## Probabilistic Models

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From DTMC to CTMCs

Time in a DTMC proceeds in discrete steps

- accurate model of (discrete) time units (e.g. clock ticks)
- or, no information assumed about the time transitions take

Continuous-time Markov chains (CTMCs): dense model of time

- transitions can occur at any (real-valued) time instant
- modelled using exponential distributions
- suits modelling of: performance/reliability (e.g. of computer networks, manufacturing systems, queueing networks), biological pathways, chemical reactions, ...
1 Exponential Distribution

2 Continuous Time Markov Chains

3 Specifying Probabilistic Properties
1 Exponential Distribution

2 Continuous Time Markov Chains

3 Specifying Probabilistic Properties
Continuous Probability Distribution
Defined by

- a cumulative distribution function: \( F(t) = Pr(X \leq t) = \int_{-\infty}^{t} f(x)dx \)

Example: uniform distribution
\( f(t) = \begin{cases} 
1/\left(b-a\right) & \text{if } a \leq t \leq b, \\
0 & \text{otherwise}.
\end{cases} \)

\( F(t) = \begin{cases} 
0 & \text{if } t \leq a, \\
\frac{t-a}{b-a} & \text{if } a \leq t \leq b, \\
1 & \text{if } t > b.
\end{cases} \)
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- where \( f \) is the probability density function
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Exponential Distribution

A continuous random variable $X$ is exponential with parameter $\lambda$ if its density function is

$$f(t) = \begin{cases} \lambda \cdot e^{-\lambda t} & \text{if } t > 0, \\ 0 & \text{otherwise.} \end{cases}$$
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Cumulative distribution function

$$F(t) = Pr(X \leq t) = \int_0^t \lambda \cdot e^{-\lambda x} dx = 1 - e^{-\lambda t}$$
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Cumulative distribution function

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F(t) = Pr(X \leq t) = \int_{0}^{t} \lambda \cdot e^{-\lambda x} \, dx = 1 - e^{-\lambda t}
\]

Other properties

- negation: \( Pr(X > t) = e^{-\lambda t} \)
- mean: \( E[X] = \int_{0}^{\infty} x \cdot \lambda \cdot e^{-\lambda x} \, dx = \frac{1}{\lambda} \)
- variance: \( Var(X) = \frac{1}{\lambda^2} \)
The more $\lambda$ increases, the faster the c.d.f. approaches 1
Exponential distribution

Adequate for modelling many real-life phenomena

- failures
  - e.g. time before machine component fails
- inter-arrival times
  - e.g. time before next call arrives to a call center
- biological systems
  - e.g. times for reactions between proteins to occur
Useful Properties

The exponential distribution is memoryless

- \( Pr(X > t_1 + t_2 | X > t_1) = Pr(X > t_2) \)
- It is the only memoryless continuous distribution
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- \( Pr(X > t_1 + t_2 | X > t_1) = Pr(X > t_2) \)
- it is the only memoryless continuous distribution
- the discrete time equivalent is the geometric distribution:

\[
P(X = k) = (1 - p)^k p
\]
Useful Properties

The minimum of two exponential distributions is an exponential distribution

- $X_1 \sim Exp(\lambda_1), \ X_2 \sim Exp(\lambda_2)$
- $Y = \min(X_1, X_2) \sim Exp(\lambda_1 + \lambda_2)$
- generalises to minimum of $n$ distributions

Comparison of two exponential distributions

The probability of $X_1 < X_2$ is given by

$$Pr(X_1 < X_2) = \frac{\lambda_1}{\lambda_1 + \lambda_2}$$
1 Exponential Distribution

2 Continuous Time Markov Chains

3 Specifying Probabilistic Properties
Continuous-time Markov Chains

Informally

- labelled transition systems, augmented with rates
- continuous time delays, exponentially distributed

Definition

A CTMC is a tuple \((S, s_0, R, L)\) where

- \(S\) is a set of states
- \(s_0 \in S\) is the initial state
- \(R : S \times S \rightarrow \mathbb{R}^+\) is the transition rate matrix
- \(L : S \rightarrow 2^{AP}\) is a labelling with atomic propositions in \(AP\)
CTMCs Semantics

