

Modeling and Verification of Probabilistic Systems

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<http://moves.rwth-aachen.de/teaching/ws-1819/movep18/>

November 27, 2018

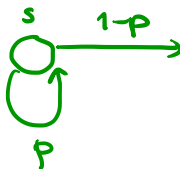
Overview

- 1 Negative exponential distribution
- 2 Continuous-time Markov chains
- 3 Summary

Time in discrete-time Markov chains

The advance of time in DTMCs

- ▶ Time in a DTMC proceeds in **discrete steps**
- ▶ Two possible interpretations:
 1. accurate model of (discrete) time units
 - ▶ e.g., clock ticks in model of an embedded device
 2. time-abstract
 - ▶ no information assumed about the time transitions take
- ▶ State residence time is **geometrically** distributed



$$p^{k-1} (1-p)$$

$$= P\{\text{stay } k \text{ steps in state } s\}$$

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Continuous-time Markov chains

- ▶ dense model of time
- ▶ transitions can occur at any (real-valued) time instant
- ▶ state residence time is **(negative) exponentially** distributed

Continuous random variables

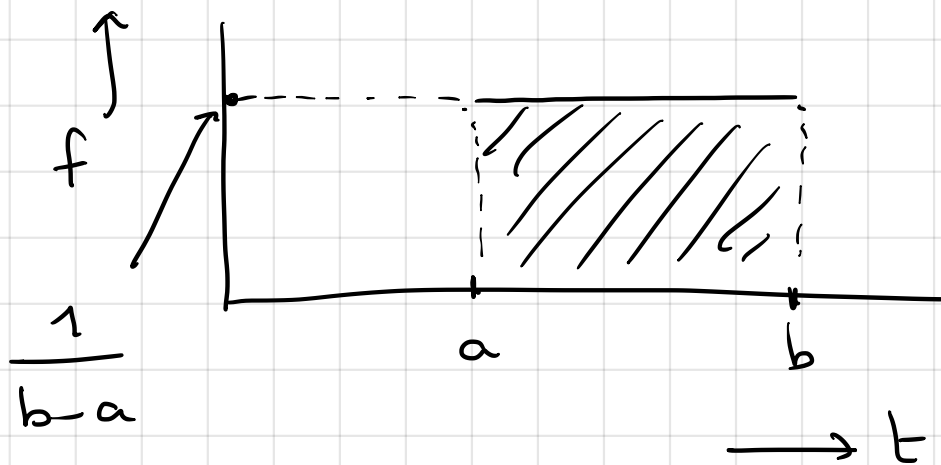
- ▶ X is a random variable (r.v., for short)
 - ▶ on a sample space with probability measure Pr
 - ▶ assume the set of possible values that X may take is dense
- ▶ X is *continuously distributed* if there exists a function $f(x)$ such that:

$$\underline{F_X(d)} = \underline{Pr\{X \leq d\}} = \int_{-\infty}^d f(x) dx \quad \text{for each real number } d$$

