

From Bisimulations to Metrics via Couplings

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A big thank to



Giorgio Bacci



Kim G. Larsen



Radu Mardare



Qiyi Tang



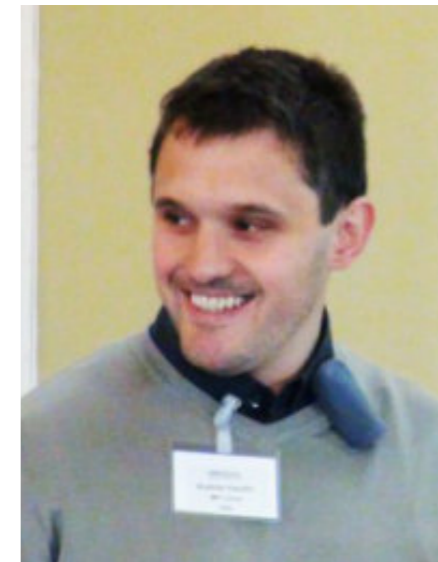
Max Tschaikowski



Mirco Tribastone



Franck van Breugel



Andrea Vandin

The Coupling Method

- It's a fundamental proof technique in probability theory
- Used to compare distributions $\mu, \nu \in D(X)$

Main Idea: construct a joint probability $\gamma \in D(X \times X)$ with marginals μ and ν where it's easier to prove the relation

Stochastic Domination & Couplings:

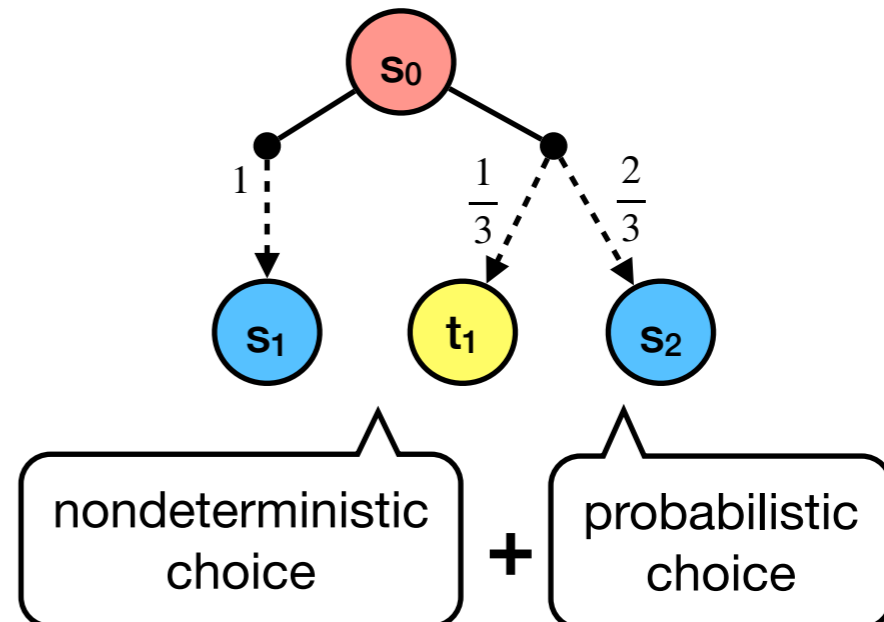
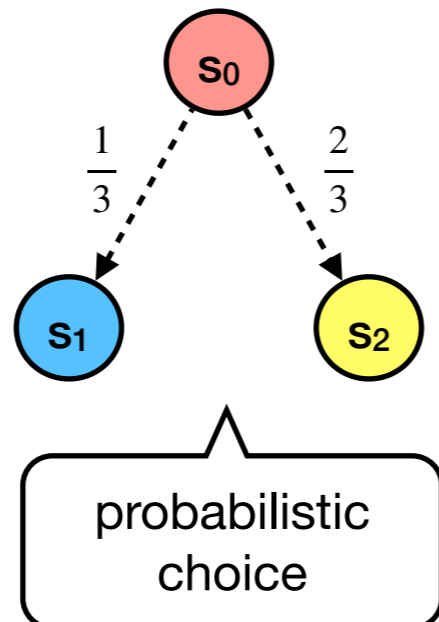
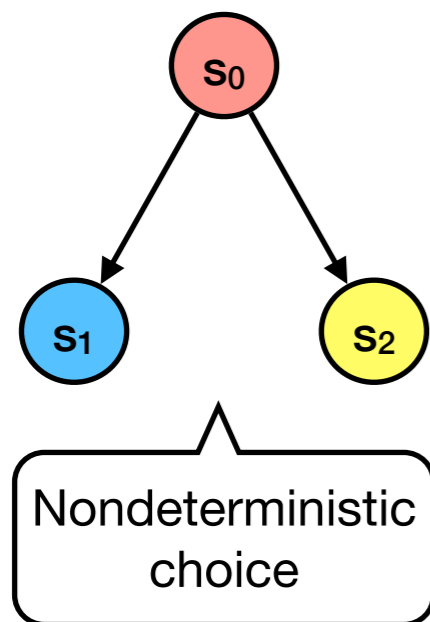
- Assume the set X has an order \sqsubseteq
- We write that $\mu \sqsupseteq_{sd} \nu$ iff $\forall a \in X. \mu[x \sqsupseteq a] \geq \nu[x' \sqsupseteq a]$

