(Bi)simulation on CTMCs

Lecture #21 of Probabilistic Models for Concurrency

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Overview Lecture #21

- Continuous-time Markov chains (CTMCs)
  - definition and race condition
- Markovian bisimulation
  - definition, quotient transition system, properties
- Weak Markovian bisimulation
- Markovian simulation
  - definition, properties, examples

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Exponential distribution

Continuous r.v. X is *exponential* with parameter $\lambda > 0$ if its density is

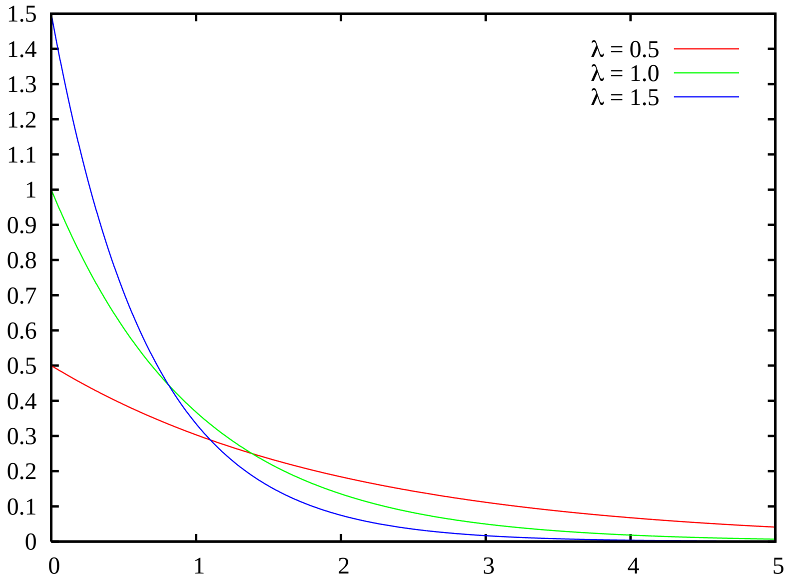
$$f(x) = \lambda \cdot e^{-\lambda \cdot x} \quad \text{for } x > 0 \quad \text{and } 0 \text{ otherwise}$$

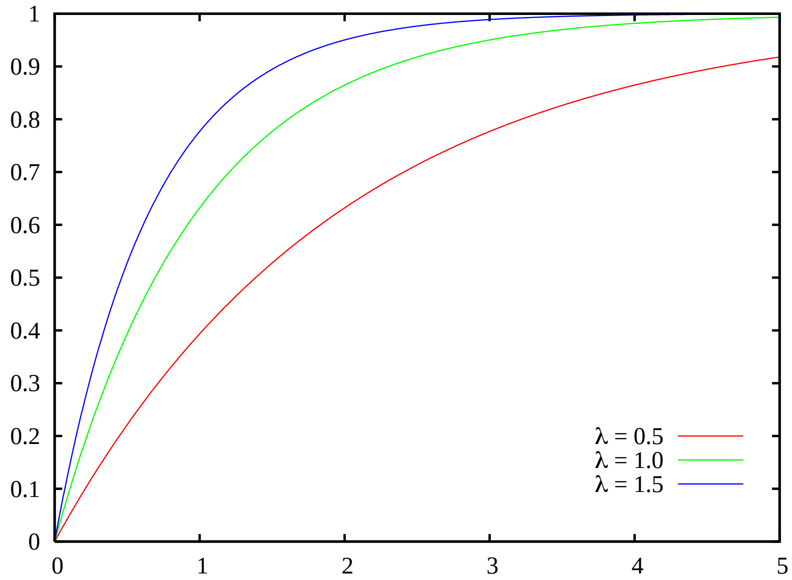
Cumulative distribution of X:

$$F_X(d) \; = \; \int_0^d \lambda \cdot e^{-\lambda \cdot x} \, dx \; = \; [-e^{-\lambda \cdot x}]_0^d \; = \; 1 - e^{-\lambda \cdot d}$$