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

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

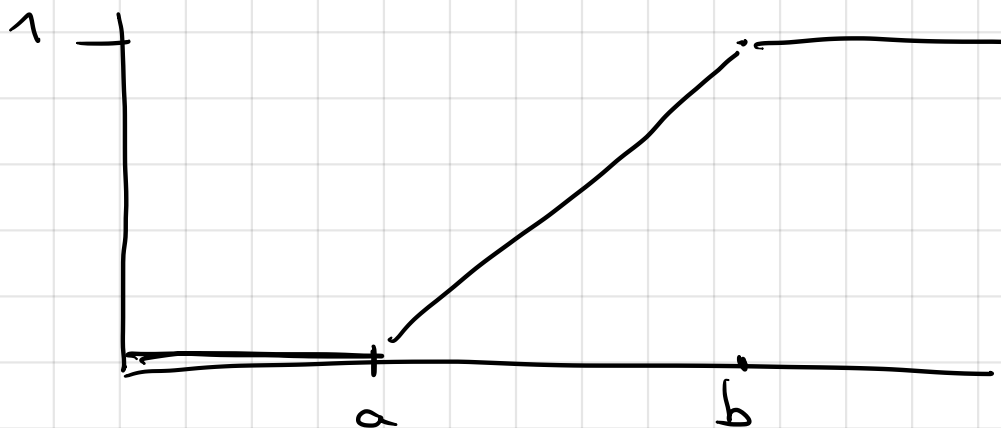
Uniform distribution on $[a, b]$



$$f(t) = \begin{cases} \frac{1}{b-a} & \text{if } a \leq t \leq b \\ 0 & \text{otherwise} \end{cases}$$

$$F(t) = \int_{-\infty}^t f(x) dx$$

$$F(t) = \begin{cases} 0 & \text{if } t < a \\ \frac{t-a}{b-a} & \text{if } a \leq t \leq b \\ 1 & \text{if } t > b \end{cases}$$



Negative exponential distribution

Density of exponential distribution

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

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

The cumulative distribution of r.v. Y with rate $\lambda \in \mathbb{R}_{>0}$ is:

$$F_Y(d) = \int_{-\infty}^d \lambda \cdot e^{-\lambda \cdot x} dx = [-e^{-\lambda \cdot x}]_0^d = 1 - e^{-\lambda \cdot d}.$$

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The rate $\lambda \in \mathbb{R}_{>0}$ uniquely determines an exponential distribution.

Variance and expectation

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

$$\blacktriangleright \text{Expectation } E[Y] = \int_0^\infty x \cdot \underbrace{\lambda \cdot e^{-\lambda \cdot x}}_{f_Y(x)} dx = \frac{1}{\lambda}$$

Negative exponential distribution

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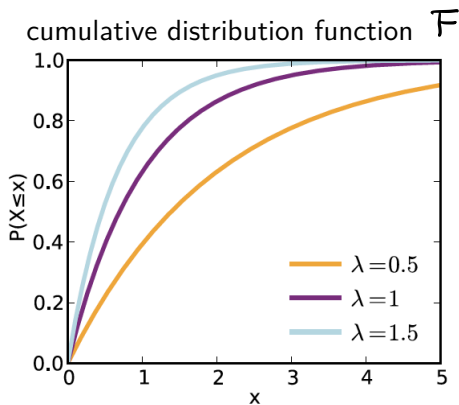
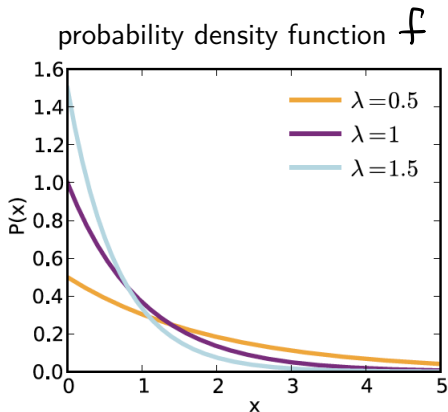
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Variance and expectation

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

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

Why exponential distributions?

- ▶ Are *adequate* for many real-life phenomena
 - ▶ the time until a radioactive particle decays
 - ▶ the time between successive car accidents
 - ▶ inter-arrival times of jobs, telephone calls in a fixed interval
- ▶ Are the continuous counterpart of the *geometric* distribution
- ▶ Heavily used in physics, performance, and reliability analysis
- ▶ Can *approximate* general distributions arbitrarily closely (Cox, 1952)

Erlang distr.



Phase-type distributions

Why exponential distributions?