Strassen's Theorem:

$\mu \sqsubseteq_{sd} \nu$ iff $\exists \gamma \in \Gamma_D(\mu, \nu)$ such that $\gamma(x, x') > 0 \implies x \sqsubseteq x'$

Systems' Behaviour & Couplings

- We want to **reason about behaviours** of systems with
 - Nondeterministic choice (e.g. transition systems)
 - Probabilistic choice (e.g., Markov chains)
 - Probabilistic + Nondeterministic choice (e.g., probabilistic automata, Markov decision processes)
- ...and more (spoiler: polynomial ODE)



Equivalences vs. Pseudometrics



EQUIVALENCE RELATION:

Reflexive: $s \sim s$

Symmetric: $s \sim t \implies t \sim s$

Transitive: $s \sim u$ and $u \sim t \implies s \sim t$

- Reason about observational equivalence
- Often used to minimise the set of states of the system
- Not informative when the equivalence is not found

PSEUDOMETRIC:

Reflexive: $d(s, s) = 0$

Symmetric: $d(s, t) = d(t, s)$

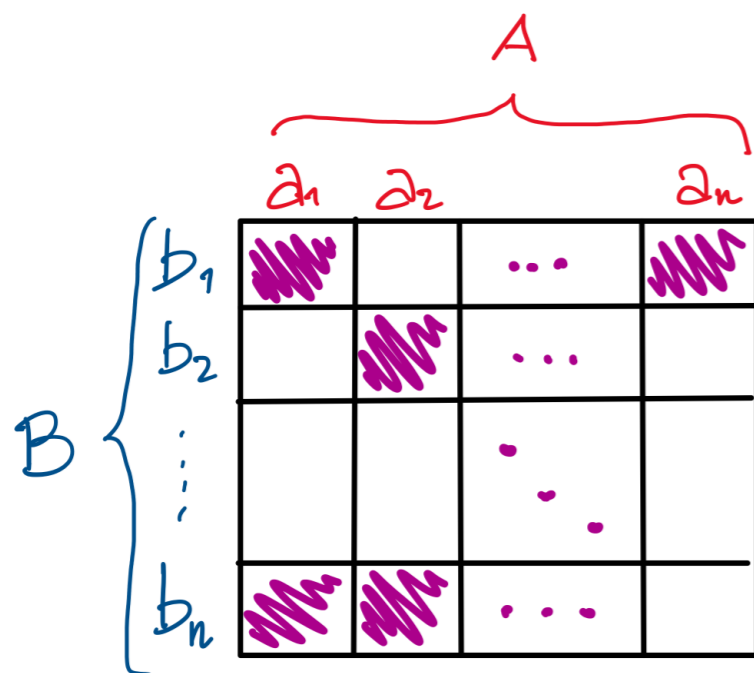
Triangular inequality: $d(s, u) + d(u, t) \leq d(s, t)$

- Measure observational dissimilarities
- May be used to minimise the set of states beyond equivalence
- Provide information about the magnitude of dissimilarity

