Markov chains and Markov decision processes in Isabelle/HOL

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Introduction

Formalize probabilistic models:

- Discrete *infinite* state spaces

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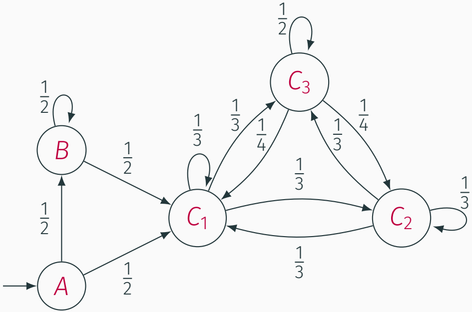
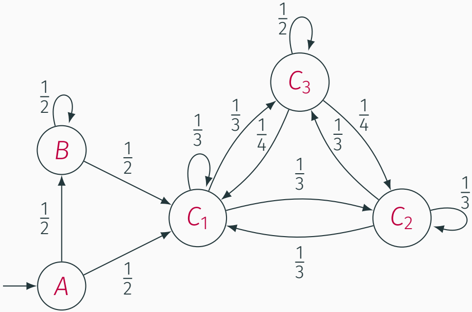
Approach:

- *Coalgebraic view* on transition systems
- *Fixed points* to define queries on trace space

Markov chains



(a) A finite process



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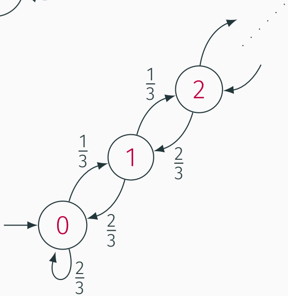
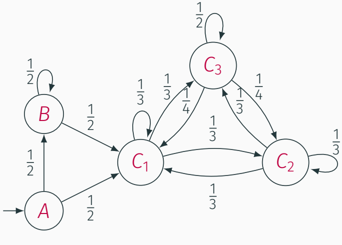


(b) An infinite birth-death process



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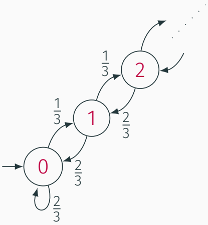
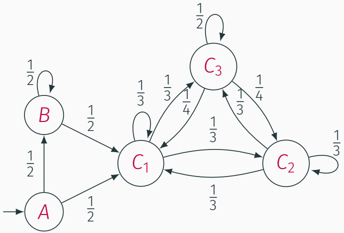


(b) An infinite birth-death process

- $\Pr_A(\Diamond C_3) = ?$



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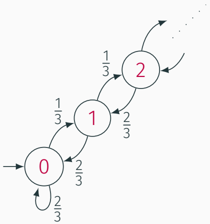

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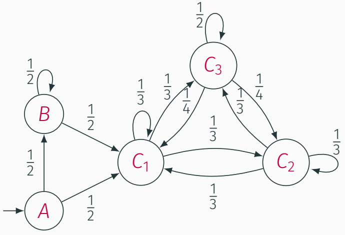

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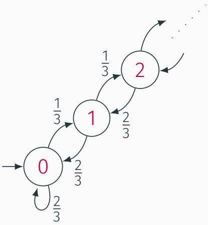

(b) An infinite birth-death process

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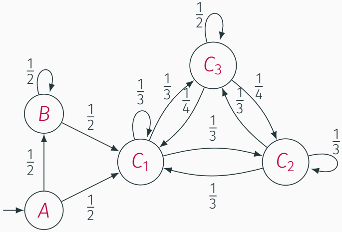

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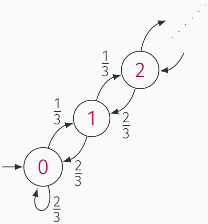

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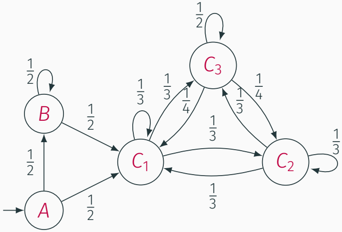