The transition rate matrix assigns rates to each pair of states

- used as a parameter to an exponential distribution
- transition between $s$ and $s'$ when $R(s, s') > 0$
- probability triggered before $t$ time units: $1 - e^{-R(s, s')t}$

Race condition
If there exists multiple $s'$ with $R(s, s') > 0$, the first transition to trigger determines the next state.
Example - Modeling 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: $S : \{s_i\}_{i=0}^{3}$ where $s_i$ indicates $i$ jobs in the queue

![Diagram of state transitions](image)
Interesting Questions for CTMCs

How long is spent in $s$ before a transition occurs?
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How long is spent in $s$ before a transition occurs?

- minimum of exponential distributions of outgoing transitions
- i.e. exponential distribution with sum of outgoing rates

Exit rate $E(s) = \sum_{s' \in S} R(s, s')$
Interesting Questions for CTMCs

How long is spent in $s$ before a transition occurs?

- minimum of exponential distributions of outgoing transitions
- i.e. exponential distribution with sum of outgoing rates

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

Note:

- the probability of leaving a state $s$ within $[0, s]$ is $1 - e^{-E(s)t}$
- $s$ is called absorbing if $E(s) = 0$ (no outgoing transitions)
Interesting Questions for CTMCs

Which transition is eventually taken from state $s$?

- Recall that $Pr(X_1 < X_2) = \frac{\lambda_1}{\lambda_1 + \lambda_2}$
- This can generalized to $Pr(X_1 = \min_{i=1\ldots n} X_i) = \frac{\lambda_1}{\sum \lambda_i}$
- Thus the probability that next state from $s$ is $s'$ is given by

$$P_R(s, s') = \begin{cases} \frac{R(s, s')}{E(s)} & \text{if } E(s) > 0, \\ 1 & \text{if } E(s) = 0 \text{ and } s = s', \\ 0 & \text{if } E(s) = 0 \text{ and } s \neq s'. \end{cases}$$
Embedded DTMC

The transition target state is independent from the time the transition occurs.

I.e. we can define a DTMC that abstracts a CTMC by describing only states transitions without time information.
Embedded DTMC

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I.e. we can define a DTMC that abstracts a CTMC by describing only states transitions without time information

**Definition**
The embedded DTMC of a CTMC \((S, s_0, R, L)\) is the DMTC \((S, s_0, P_R, L)\)
Embedded DTMC - Example

What is the embedded DTMC of

\[
\begin{align*}
\text{start} & \rightarrow s_0 & \{\text{empty}\} & \xrightarrow{3/2} s_1 & \xrightarrow{3/2} s_2 & \xrightarrow{3/2} \{\text{full}\} \\
& & & & & \\
& & 3 & & 3 & & 3 \\
\end{align*}
\]

?
Embedded DTMC - Example

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\begin{align*}
\{\text{empty}\} & \quad \frac{3}{2} & & \frac{3}{2} & & \frac{3}{2} & & \{\text{full}\} \\
\text{start} & \quad \rightarrow & s_0 & \rightarrow & s_1 & \rightarrow & s_2 & \rightarrow & s_3 \\
& & \frac{3}{2} & & \frac{3}{2} & & \frac{3}{2} & \\
\end{align*}
\]

? 

\[
\begin{align*}
\{\text{empty}\} & \quad 1 & & \frac{3/2}{3/2+3} & & \{\text{full}\} \\
\text{start} & \quad \rightarrow & s_0 & \rightarrow & s_1 & \rightarrow & s_2 & \rightarrow & s_3 \\
& & & & & \frac{3/2}{3/2+3} & & \\
\end{align*}
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What is the embedded DTMC of

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\begin{array}{cccc}
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\{\text{empty}\} & 3/2 & 3/2 & 3/2 & \{\text{full}\} \\
3 & 3 & 3 & & \\
\end{array}
\]

\[
\begin{array}{cccc}
\text{start} & s_0 & s_1 & s_2 & s_3 \\
\{\text{empty}\} & 1 & 1/3 & & \{\text{full}\} \\
& & & & \\
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Embedded DTMC - Example