Two type of Couplings

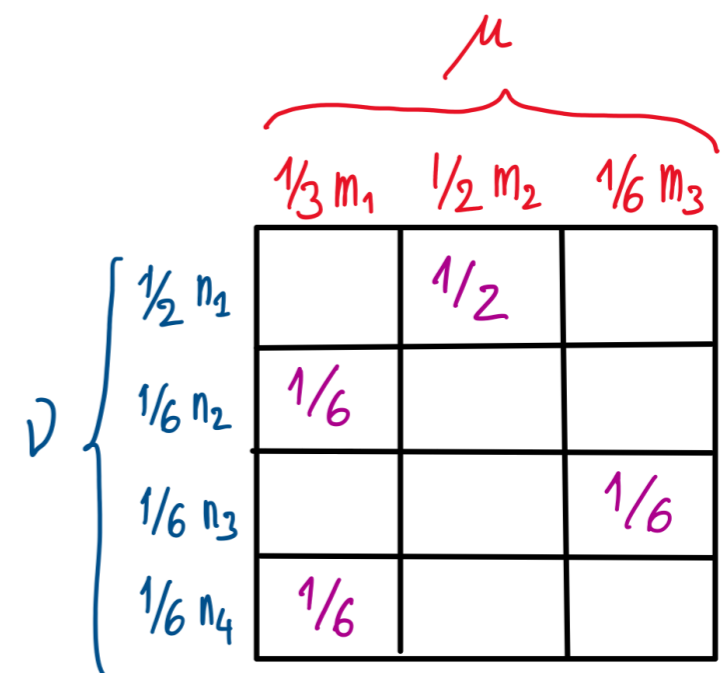
Nondeterministic Coupling

- To relate sets $A, B \subseteq S$
- Here a coupling is a **relation** $\Phi \subseteq A \times B$ such that
 - $A = \{a \in S : (a, b) \in \Phi\}$
 - $B = \{b \in S : (a, b) \in \Phi\}$
- We denote $\Gamma_S(A, B)$ the set of nondeterministic couplings for (A,B)



Probabilistic Coupling

- To relate prob. distrib. $\mu, \nu \in D(S)$,
- Here a **coupling** is a probability distribution $\gamma \subseteq D(S \times S)$ such that
 - $\forall s \in S. \mu(s) = \sum_{t \in S} \gamma(s, t)$
 - $\forall t \in S. \nu(t) = \sum_{s \in S} \gamma(s, t)$
- We denote $\Gamma_D(\mu, \nu)$ the set of probabilistic couplings for (μ, ν)



