

Probabilistic/Stochastic Transition Systems (Markov Chains)

Computational Models for Complex Systems

Paolo Milazzo

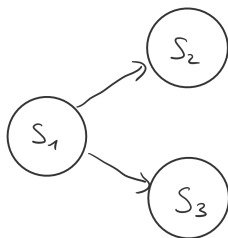
Dipartimento di Informatica, Università di Pisa
<http://pages.di.unipi.it/milazzo>
milazzo@di.unipi.it

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Introduction

Transition systems describe all the possible behaviors of a systems

Alternative behaviors are described through **non-deterministic choices**



Non-determinism allows choices between alternative behaviors to be modeled without describing the **choice criterion**

Introduction

Sometimes the choice criterion is known to be

- **probabilistic**, or
- due to a (**stochastic**) **race** between poisson processes (race condition)

This leads to the definition of

- **Probabilistic Transition Systems (PTSs)**
aka **Discrete Time Markov Chains (DTMCs)**
- **Stochastic Transition Systems (STSs)**
aka **Continuous Time Markov Chains (CTMCs)**

See also:

- Dave Parker's Lectures on **Probabilistic Model Checking**
(in particular, Lectures 2,3,8,9)

Available here:

<https://www.prismmodelchecker.org/lectures/pmc/>

Probability Example

Modeling a 6-sided dice using a fair coin

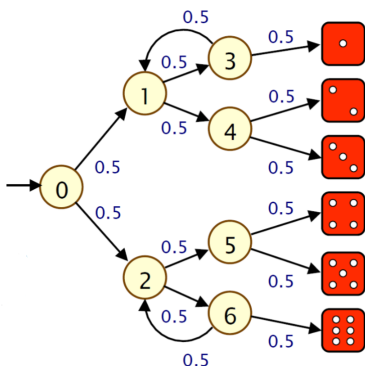
- algorithm due to Knuth/Yao
- start at 0, toss a coin
- upper branch when H
- lower branch when T
- repeat until value chosen

Is this algorithm correct?

- e.g. probability of obtaining a 4?
- Obtain as disjoint union of events
- THH, TTTHH, TTTTTHH, ...

- Probability:

$$(1/2)^3 + (1/2)^5 + (1/2)^7 + \dots = 1/6$$



Discrete Time Markov Chains (DTMCs)

Let's extend Transition Systems with probabilities...

Definition: Discrete Time Markov Chain (DTMC)

A Discrete Time Markov Chain is a pair (S, P) where

- S is a set of **states** and
- $P : S \times S \rightarrow [0, 1]$ is the **probability transition matrix** such that, for all $s \in S$ it holds:

$$\sum_{s' \in S} P(s, s') = 1$$

The probability transition matrix can be expressed equivalently as a **probabilistic transition relation** $\rightarrow \subseteq S \times [0, 1] \times S$ such that $(s, p, s') \in \rightarrow$ (or $s \xrightarrow{p} s'$) if and only if $P(s, s') = p > 0$ (if $p = 0$ the transition is usually omitted).

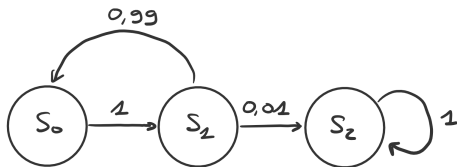
Discrete Time Markov Chains (DTMCs)

When the set of states is finite, $S = \{s_0, s_1, \dots, s_n\}$, the **probability transition matrix** can actually be represented as a **square matrix**:

$$P = \begin{bmatrix} p_{00} & p_{01} & p_{02} & \dots & p_{0n} \\ p_{10} & p_{11} & p_{12} & \dots & p_{1n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ p_{n0} & p_{n1} & p_{n2} & \dots & p_{nn} \end{bmatrix}$$

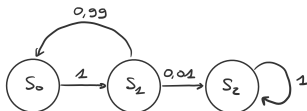
where $p_{ij} = P(s_i, s_j)$ and the **sum of each row** is equal to 1.