- ▶ Are *adequate* for many real-life phenomena
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 - ▶ inter-arrival times of jobs, telephone calls in a fixed interval
- ▶ Are the continuous counterpart of the *geometric* distribution
- ▶ Heavily used in physics, performance, and reliability analysis
- ▶ Can *approximate* general distributions arbitrarily closely
- ▶ Yield a *maximal entropy* if only the mean is known

cont. r.v. X , entropy of X

$$\text{Entropy}(X) = \int_{-\infty}^{\infty} \underbrace{f(x) \cdot \log\left(\frac{1}{f(x)}\right)}_{0 \text{ if } f(x)=0} dx$$

maximising the entropy = minimise the amount of prior information into the distribution

a. uniform distr. on $[a, b]$ has maximum entropy (among all) continuous distributions) if only it is known that the support is $[a, b]$.

b. normal (Gaussian) distribution $N(\mu, \sigma^2)$ has maximal entropy if only mean μ and variance σ^2 are known.

c. exponential distribution with rate λ has maximal entropy if only the mean $\frac{1}{\lambda}$ is known.

Memoryless property

Theorem

1. For any exponentially distributed random variable X :

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

2. Any cdf which is memoryless is a negative exponential one.

Proof:

Proof of 1. : Let λ be the rate of X 's distribution. Then we derive:

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

$$= \frac{e^{-\lambda \cdot (t+d)}}{e^{-\lambda \cdot t}} =$$

$$\begin{aligned} \Pr(X > t) &= 1 - \Pr(X \leq t) \\ &= 1 - (1 - e^{-\lambda t}) \end{aligned}$$

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Proof of 1. : Let λ be the rate of X 's distribution. Then we derive:

$$\begin{aligned} Pr\{X > t + d \mid X > t\} &= \frac{Pr\{X > t+d \cap X > t\}}{Pr\{X > t\}} = \frac{Pr\{X > t+d\}}{Pr\{X > t\}} \\ &= \frac{e^{-\lambda \cdot (t+d)}}{e^{-\lambda \cdot t}} = e^{-\lambda \cdot d} = Pr\{X > d\}. \end{aligned}$$

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

Property 1: Closure under minimum

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Minimum closure theorem

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.,:

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

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Proof:

On the blackboard.

$$\Pr \{ \min(X, Y) \leq x \}$$

$$= 1 - \Pr \{ \min(X, Y) > x \}$$

$$= 1 - \Pr \{ X > x \wedge Y > x \}$$

$$= (\text{* } X \text{ and } Y \text{ are independent *})$$

$$1 - \Pr(X > x) \cdot \Pr(Y > x)$$

=

$$1 - \left(\underbrace{1 - (1 - e^{-\lambda x})}_{e^{-\lambda x}} \right) \cdot \left(\underbrace{1 - (1 - e^{-\mu x})}_{e^{-\mu x}} \right)$$

$$= 1 - e^{-\lambda x} \cdot e^{-\mu x}$$

$$= 1 - e^{-(\lambda + \mu) \cdot x}$$

Proof

Let λ (μ) be the rate of X 's (Y 's) distribution.

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$$Pr\{\min(X, Y) \leq t\} = Pr_{X,Y}\{(x, y) \in \mathbb{R}_{\geq 0}^2 \mid \min(x, y) \leq t\}$$

Proof

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

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

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 &= \underbrace{\int_0^t \int_x^\infty \lambda e^{-\lambda x} \cdot \mu e^{-\mu y} dy dx}_{\text{min is } y} + \underbrace{\int_0^t \int_y^\infty \lambda e^{-\lambda x} \cdot \mu e^{-\mu y} dx dy}_{\text{min is } x}
 \end{aligned}$$

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 &= \int_0^t \lambda e^{-\lambda x} \cdot e^{-\mu x} dx + \int_0^t e^{-\lambda y} \cdot \mu e^{-\mu y} dy
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 &= \int_0^t \lambda e^{-\lambda x} \cdot e^{-\mu x} dx + \int_0^t e^{-\lambda y} \cdot \mu e^{-\mu y} dy \\
 &= \int_0^t \lambda e^{-(\lambda+\mu)x} dx + \int_0^t \mu e^{-(\lambda+\mu)y} dy
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 &= \int_0^t \lambda e^{-(\lambda+\mu)x} dx + \int_0^t \mu e^{-(\lambda+\mu)y} dy \\
 &= \int_0^t (\lambda+\mu) \cdot e^{-(\lambda+\mu)z} dz
 \end{aligned}$$