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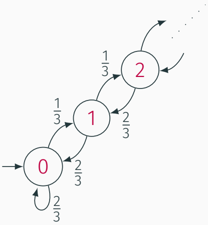

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- $\int_\omega f_0\ \omega\ d\mathcal{T}_0 = ?$ – f: first occurence

Markov Chains — A Coalgebraic View

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K – *Markov kernel*: the transitions for each state

σ – type of states

$\sigma\ pmf$ – probability mass functions (discrete distributions)

Probability Mass Function

Model probabilistic transitions!

$$\mu :: \sigma\ \mathrm{pmf} \quad \approx \quad \mu :: \sigma \Rightarrow [0,1], \quad \textstyle\sum_x \mu\, x = 1$$

$$\approx \quad \mu :: \sigma\ \mathrm{measure}, \quad \mu\, \mathcal{U} = 1, \quad \textit{discrete}$$

Similar to Audebaud & Paulin-Mohring [MPC 2006]

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Similar to Audebaud & Paulin-Mohring [MPC 2006]

- map $f\,\mu = \lambda x.\ \sum_{f\,y = x} \mu\, y$
- set $\mu = \{x \mid \mu\, x \neq 0\}$
- $\mu \ggg \nu = \lambda x.\ \sum_{y} \mu\, y \cdot \nu_y\, x$
- return $x = \lambda x'.\ \begin{cases} 1 & \text{if } x = x' \\ 0 & \text{else} \end{cases}$

- Bernoulli
- Uniform
- Binomial
- Geometric
- Poisson
- Conditional

Trace Space

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Given K construct $\mathcal{T} :: \sigma \Rightarrow \sigma\ \text{stream measure}$ where:

$$\mathcal{T}_s = \text{do}\ \{t \leftarrow K_s\ ;\ \omega \leftarrow \mathcal{T}_t\ ;\ \text{return}\ (t \cdot \omega)\}$$

Equivalently: for f Borel-measurable:

$$\int_{\omega} f(\omega)\ d\mathcal{T}_s = \int_t \left(\int_{\omega} f(t \cdot \omega)\ d\mathcal{T}_t \right)\ dK_s$$

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This construction is unique!

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- Our solution: reuse infinite product of probability spaces
  Measure space of *decisions* D:

$$D = \prod_{n::\mathbb{N}} \prod_{s::\sigma} K_s$$

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- Future Solution: Theorem by *Ionescu-Tuclea*

Queries on the trace space

Eventually ϕ: $\Diamond_{\phi}\ \omega =$

Always ϕ: $\Box_{\phi}\ \omega =$

ψ Until ϕ: ${}_{\psi}U_{\phi}\ \omega =$

First hit ϕ: $f_{\phi}\ \omega =$

Counting ϕ: $c_{\phi}\ \omega =$

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Interception: Least/Greatest Fixed Points

Monotone functions f, g

Least fixed point: $\mathrm{lfp}\, f = f\,(\mathrm{lfp}\, f) \qquad (\forall x.\; f\,x \leqslant x \implies \mathrm{lfp}\, f \leqslant x)$

$$\mathrm{lfp}\, f = \overbrace{f \circ f \circ f \circ f \circ f \circ f \circ f \circ f \circ f \circ \cdots \circ}^{\infty} \bot$$

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$\forall C \in \mathbb{N} \to X.\ \text{monotone}\ C \implies f\,(\bigsqcup_i C_i) = \bigsqcup_i f\, C_i$

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Transfer rule:

$$\sqcup\text{-continuous}\ \alpha, f, g$$

$$\frac{\alpha\ \bot = \bot \qquad \alpha \circ f = g \circ \alpha}{\alpha(\mathsf{lfp}\ f) = \mathsf{lfp}\ g}$$

$$\begin{aligned} \alpha(\mathsf{lfp}\ f) &= \alpha \circ f \circ f \circ f \circ f \circ f \circ \cdots \circ \bot \\ &= g \circ g \circ g \circ \alpha \circ f \circ f \circ \cdots \circ \bot \\ &= g \circ g \circ g \circ g \circ g \circ \cdots \circ \alpha\ \bot \\ &= \mathsf{lfp}\ g \end{aligned}$$

