

1) Basic concepts

Melih Kandemir

University of Southern Denmark Department of Mathematics and Computer Science (IMADA)

February 6, 2025

Supervised learning

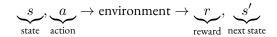
• Setup: Observation space $\mathcal X$ and label space $\mathcal Y$ and a map $f:\mathcal X\to\mathcal Y$ called a labeling function:

$$\underbrace{x}_{ ext{observation}} o \underbrace{f(\cdot)}_{ ext{labeling function}} o \underbrace{y}_{ ext{label}}$$

- Data: $\mathcal{D}_n = \{(x_i, y_i) : i = 1, \dots, n\}$ called a training set.
- *Problem:* Devise an algorithm $\mathbb{A}(\mathcal{D}_n)$ that returns a *predictor* $\hat{f}: \mathcal{X} \to \mathcal{Y}$ such that the generalization error $\mathbb{E}_x[\ell(\hat{f}(x), f(x))]$ is minimum for some loss function ℓ suitable to the output space.
- *Dilemma:* Bias (finding abstractions from individual observations) versus variance (accurately predicting individual observations)

Reinforcement learning: What?

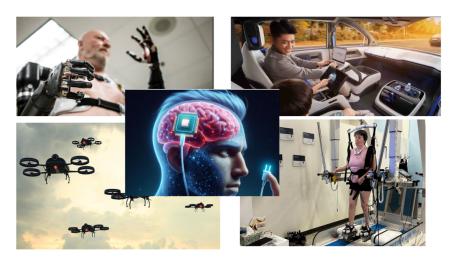
• *Setup:* State space S and action space A



- Data: $\mathcal{D}_n = \{(s_i, a_i, r_i, s_i') : i = 1, \dots, n\}$ called a replay buffer.
- *Problem:* Devise an algorithm $\mathbb{A}(\mathcal{D}_n)$ that returns a *policy (agent)* $\pi: \mathcal{S} \to \mathcal{A}$ such that the total observed reward $\mathbb{E}_s[\sum_{t=1}^{\infty} r_t]$ is maximum.
- *Dilemma:* Exploration (knowing the environment better) versus exploitation (getting maximum reward with the current environmental knowledge).
- *Synonyms:* Approximate Dynamic Programming (ADP), Neuro-Dynamic Programming (NDP)

Reinforcement Learning: Why? (user view)

We already have intelligent data processors. Next step is to have intelligent agents.



Reinforcement learning: Why? (expert view)

abilities expressed within that experience)

The reward hypothesis: All machine learning setups can be described as a reward-based learning scheme.

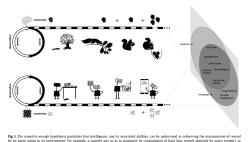


exhibit a wide variety of abilities associated with intelligence (depicted on the right as a projection from an agent's stream of experience onto a set of Figure: D. Silver et al., Reward is enough, Artif. Intl., 2021

a kitchen robot acts to maximise cleanliness (bottom, reward depicted by bubble symbol). To achieve these soals, complex behaviours are required that



History

- 1962: Checkers at human level (Arthur Samuel)
- 1992: Backgammon at super-human level (Gerald Tesauro). Uses neural networks for temporal difference learning. The model invented new openings adopted by grandmaster later.
- 1996: Chess at super-human level (IBM, Deep Blue), but NOT with RL.
- 2015: Go at super-human level (DeepMind, AlphaGo), reusing Tesauro's ideas on improved hardware.
- 2022: Continual improvement of large language models from human feedback (OpenAI, RLHF)
- 2025: Large language models with reasoning capabilities (DeepSeek, GRPO)

Discrete Dynamic Systems

$$s_{t+1} = f_t(s_t, a_t), t = 0, 1, \dots, T-1$$

where

- t is the time index
- $s_t \in \mathcal{S}_t$ is the state at time t and \mathcal{S}_t is the set of possible states at time t
- $a_t \in \mathcal{A}_t$ is the action (control variable) at time t and \mathcal{A}_t is the set of possible actions at time t
- $f_t: \mathcal{S}_t \times \mathcal{A}_t \to \mathcal{S}_{t+1}$ is the state transition function that characterizes the environment dynamics.
- ullet T>0 is the time horizon of the system.