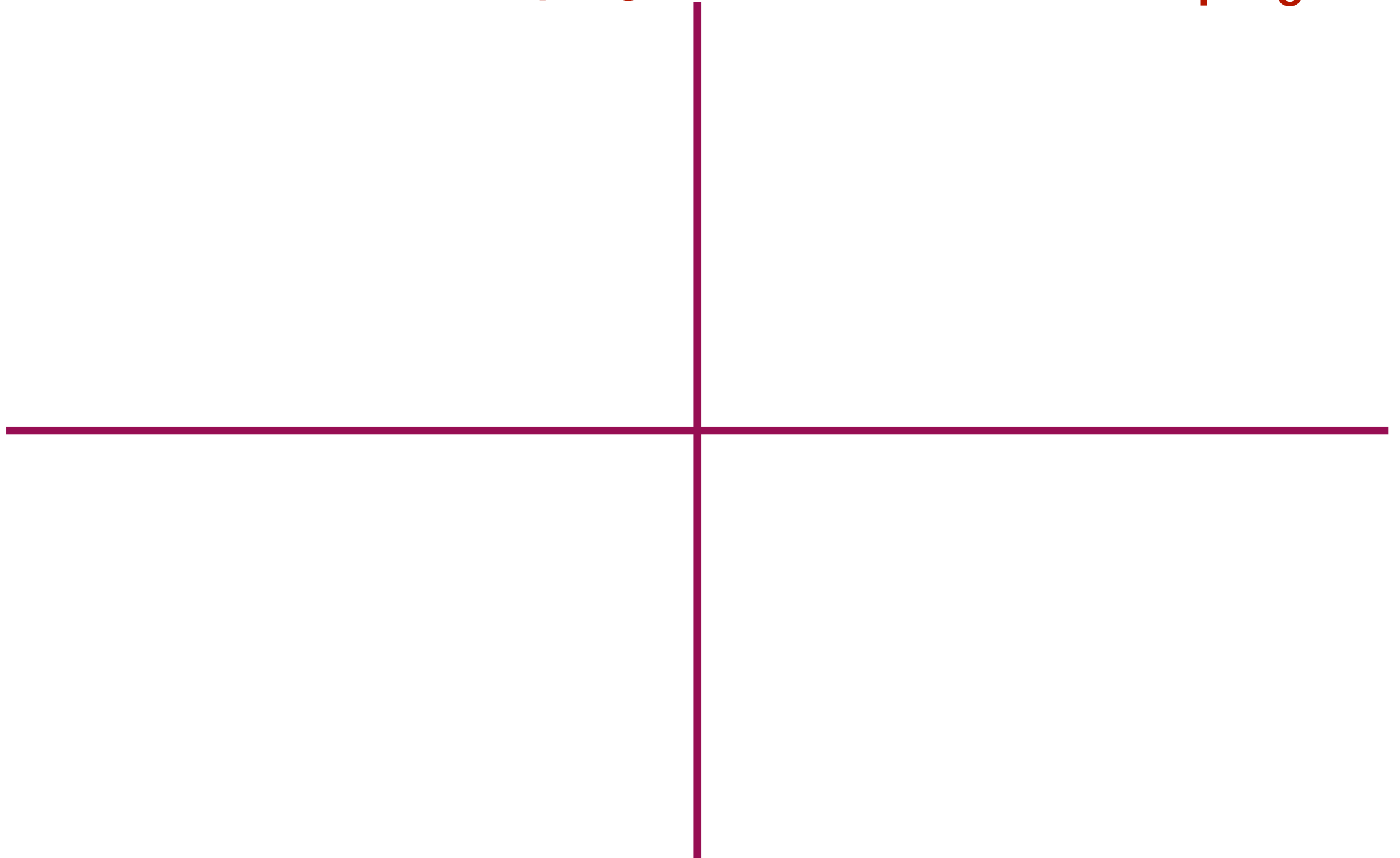
Couplings & Liftings

Nondeterministic Coupling

Probabilistic Coupling

Lifting Relations

Lifting Metrics



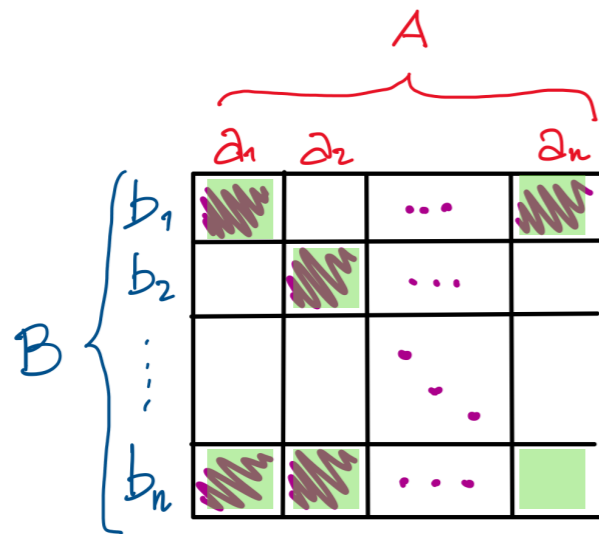
Couplings & Liftings

Nondeterministic Coupling

Probabilistic Coupling

Lifting Relations

$$S[R] = \{(A, B) : \Phi \in \Gamma_S(A, B), \Phi \subseteq R\}$$

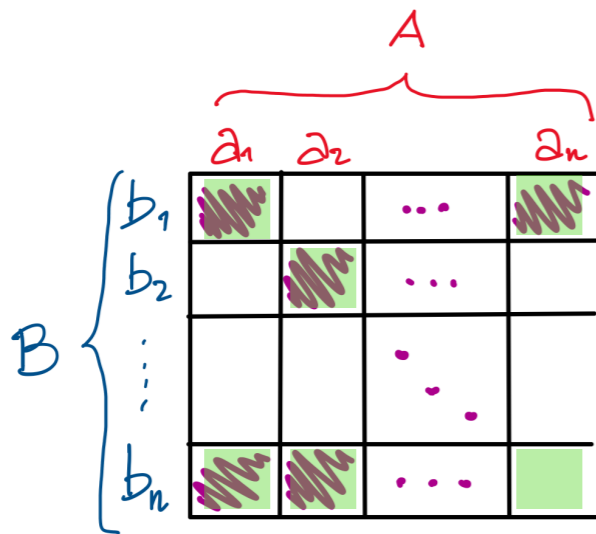


Lifting Metrics

Couplings & Liftings

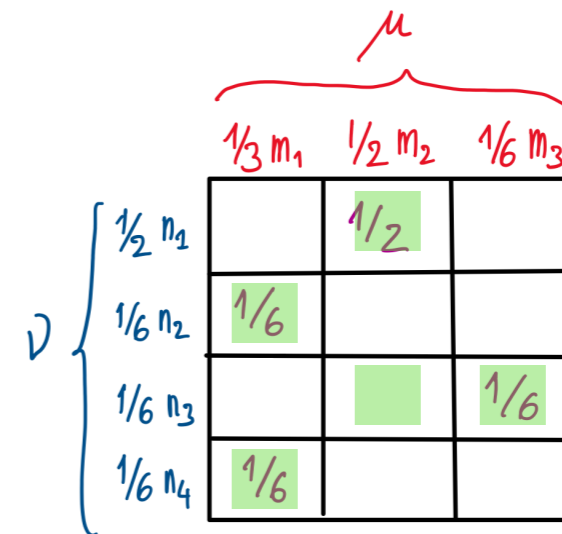
Nondeterministic Coupling

$$\mathbf{S}[R] = \{(A, B) : \Phi \in \Gamma_{\mathbf{S}}(A, B), \Phi \subseteq R\}$$