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$\alpha\ f = \int f\ d\mathcal{M}$ for f Borel-measurable

Equation for queries under integration

Example (First hitting time ϕ on states)

Define f:

$$f_{\phi} \stackrel{\text{def}}{=} \text{lfp}\ (\lambda\, f\, (s \cdot \omega).\ \lfloor \neg \phi\ s \rfloor \cdot (1 + f\ \omega))$$

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$$f_\phi\ (s{\cdot}\omega) \stackrel{\text{lfp}}{=} \begin{cases} 1 + f_\phi\ \omega & \text{if } \neg\ \phi\ s \\ 0 & \text{otherwise} \end{cases}$$

Prove computation rule by transfer rule:

$$\int_\omega f_\phi\ \omega\ d\mathcal{T}_s = lfp\ \left(\lambda g\ s.\ \int_t \lfloor \neg\phi\ t \rfloor \cdot (1 + g\ t)\ \ dK_s\right)\ s$$

Equation for queries under integration

Example (First hitting time ϕ on states)

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For finite state space: lfp is a system of linear equations!

Proofs employing fixed point reasoning

Lemma (Fairness)

$$\Pr_s\Big(\Box\Diamond t \implies \Box\Diamond(t \wedge \bigcirc t')\Big) = 1 \qquad \textit{if } t' \in K_t$$

Proof.

Show that gfp $(\lambda g\ s.\ (\neg t)\ U\ (t \cdot \neg t' \cdot g))$ has probability 0. ☐

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Proof size is reduced to $\approx 65\%$!

Stationary Distribution

N is a *stationary distribution* iff $(N \gg= K) = N$

Or: $K \times N = N$ — K as transition matrix

- When support set of N is essential (bottom SCC):

$$\int_{\omega} f_s\ \omega\ d\mathfrak{T}_s = \frac{1}{N\ s} - 1$$

- When essential and aperiodic:

$$\lim_{n \to \infty} \Pr_s(\omega_n = t) = N\ t$$

- Stationary distribution for b): $N = \mathit{geometric}\left(\frac{1}{2}\right)$

$$\text{DTMC}\ (M :: \alpha\ \text{measure})\ (X :: \text{nat} \Rightarrow \alpha \Rightarrow \sigma) =$$
$$\quad \text{prob-space}\ M \quad\wedge\quad (\forall n.\ X\ n \in M \to^{\sigma} \mathcal{U}) \quad\wedge$$
$$\quad (\exists S.\ \text{countable}\ S \wedge \forall n.\ \Pr(X\ n \in S) = 1) \quad\wedge$$

— **The stochastic process** X **is** ***memoryless*****:**

$$\Big(\forall n\ s\ t.$$
$$\quad \Pr(\forall n' \leqslant n.\ X\ n' = t\ n') \neq 0 \longrightarrow$$
$$\quad \Pr(X\ (n+1) = s \mid \forall n' \leqslant n.\ X\ n' = t\ n') =$$
$$\quad \Pr(X\ (n+1) = s \mid X\ n = t\ n)\Big) \quad\wedge$$

— **The stochastic process** X **is** ***time-homogeneous*****:**

$$\Big(\forall n\ n'\ s\ t.$$
$$\quad \Pr(X\ n = t) \neq 0 \wedge \Pr(X\ n' = t) \neq 0 \longrightarrow$$
$$\quad \Pr(X\ (n+1) = s \mid X\ n = t) = \Pr(X\ (n'+1) = s \mid X\ n' = t)\Big)$$

Markov decision processes

Markov decision process

Probabilistic & non-deterministic transitions

Probabilistic & non-deterministic transitions

- Kernels (coalgebras) of MDPs:

$$\boxed{K :: \sigma \Rightarrow \sigma \text{ pmf set}, \quad K_s \neq \emptyset}$$