Example: Linear dynamic systems

$$s_{t+1} = As_t + Ba_t \tag{I}$$

where $s_t \in \mathbb{R}^n$, $a_t \in \mathbb{R}^m$, $A \in \mathbb{R}^{n \times n}$, and $A \in \mathbb{R}^{n \times m}$.

Basic concepts

• The above system is *time-varying* because f_t , S_t , A_t depend on t. A *time-invariant* system would look as below:

$$s_{t+1} = f(s_t, a_t), t = 0, 1, \dots, T-1$$

where $s_t \in \mathcal{S}$ and $a_t \in \mathcal{A}$.

• The state-action space is *finite (a.k.a. discrete or tabular)* if

$$S_t = \{1, 2, \dots, n_t\}$$
 and $A_t(s) = \{1, 2, \dots, m_t(s)\}, s \in S_t$

for all time steps t.

• A sequence $h_T = (s_0, a_0, \dots, s_{T-1}, a_{T-1}, s_T)$ such that $a_t \in \mathcal{A}_t$ and $s_{t+1} = f_t(s_t, a_t)$ for $t \in \{0, \dots, T-1\}$ is called a *feasible path*.

Feasible path

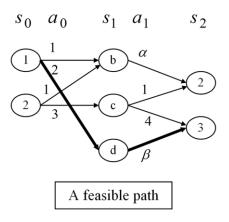


Figure is taken from Mannor et al.

Finite horizon decision problem

Total reward: (a.k.a. cumulative reward) Given a feasible path h_t

$$V_t(h_t) := \sum_{t=0}^{T-1} r_t(s_t, a_t) + r_T(s_T)$$

where

- $r_t(s_t, a_t)$ is the instantaneous (single-stage) reward at stage t,
- r_T is the *terminal* reward.

T-stage finite horizon problem: Find a feasible h_T^st such that

$$h_T^* = \arg\max_{h_T} V_T(h_T).$$

Such h_T^* is called an *optimal path* from s_0 .

Policy

A *deterministic* control policy is

- History-dependent if $a_t = \pi_t(h_t)$ such that $\pi_t \in \Pi_{HD}$
- *Markov* if $a_t = \pi_t(s_t)$ such that $\pi_t \in \Pi_{MD}$
- Stationary if $a_t = \pi(s_t)$ such that $\pi \in \Pi_{SD}$
- Note that $\Pi_{HD} \supset \Pi_{MD} \supset \Pi_{SD}$.

A stochastic (a.k.a. randomized, probabilistic) control policy is

- History-dependent if $P(a_t = a|h_t) = \pi_t(a|h_t)$ such that $\pi_t \in \Pi_{HS}$
- Markov if $P(a_t = a|s_t) = \pi_t(a|s_t)$ such that $\pi_t \in \Pi_{MS}$
- Stationary if $P(a_t = a|s_t) = \pi(a|s_t)$ such that $\pi \in \Pi_{SS}$
- Note that $\Pi_{HS} \supset \Pi_{MS} \supset \Pi_{SS}$.

where $P(\cdot|\cdot)$ defines conditional probability.

Policy versus a feasible path

- Policy specifies an action for each state.
- Path specifies an action only for the states on the path.
- Induced path of a policy π_t is a path h_T^{π} such that $a_t = \pi_t(h_t)$ for all $t \in [T]$.

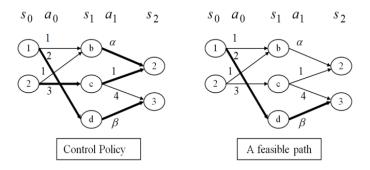


Figure is taken from Mannor et al.

Notation: $[T] = \{0, 1, 2, \dots, T-1\}.$

Reduction between policy classes

Define state-action probability of time step t induced by a policy π as

$$\rho_t^{\pi}(s, a) := P(a_t = a, s_t = s | h_{t-1}^{\pi})$$
$$= \mathbb{E}_{h_{t-1}^{\pi}} [\mathbb{I}(s_t = s, a_t = a) | h_{t-1}^{\pi}]$$

and plug into the definition of total reward

$$\mathbb{E}[V_T(h_T^{\pi})] = \sum_{t=0}^{T-1} \sum_{(s,a)\in\mathcal{S}_t\times\mathcal{A}_t} r_t(s,a) \rho_t^{\pi}(s,a)$$
$$=: \mathbb{E}[V^{\pi}(s_0)]$$

where $V^{\pi}(s_0)$ is the *reward-to-go* for state s_0 at time 0 when policy π is executed. Hence, the expected total reward of two policies π and π' will be equal if and only if $\rho_t^{\pi}(s,a) = \rho_t^{\pi'}(s,a)$.

