Probabilistic Programming Lecture #3: Markov Chains

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RWTH Lecture Series on Probabilistic Programming 2018

Overview







Overview

1 Markov Chains

2 State classification



Probability distribution

Probability distribution A probability distribution on countable set X is a function $\mu: X \to [0, 1] \subseteq \mathbb{R}$ such that $\sum_{x \in X} \mu(x) = 1$.

The set $\{x \mid \mu(x) > 0\}$ is the support set of probability distribution μ . Let Dist(X) denote the set of all probability measures on X.

Andrei Andrejewitsch Markow



Markov chains
$$\mathcal{P}(\sigma, \sigma') = \frac{1}{2}$$

 $\mathcal{P}(\sigma, \cdot) \in \mathcal{D}$ is $\mathcal{V}(\Sigma) = \mathcal{P}(\sigma, \sigma^*)$

Markov chain

- A Markov chain (MC) D is a triple (Σ , σ_I , **P**) with:
 - Σ being a countable set of states
 - $\sigma_I \in \Sigma$ the initial state, and
 - ▶ $\mathbf{P}: \Sigma \rightarrow Dist(\Sigma)$ the transition probability function

where $Dist(\Sigma)$ is a (discrete) probability measure on Σ .

A state $\sigma \in \Sigma$ for which $\mathbf{P}(\sigma, \sigma) = 1$ is called absorbing.

Transition probability matrix

For MC D with finite state space Σ , function P is called the *transition* probability matrix of D. $P(\sigma_1, \cdot) \in Dist(\Sigma)$

Properties:

- 1. **P** is a (right) *stochastic* matrix, i.e., it is a square matrix, all its elements are in [0, 1], and each row sum equals one.
- 2. P has an eigenvalue of one, and all its eigenvalues are at most one.
- 3. For all $n \in \mathbb{N}$, \mathbf{P}^n is a stochastic matrix.



Paths

Paths

Path $\pi = \sigma_0 \sigma_1 \dots$ is a *path* through MC *D* whenever $\mathbf{P}(\sigma_i, \sigma_{i+1}) > 0$ for all natural *i*.

Let Paths(D) denotes the set of paths in D that start in its initial state σ_I .



Cylinder sets

Cylinder set

The *cylinder set* of finite path $\hat{\pi} = \sigma_0 \sigma_1 \dots \sigma_n$ in MC *D* is defined by:

$$Cyl(\hat{\pi}) = \{\pi \in Paths(D) \mid \hat{\pi} \text{ is a prefix of } \pi\}$$

The cylinder set spanned by finite path $\hat{\pi}$ consists of all infinite paths that have prefix $\hat{\pi}$.

Probability measure on sets of infinite paths $Pr(C_1 \uplus \overline{C_2}) = Pr(C_1) + (1 - Pr(C_1))$

Probability measure

Pr is the unique *probability distribution* defined on cylinder sets by:

$$Pr(Cyl(\sigma_0...\sigma_n)) = \prod_{0 \le i < n} \mathbf{P}(\sigma_i, \sigma_{i+1})$$

for
$$n > 0$$
 and $\mathbf{P}(\sigma_0) = 1$ iff $\sigma_0 = \sigma_I$.

of infinite paths By standard results in probability theory, Pr is a distribution on all sets that are countable unions and/or complements of cylinder sets.

$$\mathcal{P}(\boldsymbol{\tau}_{0},\boldsymbol{\tau}_{1}), \mathcal{P}(\boldsymbol{\tau}_{1},\boldsymbol{\tau}_{2}), \ldots, \mathcal{P}(\boldsymbol{\tau}_{n-1},\boldsymbol{\tau}_{n})$$

Reachability

Reachability

Let MC *D* with countable state space Σ and $G \subseteq \Sigma$ the set of *goal* states. The event *eventually reaching G* is defined by:

$$\diamond G = \{ \pi \in Paths(D) \mid \exists i \in \mathbb{N}. \pi[i] \in G \}$$

where $\pi[i] = \sigma_i$ for $\pi = \sigma_0 \sigma_1 \dots$

The event $\diamond G$ is measurable, i.e., the probability $Pr(\diamond G)$ is well defined.

► Consider the event ♦4



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- We have:





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$$Pr(\diamond 4) = \sum_{s_0 \dots s_n \in (\Sigma \setminus 4^*)4} \mathbf{P}(s_0 \dots s_n)$$





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• This yields:

$$P(s_0s_2s_54) + P(s_0s_2s_6s_2s_54) + \dots$$

• Or:
$$\sum_{k=0}^{\infty} \mathbf{P}(s_0 s_2(s_6 s_2)^k s_5 4)$$



Consider the event \$\$4

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Or:
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Or:
$$\frac{1}{8} \cdot \sum_{k=0}^{\infty} (\frac{1}{4})^k$$

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• Geometric series: $\frac{1}{8} \cdot \frac{1}{1 - \frac{1}{4}} = \frac{1}{8} \cdot \frac{4}{3} = \frac{1}{6}$





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Geometric series:
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For finite state spaces, reachability probabilities can be obtained algorithmically.