Probabilistic & non-deterministic transitions

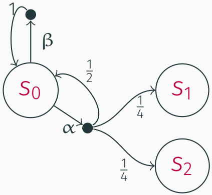
- Kernels (coalgebras) of MDPs:

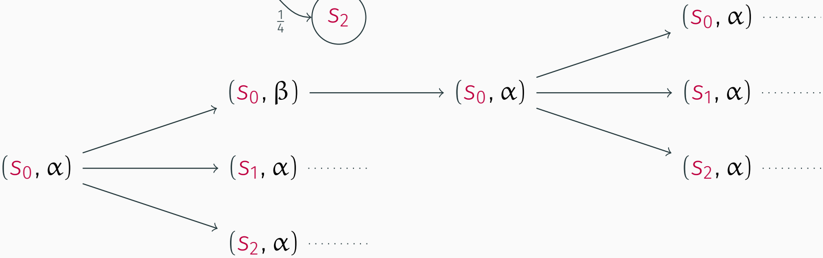
$$\boxed{K :: \sigma \Rightarrow \sigma \text{ pmf set}, \quad K_s \neq \emptyset}$$

- Traditional definition of schedulers:

$$sc :: \sigma \text{ list} \Rightarrow \sigma \text{ pmf}, \quad sc\ (h \cdot s) \in K_s$$

Configurations





Attention: the configuration includes the entire tree!

Configurations on MDPs

$$\texttt{codatatype}\ \sigma\ \mathit{cfg} = \mathit{Cfg}\ (\mathit{state} :\ \sigma)\ (\mathit{act} :\ \sigma\ \mathrm{pmf})\ (\mathit{cont} :\ \sigma \Rightarrow \sigma\ \mathrm{cfg})$$
$$\texttt{where}\ \mathit{state}\ (\mathit{cont}\ c\ s) = s$$

- Induces a *Markov chain*:

$$K^{MC} :: \sigma\ \mathrm{cfg} \Rightarrow \sigma\ \mathrm{cfg}\ \mathrm{pmf}$$
$$K^{MC}{}_c = \mathit{map}\ (\mathit{cont}\ c)\ (\mathit{act}\ c)$$

- Trace space: $\mathcal{T}_c = \mathit{map}_{\mathit{measure}}\ (\mathit{map}_{\mathit{stream}}\ \mathit{state})\ \mathcal{T}^{MC}{}_c$
- Valid Configuration: *act* is always compatible with K

Definition (Minimal Expectation)

$$\mathbb{E}^{\mathrm{min}}{}_{s}\left[f\right] = \prod_{c \in valid_s} \int f \, d\mathcal{T}_c$$

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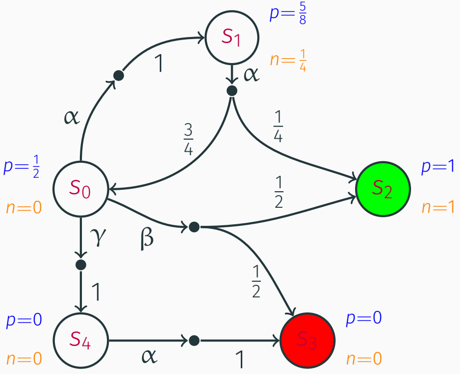
Lemma (Iteration Rule)

$$\mathbb{E}^{\min}{}_{s}[f] = \prod_{D \in K_s} \int_t \mathbb{E}^{\min}{}_{s}[f\,(t \cdot \omega)] \; dD$$

Application: Reachability Problem Example



p is $\Pr_s^{\max}(S_1\ U\ S_2)$, n is $\Pr_s^{\min}(S_1\ U\ S_2)$

Application: Reachability problems on MDPs

Goal: certify solutions to reachability problems in MDPs

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$\Longrightarrow$ Import results by executing algorithm in Isabelle/HOL