Notation: $\mathbb{I}(\cdot)$ is the indicator function and $\mathbb{E}[\cdot]$ is the expectation.

From Π_{HS} to Π_{MS}

Theorem

For any stochastic history-dependent policy $\pi \in \Pi_{HS}$ there exists a stochastic Markov policy $\pi' \in \Pi_{MS}$ such that $\rho_t^{\pi}(s, a) = \rho_t^{\pi'}(s, a)$ for all $(s, a) \in \mathcal{S}_t \times \mathcal{A}_t$, which implies

$$\mathbb{E}[V^{\pi}(s_0)] = \mathbb{E}[V^{\pi'}(s_0)]$$

Proof sketch. Choose

$$\pi'_t(a|s) = \frac{\rho_t^{\pi}(s, a)}{\sum_{a' \in \mathcal{A}_t} \rho_t^{\pi}(s, a')},$$

define $ho_t^\pi(s_0) := P(s_t = s | h_{t-1}^\pi)$ and apply induction.

From Π_{MS} to Π_{MD}

Theorem

For any stochastic Markov policy $\pi \in \Pi_{MS}$ there exists a better deterministic Markov policy $\pi' \in \Pi_{MD}$ in the sense that

$$\mathbb{E}[V^{\pi}(s_0)] \le \mathbb{E}[V^{\pi'}(s_0)].$$

Proof sketch. Backward induction by claim: For any policy $\pi \in \Pi_{MS}$ which is deterministic in [t+1,T] there is a policy $\pi' \in \Pi_{MS}$ which is deterministic in [t,T] and $\mathbb{E}[V^{\pi}(s_0)] \leq \mathbb{E}[V^{\pi'}(s_0)]$. Base case t=T holds trivially. In the induction step do

$$\pi'_t(s_t) = \arg\max_{a \in \mathcal{A}_t} r_t(s_t, a) + V^{\pi}(f_t(s_t, a))$$

which would satisfy

$$\mathbb{E}[V^{\pi}(s_t)] = \mathbb{E}_{h_t^{\pi}}[\mathbb{E}_{a_t \sim \pi}[r_t(s_t, a_t) + V^{\pi}(f_t(s_t, a_t))]]$$

$$\leq \mathbb{E}_{h_t^{\pi}}\left[\max_{a_t \in \mathcal{A}_t} r_t(s_t, a_t) + V^{\pi}(f_t(s_t, a_t))\right] = \mathbb{E}[V^{\pi'}(s_t)].$$

Optimal control policies

Definition

A control policy $\pi \in \Pi_{MD}$ is called *optimal* if for each $s_0 \in \mathcal{S}_0$ it holds that $V^{\pi}(s_0) \geq V^{\pi'}(s_0)$ for any other $\pi' \in \Pi_{MD}$.

T-stage finite-horizon planning problem: Find the optimal π for a T-stage deterministic dynamical system.

Brute-force search: Assume $|\mathcal{S}_t|=n$ and $|\mathcal{A}_t(s)|=m$. Then we need to consider m^{nT} policies. When T=n=m=10, this amounts to 10^{100} policies! Dynamic programming will speed up the search.

Finite horizon dynamic programming

- Dynamic Programming (DP) breaks down the T-stage problem into T sequential single-stage optimization problems.
- DP builds on Bellman's Principle of Optimality:

The tail of an optimal policy is optimal for the tail problem.

- The same principle does not hold for the head problem!
- The essence of DP is to apply this principle recursively from the last stage backwards.

Remark: Tail problem is defined with respect to a single starting state.

The DP algorithm

Algorithm Finite-horizon Dynamic Programming

- 1: $V_T(s) = r_T(s)$ for all $s \in \mathcal{S}_T$
- 2: **for all** $t = T 1, \dots, 0$ **do**
- 3: Compute $V_t(s) = \max_{a \in \mathcal{A}_t} \left\{ r_t(s, a) + V_{t+1}(f_t(s, a)) \right\}$ for all $s \in \mathcal{S}_t$
- 4: end for
- 5: **return** $\pi_t^*(s) \in \arg \max_{a \in \mathcal{A}_t} \{ r_t(s, a) + V_{t+1}(f_t(s, a)) \}$ for $t \in [T]$.