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 &= \int_0^t \lambda e^{-\lambda x} \cdot e^{-\mu x} dx + \int_0^t e^{-\lambda y} \cdot \mu e^{-\mu y} dy \\
 &= \int_0^t \lambda e^{-(\lambda+\mu)x} dx + \int_0^t \mu e^{-(\lambda+\mu)y} dy \\
 &= \int_0^t (\lambda+\mu) \cdot e^{-(\lambda+\mu)z} dz = 1 - e^{-(\lambda+\mu)t}
 \end{aligned}$$

Property 1: Closure under minimum

Minimum closure theorem for several exponentially distributed r.v.'s

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

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

z

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

Proof:

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

Exponential distributions are not closed
under max

$$\Pr \{ \max(X, Y) \leq x \} =$$

$$\Pr \{ X \leq x \wedge Y \leq x \}$$

$$= \Pr \{ X \leq x \} \cdot \Pr \{ Y \leq x \}$$

$$= (1 - e^{-\lambda x}) \cdot (1 - e^{-\mu x})$$

$$= \underbrace{1 - e^{-\lambda x} - e^{-\mu x} + e^{-(\lambda + \mu)x}}$$

not an exp. distribution.

Property 2: Winning the race with two competitors

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:

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

$$\lambda = 10$$

$$\mu = 20$$

Proof:

On the blackboard.

$$\Pr\{X \leq Y\} = \frac{10}{30} = \frac{1}{3}$$

$$Y \sim \exp(\mu)$$

$$X \sim \exp(\lambda)$$

$$\Pr \{ X = \min(X, Y) \}$$

$$= \Pr \{ X \leq Y \}$$

$$= \int_0^{\infty} \underbrace{\Pr \{ Y = y \}}_{\text{density}} \cdot \underbrace{\Pr \{ X \leq y \}}_{\text{cdf}} dy$$

$$= \int_0^{\infty} \mu \cdot e^{-\mu y} \cdot (1 - e^{-\lambda y}) dy$$

$$= \int_0^{\infty} \mu e^{-\mu y} - \mu e^{-(\lambda + \mu)y} dy$$

$$= \left[-e^{-\mu y} + \frac{\mu}{\lambda + \mu} \cdot e^{-(\lambda + \mu)y} \right]_0^{\infty}$$

$$= \left(-e^{-\mu \cdot \infty} + \frac{\mu}{\lambda + \mu} e^{-(\lambda + \mu) \cdot \infty} - \left(-e^{-\mu \cdot 0} + \frac{\mu}{\lambda + \mu} e^{-(\lambda + \mu) \cdot 0} \right) \right)$$

$$= -\left(-1 + \frac{\mu}{\mu + \lambda} \right) = 1 - \frac{\mu}{\mu + \lambda} = \frac{\lambda}{\lambda + \mu} \quad \square$$

Proof

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

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

Property 2: Winning the race with many competitors

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

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

$$Pr\{\textcolor{red}{X}_i = \min(X_1, \dots, X_n)\} = \frac{\textcolor{red}{\lambda}_i}{\sum_{j=1}^n \lambda_j}.$$

Proof:

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

Overview

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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

$\text{exp-time} = \frac{1}{4}$ $\bigcirc s$ $r(s) = 4$
 $\frac{1}{2}$ $\bigcirc s'$ $r(s') = 2$