- $\Pr\{X > d\} = e^{-\lambda \cdot d}$
- expectation $E[X] = \int_0^\infty x \cdot \lambda \cdot e^{-\lambda \cdot x} \, dx = \frac{1}{\lambda}$
- variance *Var*$[X] = \frac{1}{\lambda^2}$

Exponential pdf and cdf





the higher λ, the faster the cdf approaches 1

Exponential distributions

- Have *nice mathematical* properties (cf. next slide)
- Are *adequate* for many real-life phenomena
  - the time until a radioactive particle decays
  - the constant hazard rate portion of the bathtub curve in reliability theory
  - the time it takes before your next telephone call
  - times for reactions between proteins to occur
- Can *approximate* general distributions arbitrarily closely
  - phase-type distributions
- Maximal *entropy* probability distribution if just the mean is known

Properties

- An exponential distribution possesses the *memory-less property*

$$\Pr\{X > t + d \mid X > t\} \;=\; \Pr\{X > d\}$$

  - exponential distributions are the only memoryless continuous distributions

- Let X and Y be exponential random variables with rate λ and μ
- $\min(X, Y)$ is exponentially distributed with rate $\lambda{+}\mu$
- $\Pr\{X = \min(X, Y)\} = \frac{\lambda}{\lambda+\mu}$
- $\max(X, Y)$ is not an exponential, but a phase-type distribution

$\Rightarrow$ *exponential distributions are closed under* $\min$*, but not under* $\max$

CTMC definition

A *continuous-time Markov chain* (CTMC) is a tuple $(S, \mathbf{R})$ where:

- S is a countable set of states
- $\mathbf{R} : S \times S \to \mathbb{R}_{\geqslant 0}$, a *rate matrix*
  - $\mathbf{R}(s, s') = \lambda$ means that the average speed of going from s to s' is $\frac{1}{\lambda}$
- $E(s) = \sum_{s' \in S} \mathbf{R}(s, s') = \mathbf{R}(s, S)$ is the *exit rate* of state s
  - s is called *absorbing* when $E(s) = 0$

a CTMC is a transition system (unlabeled transitions)
where transitions are equipped with continuous probabilities

Interpretation

- The probability that transition $s \longrightarrow s'$ is *enabled* in $[0, t]$:

$$1 - e^{-\mathbf{R}(s,s')\cdot t}$$

- The probability to *move* from non-absorbing s to s' in $[0, t]$ is:

$$\frac{\mathbf{R}(s, s')}{E(s)} \cdot \left(1 - e^{-E(s)\cdot t}\right)$$

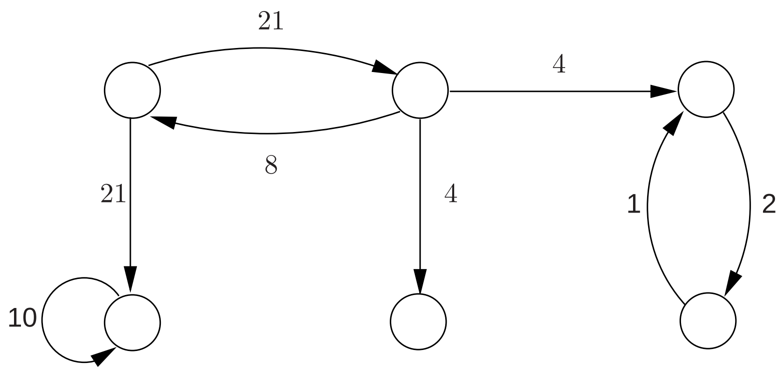
- The probability to take an outgoing transition from s within $[0, t]$ is:

$$1 - e^{-E(s)\cdot t}$$

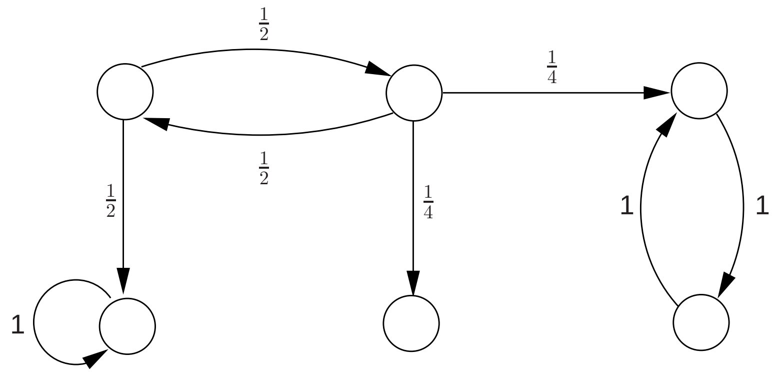
Embedded DTMC

The *embedded* DTMC of the CTMC $(S, \mathbf{R})$ is $(S, \mathbf{P})$ where

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

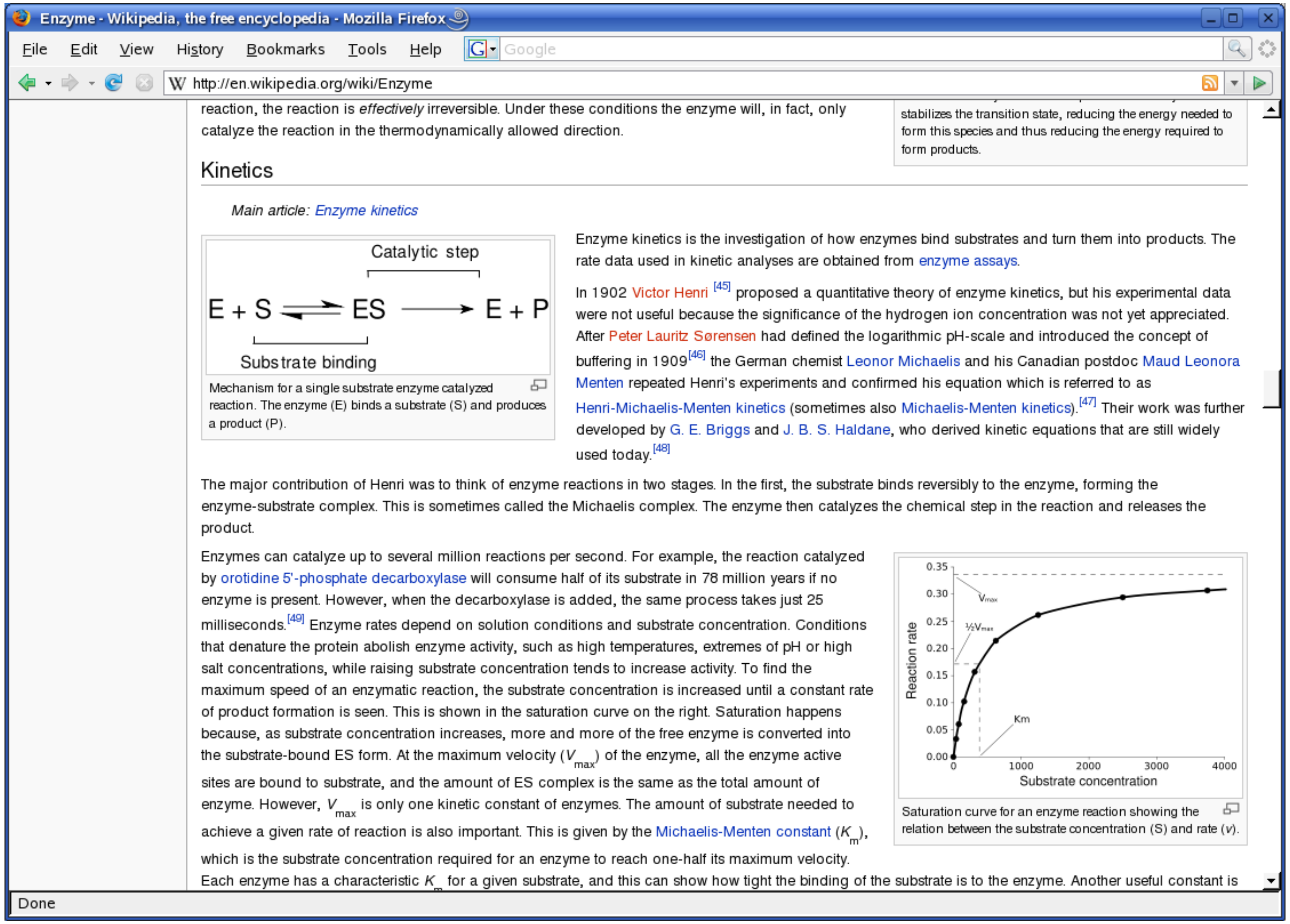


a CTMC



iits embedded DTMC

Enzyme-catalysed substrate conversion



Enzyme - Wikipedia, the free encyclopedia - Mozilla Firefox

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http://en.wikipedia.org/wiki/Enzyme

reaction, the reaction is *effectively* irreversible. Under these conditions the enzyme will, in fact, only catalyze the reaction in the thermodynamically allowed direction.

stabilizes the transition state, reducing the energy needed to form this species and thus reducing the energy required to form products.

Kinetics

Main article: Enzyme kinetics

Mechanism for a single substrate enzyme catalyzed reaction. The enzyme (E) binds a substrate (S) and produces a product (P).

Enzyme kinetics is the investigation of how enzymes bind substrates and turn them into products. The rate data used in kinetic analyses are obtained from enzyme assays.