What is the embedded DTMC of

\[ \text{start} \rightarrow \quad \{\text{empty}\} \quad \frac{3}{2} \quad \frac{3}{2} \quad \frac{3}{2} \quad \{\text{full}\} \]

? 

\[ \text{start} \rightarrow \quad \{\text{empty}\} \quad 1 \quad \frac{1}{3} \quad \frac{1}{3} \quad \{\text{full}\} \]
Interesting Question

What is the probability of being in state $s_j$ at time $t$ starting in $s_i$?

Define

$$P(t) = \begin{pmatrix} P_{11}(t) & \cdots & P_{1n}(t) \\ & \ddots & \\ P_{n1}(t) & \cdots & P_{nn}(t) \end{pmatrix}$$

with $P_{ij}(t) = Pr(s(t) = s_j | s(t = 0) = s_i)$
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and the infinitesimal generator matrix $Q$

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with $Q_{ij} = \begin{cases} R(s_i, s_j) & \text{if } i \neq j, \\ -\sum_{k \neq i} R(s_i, s_k) & \text{if } i = j. \end{cases}$
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Then one can show that \( P(t) \) satisfies the linear ODE:

\[
\dot{P}(t) = P(t)'Q, \quad P(0) = I
\]
Simple Example

\[ C = (S, s_{\text{init}}, R, L) \]
\[ S = \{s_0, s_1, s_2, s_3\} \]
\[ s_{\text{init}} = s_0 \]

\[ AP = \{\text{empty, full}\} \]
\[ L(s_0) = \{\text{empty}\}, \ L(s_1) = L(s_2) = \emptyset \text{ and } L(s_3) = \{\text{full}\} \]

\[ R = \begin{bmatrix} 0 & 3/2 & 0 & 0 \\ 3 & 0 & 3/2 & 0 \\ 0 & 3 & 0 & 3/2 \\ 0 & 0 & 3 & 0 \end{bmatrix} \]

\[ p_{\text{emb}}(C) = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 2/3 & 0 & 1/3 & 0 \\ 0 & 2/3 & 0 & 1/3 \\ 0 & 0 & 1 & 0 \end{bmatrix} \]

\[ Q = \begin{bmatrix} -3/2 & 3/2 & 0 & 0 \\ 3 & -9/2 & 3/2 & 0 \\ 0 & 3 & -9/2 & 3/2 \\ 0 & 0 & 3 & -3 \end{bmatrix} \]
A path $\omega$ is a sequence $s_0t_0s_1t_1s_2t_2...$ such that

- $\forall i, R(s_i, s_{i+1}) \in \mathbb{R}_{>0}$ and $t_i \in \mathbb{R}_{>0}$
- $t_i$ is the time spent in $s_i$

The path $\omega$ is finite if for some $k$, the state $s_k$ is absorbing (i.e. $R(s, s') =$)

Path($s$) denotes all paths starting in $s$. 
Simulation Algorithm

Main Idea
As the next state probability is independent from the time when the transition takes place, use **two independent stochastic processes for** $s_i$ and $t_i$.

1. **Init** $i = 0, s_i = s_0$
2. **loop**
3. Pick $t_i \in \mathbb{R}_{>0}$ using exponential distribution with rate $E(s)$
4. Pick $s_{i+1}$ using discrete distribution $P_R(s_i, s')$ of embedded DTMCs
5. $i = i + 1$
6. **end loop**

Sometimes referred as Gillespie’s algorithm, and used by its author for stochastic simulation of chemical reactions
Example: A Chemical Reaction

- Three species: $A$, $B$ and $AB$, three reactions:
  - $A$ and $B$ collide and produce $AB$: $A + B \xrightarrow{k_1} AB$
  - $AB$ breaks into $A$ and $B$: $AB \xrightarrow{k_2} A + B$
  - Degradation of $A$: $A \xrightarrow{k_3} \emptyset$
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- CTMC with state-space $(\#A, \#B, \#AB)$

```
2,2,0 1,1,1 0,0,2
- 2k_1 2k_2 2k_3

1,2,0 0,1,1 0,2,0
- k_2 k_3 k_3
```
Example: A Chemical Reaction