Reachability probabilities

Problem statement

Let D be an MC with finite state space Σ , $\sigma \in \Sigma$, and $G \subseteq \Sigma$.

Aim: determine $Pr(\sigma \models \diamondsuit G) = Pr_{\sigma}(\diamondsuit G)$

Reachability probabilities

Problem statement

Let *D* be an MC with finite state space Σ , $\sigma \in \Sigma$, and $G \subseteq \Sigma$. Aim: determine $Pr(\sigma \models \Diamond G) = Pr_{\sigma}(\Diamond G) = Pr\{\pi \in Paths(D_{\sigma}) \mid \pi \in \Diamond G\}$ where D_{σ} is the MC *D* with initial state σ .



Characterisation of reachability probabilities

Let variable $x_{\sigma} = Pr(\sigma \models \diamondsuit G)$ for any state σ be defined by:



Characterisation of reachability probabilities

Let variable $x_{\sigma} = Pr(\sigma \models \diamondsuit G)$ for any state σ be defined by:

- if $\sigma \notin Pre^*(G)$, then $x_{\sigma} = 0$
- ▶ if $\sigma \in \mathbf{G}$, then $x_{\sigma} = 1$
- otherwise:

Characterisation of reachability probabilities

Let variable $x_{\sigma} = Pr(\sigma \models \diamondsuit G)$ for any state σ be defined by:



 $Pre^*(G)$ is the set of states in Σ from which G is reachable, i.e., $\{\sigma \in \Sigma \mid Pr(\sigma \models \diamondsuit G) > 0\}.$

► Consider the event ♦4





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- > The previous characterisation yields:

$$x_1 = x_2 = x_3 = x_5 = x_6 = 0$$
 and $x_4 = 1$



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$$x_{s_{1}} = x_{s_{3}} = x_{s_{4}} = 0$$

$$x_{s_{0}} = \frac{1}{2}x_{s_{1}} + \frac{1}{2}x_{s_{2}}$$

$$P(s_{0}, s_{1}) = 0$$

$$P(s_{0}, s_{1})$$



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$$P(s_{2}, \Xi) = 0$$

$$\sum_{\tau \in \Sigma \setminus G} P(s_{2}, \tau) \cdot x_{\tau} < \tau = s_{t}$$



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$$x_{s_{5}} = \frac{1}{2}x_{5} + \frac{1}{2}x_{4} = \frac{1}{2}x_{5} + \frac{1}{2}$$

$$\sum P(s_{5}, \tau) + \sum P(s_{5}, \tau)$$

$$r \in \Sigma \setminus G \qquad \qquad r \in G$$

$$= P(s_{5}, \tau) = \frac{1}{2}$$



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Gaussian elimination yields:

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Linear equation system

• Let $\Sigma_7 = Pre^*(G) \setminus G$, the states that can reach G by > 0 steps

non 0,1 cases

Linear equation system

• Let $\Sigma_{?} = Pre^{*}(G) \setminus G$, the states that can reach G by > 0 steps

► **A** = $(\mathbf{P}(\sigma, \tau))_{\sigma, \tau \in \Sigma_2}$, the transition probabilities in Σ_2 ?

Linear equation system

- Let $\Sigma_{?} = Pre^{*}(G) \setminus G$, the states that can reach G by > 0 steps
- **A** = $(\mathbf{P}(\sigma, \tau))_{\sigma, \tau \in \Sigma_2}$, the transition probabilities in Σ_2
- **b** = $(b_{\sigma})_{\sigma \in \Sigma_{\gamma}}$, the probes to reach *G* in 1 step, i.e., $b_{\sigma} = \sum_{\gamma \in G} \mathbf{P}(\sigma, \gamma)$
Linear equation system

Let $\Sigma_{?} = Pre^{*}(G) \setminus G$, the states that can reach G by > 0 steps

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Theorem

The vector $\mathbf{x} = (x_{\sigma})_{\sigma \in \Sigma_{\gamma}}$ with $x_{\sigma} = Pr(\sigma \models \diamondsuit G)$ is the unique solution of the linear equation system:

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Theorem

The vector $\mathbf{x} = (x_{\sigma})_{\sigma \in \Sigma_{?}}$ with $x_{\sigma} = Pr(\sigma \models \diamondsuit G)$ is the unique solution of the linear equation system:

 $\mathbf{x} = \mathbf{A} \cdot \mathbf{x} + \mathbf{b}$ or, equivalently $(\mathbf{I} - \mathbf{A}) \cdot \mathbf{x} = \mathbf{b}$

where **I** is the identity matrix of cardinality $|\Sigma_{?}| \cdot |\Sigma_{?}|$.