In 1902 Victor Henri [45] proposed a quantitative theory of enzyme kinetics, but his experimental data were not useful because the significance of the hydrogen ion concentration was not yet appreciated. After Peter Lauritz Sørensen had defined the logarithmic pH-scale and introduced the concept of buffering in 1909[46] the German chemist Leonor Michaelis and his Canadian postdoc Maud Leonora Menten repeated Henri's experiments and confirmed his equation which is referred to as Henri-Michaelis-Menten kinetics (sometimes also Michaelis-Menten kinetics).[47] Their work was further developed by G. E. Briggs and J. B. S. Haldane, who derived kinetic equations that are still widely used today.[48]

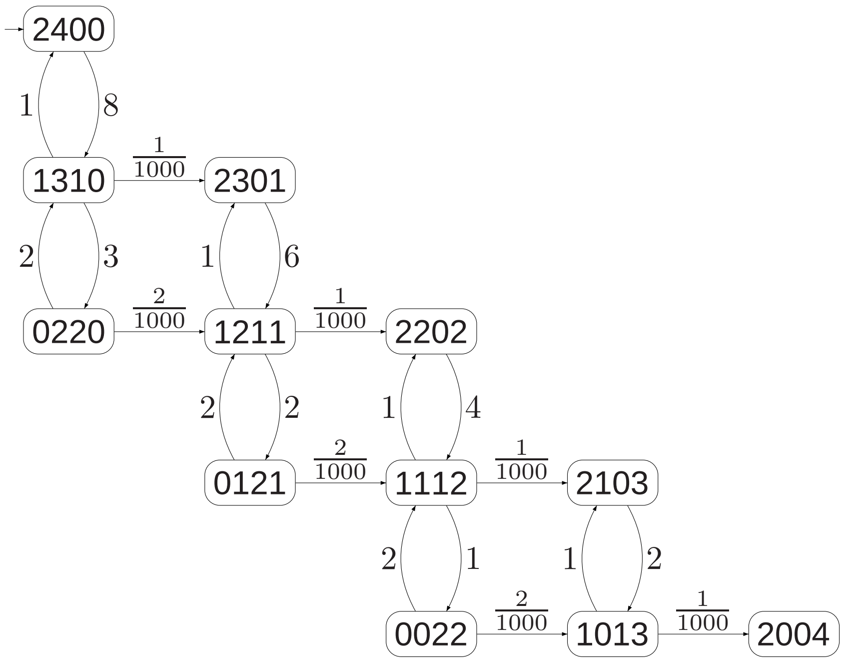
The major contribution of Henri was to think of enzyme reactions in two stages. In the first, the substrate binds reversibly to the enzyme, forming the enzyme-substrate complex. This is sometimes called the Michaelis complex. The enzyme then catalyzes the chemical step in the reaction and releases the product.

