Modeling and Verification of Probabilistic Systems

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http://moves.rwth-aachen.de/teaching/ws-1516/movep15/

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Overview

Time in discrete-time Markov chains

The advance of time in DTMCs

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Continuous random variables

- X is a random variable (r.v., for short)
  - on a sample space with probability measure Pr
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- X is a random variable (r.v., for short)
  - on a sample space with probability measure Pr
  - assume the set of possible values that X may take is dense
- X is *continuously distributed* if there exists a function $f(x)$ such that:

$$F_x(d) \;=\; Pr\{X \leqslant d\} \;=\; \int_{-\infty}^{d} f(x)\; dx \quad \text{for each real number } d$$

where f satisfies: $f(x) \geqslant 0$ for all x and $\displaystyle\int_{-\infty}^{\infty} f(x)\; dx = 1$

- $F_X(d)$ is the *(cumulative) probability distribution function*
- $f(x)$ is the *probability density function*

Negative exponential distribution

Negative exponential distribution

Density of exponential distribution

The density of an *exponentially distributed* r.v. Y with *rate* $\lambda \in \mathbb{R}_{>0}$ is:

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

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Let r.v. Y be exponentially distributed with rate $\lambda \in \mathbb{R}_{>0}$. Then:

- Expectation $E[Y] = \int_0^\infty x \cdot \lambda \cdot e^{-\lambda \cdot x} \; dx \; = \; \frac{1}{\lambda}$

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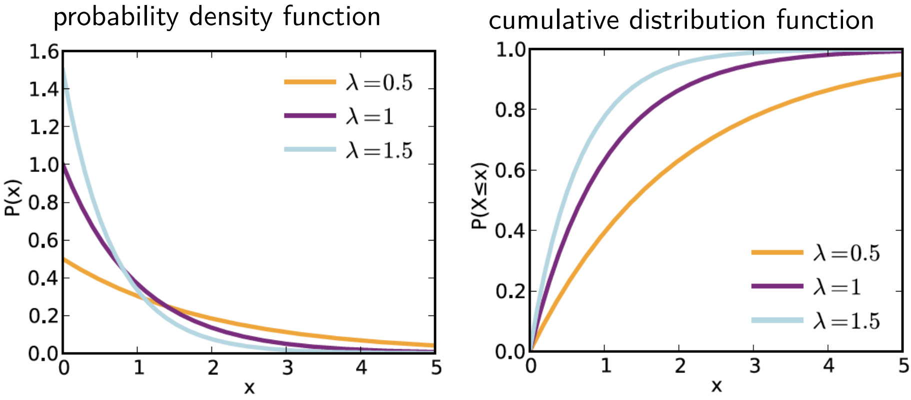
- Expectation $E[Y] = \int_0^\infty x \cdot \lambda \cdot e^{-\lambda \cdot x} \; dx \;=\; \frac{1}{\lambda}$
- Variance $Var[Y] = \int_0^\infty (x - E[X])^2 \lambda \cdot e^{-\lambda \cdot x} \; dx \;=\; \frac{1}{\lambda^2}$

Exponential pdf and cdf



The higher λ, the faster the cdf approaches 1.

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- Can *approximate* general distributions arbitrarily closely
- Yield a *maximal entropy* if only the mean is known

Memoryless property

Theorem

1. For any exponentially distributed random variable X:

$$Pr\{X > t + d \mid X > t\} \;=\; Pr\{X > d\} \text{ for any } t, d \in \mathbb{R}_{\geqslant 0}.$$

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Proof of 2. : By contraposition, using the total law of probability.

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Minimum closure theorem

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For independent, exponentially distributed random variables X and Y with rates $\lambda, \mu \in \mathbb{R}_{>0}$, the r.v. $\min(X, Y)$ is exponentially distributed with rate $\lambda+\mu$, i.e.,:

$$Pr\{\min(X, Y) \leqslant t\} \;=\; 1 - e^{-(\lambda+\mu)\cdot t} \quad \text{for all } t \in \mathbb{R}_{\geqslant 0}.$$

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$$Pr\{\min(X, Y) \leqslant t\} = Pr_{X,Y}\{(x, y) \in \mathbb{R}^2_{\geqslant 0} \mid \min(x, y) \leqslant t\}$$
$$= \int_0^\infty \left(\int_0^\infty \mathbf{I}_{\min(x,y)\leqslant t}(x, y) \cdot \lambda e^{-\lambda x} \cdot \mu e^{-\mu y} \, dy \right) dx$$

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&= \int_0^t \int_x^\infty \lambda e^{-\lambda x} \cdot \mu e^{-\mu y} \, dy \, dx + \int_0^t \int_y^\infty \lambda e^{-\lambda x} \cdot \mu e^{-\mu y} \, dx \, dy
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Minimum closure theorem for several exponentially distributed r.v.'s

For independent, exponentially distributed random variables $X_1, X_2, \ldots, X_n$ with rates $\lambda_1, \lambda_2, \ldots, \lambda_n \in \mathbb{R}_{>0}$ the r.v. $\min(X_1, X_2, \ldots, X_n)$ is exponentially distributed with rate $\sum_{0<i\leqslant n} \lambda_i$, i.e.,:

$$Pr\{\min(X_1, X_2, \ldots, X_n) \leqslant t\} \;=\; 1 - e^{-\sum_{0<i\leqslant n} \lambda_i \cdot t} \quad \text{for all } t \in \mathbb{R}_{\geqslant 0}.$$

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Proof:

Generalization of the proof for the case of two exponential distributions.