Continuous-time Markov chain

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

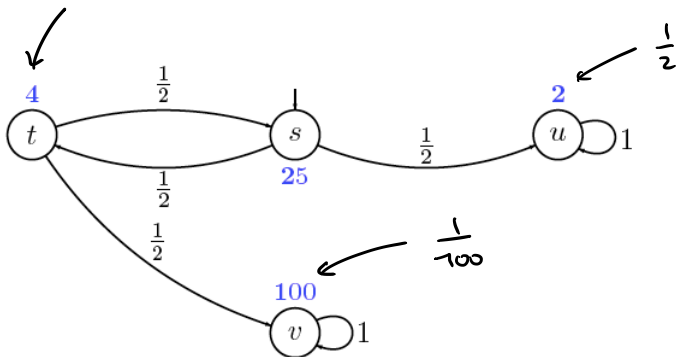
- ▶ $(S, \mathbf{P}, \ell_{\text{init}}, AP, L)$ is a DTMC, and
- ▶ $r : S \rightarrow \mathbb{R}_{>0}$, the **exit-rate function**

Interpretation

- ▶ **residence** time in state s is exponentially distributed with **rate** $r(s)$.
- ▶ 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 .

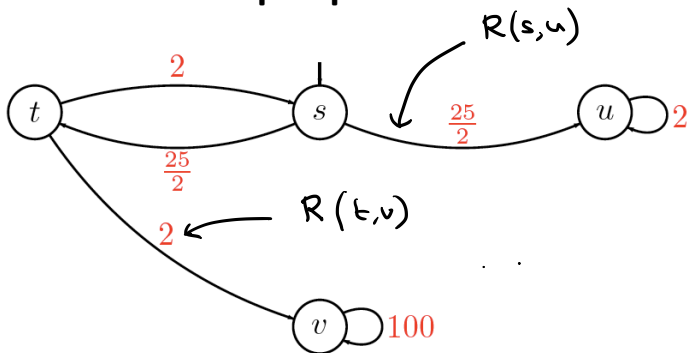
Example

$$\Pr \{ \text{stay in state } t \text{ for } \leq d \text{ time} \} = 1 - e^{4 \cdot d}$$



$$r(s) = 25, r(t) = 4, r(u) = 2 \text{ and } r(v) = 100$$

Example: a classical perspective

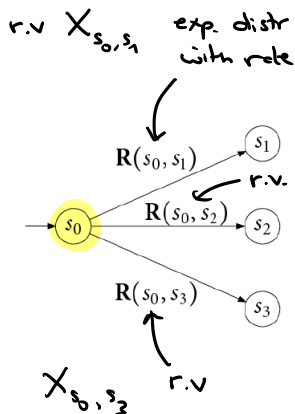


$$r(s) = 25, r(t) = 4, r(u) = 2 \text{ and } r(v) = 100$$

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

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

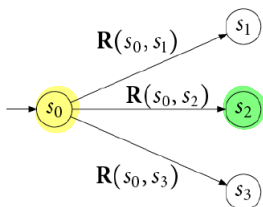
CTMC semantics by example



CTMC semantics

- Transition $s \rightarrow s' := \text{r.v. } X_{s, s'}$ with rate $R(s, s')$

CTMC semantics by example



CTMC semantics

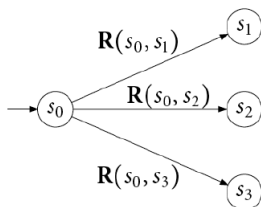
- ▶ Transition $s \rightarrow s' := \text{r.v. } X_{s,s'}$ with rate $R(s, s')$
- ▶ Probability to go from state s_0 to, say, state s_2 is:

$$\Pr\{X_{s_0,s_2} \leq X_{s_0,s_1} \cap X_{s_0,s_2} \leq X_{s_0,s_3}\}$$

=

$$\Pr\{X_{s_0,s_2} = \min(X_{s_0,s_1}, X_{s_0,s_2}, X_{s_0,s_3})\}$$

CTMC semantics by example



CTMC semantics

- ▶ Transition $s \rightarrow s' := \text{r.v. } X_{s,s'}$ with rate $R(s, s')$
- ▶ Probability to go from state s_0 to, say, state s_2 is:

$$\begin{aligned}
 & Pr\{X_{s_0, s_2} \leq X_{s_0, s_1} \cap X_{s_0, s_2} \leq X_{s_0, s_3}\} \\
 &= \\
 & \frac{R(s_0, s_2)}{R(s_0, s_1) + R(s_0, s_2) + R(s_0, s_3)} = \frac{R(s_0, s_2)}{r(s_0)}
 \end{aligned}$$