Application: pGCL semantics

Present the pGCL semantics similar to [Gretz, Katoen, McIver (2014)]:

$$
\begin{aligned}
\text{pgcl} \quad := \quad & \text{Skip} \\
| \quad & \text{Abort} \\
| \quad & \text{Assign } (\sigma \Rightarrow \sigma) \\
| \quad & \text{Seq pgcl pgcl} \\
| \quad & \text{Par pgcl pgcl} \\
| \quad & \text{If } (\sigma \Rightarrow \mathrm{bool}) \text{ pgcl pgcl} \\
| \quad & \text{Prob } [0,1] \text{ pgcl pgcl} \\
| \quad & \text{While } (\sigma \Rightarrow \text{bool}) \text{ pgcl pgcl}
\end{aligned}
$$

Weakest pre-expectation transformer

$$\text{wp} :: \text{pgcl} \Rightarrow \left(\sigma \Rightarrow \mathbb{R}^{\infty}_{\geqslant 0}\right) \Rightarrow \left(\sigma \Rightarrow \mathbb{R}^{\infty}_{\geqslant 0}\right)$$

$$\begin{aligned}
\text{wp Skip } f &= f \\
\text{wp Abort } f &= \bot \\
\text{wp (Assign } u\text{) } f &= f \circ u \\
\text{wp (Seq } c_1\ c_2\text{) } f &= \text{wp } c_1\ (\text{wp } c_2\ f) \\
\text{wp (Par } c_1\ c_2\text{) } f &= \text{wp } c_1\ f \sqcap \text{wp } c_2\ f \\
\text{wp (If } b\ c_1\ c_2\text{) } f &= \lambda s.\ \text{if } b\ s \text{ then wp } c_1\ f\ s \text{ else wp } c_2\ f\ s \\
\text{wp (Prob } p\ c_1\ c_2\text{) } f &= \lambda s.\ p \cdot \text{wp } c_1\ f\ s + (1 - p) \cdot \text{wp } c_2\ f\ s \\
\text{wp (While } b\ c\text{) } f &= \text{lfp } (\lambda g\ s.\ \text{if } b\ s \text{ then wp } c\ g\ s \text{ else } f\ s)
\end{aligned}$$

Operational semantics as MDP

$$K :: (\text{pgcl} \times \sigma) \Rightarrow (\text{pgcl} \times \sigma)\ \text{pmf set}$$

$$\begin{aligned}
K\ (\text{Skip}, s) &= \ll \text{Skip}, s \gg \\
K\ (\text{Abort}, s) &= \ll \text{Abort}, s \gg \\
K\ (\text{Assign}\ u, s) &= \ll \text{Skip}, u\ s \gg \\
K\ (\text{Seq}\ c_1\ c_2, s) &= \\
&\quad K(c_1, s) \left[\lambda(c_1', s').\ \left\{ \begin{array}{ll} (\text{Seq}\ c_1'\ c_2, s') & \text{if } c_1' \neq \text{Skip} \\ (c_2, s') & \text{else} \end{array} \right\} \right] \\
K\ (\text{Par}\ c_1\ c_2, s) &= \ll c_1, s \gg \cup \ll c_2, s \gg \\
K\ (\text{If}\ b\ c_1\ c_2, s) &= \text{if } b\ s \text{ then } K\ (c_1, s) \text{ else } K\ (c_2, s) \\
K\ (\text{Prob}\ p\ c_1\ c_2, s) &= \{\{(c_1, s) \mapsto p, (c_2, s) \mapsto (1 - p)\}\} \\
K\ (\text{While}\ g\ c, s) &= \begin{cases} \ll \text{Seq}\ c\ (\text{While}\ g\ c), s \gg & \text{if } g\ s \\ \ll \text{Skip}, s \gg & \text{else} \end{cases}
\end{aligned}$$

Definition (Result of a Trace)

$$r\ f\ ((c, s)\cdot\omega) \stackrel{\text{lfp}}{=} \begin{cases} r\ f\ \omega & \text{if } c \neq \mathsf{Skip} \\ f\ s & \text{else} \end{cases}$$