A simple DTMC example



$$S = \{s_0, s_1, s_2\} \quad P = \begin{bmatrix} 0 & 1 & 0 \\ 0.99 & 0 & 0.01 \\ 0 & 0 & 1 \end{bmatrix}$$

Some notes



In DTMC we usually have an **initial state** or (more generally) a **probability distribution of initial states**, represented as a vector

- $[1, 0, 0]$ means that s_0 is the initial state
- $[0.5, 0.5, 0]$ means that s_0 and s_1 are equally likely to be initial states

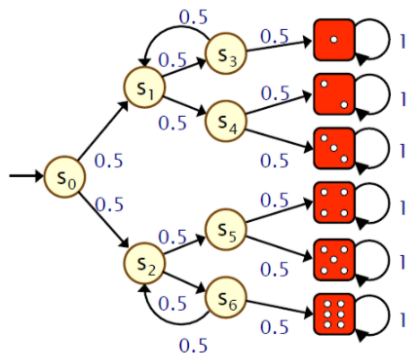
The constraint $\sum_{s' \in S} P(s, s') = 1$ implies that

- every state has **at least one outgoing transition** (otherwise the sum would be 0)
- hence, **deadlocks** correspond to states with a **self-loop**



Coins and dice example as a DTMC

Let's reformulate Knuth/Yao's algorithm as a DTMC:



$$S = \{s_0, s_1, \dots, s_6, 1, 2, \dots, 6\}$$

$$s_{init} = s_0$$

$$P = \begin{bmatrix} 0 & 0.5 & 0.5 & \dots \\ 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

Paths and their probabilities

A **path** of a DTMC is the analogous of a (maximal) **trace** for a Transition System

Definition: Path

A path π of a DTMC (S, P) with initial state s_0 , is a (possibly infinite) sequence of states $\pi = s_0, s_1, s_2, \dots$ such that for each s_{i+1} with $i \in \mathbb{N}$ in π it holds $P(s_i, s_{i+1}) > 0$.

The **probability of a path** is simply the **product** of the probabilities of its transitions:

$$\text{Prob}(s_0, s_1, s_2, \dots, s_n) = \prod_{i=0}^{n-1} P(s_i, s_{i+1})$$

$$\text{Prob}(s_0, s_1, s_2, \dots) = \prod_{i \in \mathbb{N}} P(s_i, s_{i+1})$$

Probabilistic reachability

In a DTMC it is possible to compute the probability that the system will reach a given state

- **Reachability** = **property** expressing whether a given state **can be reached** (there exists a path leading to it)
- **Probabilistic reachability** = **probability** of reaching a given state (probabilities of **all the paths** leading to it)

Paths are independent events: their probabilities can be summed!

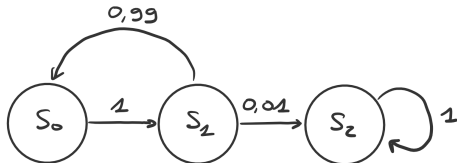
Definition: Probabilistic Reachability

The **probability of reaching** state s of a DTMC (S, \rightarrow) from the initial state s_0 , is the **sum of the probabilities** of all paths leading to it.

$$ProbReach(s_0, s) = \sum_{\pi \in Reach(s_0, s)} Prob(\pi)$$

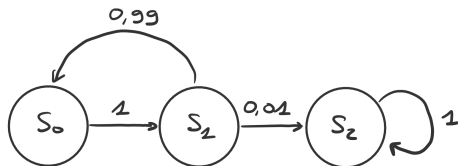
where $Reach(s_0, s)$ is the (**possibly infinite**) set of paths reaching s .

Probabilistic reachability: example



$$\begin{aligned} \text{ProbReach}(s_0, s_2) &= 1 \cdot 0.01 \\ &+ 1 \cdot 0.99 \cdot 1 \cdot 0.01 \\ &+ (1 \cdot 0.99)^2 \cdot 1 \cdot 0.01 \\ &\vdots \\ &+ (1 \cdot 0.99)^n \cdot 1 \cdot 0.01 \\ &\vdots \\ &= 1 \end{aligned}$$

Probabilistic reachability: example



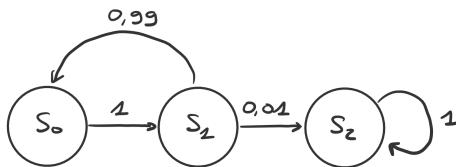
In this example, the infinite sum can be avoided by observing that the only path not leading to s_2 is the infinite path $\pi_{01} = s_0, s_1, s_0, s_1, s_0, \dots$

So, $ProbReach(s_0, s_2) = 1 - Prob(\pi_{01})$

But π_{01} is a single **infinite path** with a loop containing a transition with a probability **strictly smaller than 1**

- $P(\pi_{01}) = (0.99 \cdot 1)^\infty = 0$
- $ProbReach(s_0, s_2) = 1 - Prob(\pi_{01}) = 1$

Probabilistic reachability: example

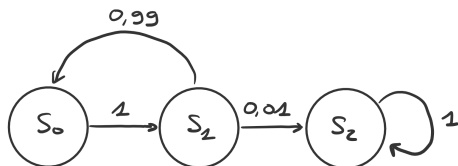


Another (more general) way to avoid the infinite summation, is by reformulating *ProbReach* in terms of a **linear system of equations**

The idea:

- the probability of reaching s_2 from s_2 is 1
- the probability of reaching s_2 from s_1 is 0.01 plus the probability of reaching s_0 in one step, and then of reaching s_2 from there
- the probability of reaching s_2 from s_0 is the probability of reaching s_1 in one step, and then of reaching s_2 from there

Probabilistic reachability: example

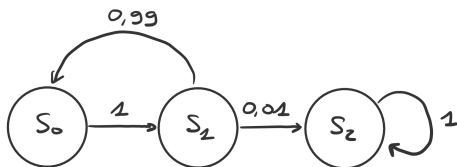


Another (more general) way to avoid the infinite summation, is by reformulating *ProbReach* in terms of a **linear system of equations**

This leads to a mutually recursive reformulation of *ProbReach*:

- $ProbReach(s_2, s_2) = 1$
- $ProbReach(s_1, s_2) = 0.01 \cdot ProbReach(s_2, s_2) + 0.99 \cdot ProbReach(s_0, s_2)$
- $ProbReach(s_0, s_2) = 1 \cdot ProbReach(s_1, s_2)$

Probabilistic reachability: example



Another (more general) way to avoid the infinite summation, is by reformulating *ProbReach* in terms of a **linear system of equations**

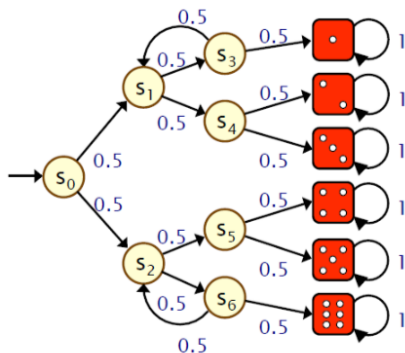
Let's denote $ProbReach(s, s_2)$ as x_s to obtain:

$$\begin{cases} x_{s_2} = 1 \\ x_{s_1} = 0.01x_{s_2} + 0.99x_{s_0} \\ x_{s_0} = x_{s_1} \end{cases}$$

From which we obtain easily $x_{s_0} = 1$

Probabilistic reachability: coins and dice example

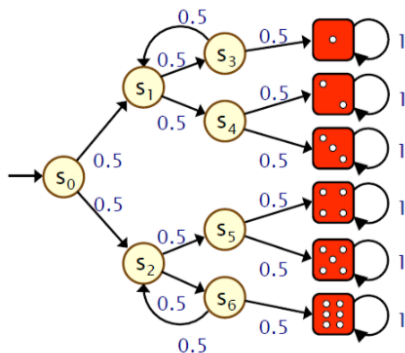
Let's compute the probability of **rolling a 6**



$$\begin{cases} x_6 = 1 \\ x_{s_6} = \frac{1}{2}x_{s_2} + \frac{1}{2}x_6 \\ x_{s_2} = \frac{1}{2}x_{s_6} + \frac{1}{2}x_{s_5} \\ x_{s_5} = 0 \\ x_{s_0} = \frac{1}{2}x_{s_2} + \frac{1}{2}x_{s_1} \\ x_{s_1} = 0 \end{cases}$$

Probabilistic reachability: coins and dice example

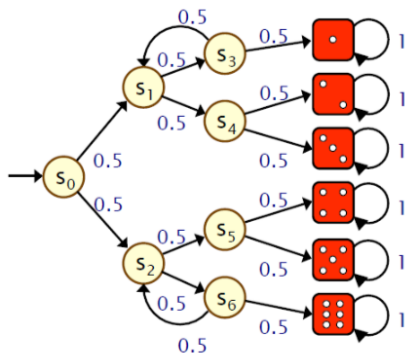
Let's compute the probability of **rolling a 6**



$$\begin{cases} x_{s_6} = \frac{1}{2}x_{s_2} + \frac{1}{2} \\ x_{s_2} = \frac{1}{2}x_{s_6} \\ x_{s_0} = \frac{1}{2}x_{s_2} \end{cases}$$

Probabilistic reachability: coins and dice example

Let's compute the probability of rolling a 6



$$\begin{cases} x_{s_6} = \frac{2}{3} \\ x_{s_2} = \frac{1}{3} \\ x_{s_0} = \frac{1}{6} \end{cases}$$

Computing probabilistic reachability

We have seen that computing probabilistic reachability amounts to solving a system of linear equations

This corresponds to solving the following equation in matrix form:

$$X = P \cdot X$$

where P is the **probability transition matrix of the DTMC**

This can be done by applying computational algebra methods

Continuous Time Markov Chains (CTMCs)

This time let's extend Transition Systems with stochastic rates...