- Three species: $A$, $B$ and $AB$, three reactions:
  - $A$ and $B$ collide and produce $AB$ \( A + B \xrightleftharpoons[k_1]{k_2} AB \)
  - $AB$ breaks into $A$ and $B$ \( AB \xrightarrow[k_3]{k_2} A + B \)
  - degradation of $A$ \( A \xrightarrow[k_3]{k_3} \emptyset \)

- CTMC with state-space \((\#A, \#B, \#AB)\)

- $A$ and $B$ collide at rate $k_1 \#A \#B$
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Example: A Chemical Reaction

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- CTMC with state-space $(\#A, \#B, \#AB)$

- $A$ and $B$ collide at rate $k_1 \#A \#B$
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How many states does a CTMC of a chemical reaction have?
CTMCs for Chemical Reactions

How many states does a CTMC of a chemical reaction have?

It depends on:

- The number of reactions
- The number species types
- The initial number of each specie
CTMCs for Chemical Reactions

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- The initial number of each specie

If there is a production reaction, e.g., $\emptyset \rightarrow A$, the number can be infinite
Stochastic versus deterministic models of chemical reactions

Recall that we can formulate ODE to describe a deterministic evolution of the number of molecules (using mass-action laws)
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The stochastic (CTMC) model is believed to be more realistic, but can be quickly intractable.
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Recall that we can formulate ODE to describe a deterministic evolution of the number of molecules (using mass-action laws).

The stochastic (CTMC) model is believed to be more realistic, but can be quickly intractable. In general,

- For large populations of molecules the deterministic model is used.
- For small populations use the stochastic model.
1. Exponential Distribution

2. Continuous Time Markov Chains

3. Specifying Probabilistic Properties
Temporal logic for describing properties of CTMCs
  - CSL = Continuous Stochastic Logic [ASSB00,BHHK03]
  - extension of (non-probabilistic) temporal logic CTL
  - transient, steady-state and path-based properties

Key additions:
  - probabilistic operator $P$ (like PCTL)
  - steady state operator $S$

Example: down $\rightarrow P_{>0.75} \ [\neg \text{fail } U^{[1,2.5]} \text{ up} ]$
  - when a shutdown occurs, the probability of a system recovery
    being completed between 1 and 2.5 hours without further
    failure is greater than 0.75

Example: $S_{<0.1} [\text{insufficient_routers} ]$
  - in the long run, the chance that an inadequate number of
    routers are operational is less than 0.1
CSL Syntax (slides: David Parker)

- **CSL syntax:**

  - $\phi ::= \text{true} \mid a \mid \phi \land \phi \mid \neg \phi \mid P_{=\sim p}[\psi] \mid S_{=\sim p}[\phi]$ (state formulae)

  - $\psi ::= X \phi \mid \phi \mathbf{U} \phi$ (path formulae)

  - where $a$ is an atomic proposition, $I$ interval of $\mathbb{R}_{\geq 0}$, $p \in [0, 1]$, and $\sim \in \{<, >, \leq, \geq\}$

  - unbounded until $U$ is a special case: $\phi_1 U \phi_2 \equiv \phi_1 U^{[0, \infty)} \phi_2$

- **Quantitative properties:** $P_{=\sim}[\psi]$ and $S_{=\sim}[\phi]$

  - where $P/S$ is the outermost operator
CSL Semantics (slides: David Parker)

- **CSL formulae interpreted over states of a CTMC**
  - \( s \models \phi \) denotes \( \phi \) is “true in state \( s \)” or “satisfied in state \( s \)”

- **Semantics of state formulae:**
  - for a state \( s \) of the CTMC \((S, s_{init}, R, L)\):

