



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

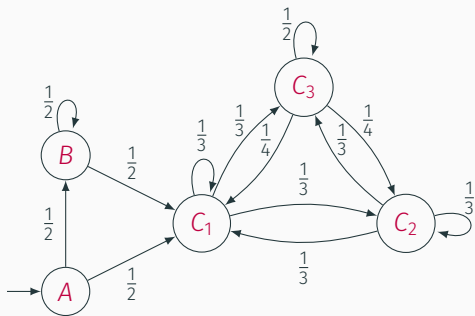
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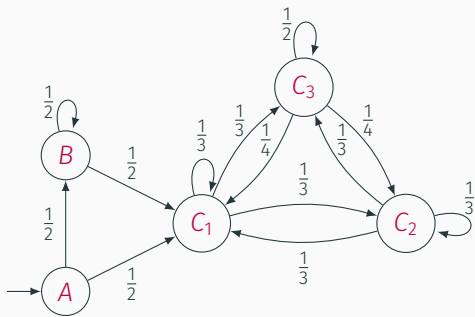
Approach:

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

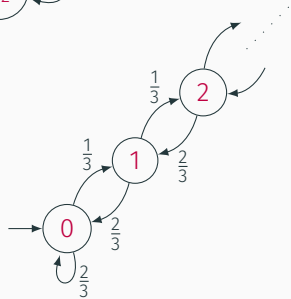
Markov chains



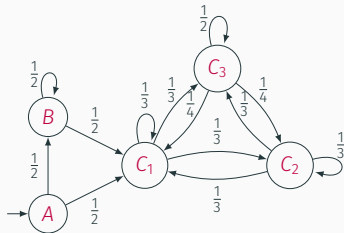
(a) A finite process



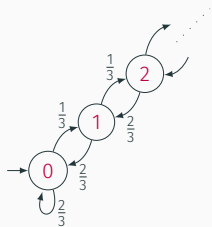
(a) A finite process



(b) An infinite birth-death process

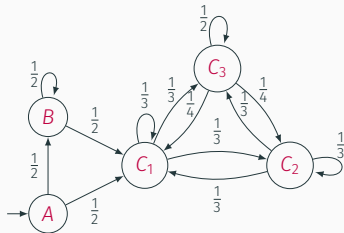


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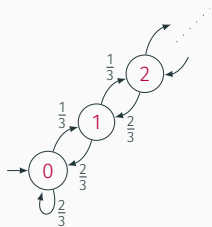


(b) An infinite birth-death process

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

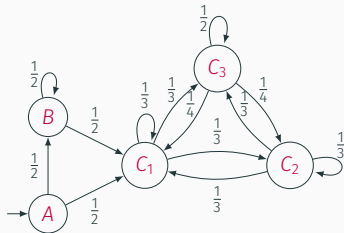


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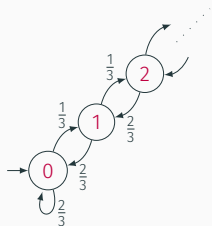


(b) An infinite birth-death process

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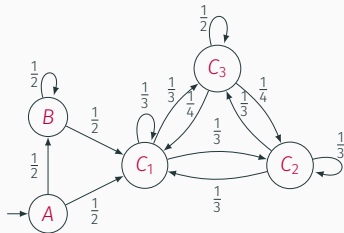


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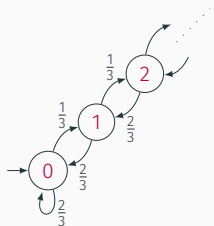


(b) An infinite birth-death process

- $\Pr_A(\diamond C_3) = ?$
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- $\Pr_A(\square \diamond \{C_1, C_2, C_3\}) = ?$



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- $\Pr_A(\diamond C_3) = ?$
- $\Pr_A(\square \neg C_3) = ?$
- $\Pr_A(\square \diamond \{C_1, C_2, C_3\}) = ?$
- $\lim_{n \rightarrow \infty} \Pr_A(\omega_n = C_3) > \lim_{n \rightarrow \infty} \Pr_A(\omega_n = C_2) ?$
- $\int_{\omega} f_0 \omega d\mathcal{T}_0 = ?$ - f : first occurrence

How to represent Markov chains?