Property 2: Winning the race with two competitors

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The minimum of two exponential distributions

For independent, exponentially distributed random variables X and Y with rates $\lambda, \mu \in \mathbb{R}_{>0}$, it holds:

$$Pr\{X \leqslant Y\} = \frac{\lambda}{\lambda+\mu}.$$

Proof:

On the blackboard.

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Proof

Let λ (μ) be the rate of X's (Y's) distribution. Then we derive:

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Pr\{X \leqslant Y\} &= Pr_{X,Y}\{(x,y) \in \mathbb{R}^2_{\geqslant 0} \mid x \leqslant y\} \\
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&= 1 - \int_0^\infty \mu e^{-\mu y} \cdot e^{-\lambda y} \, dy \;=\; 1 - \int_0^\infty \mu e^{-(\mu+\lambda) y} \, dy \\
&= 1 - \frac{\mu}{\mu+\lambda} \cdot \underbrace{\int_0^\infty (\mu+\lambda) e^{-(\mu+\lambda) y} \, dy}_{=1}
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\end{aligned}
$$

Proof

Let λ (μ) be the rate of X's (Y's) distribution. Then we derive:

$$
\begin{aligned}
Pr\{X \leqslant Y\} &= Pr_{X,Y}\{(x,y) \in \mathbb{R}^2_{\geqslant 0} \mid x \leqslant y\} \\
&= \int_0^\infty \mu e^{-\mu y} \left(\int_0^y \lambda e^{-\lambda x} \, dx \right) dy \\
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Property 2: Winning the race with many competitors

The minimum of several exponentially distributed r.v.'s

For independent, exponentially distributed random variables $X_1, X_2, \ldots, X_n$ with rates $\lambda_1, \lambda_2, \ldots, \lambda_n \in \mathbb{R}_{>0}$ it holds:

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Proof:

Generalization of the proof for the case of two exponential distributions.

Overview

Continuous-time Markov chains

- Continuous-time Markov chains
  - labeled transition systems augmented with rates
  - discrete state space
  - continuous time steps
  - delays exponentially distributed
- Suited to modelling
  - reliability models
  - control systems
  - queueing networks
  - biological pathways
  - chemical reactions
  - ...

Continuous-time Markov chain

Continuous-time Markov chain

A CTMC is a tuple $(S, \mathbf{P}, r, \iota_{\text{init}}, AP, L)$ where

- $(S, \mathbf{P}, \iota_{\text{init}}, AP, L)$ is a DTMC, and
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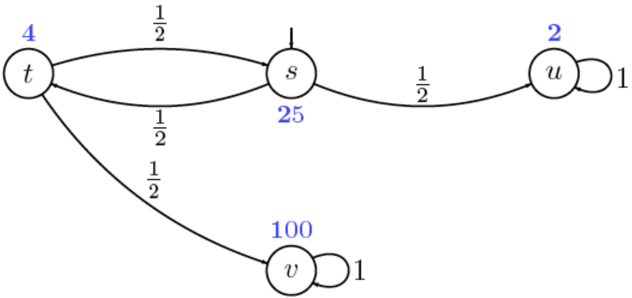
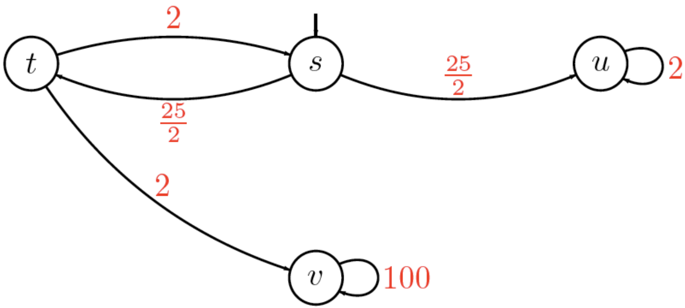
- phrased alternatively, the average residence time of state s is $\frac{1}{r(s)}$.
- thus, the higher the rate $r(s)$, the shorter the average residence time in s.

Example



$r(s) = 25$, $r(t) = 4$, $r(u) = 2$ and $r(v) = 100$

Example: a classical perspective



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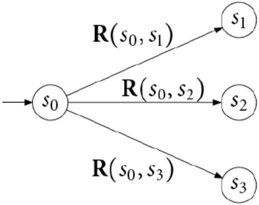
The transition rate $\mathbf{R}(s, s') = \mathbf{P}(s, s') \cdot r(s)$

We use $(S, \mathbf{P}, r, \iota_{\text{init}}, AP, L)$ and $(S, \mathbf{R}, \iota_{\text{init}}, AP, L)$ interchangeably.