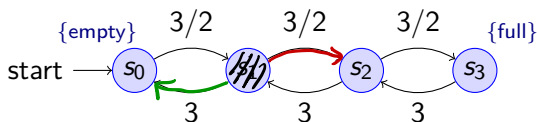
- ▶ Probability of staying at most t time in s_0 is:

$$\begin{aligned}
 & Pr\{\min(X_{s_0, s_1}, X_{s_0, s_2}, X_{s_0, s_3}) \leq t\} \\
 &= \\
 & 1 - e^{-(R(s_0, s_1) + R(s_0, s_2) + R(s_0, s_3)) \cdot t} = 1 - e^{-r(s_0) \cdot t}
 \end{aligned}$$

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 $S = \{s_i \mid 0 \leq i \leq 3\}$ where s_i indicates i jobs in queue.



$$\Pr(s_1 \xrightarrow{\text{green}} s_0) = \frac{3}{3 + \frac{3}{2}}$$

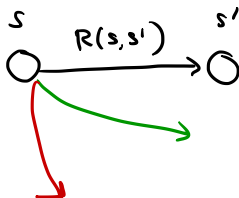
$$\begin{aligned} \Pr(\text{leave } s_1 \leq 7 \text{ time}) &= 1 - e^{-(3 + \frac{3}{2}) \cdot 7} \end{aligned}$$

CTMC semantics

CTMC semantics

Enabledness

The probability that transition $s \rightarrow s'$ is *enabled* in $[0, t]$ is $1 - e^{-R(s,s') \cdot t}$.



↑
possible to take

CTMC semantics

Enabledness

The probability that transition $s \rightarrow s'$ is *enabled* in $[0, t]$ is $1 - e^{-R(s,s') \cdot t}$.

State-to-state timed transition probability

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

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

Residence time distribution

The probability to *take some* outgoing transition from s in $[0, t]$ is:

$$\int_0^t r(s) \cdot e^{-r(s) \cdot x} dx = 1 - e^{-r(s) \cdot t}$$

CTMC semantics

State-to-state timed transition probability

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

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

Proof:

On the blackboard.

$$\Pr \{ s \rightarrow s' \text{ wins the race } \leq t \mid \text{ in } s \text{ at time } 0 \}$$

$$= \int_0^t \underbrace{\Pr \{ s \rightarrow s' \text{ at time } x \}}_{\text{density}} \cdot \underbrace{\Pr \{ \text{earliest time to take } s \rightarrow s'' \text{ (} s'' \neq s' \text{)} > x \}}_{\text{density}} dx$$

$$= \int_0^t R(s, s') \cdot e^{-R(s, s') \cdot x} \cdot \prod_{\substack{s'' \in \text{Post}(s) \\ s'' \neq s'}} \underbrace{e^{-R(s, s'') \cdot x}}_{1 - (1 - e^{-R(s, s'') \cdot x})} dx$$

$$= \int_0^t R(s, s') \cdot \prod_{s'' \in \text{Post}(s)} e^{-R(s, s'') \cdot x} dx$$

$$\underbrace{e^{-\sum_{s''} R(s, s'')}}_{e^{-r(s)}}$$

$$\begin{aligned}
 & \int_0^t R(s, s') \cdot e^{-r(s) \cdot x} dx \\
 = & \boxed{\frac{R(s, s')}{r(s)} (1 - e^{-r(s) \cdot t})} \quad \square
 \end{aligned}$$

Remark:

summing over all successor states s'
we obtain

$$\begin{aligned}
 & \sum_{s' \in S} \frac{R(s, s')}{r(s)} (1 - e^{-r(s) \cdot t}) \\
 = & \frac{r(s)}{r(s)} \cdot (1 - e^{-r(s) \cdot t}) \\
 = & 1 - e^{-r(s) \cdot t}
 \end{aligned}$$

CTMC semantics

Residence time distribution

The probability to *take some* outgoing transition from s in $[0, t]$ is:

$$\int_0^t r(s) \cdot e^{-r(s) \cdot x} dx = 1 - e^{-r(s) \cdot t}$$

Proof:

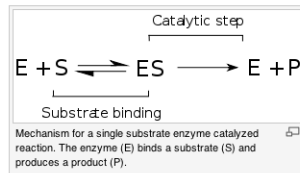
On the blackboard.