Enzymes can catalyze up to several million reactions per second. For example, the reaction catalyzed by orotidine 5'-phosphate decarboxylase will consume half of its substrate in 78 million years if no enzyme is present. However, when the decarboxylase is added, the same process takes just 25 milliseconds.[49] Enzyme rates depend on solution conditions and substrate concentration. Conditions that denature the protein abolish enzyme activity, such as high temperatures, extremes of pH or high salt concentrations, while raising substrate concentration tends to increase activity. To find the maximum speed of an enzymatic reaction, the substrate concentration is increased until a constant rate of product formation is seen. This is shown in the saturation curve on the right. Saturation happens because, as substrate concentration increases, more and more of the free enzyme is converted into the substrate-bound ES form. At the maximum velocity (V_{max}) of the enzyme, all the enzyme active sites are bound to substrate, and the amount of ES complex is the same as the total amount of enzyme. However, V_{max} is only one kinetic constant of enzymes. The amount of substrate needed to achieve a given rate of reaction is also important. This is given by the Michaelis-Menten constant (K_m), which is the substrate concentration required for an enzyme to reach one-half its maximum velocity. Each enzyme has a characteristic K_m for a given substrate, and this can show how tight the binding of the substrate is to the enzyme. Another useful constant is

Saturation curve for an enzyme reaction showing the relation between the substrate concentration (S) and rate (v).

Done

Enzyme-catalysed substrate conversion as a CTMC



		init	*goal*
States:	enzymes	2	2
	substrate molecules	4	0
	complex molecules	0	0
	product molecules	0	4

Transitions: $E + S \underset{1}{\overset{1}{\rightleftharpoons}} C \xrightarrow{0.001} E + P$

e.g., $(x_E, x_S, x_C, x_P) \xrightarrow{0.001 \cdot x_C} (x_E + 1, x_S, x_C - 1, x_P + 1)$ for $x_C > 0$

Transient distribution of a CTMC

Probability to be in state s at time t:

$$\begin{aligned} p_s(t) &= \Pr\{ X(t) = s \} \\ &= \sum_{s' \in S} \Pr\{ X(0) = s' \} \cdot \Pr\{ X(t) = s \mid X(0) = s' \} \end{aligned}$$

Using $\underline{p}(t) = (p_{s_0}(t), p_{s_1}(t), \ldots, p_{s_k}(t))$ we obtain in matrix form:

$$\underline{p}'(t) = \underline{p}(t) \cdot \mathbf{Q} \quad \text{given} \quad \underline{p}(0)$$

where $\mathbf{Q} = \mathbf{R} - \mathit{diag}(E)$ is the infinitesimal generator matrix

$\underline{p}(t)$ is the transient-state probability vector at time t

Steady-state distribution of a CTMC

Assuming a stationary distribution exists (e.g., finite and irreducible):

$$p_s \;=\; \lim_{t\to\infty} p_s(t) \quad\Leftrightarrow\quad \lim_{t\to\infty} p'_s(t) \;=\; 0 \quad\Leftrightarrow\quad \lim_{t\to\infty} p_s(t)\cdot\mathbf{Q} \;=\; 0$$

Using $\underline{p} = (p_{s_0}, p_{s_1}, \ldots, p_{s_k})$ we obtain in matrix form:

$$\underline{p}\cdot\mathbf{Q} \;=\; 0 \quad \text{where} \quad \textstyle\sum_{s\in S} p_s = 1$$

$\underline{p}$ is the steady-state probability vector

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Markovian bisimulation

- Let $\mathcal{C} = (S, \mathbf{R})$ be a CTMC and R an equivalence relation on S
- R is a *Markovian bisimulation* on S if for any $(s, s') \in R$:

$$\underbrace{\mathbf{P}(s, C) \;=\; \mathbf{P}(s', C) \quad \text{for all} \quad C \in S/R \quad \text{and} \quad E(s) \;=\; E(s')}_{\mathbf{R}(s,C) \,=\, \mathbf{R}(s',C)}$$

- s and s' are *Markovian bisimilar* (or: lumping equivalent), $s \sim_m s'$, if:

  $\exists$ a Markovian bisimulation R on S with $(s, s') \in R$

Quotient transition system

For $\mathcal{C} = (S, \mathbf{R})$ and probabilistic bisimulation $\sim_m \subseteq S \times S$ let

$$\mathcal{C}/\sim_m = (S', \mathbf{R}'), \quad \text{the quotient of } \mathcal{C} \text{ under } \sim_m$$

where

- $S' = S/\sim_m = \{ [s]_{\sim_m} \mid s \in S \}$ with $[s]_{\sim_m} = \{ s' \in S \mid s \sim_m s' \}$
- $\mathbf{R}' : S' \times S' \to \mathbb{R}_{\geqslant 0}$ is defined such that for each $s \in S$ and $C \in S'$:

$$\mathbf{R}'([s]_{\sim_m}, C) = \mathbf{R}(s, C)$$

Preservation of state probabilities

- Let $\mathcal{C} = (S, \mathbf{R})$ be a CTMC with initial distribution $\underline{p}(0)$ and $\mathcal{C}/\sim_m$ the quotient under $\sim_m$

- For any $C \in S_0/\sim_m$ we have:

$$\underline{p'}_C(t) = \sum_{s \in C} \underline{p}_s(t) \quad \text{for any } t \geqslant 0$$

- If the steady-state distribution exists, then it follows:

$$\underline{p'}_C = \lim_{t \to \infty} \underline{p'}_C(t) = \lim_{t \to \infty} \sum_{s \in C} \underline{p}_s(t) = \sum_{s \in C} \underline{p}_s$$

Example

Probabilistic timed reachability

For any $C \in S/\sim_m$:

$$s \sim_m s' \;\Rightarrow\; \underbrace{\Pr\left\{ s \overset{\leqslant t}{\rightsquigarrow} C \right\}}_{p(s,t,C)} = \Pr\left\{ s' \overset{\leqslant t}{\rightsquigarrow} C \right\} \quad \text{for any } t \geqslant 0$$

where $p(s,t,C) = \lim_{n \to \infty} p(s,t,n,C)$ with:

$$p(s,t,n,C) = \begin{cases} 1 & \text{if } s \in C \\ \displaystyle\int_0^t \sum_{s' \in S} \mathbf{R}(s,s') \cdot e^{-E(s)\cdot x} \cdot p(s', t{-}x, n{-}1, C)\, dx & \text{if } s \notin C \text{ and } n > 0 \\ 0 & \text{otherwise} \end{cases}$$

generalization possible by forbidding paths visiting $B \in S/\sim_m$

Weak Markovian bisimulation

- Let $\mathcal{C} = (S, \mathbf{R})$ be a CTMC and R an equivalence relation on S
- R is a *weak Markovian bisimulation* on S if for any $(s, s') \in R$:

$$\mathbf{R}(s, C) \;=\; \mathbf{R}(s', C) \qquad \text{for all } C \in S/R \text{ with } C \neq [s]_R \text{ and } C \neq [s']_R$$

- s and s' are *weak Markovian bisimilar* $s \approx_m s'$, if:

  $\exists$ a weak Markovian bisimulation R on S with $(s, s') \in R$

obviously we have: $s \sim_m s' \;\Rightarrow\; s \approx_m s'$

Example

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$\Rightarrow$ Markovian simulation

  - definition, properties, examples

Alternative definition of Markovian bisimulation

- Let $\mathcal{C} = (S, \mathbf{R})$ be a CTMC and R an equivalence relation on S
- R is a *Markovian bisimulation* on S if for any $(s, s') \in R$:

$$\underbrace{\mathbf{P}(s, \cdot) \;\equiv_R\; \mathbf{P}(s', \cdot) \quad \text{and} \quad E(s) = E(s')}_{\mathbf{R}(s,\cdot) \,\equiv_R\, \mathbf{R}(s',\cdot)}$$

where $\equiv_R$ denotes the lifting of R on *Distr*(S) defined by:

$$\mu \;\equiv_R\; \mu' \quad \text{iff} \quad \mu(C) = \mu'(C) \quad \text{for all} \quad C \in S/R$$

