceil s_2 \log s_2 \rceil$.

Remark: Other example:

$X_n \stackrel{i.i.d}{\sim} N(1,1)$, $S_n = \sum_{i=1}^n X_i$. Then near $n = d$:



$p(S_n > n)$ will decrease at order $O(1/n)$, if d is large enough.

Denote: $A(n) = \|Z_n - z\|$.

Def: Random time T is strong stationary time

if: i) T is stopping time

ii) X_T indept with T .

iii) $X_T \sim \pi$, stationary dist.

Lemma. If T is strong stationary time for (X_n) .

Then: $\|Z_n - Z\| \leq P(T \geq n)$. $\forall n$.

Pf: 1') Show: $P(T \leq n, X_n \in A) = P(T \leq n) Z(A)$.

$$\text{LHS} = \sum_{k=1}^n P(T=k, X_n \in A)$$

$$= \sum_k \sum_i P(T=k, X_k=i, X_n \in A)$$

$$= \sum_k \sum_i P^{n-k}(i, A) P(T=k, X_T=i)$$

$$= P(T \leq n) Z(A).$$

$$2') \forall A \subseteq S. \quad Z(A) - Z_n(A) =$$

$$Z(A) - P(X_n \in A, T \leq n) - P(X_n \in A, T > n)$$

$$= Z(A) P(T > n) - P(X_n \in A, T > n)$$

$$\Rightarrow |Z(A) - Z_n(A)| \leq \max\{\square, \square\} \leq P(T \geq n)$$

Thm: $\Delta(\lambda \log \lambda + c\lambda) \leq P(T > \lambda \log \lambda + c\lambda) \leq e^{-c}$. $\forall c \geq 0, \lambda \geq 2$.

Pf: $T \sim \text{Geo}(1/\lambda) \oplus \dots \oplus \text{Geo}(\lambda/\lambda)$

(Famous Dist. in Coupons collector Problem)

$$\{T > n\} = \bigcup_{k=1}^{\lambda} \{k^{\text{th}} \text{ coupon isn't collected at time } n\}$$
$$\stackrel{\Delta}{=} \bigcup_{k=1}^{\lambda} A_k.$$

$$\Rightarrow P(T > n) \leq \sum P(A_k) = \sum_{k=1}^{\lambda} \left(\frac{\lambda-1}{\lambda}\right)^n \leq \lambda e^{-n/\lambda}$$

rmk: Fix c . if λ is large enough, then $c\lambda$.

is small relative to $\lambda \log \lambda$

So it will have an abrupt decrease near

$\lambda \log \lambda$. When c changes a lot.

Thm. $k(n) = n \log n - c n$. (c) $\nearrow \infty$ as $n \rightarrow \infty$.

Then: $\| \pi_{k(n)}^{(n)} - \pi^{(n)} \| \xrightarrow{n \rightarrow \infty} 1$. index "(n)" means

list, π , is relative to deck size n .

Pf: We want to find event $A \in \mathcal{S}$ st.

$\pi_{k(n)}^{(n)}(A)$ is large (≈ 1). $\pi^{(n)}(A)$ is small.

Consider: $A_{n,n} = \{ \text{Card } n-n+1 \sim n \text{ are still in their origin order} \}$

$\pi(A_{n,n}) = 1/n!$ (permute first n cards)

Note: $A_{n,n} = \{ \text{Card } n-n+1 \text{ isn't at top yet} \}$

$\Rightarrow \pi_k(A_{n,n}) \geq p(k > k)$.

k is number of shufflings required for card $n-n+1$ to rise to top.

$k \sim \text{Geo}(n/n) \oplus \dots \oplus \text{Geo}(n-1/n)$

$$\begin{cases} E(k) = n(\log n - \log e + o(1)) \\ \text{Var}(k) \leq n^2(\frac{1}{n} + \dots) = O(\frac{1}{n})n^2 \quad (\text{Var}(\text{Geo}(p)) = \frac{1-p}{p^2}) \end{cases}$$

$$S_0 = p(k > k(n)) = p(k - E(k) > -n(\log n - \log e + o(1)))$$

$$\geq 1 - \text{Var}(k) / n^2 (\square)$$

choose $a_n = e^{cn/2}$. ($c = a_n$ depend on n)

Prk: By the two Thms. above. We know:

$\left(\frac{n \log n}{2} \right)$ a subtle interval of $n \log n$

contains a abrupt decrease!