Probabilistic Coupling

$$\mathbf{D}[R] = \{(\mu, \nu) : \gamma \in \Gamma_{\mathbf{D}}(\mu, \nu), \text{supp}(\gamma) \subseteq R\}$$



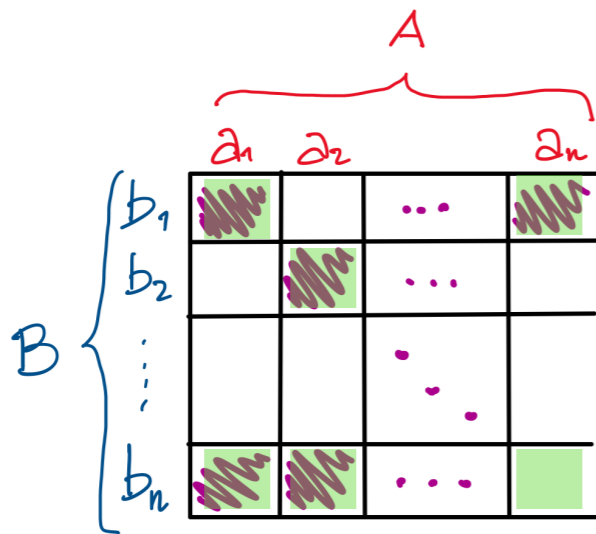
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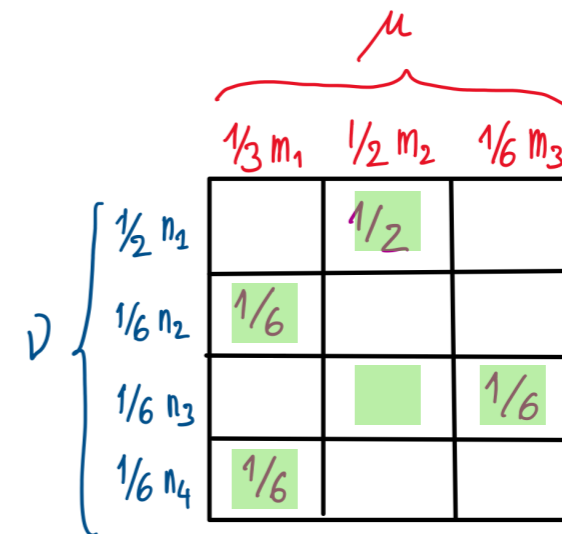
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$$\mathbf{H}(d)(A, B) = \min_{\Phi \in \Gamma_{\mathbf{S}}(A, B)} \max_{(a, b) \in \Phi} d(a, b)$$

Hausdorff distance!
(see Mémoli'11)

Lifting Relations

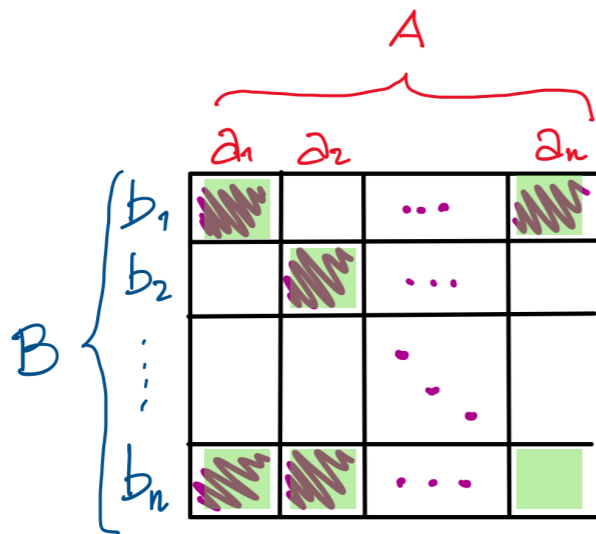
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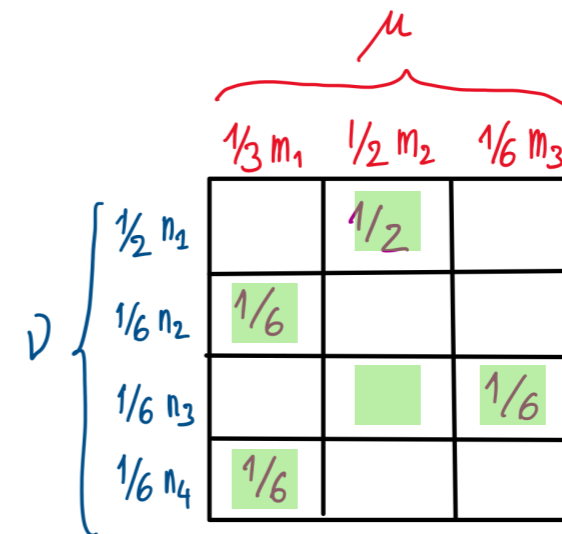
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Lifting Metrics