In the algorithm above

- ullet $V_t: \mathcal{S}_t o \mathbb{R}$ are called the *value functions* that are calculated recursively.
- Thanks to the value functions, the algorithm visits each state exactly once!
- The step $V_t(s) = \max_{a \in \mathcal{A}_t} \{ r_t(s, a) + V_{t+1}(f_t(s, a)) \}$ is called the Bellman equation.
- It is guaranteed that (π_t^*) is optimal and $V_0(s) = \max_{\pi} V^{\pi}(s), \forall s \in \mathcal{S}_0$.

Example: Run the algorithm on this decision graph

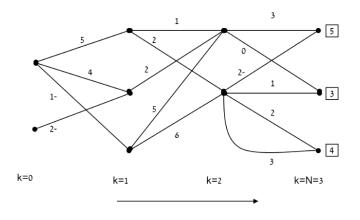


Figure taken from Mannor et al.

Average reward criteria

The aim is to maximize the expectation of:

$$R_{avg} = \lim_{T \to \infty} \frac{1}{T} \sum_{t=0}^{T} r_t(s_t, a_t).$$

Any finite prefix has no influence on the final average reward. For any DDP, the optimal average reward is reached by a policy that cycles around a simple cycle. The maximum average reward is the total reward of this simple cycle.

Linear quadratic regulator (LQR)

This is a continuous optimal control method that assumes that dynamics are linearly and costs are quadratically dependent on the states and actions:

$$\min_{a_0,...,a_T} \sum_{t=0}^{T} c_t(s_t, a_t),$$
s.t. $s_{t+1} = A_t s_t + B_t a_t,$

$$c_t = s_t^{\top} Q_t s_t + a_t^{\top} R_t a_t, \quad \forall t = 0, ..., T-1,$$

$$c_T = s_T^{\top} Q_T s_T.$$

where s_0 is given, $Q_t = Q_t^{\top} \ge 0$ is a symmetric non-negative definite state-cost matrix (i.e. $v^{\top}Q_tv \ge 0, \forall v \in \mathbb{R}^n$), and $R_t = R_t^{\top} > 0$ is a symmetric positive definite control-cost matrix (i.e. $v^{\top}R_tv > 0, \forall v \in \mathbb{R}^m$). Let $V_t(s)$ denote the value function of a state at time t, that is,

$$V_t(s) = \min_{a_t, \dots, a_T} \sum_{t'=t}^T c_{t'}(s_{t'}, a_{t'}) \quad \text{s.t.} \quad s_t = s. \label{eq:vt}$$

DP solution to LQR

Theorem

The value function has a quadratic form: $V_t(s) = s^{\top} P_t s$, and $P_t = P_t^{\top}$.

Proof.

For t = T, by definition, as $V_T(s) = s^{\top}Q_Ts$. Assume $V_{t+1}(s) = s^{\top}P_{t+1}s$, then

$$V_{t}(s) = \min_{a_{t}} s^{\top} Q_{t} s + a_{t}^{\top} R_{t} a_{t} + V_{t+1} (A_{t} s + B_{t} a_{t})$$

$$= \min_{a_{t}} s^{\top} Q_{t} s + a_{t}^{\top} R_{t} a_{t} + (A_{t} s + B_{t} a_{t})^{\top} P_{t+1} (A_{t} s + B_{t} a_{t})$$

$$= s^{\top} Q_{t} s + (A_{t} s)^{\top} P_{t+1} (A_{t} s)$$

$$+ \min_{a_{t}} a_{t}^{\top} (R_{t} + B_{t}^{\top} P_{t+1} B_{t}) a_{t} + 2(A_{t} s)^{\top} P_{t+1} (B_{t} a_{t})$$

Solving the minimization gives $a_t^* = -(R_t + B_t^\top P_{t+1} B_t)^{-1} B_t^\top P_{t+1} A_t s$. Substituting back a_t^* into $V_t(s)$ gives a quadratic expression in s.

Markov Chains

Definition

A Markov chain $\{X_t: t\in \mathbb{N}^+\}$, with $X_t\in \mathcal{X}$, is a discrete-time stochastic, process, over a finite or countable state-space \mathcal{X} , that satisfies the following Markov property:

$$P(X_{t+1} = j | X_t = i, X_{t-1}, \dots X_0) = P(X_{t+1} = j | X_t = i)$$

We focus on time-homogeneous Markov chains, where:

$$P(X_{t+1} = j | X_t = i) = P(X_1 = j | X_0 = i) \stackrel{\Delta}{=} p_{ij}.$$

Define $p_{ij}^{(m)} = P(X_m = j | X_0 = i)$, the m-step transition probabilities, then

$$p_{ij}^{(m)} = [P^m]_{ij}$$

where P^m is the m-th power of the matrix P.