Markov Chains — A Coalgebraic View

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

σ – type of states

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

Probability Mass Function

Model probabilistic transitions!

$$\begin{aligned}\mu :: \sigma \text{ pmf} &\approx \mu :: \sigma \Rightarrow [0, 1], \sum_x \mu x = 1 \\ &\approx \mu :: \sigma \text{ measure}, \mu \mathcal{U} = 1, \text{ discrete}\end{aligned}$$

Similar to Audebaud & Paulin-Mohring [MPC 2006]

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- map $f \mu = \lambda x. \sum_{f y=x} \mu y$
 - set $\mu = \{x \mid \mu x \neq 0\}$
 - $\mu \gg \nu = \lambda x. \sum_y \mu y \cdot \nu_y x$
 - return $x = \lambda x'. \begin{cases} 1 & \text{if } x = x' \\ 0 & \text{else} \end{cases}$
- Bernoulli
 - Uniform
 - Binomial
 - Geometric
 - Poisson
 - Conditional

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Trace Space

Necessary to define $\int_{\omega} d\mathcal{T}_s$ (and $\text{Pr}_s(P \ \omega)$)

$$\text{codatatype } \sigma \text{ stream} = \sigma \cdot (\sigma \text{ stream}) \quad \approx \mathbb{N} \Rightarrow \sigma$$

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 :

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

$$\text{run}(s, d \cdot X) = s \cdot \text{run}(d s, X)$$

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- Future Solution: Theorem by *Ionescu-Tuclea*

Queries on the trace space

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

Always ϕ : $\square_{\phi} \omega =$

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: $\text{lfp } f = f(\text{lfp } f)$ $(\forall x. f x \leq x \implies \text{lfp } f \leq x)$



$\text{lfp } f = \overbrace{f \circ f \circ f \circ f \circ f \circ f \circ f \circ f \circ f \circ \dots}^{\infty} \circ \perp$

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

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\sqcup -continuous α, f, g

Transfer rule:
$$\frac{\alpha \perp = \perp \quad \alpha \circ f = g \circ \alpha}{\alpha(\text{lfp } f) = \text{lfp } g}$$

$$\begin{aligned} \alpha(\text{lfp } f) &= \alpha \circ f \circ f \circ f \circ f \circ f \circ \dots \circ \perp \\ &= g \circ g \circ g \circ \alpha \circ f \circ f \circ \dots \circ \perp \\ &= g \circ g \circ g \circ g \circ g \circ \dots \circ \alpha \perp \\ &= \text{lfp } g \end{aligned}$$

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

Equation for queries under integration

Example (First hitting time ϕ on states)

Define f :

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

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

Proofs employing fixed point reasoning

Lemma (Fairness)

$$\Pr_s(\Box\Diamond t \implies \Box\Diamond(t \wedge \bigcirc t')) = 1 \quad \text{if } t' \in K_t$$

Proof.

Show that $\text{gfp } (\lambda g \text{ s. } (\neg t) \cup (t \cdot \neg t' \cdot g))$ has probability 0. □

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Lemma (Finite hitting time)

$$\int_{\omega} f_t \omega \, d\mathcal{T}_s < \infty \quad \text{if } \Pr_s(\Diamond t) = 1 \text{ and finite state space}$$

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Lemma (Finite hitting time)

$$\int_{\omega} f_t \omega \, d\mathcal{T}_s < \infty \quad \text{if } \Pr_s(\Diamond t) = 1 \text{ and finite state space}$$

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):

$$\int_{\omega} f_s \omega d\mathcal{T}_s = \frac{1}{N_s} - 1$$

- When essential and aperiodic:

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

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

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

– The stochastic process X is *memoryless*:

($\forall n\ s\ t.$

$\text{Pr}(\forall n' \leq n. X\ n' = t\ n') \neq 0 \longrightarrow$

$\text{Pr}(X\ (n + 1) = s \mid \forall n' \leq n. X\ n' = t\ n') =$

$\text{Pr}(X\ (n + 1) = s \mid X\ n = t\ n)) \wedge$

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

($\forall n\ n'\ s\ t.$

$\text{Pr}(X\ n = t) \neq 0 \wedge \text{Pr}(X\ n' = t) \neq 0 \longrightarrow$

$\text{Pr}(X\ (n + 1) = s \mid X\ n = t) = \text{Pr}(X\ (n' + 1) = s \mid X\ n' = t))$

Markov decision processes

Probabilistic & non-deterministic transitions

Probabilistic & non-deterministic transitions

- Kernels (coalgebras) of MDPs:

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

Probabilistic & non-deterministic transitions

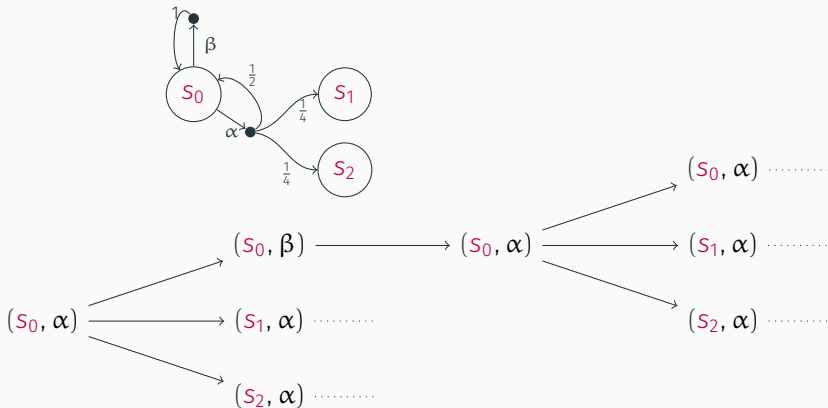
- Kernels (coalgebras) of MDPs:

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

- Traditional definition of schedulers:

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

Configurations



Attention: the configuration includes the entire tree!

Configurations on MDPs

```
codatatype  $\sigma$  cfg = Cfg (state :  $\sigma$ ) (act :  $\sigma$  pmf) (cont :  $\sigma \Rightarrow \sigma$  cfg)
  where state (cont c s) = s
```

- Induces a *Markov chain*:

$$K^{MC} :: \sigma \text{ cfg} \Rightarrow \sigma \text{ cfg pmf}$$
$$K_c^{MC} = \text{map} (\text{cont } c) (\text{act } c)$$

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

Definition (Minimal Expectation)

$$\mathbb{E}_s^{\min} [f] = \bigcap_{c \in \text{valid}_s} \int f d\mathcal{T}_c$$

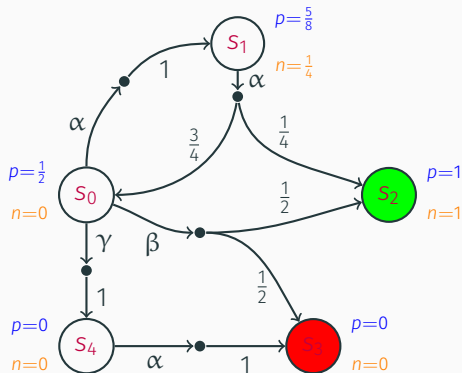
Definition (Minimal Expectation)

$$\mathbb{E}^{\min}_s[f] = \prod_{c \in \text{valid}_s} \int f d\mathcal{T}_c$$

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

Application: Reachability problems on MDPs

Goal: certify solutions to reachability problems in MDPs

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⇒ Formalize MDPs and reachability problems

$$\Pr_s^{\min}(S_1 \ U \ S_2) = \text{lfp}(\dots)$$

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⇒ Implement and verify certification algorithm