CTMC semantics by example



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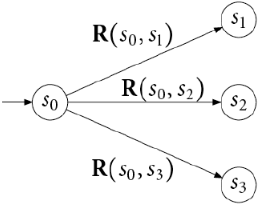

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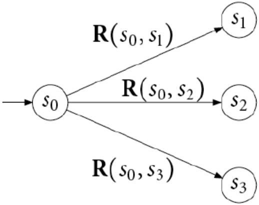

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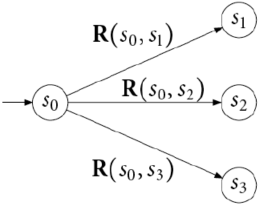

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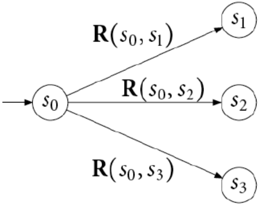

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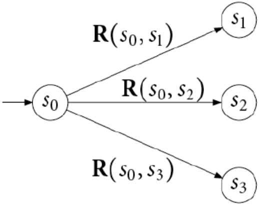

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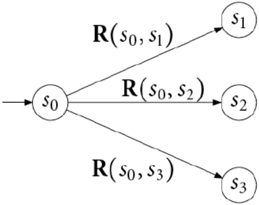

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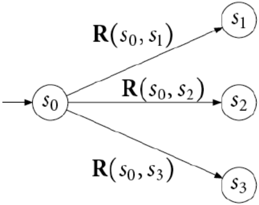

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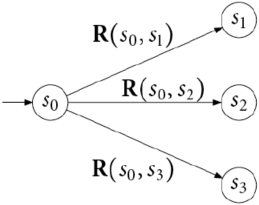

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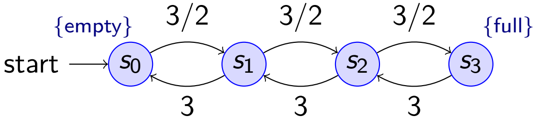
Simple CTMC example

Modelling a queue of jobs

- initially the queue is empty
- jobs arrive with rate 3/2 (i. e., mean inter-arrival time is 2/3)
- jobs are served with rate 3 (i. e., mean service time is 1/3)
- maximum size of the queue is 3
- state space $S = \{s_i \mid 0 \leqslant i \leqslant 3\}$ where s_i indicates i jobs in queue.



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

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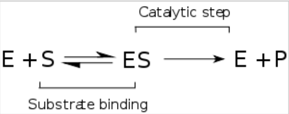
Enzyme-catalysed substrate conversion

Kinetics

[edit]

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 commonly obtained from enzyme assays, where since the 90s, the dynamics of many enzymes are studied on the level of individual molecules.

In 1902 Victor Henri[57] 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[58] 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 (termed also Michaelis-Menten kinetics).[59] Their work was further developed by G. E. Briggs and J. B. S. Haldane, who derived kinetic equations that are still widely considered today a starting point in solving enzymatic activity.[60]

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. Note that the simple Michaelis Menten mechanism for the enzymatic activity is considered today a basic idea, where many examples show that the enzymatic activity involves structural dynamics. This is incorporated in the enzymatic mechanism while introducing several Michaelis Menten pathways that are connected with fluctuating rates [44][45][46]. Nevertheless, there is a mathematical relation connecting the behavior obtained from the basic Michaelis Menten mechanism (that was indeed proved correct in many experiments) with the generalized Michaelis Menten mechanisms involving dynamics and activity; [61] this means that the measured activity of enzymes on the level of many enzymes may be explained with the simple Michaelis-Menten equation, yet, the actual activity of enzymes is richer and involves structural dynamics.

Source: wikipedia (June 2011)

Stochastic chemical kinetics

- Types of reaction described by stochiometric equations:

$$E + S \underset{k_2}{\overset{k_1}{\rightleftharpoons}} ES \xrightarrow{k_3} E + P$$

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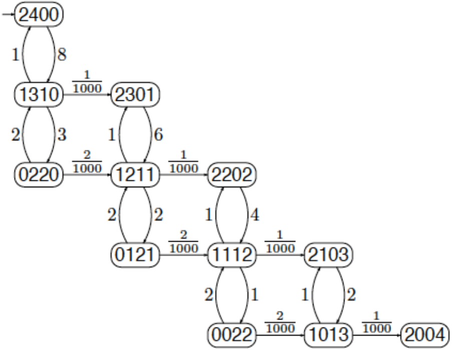
- This process is a continuous-time Markov chain.

Enzyme-catalyzed substrate conversion as a CTMC



States:	*init*	*goal*
enzymes	2	2
substrates	4	0
complex	0	0
products	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 $x_C > 0$

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CTMCs are one of the most prominent models in performance analysis

Overview

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- The probability to win a race amongst several exponential distributions only depends on their rates.
- A CTMC is a DTMC where state residence times are exponentially distributed.
- CTMC semantics distinguishes between enabledness and taking a transition.
- CTMCs are frequently used as semantical model for high-level formalisms.