Some definitions

Definition

State j is **accessible** (or reachable) from i (denoted by $i \to j$) if $p_{ij}^{(m)} > 0$ for some $m \ge 1$.

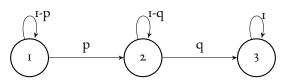
Construct a directed graph G(X, E) where $E = \{(i, j) : p_{ij} > 0\}$ and find a directed path from i to j. Remarks:

- The relation is transitive. If $i \to j$ and $j \to k$ then $i \to k$.
- If $i \to j$ then $\exists m_1$ s.t. $p_{ij}^{(m_1)} > 0$. When $j \to k$ where $\exists m_2$ s.t. $p_{jk}^{(m_2)} > 0$, we also have $p_{ik}^{(m_1+m_2)} \ge p_{ij}^{(m_1)} p_{jk}^{(m_2)} > 0$.

States i and j are **communicating** states if $i \rightarrow j$ and $j \rightarrow i$.

Example

Transition diagram:



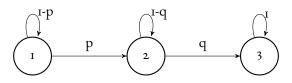
Adjacency matrix:

$$P = \begin{pmatrix} 1 - p & p & 0 \\ 0 & 1 - q & q \\ 0 & 0 & 1 \end{pmatrix}$$

where $P(s_{t+1} = j | s_t = i) = [P]_{ij} =: p_{ij}$.

$$P(s_{t+2} = j | s_t = i) = \sum_k P(s_{t+2} = j | s_{t+1} = k) P(s_{t+1} = k | s_t = i)$$
$$= p_{ik} p_{kj}$$

Then the matrix of $P(s_{t+2} = j | s_t = i)$'s can be expressed as $P \cdot P = P^2$.



$$P^{2} = \begin{pmatrix} (1-p)^{2} & p(2-p-q) & pq \\ 0 & (1-q)^{2} & q(2-q) \\ 0 & 0 & 1 \end{pmatrix}$$

hence

- 3 is accessible from 1 as pq > 0.
- As the matrix is triangular, no pair of states are communicating.

Notation:
$$p_{ij}^{(2)} := [P_{ij}^2].$$

Some definitions

Definition

A **communicating class** (or just class) is a maximal collection of states that communicate.

Definition

The Markov chain is **irreducible** if all states belong to a single class (i.e., all states communicate with each other).

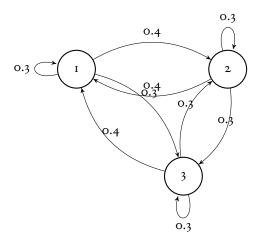
Definition

State i is **recurrent** if $\exists m$ such that $p_{ii}^{(m)} = 1$. Otherwise, state i is **transient**.

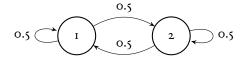
Definition

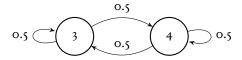
State i has a **period** $d_i = \text{GCD}\{m \ge 1 : p_{ii}^{(m)} > 0\}$, where GCD is the greatest common divisor. A state is **aperiodic** if $d_i = 1$.

Irreducible aperiodic



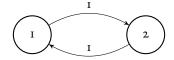
Non-irreducible



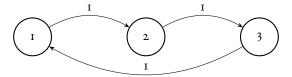


Periodic

Period 2



Period 3



Some results

Theorem

State i is transient if and only if $\sum_{m=1}^{\infty} p_{ii}^{(m)} < \infty$ and recurrent if and only if $\sum_{m=1}^{\infty} p_{ii}^{(m)} = \infty$.

Theorem

Recurrence is a class property in the sense that if i and j are communicating and i is recurrent, then j is also recurrent.

Theorem

If i and j are in the same recurrent class, then $\exists m$ such that $p_{ij}^{(m)} = 1$.

Theorem

For any two states i and j with periods d_i and d_j , in the same communicating class, we have $d_i = d_j$.