Currently: $v \leq \Pr^{\min}(S_1 \cup S_2)$ and $\Pr^{\max}(S_1 \cup S_2) \leq v$

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⇒ Import results by executing algorithm in Isabelle/HOL

Application: pGCL semantics

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

```
pgcl := Skip
      | Abort
      | Assign ( $\sigma \Rightarrow \sigma$ )
      | Seq pgcl pgcl
      | Par pgcl pgcl
      | If ( $\sigma \Rightarrow \text{bool}$ ) pgcl pgcl
      | Prob [0, 1] pgcl pgcl
      | While ( $\sigma \Rightarrow \text{bool}$ ) pgcl pgcl
```

Weakest pre-expectation transformer

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

$\text{wp} \text{ Skip } f = f$

$\text{wp} \text{ Abort } f = \perp$

$\text{wp} (\text{Assign } u) f = f \circ u$

$\text{wp} (\text{Seq } c_1 c_2) f = \text{wp } c_1 (\text{wp } c_2 f)$

$\text{wp} (\text{Par } c_1 c_2) f = \text{wp } c_1 f \sqcap \text{wp } c_2 f$

$\text{wp} (\text{If } b c_1 c_2) f = \lambda s. \text{ if } b s \text{ then } \text{wp } c_1 f s \text{ else } \text{wp } c_2 f s$

$\text{wp} (\text{Prob } p c_1 c_2) f = \lambda s. p \cdot \text{wp } c_1 f s + (1 - p) \cdot \text{wp } c_2 f s$

$\text{wp} (\text{While } b c) f = \text{lfp } (\lambda g s. \text{ if } b s \text{ then } \text{wp } c g s \text{ else } f s)$

Operational semantics as MDP

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

$K(\text{Skip}, s) = \ll \text{Skip}, s \gg$

$K(\text{Abort}, s) = \ll \text{Abort}, s \gg$

$K(\text{Assign } u, s) = \ll \text{Skip}, u s \gg$

$K(\text{Seq } c_1 c_2, s) =$

$$K(c_1, s) \left[\lambda(c'_1, s'). \left\{ \begin{array}{ll} (\text{Seq } c'_1 c_2, s') & \text{if } c'_1 \neq \text{Skip} \\ (c_2, s') & \text{else} \end{array} \right\} \right]$$

$K(\text{Par } c_1 c_2, s) = \ll c_1, s \gg \cup \ll c_2, s \gg$

$K(\text{If } b c_1 c_2, s) = \text{if } b s \text{ then } K(c_1, s) \text{ else } K(c_2, s)$

$K(\text{Prob } p c_1 c_2, s) = \{ \{(c_1, s) \mapsto p, (c_2, s) \mapsto (1 - p)\} \}$

$K(\text{While } g c, s) = \begin{cases} \ll \text{Seq } c (\text{While } g c), s \gg & \text{if } g s \\ \ll \text{Skip}, s \gg & \text{else} \end{cases}$

Definition (Result of a Trace)

$$rf((c, s) \cdot \omega) \stackrel{\text{IfP}}{=} \begin{cases} rf\omega & \text{if } c \neq \text{Skip} \\ fs & \text{else} \end{cases}$$

Definition (Result of a Trace)

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

Theorem (Operational semantics equals denotational semantics)

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

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

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

$$\mathbb{E}^{\min}_{(\text{Seq } c_1 c_2, s)}(rf) = \mathbb{E}^{\min}_{(c_1, s)}(r (\lambda s'. \mathbb{E}^{\min}_{(c_2, s')}(rf)))$$

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

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

Probabilistic Hierarchy

Zoo of Probabilistic System Types

H., Traytel & Lochbihler [ITP 2015]