Reachability probabilities: Knuth-Yao's die $(I - A) \cdot x = b$

► Consider the event ♦4





Consider the event \$\$4

$$\Sigma_{?} = \{ s_0, s_2, s_5, s_6 \}$$



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Consider the event \$\$4

$$\Sigma_{?} = \{ s_{0}, s_{2}, s_{5}, s_{6} \}$$

$$\begin{pmatrix} 1 & -\frac{1}{2} & 0 & 0 \\ 0 & 1 & -\frac{1}{2} & -\frac{1}{2} \\ 0 & 0 & 1 & 0 \\ 0 & -\frac{1}{2} & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} x_{s_{0}} \\ x_{s_{2}} \\ x_{s_{5}} \\ x_{s_{6}} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \\ 0 \\ s_{5} \\ s_{6} \end{pmatrix}$$



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Gaussian elimination yields:

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Computing reachability probabilities

Polynomial complexity

Reachability probabilities in finite MCs can be computed in polynomial time.

Overview

Markov Chains

2 State classification



Probabilistic Programming	State classification		
First visit probabilities	90	0 T	
First visit probabilities			
For states $\sigma, \tau \in \Sigma$, let			
$f_{\sigma,\tau}^{(n)} = Pr\{\text{first visit to } \tau \text{ after exactly } n \text{ steps from } \sigma\}$			
(This differs from the probability to move from τ to σ in <i>n</i> steps.)			
We have: $\mathbf{P}^{n}(\sigma,\tau) = \sum_{\ell=1}^{n}$	$f_{\sigma,\tau}^{(\ell)} \cdot \mathbf{P}^{n-\ell}(\tau,\tau)$	repetitive visits to T	
The probability to reach $ au$ from state σ equals:			

$$Pr(\sigma \models \diamondsuit \tau) = f_{\sigma,\tau} = \sum_{n=1}^{\infty} f_{\sigma,\tau}^{(n)}$$

State classification

Return probabilities

$$abla =
abla$$



_ steps

Return probabilities

For state $\sigma \in \Sigma$, let

$$f_{\sigma}^{(n)} = Pr\{\text{first return to } \sigma \text{ after exactly } n\}$$

We have:

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The return probability to state σ equals: $Pr(\sigma \models \Diamond \sigma) = f_{\sigma} = \sum_{n=1}^{\infty} f_{\sigma}^{(n)}$.

Transient and recurrent states $\chi_{=P_{r=1}}$

The return probability to σ equals: $Pr(\sigma \models \Diamond \sigma) = f_{\sigma} = \sum_{\sigma \in \mathcal{T}} f_{\sigma}$

Transient and recurrent states

State σ is called *recurrent* if $f_{\sigma} = 1$, i.e., with probability one (aka: almost surely) the MC returns to σ .

State σ is called *transient* otherwise, i.e., if $f_{\sigma} < 1$. With a positive probability, the MC does not return to a transient state.

Example on the black board.

State classification

Null and positive recurrence

Let σ be a recurrent state, i.e., $Pr(\sigma \models \diamondsuit \sigma) = f_{\sigma} = 1$.

Mean recurrence time

The mean recurrence time of recurrent state σ equals

$$m_{\sigma} = \sum_{n=1}^{\infty} n \cdot f_{\sigma}^{(n)}$$

This is the expected number of steps between two successive visits to σ .

Null and positive recurrent states

State σ is called positive recurrent whenever $m_{\sigma} < \infty$. Otherwise, state σ is called null recurrent; then $m_{\sigma} = \infty$.

Example on the black board.

Joost-Pieter Katoen





Null and positive recurrence in finite MC

- 1. Every state in a finite MC is either positive recurrent or transient.
- 2. At least one state in a finite MC is positive recurrent.
- 3. A finite MC has no null recurrent states.

Foster's theorem

- A countable Markov chain is "non-dissipative"
- if almost every infinite path eventually enters
- and remains in positive recurrent states.

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A sufficient condition for being non-dissipative is:

$$\sum_{j\geq 0} j \cdot \mathbf{P}(i, j) \leq i \quad \text{for all states } i$$

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Frederic Gordon Foster Markoff chains with an enumerable number of states and a class of cascade processes

1951

Periodicity and ergodicity

Periodic state

A state σ is called *periodic* if

$$f_{\sigma}^{(n)} > 0$$
 implies $n = k \cdot d$ where period $d > 1$.

A state is aperiodic otherwise.

A state is ergodic if it is positive recurrent and aperiodic. An MC is ergodic if all its states are ergodic.



xample on the black board.