  - \( s \models a \) \( \iff \) \( a \in L(s) \)
  - \( s \models \phi_1 \land \phi_2 \) \( \iff \) \( s \models \phi_1 \) and \( s \models \phi_2 \)
  - \( s \models \neg \phi \) \( \iff \) \( s \models \phi \) is false
  - \( s \models P_{\sim p} [\psi] \) \( \iff \) \( \text{Prob}(s, \psi) \sim p \)
  - \( s \models S_{\sim p} [\phi] \) \( \iff \) \( \sum_{s'} \models \phi \ \pi_s(s') \sim p \)

---

Probability of, starting in state \( s \), satisfying the path formula \( \psi \)

Probability of, starting in state \( s \), being in state \( s' \) in the long run
CSL Semantics (slides: David Parker)

- Prob(s, ψ) is the probability, starting in state s, of satisfying the path formula ψ
  - Prob(s, ψ) = Pr_s {ω ∈ Path_s | ω ⊨ ψ }

- Semantics of path formulae:
  - for a path ω of the CTMC:
    - ω ⊨ X ϕ ⇔ ω(1) is defined and ω(1) ⊨ ϕ
    - ω ⊨ ϕ_1 U^l ϕ_2 ⇔ ∃t ∈ I. ( ω@t ⊨ ϕ_2 ∧ ∀t’<t. ω@t’ ⊨ ϕ_1 )

    there exists a time instant in the interval I where ϕ_2 is true and ϕ_1 is true at all preceding time instants

if ω(0) is absorbing, ω(1) not defined
 CSL Example (slides: David Parker)

- **Case study:** Cluster of workstations [HHK00]
  - two sub-clusters (N workstations in each cluster)
  - star topology with a central switch
  - components can break down, single repair unit

  ![Diagram of a clustered workstations with a central switch and sub-clusters]

  - **minimum QoS:** at least $\frac{3}{4}$ of the workstations operational and connected via switches
  - **premium QoS:** all workstations operational and connected via switches
CSL Example (slides: David Parker)

- $S \Rightarrow \mathsf{minimum}$
  - the probability in the long run of having minimum QoS

- $P \Rightarrow F[t,t] \mathsf{minimum}$
  - the (transient) probability at time instant $t$ of minimum QoS

- $P_{<0.05} \left[ F[0,10] \neg \mathsf{minimum} \right]$
  - the probability that the QoS drops below minimum within 10 hours is less than 0.05

- $\neg \mathsf{minimum} \rightarrow P_{<0.1} \left[ F[0,2] \neg \mathsf{minimum} \right]$
  - when facing insufficient QoS, the chance of facing the same problem after 2 hours is less than 0.1
CSL Example (slides: David Parker)

- \( \text{minimum} \rightarrow P_{>0.8} [ \text{minimum } U^{[0,t]} \text{ premium } ] \)
  - the probability of going from minimum to premium QoS within \( t \) hours without violating minimum QoS is at least 0.8

- \( P_{=?} [ \neg \text{minimum } U^{[t,\infty)} \text{ minimum } ] \)
  - the chance it takes more than \( t \) time units to recover from insufficient QoS

- \( \neg r\_\text{switch}\_up \rightarrow P_{<0.1} [\neg r\_\text{switch}\_up U \neg l\_\text{switch}\_up ] \)
  - if the right switch has failed, the probability of the left switch failing before it is repaired is less than 0.1

- \( P_{=?} [ F^{[2,\infty)} S_{>0.9} [ \text{minimum } ] ] \)
  - the probability of it taking more than 2 hours to get to a state from which the long-run probability of minimum QoS is >0.9
CSL Model Checking

(See PRISM literature for more details...)

- For untimed operators, equivalent to PCTL on embedded DTMCs
- For timed operators, can be reduced to computation of transient probabilities (such as matrix $P(t)$) - complex
- An alternative is using Statistical Model Checking, approximate but more scalable
Statistical Model Checking

Assume we can decide $\omega \models \phi$. Based on simulations, decide hypothesis $H_1 : Pr_{\geq \theta}(\omega \models \phi)$ against $H_0 : Pr_{< \theta}(\omega \models \phi)$

Bounds on the error of choosing $H_1$ instead of $H_0$, depending on the number of positive runs