Markovian simulation

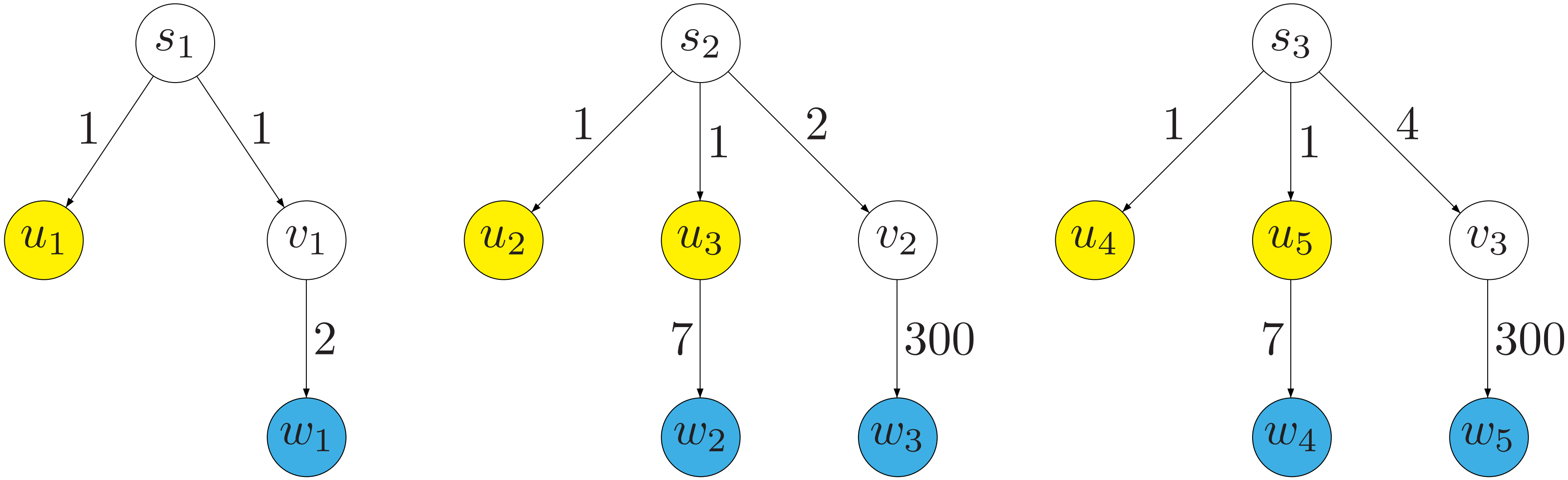
- Let $\mathcal{C} = (S, \mathbf{R})$ be a CTMC and R a binary relation on S
- R is a *Markovian simulation* on S if for all $(s, s') \in R$:

$$\mathbf{P}(s, \cdot) \sqsubseteq_R \mathbf{P}(s', \cdot) \quad \text{and} \quad E(s) \leqslant E(s')$$

- s' simulates s, denoted $s \sqsubseteq_m s'$, if

  $\exists$ a Markovian simulation R on S such that $(s, s') \in R$

Example



$s_1 \sqsubseteq_m s_2$ but $s_2 \not\sqsubseteq_m s_3$

Probabilistic timed reachability

For any $C \subseteq S$ such that $C = C\!\uparrow_{\sqsubseteq_m}$:

$$s \sqsubseteq_m s' \quad \Rightarrow \quad \underbrace{\Pr\left\{s \overset{\leqslant t}{\rightsquigarrow} C\right\}}_{p(s,t,C)} \leqslant \Pr\left\{s' \overset{\leqslant t}{\rightsquigarrow} C\right\} \qquad \text{for any } t \geqslant 0$$

where $p(s, t, C) = \lim_{n \to \infty} p(s, t, n, C)$ with:

$$p(s,t,n,C) = \begin{cases} 1 & \text{if } s \in C \\ \displaystyle\int_0^t \sum_{s' \in S} \mathbf{R}(s,s') \cdot e^{-E(s) \cdot x} \cdot p(s', t-x, n-1, C)\, dx & \text{if } s \notin C \text{ and } n > 0 \\ 0 & \text{otherwise} \end{cases}$$