Equate wp and K

Definition (Result of a Trace)

$$r\ f\ ((c, s)\cdot\omega) \stackrel{\text{lfp}}{=} \begin{cases} r\ f\ \omega & \text{if } c \neq \mathrm{Skip} \\ f\ s & \text{else} \end{cases}$$

Theorem (Operational semantics equals denotational semantics)

$$\mathbb{E}^{\min}{}_{(c,s)}(r\ f) = \mathrm{wp}\ \ c\ f\ s$$

Proof

$$\mathbb{E}^{\min}{}_{(c,s)}\,(r\,f) = \mathrm{lfp}\left(\lambda g\ s.\ \prod_{\mu \in K_{(c,s)}} \int_{(c,s)} \begin{cases} g\ (c,s) & \text{if } c \neq \mathrm{Skip} \\ f\ s & \text{else} \end{cases} d\mu\right)\ (c,s)$$

Case $c = \mathrm{Seq}\ c_1\ c_2$:

$$\mathbb{E}^{\min}{}_{(\mathrm{Seq}\ c_1\ c_2,s)}(r\,f) = \mathbb{E}^{\min}{}_{(c_1,s)}\left(r\ \left(\lambda s'.\ \mathbb{E}^{\min}{}_{(c_2,s')}(r\,f)\right)\right)$$

Case $c = \mathrm{While}\ b\ c'$: $\mathbb{E}^{\min}{}_{(\mathrm{While}\ g\ c',s)}(r\,f) = \mathrm{lfp}\ w\ s$

$$w\ g\ s = \prod_{\mu \in K_s} \int_{(d,t)} \begin{cases} g\ (d,t) & \text{if } d \neq \mathrm{Skip} \\ g\ (c',t) & \text{if } b\ t \\ f\ t & \text{else} \end{cases} d\mu$$

Probabilistic Hierarchy

Zoo of Probabilistic System Types

H., Traytel & Lochbihler [ITP 2015]

Ana Sokolva – Coalgebraic Analysis of Probabilistic Systems (2005):

4.4 The hierarchy 107

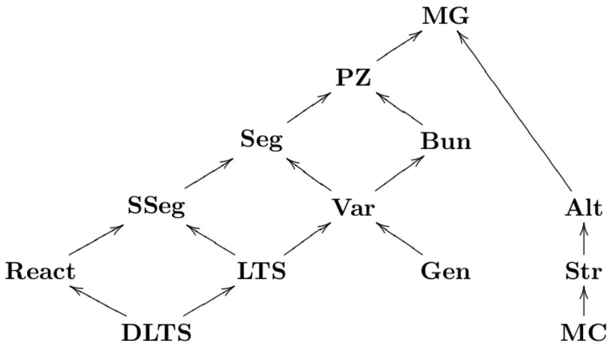

Figure 4.2: Hierarchy of probabilistic system types

Hierarchy of Probabilistic Systems Types

How to ...

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How to …

…model system types?

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How to …

…model system types?

…compare systems of same type?

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…formalize it in Isabelle/HOL?

Hierarchy of Probabilistic Systems Types

How to ...

...model system types?	Coalgebras
...compare systems of same type?	Bisimulation
...compare different system types?	Embedding respecting bisimulation
...formalize it in Isabelle/HOL?	**codatatype** + Probability Mass Func.

Coalgebras as Codatatypes in Isabelle/HOL

Idea: Analyse transition systems modulo *bisimulation*!

$$\text{Equality} :\Longleftrightarrow \text{Bisimulation}$$

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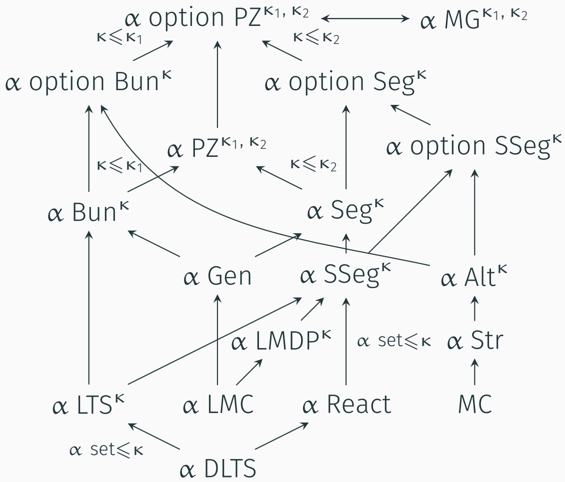
Example (Labeled Markov Chains where $F = \alpha \times \Box\ \mathsf{pmf}$):