$$\mathbf{H}(d)(A, B) = \min_{\Phi \in \Gamma_{\mathbf{S}}(A, B)} \max_{(a, b) \in \Phi} d(a, b)$$

Hausdorff distance!
(see Mémoli'11)

$$\mathbf{K}(d)(\mu, \nu) = \min_{\gamma \in \Gamma_{\mathbf{D}}(\mu, \nu)} \sum_{s, t \in S} d(s, t) \cdot \gamma(s, t)$$

Kantorovich distance!

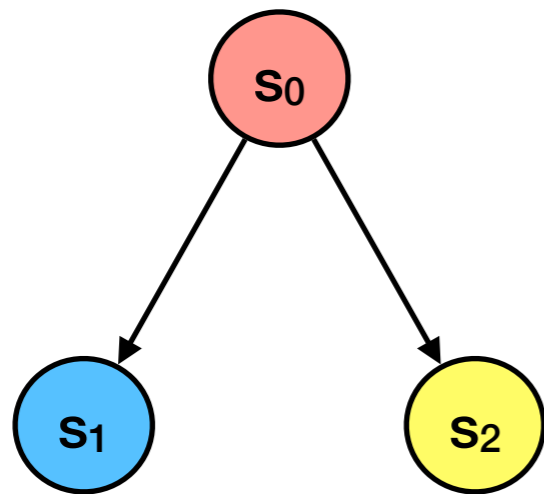
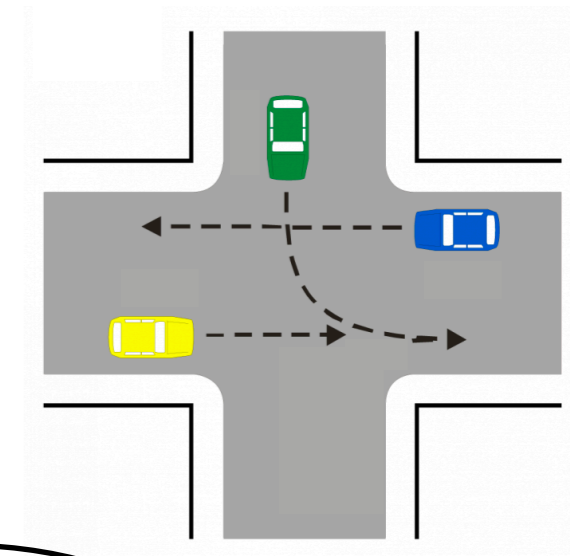
Transition Systems