Connected states are of the same "type"

ab

Let σ and τ be mutually reachbeine from each other. Then:

σ is transient	iff	au is transient
σ is null-recurrent	iff	au is null-recurrent
σ is positive recurrent	iff	τ is positive recurrent
σ has period d	iff	tad has period d
		τ

Irreducibility



Irreducible

A MC is irreducible if it is strongly connected, i.e., all states are mutually reachable.

Markov's theorem

A finite, irreducible MC D is (1) positive recurrent, and (2) ergodic provided D is aperiodic. In the latter case, we have

$$\mathbf{P}^{\infty} = \lim_{n \to \infty} \mathbf{P}^n = \begin{pmatrix} v \\ \cdot \\ \cdot \\ v \end{pmatrix} \quad \text{where} \quad v = \left(\frac{1}{m_1}, \dots, \frac{1}{m_k}\right)$$

where $k = |\Sigma|$.





Stationary distribution

Stationary distribution

A probability vector **x** satisfying $\mathbf{x} = \mathbf{x} \cdot \mathbf{P}$ is called a stationary distribution of MC *D*.

$$x_{\sigma} = \sum_{\tau \in \Sigma} x_{\tau} \cdot \mathbf{P}(\tau, \sigma) \quad \text{iff} \quad \underbrace{x_{\sigma} \cdot (1 - \mathbf{P}(\sigma, \sigma))}_{\text{outflow of } \sigma} = \underbrace{\sum_{\tau \neq \sigma} x_{\tau} \cdot \mathbf{P}(\tau, \sigma)}_{\text{inflow of } \sigma}$$

An irreducible, positive recurrent MC has a unique stationary distribution satisfying $x_{\sigma} = \frac{1}{m_{\sigma}}$ for every state σ .

Limiting distribution

Ergodic stochastic matrix

Stochastic matrix **P** is called *ergodic* if:

$$\mathbf{P}^{\infty} = \lim_{n \to \infty} \mathbf{P}^{n}$$
 exists and has identical rows

Limiting distribution

If **P** is ergodic, then each row of \mathbf{P}^{∞} equals the limiting distribution.

Limiting = stationary distribution

For ergodic (aka: aperiodic and positive recurrent) MCs, the stationary and limiting distribution are equal.

Overview

Markov Chains

2 State classification



To reason about resource usage in MCs: use rewards.

MC with rewards

A reward MC is a pair (D, r) with D an MC with state space Σ and $r: \Sigma \to \mathbb{R}$ a function assigning a real reward to each state.

The reward $r(\sigma)$ stands for the reward earned on leaving state σ .

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Cumulative reward for reachability

Let $\pi = \sigma_0 \dots \sigma_n$ be a finite path in (D, r) and $G \subseteq \Sigma$ a set of target states with $\pi \in \diamondsuit G$. The cumulative reward along π until reaching G is:

$$r_G(\pi) = r(\sigma_0) + \ldots + r(\sigma_{k-1})$$
 where $\sigma_i \notin G$ for all $i < k$ and $\sigma_k \in G$.

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$$r_G(\pi) = r(\sigma_0) + \ldots + r(\sigma_{k-1})$$
 where $\sigma_i \notin G$ for all $i < k$ and $\sigma_k \in G$.

If $\pi \notin \diamondsuit G$, then $r_G(\pi) = 0$.

Expected reward reachability

Expected reward for reachability

The expected reward until reaching $G \subseteq \Sigma$ from $\sigma \in \Sigma$ is:

$$\mathsf{ER}(\sigma, \diamondsuit G) = \sum_{\pi \models \diamondsuit G} \Pr(\widehat{\pi}) \cdot r_G(\widehat{\pi})$$

where $\widehat{\pi} = \sigma_0 \dots \sigma_k$ is the shortest prefix of π such that $\sigma_k \in G$ and $\sigma_0 = \sigma$.





Expected reward reachability

Expected reward for reachability

The expected reward until reaching $G \subseteq \Sigma$ from $\sigma \in \Sigma$ is:

$$\mathsf{ER}(\sigma, \diamondsuit G) = \sum_{\pi \models \diamondsuit G} \Pr(\widehat{\pi}) \cdot r_G(\widehat{\pi})$$

where $\hat{\pi} = \sigma_0 \dots \sigma_k$ is the shortest prefix of π such that $\sigma_k \in G$ and $\sigma_0 = \sigma$.

Conditional expected reward

Let $ER(\sigma, \diamondsuit G \mid \neg \diamondsuit F)$ be the conditional expected reward until reaching G under the condition that no states in $F \subseteq \Sigma$ are visited.

Expected rewards in finite Markov chains

Polynomial complexity

Expected rewards in finite MCs can be computed in polynomial time.