$$\textbf{codatatype } \alpha\ \mathsf{mc} = \mathsf{MC}\ (\alpha \times \alpha\ \mathsf{mc}\ \mathsf{pmf})$$

System Types

Name	Functor	Codatatype
Markov chain	σ pmf	MC
Labeled MC	$\alpha \times \sigma$ pmf	α LMC
Labeled MDP	$\alpha \times \sigma$ pmf set_1^{κ}	α LMDP^{κ}
Det. automaton	$\alpha \Rightarrow \sigma$ option	α DLTS
Non-det. automaton	$(\alpha \times \sigma)$ set^{κ}	α LTS^{κ}
Reactive system	$\alpha \Rightarrow \sigma$ pmf option	α React
Generative system	$(\alpha \times \sigma)$ pmf option	α Gen
Stratified system	σ pmf $+$ $(\alpha \times \sigma)$ option	α Str
Alternating system	σ pmf $+$ $(\alpha \times \sigma)$ set^{κ}	α Alt^{κ}
Simple Segala system	$(\alpha \times \sigma$ pmf$)$ set^{κ}	α SSeg^{κ}
Segala system	$(\alpha \times \sigma)$ pmf set^{κ}	α Seg^{κ}
Bundle system	$(\alpha \times \sigma)$ set^{κ} pmf	α Bun^{κ}
Pnueli-Zuck system	$(\alpha \times \sigma)$ set^{κ_1} pmf set^{κ_2}	α $\text{PZ}^{\kappa_1,\kappa_2}$
Most general system	$(\alpha \times \sigma + \sigma)$ set^{κ_1} pmf set^{κ_2}	α $\text{MG}^{\kappa_1,\kappa_2}$

Hierarchy


α option PZ^κ1,κ2
α MG^κ1,κ2
κ⩽κ1
κ⩽κ2
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α option Seg^κ
α PZ^κ1,κ2
α option SSeg^κ
κ⩽κ1
κ⩽κ2
α Bun^κ
α Seg^κ
α Gen
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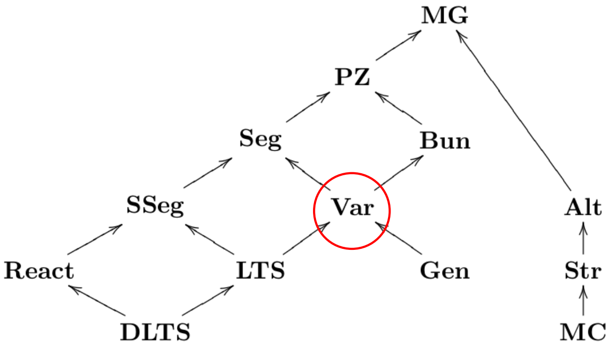

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Conclusion

Related Work

Formalizing probabilistic trace spaces:

- Formal verification of probabilistic algorithms
  Hurd [thesis 2002]
- Formal reasoning about classified Markov chains in HOL
  Liu, Hasan, Aravantinos, and Tahar [ITP 2013]

Formalizing probabilistic transition systems:

- Probabilistic guarded commands mechanized in HOL
  Hurd, McIver, and Morgan [Theor. Comput. Sci. 2005]
- Proofs of randomized algorithms in Coq
  Audebaud and Paulin-Mohring [MPC 2006]
- Verifying probabilistic correctness in Isabelle with pGCL
  Cock [SSV 2012]

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- Future Work:
  Average Runtime Analysis, Probabilistic Programming