$$\mathcal{T} = (S, \delta, \ell)$$

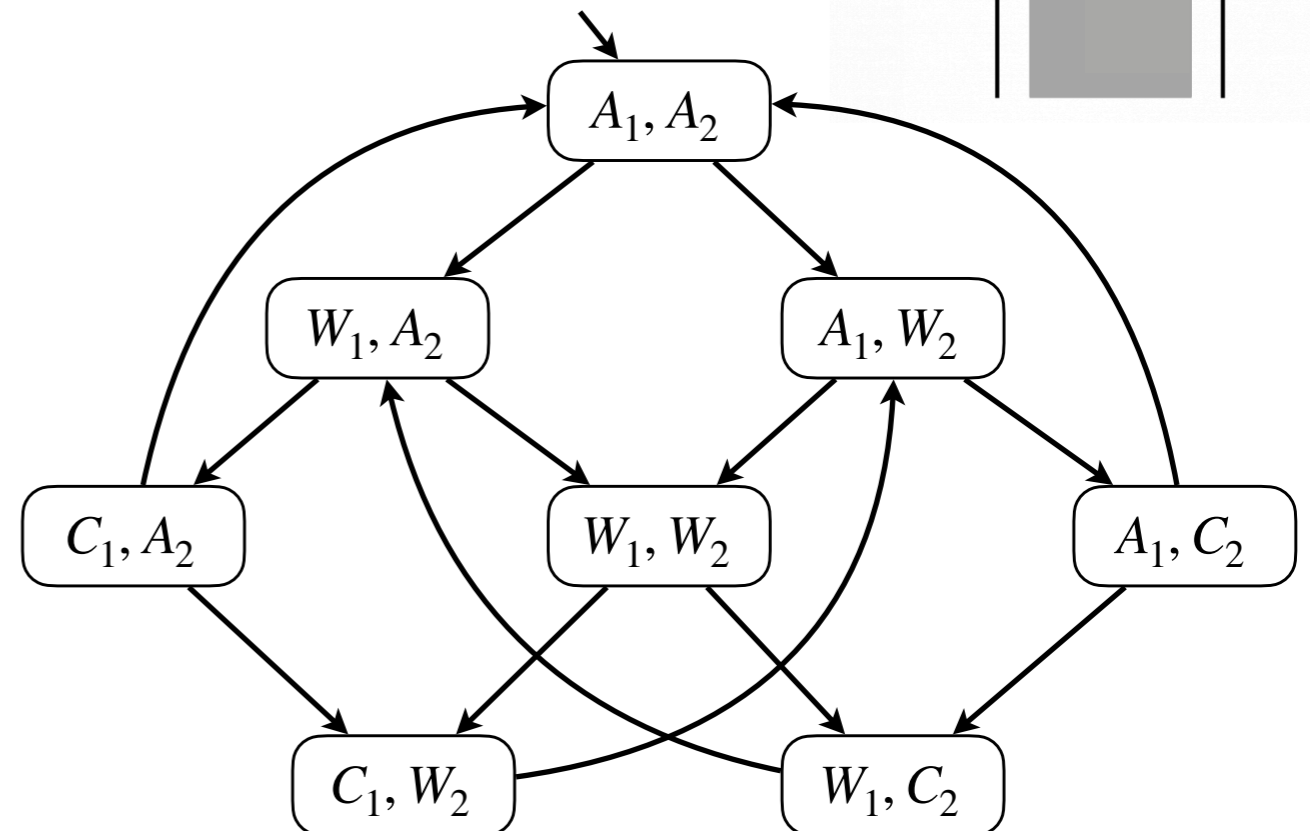
States

Labelling function $\delta: S \rightarrow L$

Successor function $\delta: S \rightarrow 2^S$

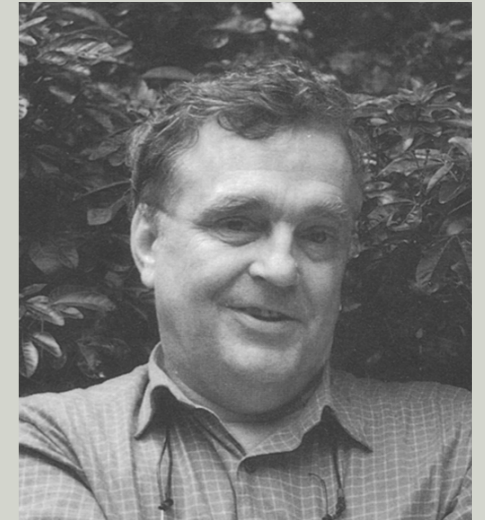


Nondeterministic choices



Bisimulation

- Initially formulated by Robin Milner under the name “observation equivalence” in 1980
- Perfected by David Park with a fixed point characterisation.



Definition:

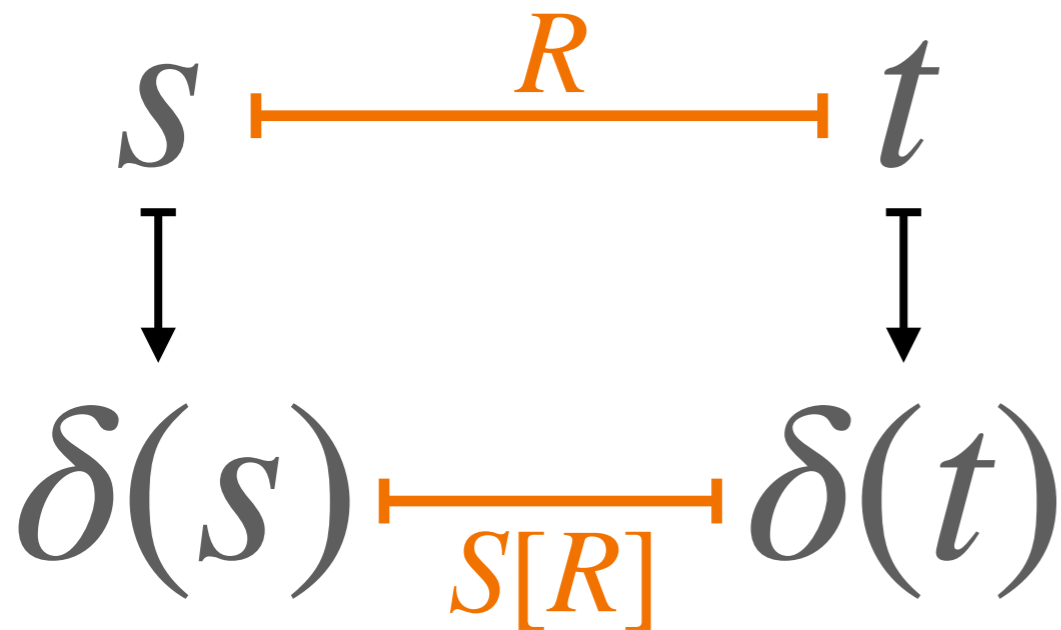
$R \subseteq S \times S$ is a *bisimulation* if whenever $(s, t) \in R$ then