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

4.4 The hierarchy

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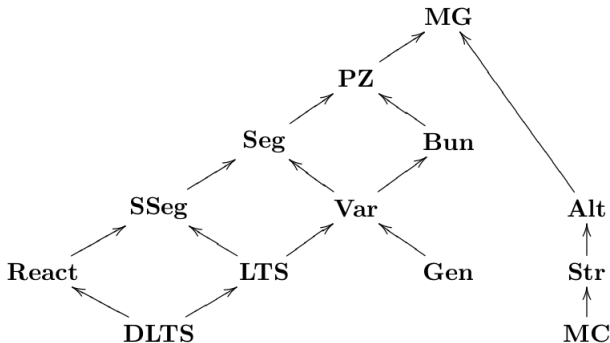


Figure 4.2: Hierarchy of probabilistic system types

Hierarchy of Probabilistic Systems Types

How to ...

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How to ...

...model system types?

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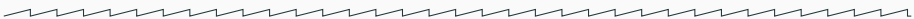
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codatatype +
Probability Mass Func.

Coalgebras as Codatatypes in Isabelle/HOL

Idea: Analyse transition systems modulo *bisimulation*!

Equality $:\Leftrightarrow$ Bisimulation

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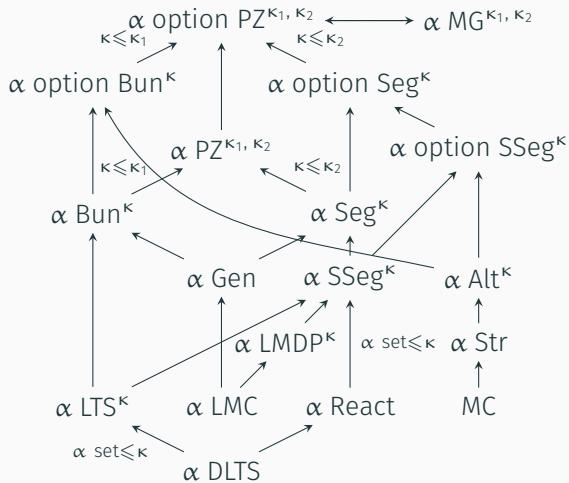
Example (Labeled Markov Chains where $F = \alpha \times \square \text{ pmf}$):

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

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^k	α LMDP ^k
Det. automaton	$\alpha \Rightarrow \sigma$ option	α DLTS
Non-det. automaton	$(\alpha \times \sigma)$ set^k	α LTS ^k
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^k	α Alt ^k
Simple Segala system	$(\alpha \times \sigma$ pmf) set^k	α SSeg ^k
Segala system	$(\alpha \times \sigma)$ pmf set^k	α Seg ^k
Bundle system	$(\alpha \times \sigma)$ set^k pmf	α Bun ^k
Pnueli-Zuck system	$(\alpha \times \sigma)$ set^{k_1} pmf set^{k_2}	α PZ ^{k₁, k₂}
Most general system	$(\alpha \times \sigma + \sigma)$ set^{k_1} pmf set^{k_2}	α MG ^{k₁, k₂}

Hierarchy



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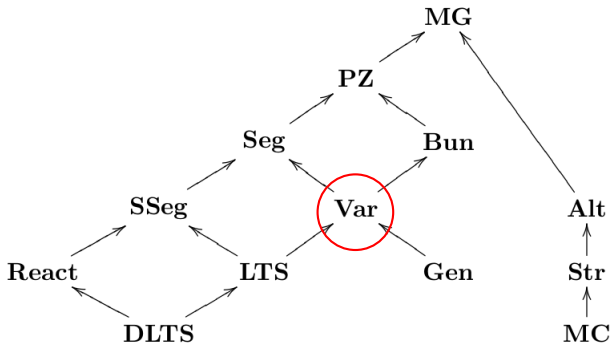


Figure 4.2: Hierarchy of probabilistic system types

Conclusion

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