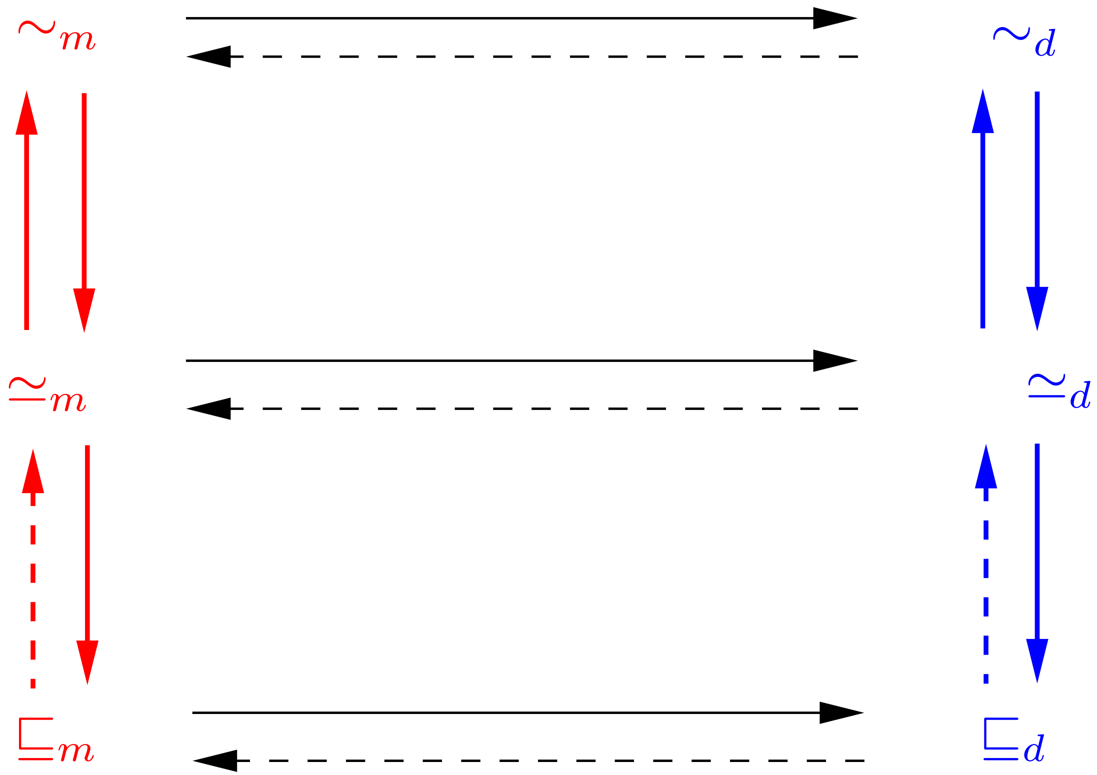
generalization possible by forbidding paths visiting $B \subseteq S$ with $B = B\!\uparrow_{\sqsubseteq_m}$

Proof

Properties

- $s \approx_m s'$ implies $s \sim_m s'$ and $s \sim_m s'$ implies $s \sqsubseteq_m s'$
- Markovian simulation equivalence $\simeq_m$ coincides with $\sim_m$
- relationship to the embedded DTMC:
  - $s \sim_m s'$ in CTMC $\mathcal{C}$ implies $s \sim_p s'$ in *emb*$(\mathcal{C})$
  - $s \sqsubseteq_m s'$ in CTMC $\mathcal{C}$ implies $s \sqsubseteq_p s'$ in *emb*$(\mathcal{C})$
  - $s \approx_m s'$ in CTMC $\mathcal{C}$ implies $s \approx_p s'$ in *emb*$(\mathcal{C})$
- if $E(s) = E$ for any s we have:
  - the reverse implications for *emb*$(\mathcal{C})$ also hold
  - $\sim_m$ and $\approx_m$ coincide, as well as $\sim_m$ and $\sqsubseteq_m$

Relating (bi)simulation on CTMCs and DTMCs



$R \longrightarrow R'$ means that R is coarser than R'