Enzyme-catalysed substrate conversion

Kinetics

[\[edit\]](#)

Main article: [Enzyme kinetics](#)



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

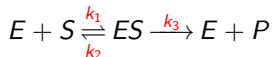
equations that are still widely considered today a starting point in solving enzymatic activity.^[60]

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 **stoichiometric equations**:



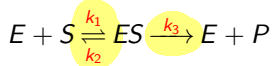
- N different types of molecules that **randomly collide**
where state $X(t) = (x_1, \dots, x_N)$ with $x_i = \#$ molecules of sort i

$$\text{sorts} = \{E, S, ES, P\}$$

$$N = 4$$

Stochastic chemical kinetics

- Types of reaction described by **stoichiometric equations**:



- N different types of molecules that **randomly collide**
where state $X(t) = (x_1, \dots, x_N)$ with $x_i = \#$ molecules of sort i

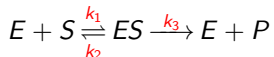
- Reaction probability** within infinitesimal interval $[t, t+\Delta)$:
reaction 1, 2 or 3

$$\alpha_m(\vec{x}) \cdot \Delta = \Pr\{\text{reaction } m \text{ in } [t, t+\Delta) \mid X(t) = \vec{x}\} \text{ where}$$

$$\alpha_m(\vec{x}) = k_m \cdot \# \text{ possible combinations of reactant molecules in } \vec{x}$$

Stochastic chemical kinetics

- Types of reaction described by **stoichiometric equations**:



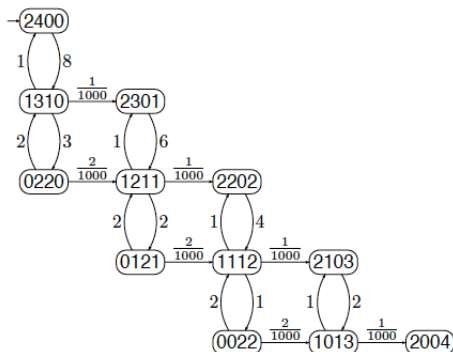
- N different types of molecules that **randomly collide**
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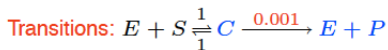
$$\alpha_m(\vec{x}) = k_m \cdot \# \text{ possible combinations of reactant molecules in } \vec{x}$$

- This process is a **continuous-time Markov chain**.

Enzyme-catalyzed substrate conversion as a CTMC



States:	<i>init</i>	<i>goal</i>
enzymes	2	2
substrates	4	0
complex	0	0
products	0	4



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 $x_C > 0$

CTMCs are omnipresent!

- ▶ Markovian queueing networks

(Kleinrock 1975)

CTMCs are omnipresent!

- ▶ Markovian queueing networks (Kleinrock 1975)
- ▶ Stochastic Petri nets (Molloy 1977)
- ▶ Stochastic activity networks (Meyer & Sanders 1985)
- ▶ Stochastic process algebra (Herzog *et al.*, Hillston 1993)
- ▶ Probabilistic input/output automata (Smolka *et al.* 1994)
- ▶ Calculi for biological systems (Priami *et al.*, Cardelli 2002)

CTMCs are one of the most prominent models in performance analysis

Overview

- 1 Negative exponential distribution
- 2 Continuous-time Markov chains
- 3 **Summary**

Summary

Main points

- ▶ Exponential distributions are closed under minimum.
- ▶ 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.