Definition: Continuous Time Markov Chain (CTMC)

A Continuous Time Markov Chain is a pair (S, R) where

- S is a set of states and
- $R : S \times S \rightarrow \mathbb{R}^{\geq 0}$ is the transition rate matrix

The transition rate matrix can be expressed equivalently as a stochastic transition relation $\rightarrow \subseteq S \times \mathbb{R}^{\geq 0} \times S$ such that $(s, r, s') \in \rightarrow$ (or $s \xrightarrow{r} s'$) if and only if $R(s, s') = r > 0$ (if $r = 0$ the transition is usually omitted).

Race conditions

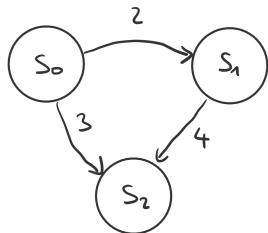
What happens when there exist multiple s' with $R(s, s') > 0$?

- **race condition**: the “fastest” transition determines the next state of the system
- Two questions:
 - ▶ 1) How long is spent in s before a transition occurs?
 - ▶ 2) Which transition is eventually taken?

1) Time spent in a state before a transition

- **minimum** of exponential distributions
- exponential with parameter given by the summation:

$$E(s) = \sum_{s' \in S} R(s, s')$$



- $E(s)$ is called **exit rate** of state s

Race conditions

2) Which transition is taken from state s ?

- the choice is **independent** from the time at which it occurs
- the probability is **proportional to the rate** of each transition

More generally, the probability of the next transition to occur is given by the **embedded DTMC** of the CTMC...

Embedded DTMC of a CTMC

The embedded DTMC of a CTMC describes the state changes of the CTMC by ignoring time

It is obtained by **normalizing** the transition rates of the CTMC with respect to the **exit rate** of each state

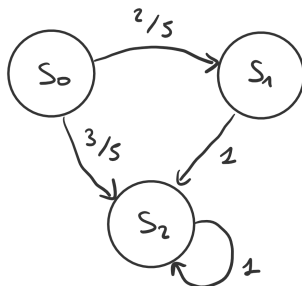
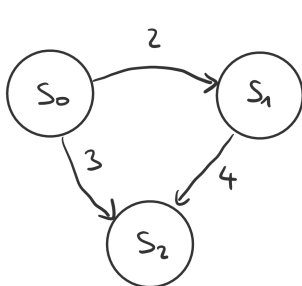
Definition: Embedded DTMC

Given a CTMC (S, R) , its embedded DTMC is the DTMC (S, P) where, for any $s, s' \in S$

$$P(s, s') = \begin{cases} R(s, s')/E(s) & \text{if } E(s) > 0 \\ 1 & \text{if } E(s) = 0 \text{ and } s = s' \\ 0 & \text{otherwise} \end{cases}$$

Embedded DTMC of a CTMC

An example:



Time Independent Probabilistic Reachability on CTMCs

Given a CTMC, what is the probability of reaching a state s at any time?

- It corresponds to probabilistic reachability of the same state in the embedded DTMC
- So, it can be computed by applying computational algebra methods based on the transition probability matrix P of the embedded DTMC

Transient (Time-dependent) Probabilistic Reachability on CTMCs

Given a **CTMC**, what is the probability of the system to be in a state s **at a given time**?

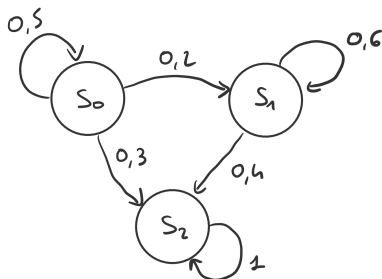
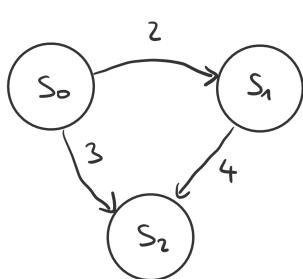
This can be answered by introducing **uniformised DTMCs**

Uniformisation

Given a CTMC, its **uniformised DTMC** is obtained by choosing a **uniformisation rate q** bigger or equal to all the rates of the CTMC

- each rate r of the CTMC is transformed into probability r/q
- self-loops are added where necessary

Example (with $q = 10$):



Uniformisation

Some notes:

- a transition in the uniformised DTMC describes a step with duration $1/q$
- q should be chosen big enough to assume that **at most one transition** can occur during a $1/q$ time interval

Transient probabilistic reachability of a **CTMC** can now be computed as **probabilistic reachability** in the **uniformised DTMC**, by taking the length of the paths in the DTMC into account.

- again, can be computed by performing matrix computations on the transition probability matrix of the DTMC

Application to chemical reactions

Now, we could apply reachability analysis to chemical reactions...