Stationary distribution

The probability vector $\mu = (\mu_i)$ is an *invariant distribution* (or *stationary distribution* or *steady-state distribution*) for the Markov chain if $\mu^{\top}P = \mu^{\top}$:

$$\mu_j = \sum_i \mu_i p_{ij}, \quad \forall j.$$

In this case, if $X_t \sim \mu$ then $X_{t+1} \sim \mu$. If $X_0 \sim \mu$, then the Markov chain (X_t) is a stationary stochastic process.

Theorem

Let (X_t) be an irreducible and aperiodic Markov chain over a finite state space \mathcal{X} with transition matrix P. Then there is a unique distribution μ such that $\mu^\top P = \mu^\top > 0$.

Convergence of visitation counts

We define the average fraction that a state $j \in X$ occurs, given that we start with an initial state distribution x_0 , as follows:

$$\pi_j^{(m)} = \frac{1}{m} \sum_{t=1}^m \mathbb{I}(X_t = j).$$
 (2)

Theorem

Let (X_t) be an irreducible and aperiodic Markov chain over a finite state space X with transition matrix P. Let μ be the stationary distribution of P. Then, for any $j \in X$ we have,

$$\mu_j = \lim_{m \to \infty} \mathbb{E}[\pi_j^{(m)}] = \frac{1}{\mathbb{E}[T_j]}.$$
 (3)

where T_i is the return time to state i (number of steps until its next visit).

Note that if *i* is a recurrent state, then $T_i < \infty$ with probability (w.p.) 1.

Key properties of finite Markov chains

Theorem

Let (X_t) be an irreducible, aperiodic Markov chain over a finite state space X. Then the following properties hold:

- All states are positive recurrent, i.e., $\mathbb{E}[T_i] < \infty, \forall i \in \mathcal{S}$.
- There exists a unique stationary distribution μ , where $\mu(i) = 1/\mathbb{E}[T_i]$.
- Convergence to the stationary distribution: $\lim_{t\to\infty} P[X_t=j] = \mu_j \ (\forall j)$
- Ergodicity: For any finite $f: \lim_{t \to \infty} \frac{1}{t} \sum_{s=0}^{t-1} f(X_s) = \sum_i \mu_i f(i) \stackrel{\Delta}{=} \pi \cdot f$.

Remark: A state i with $\mathbb{E}[T_i] = \infty$ is called *null recurrent*.

Reversible Markov chains

Suppose there exists a probability vector $\mu=(\mu_i)$ so that

$$\mu_i p_{ij} = \mu_j p_{ji}, \quad i, j \in X.$$

These equations are called the **detailed balance equations**. It is then easy to verify by direct summation that μ is an invariant distribution for the Markov chain defined by $(p_{i,j})$. This follows since

$$\sum_{i} \mu_i p_{ij} = \sum_{i} p_{ji} \mu_j = \mu_j$$

A Markov chain that satisfies these equations is called **reversible**.

Mixing time

The mixing time measures how fast the Markov chain converges to the steady state distribution. We first define the *Total Variation (TV) distance* between distributions D_1 and D_2 as:

$$||D_1 - D_2||_{TV} = \max_{B \subseteq \mathcal{X}} \{D_1(B) - D_2(B)\} = \frac{1}{2} \sum_{x \in \mathcal{X}} |D_1(x) - D_2(x)|$$

The mixing time τ is defined as the time to reach a total variation of at most 1/4:

$$||s_0 P^{\tau} - \mu||_{TV} = ||p^{(\tau)} - \mu||_{TV} \le \frac{1}{4} ||s_0 - \mu||_{TV}$$

where μ is the steady state distribution and $p^{(\tau)}$ is the state distribution after τ steps starting with an initial state distribution s_0 .

Note that after 2τ time steps we have

$$||s_0 P^{2\tau} - \mu||_{TV} = ||p^{(\tau)} P^{\tau} - \mu||_{TV} \le \frac{1}{4} ||p^{(\tau)} - \mu||_{TV} \le \frac{1}{4^2} ||s_0 - \mu||_{TV}.$$

Mixing time

After $k\tau$ time steps we have

$$||s_0 P^{k\tau} - \mu||_{TV} = ||p^{((k-1)\tau)} P^{\tau} - \mu||_{TV}$$

$$\leq \frac{1}{4} ||p^{((k-1)\tau)} - \mu||_{TV}$$

$$\leq \frac{1}{4^k} ||s_0 - \mu||_{TV}.$$

where the formal proof is by induction on $k \geq 1$.