- (i) **What we observe in the two states is the same, i.e., $\ell(s) = \ell(t)$**
- (ii) **Each transition of one can be matched by some transition of the other and vice versa, formally:**
 - $\forall s' \in \delta(s) \exists t' \in \delta(t)$ such that $(s', t') \in R$
 - $\forall t' \in \delta(t) \exists s' \in \delta(s)$ such that $(s', t') \in R$

Fixed point characterisation

...just rephrasing Park's idea

$$\mathcal{B}(R) = \{ (s, t) \in S \times S \mid (\delta(s), \delta(t)) \in S[R] \}$$



Theorem (Fixed point):

For any $R \subseteq S \times S$

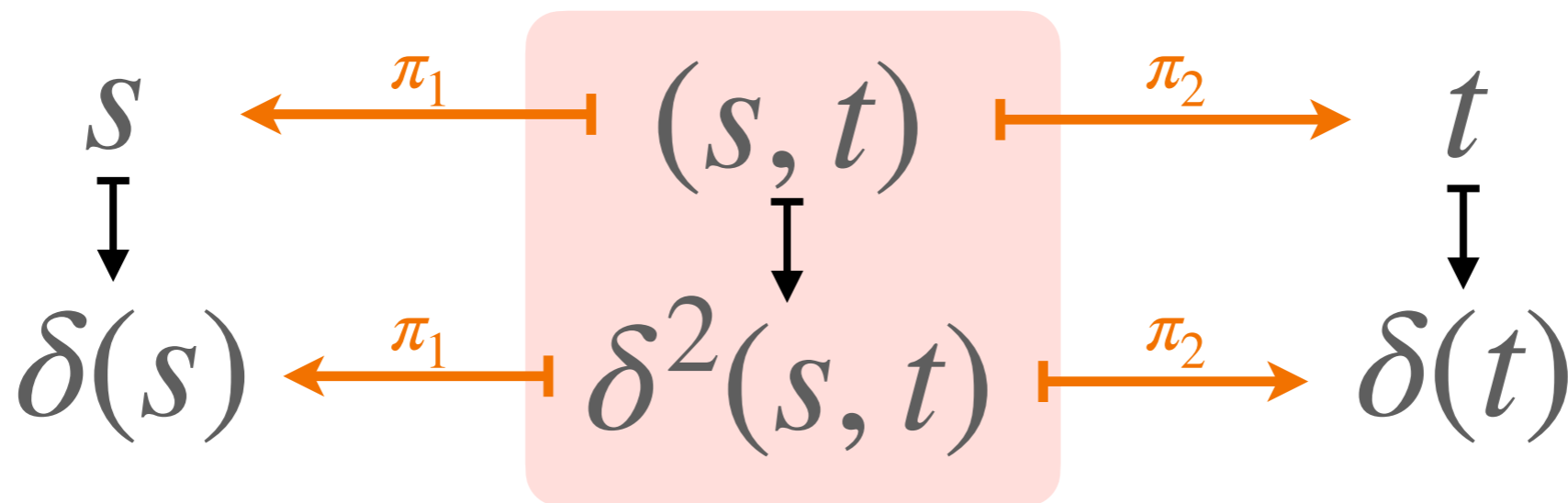
- (1) $R \subseteq \mathcal{B}(R)$ iff R is a bisimulation
- (2) $\text{gfp}(\mathcal{B})$ coincides with bisimilarity

$$S[R] = \{ (A, B) : \Phi \in \Gamma_S(A, B) \text{ and } \Phi \subseteq R \}$$

Coupled system

Given the TS \mathcal{T} , a $\mathcal{T}^2 = (S^2, \delta^2, \{eq, neq\}, \ell^2)$ is a “coupled” system for \mathcal{T} if

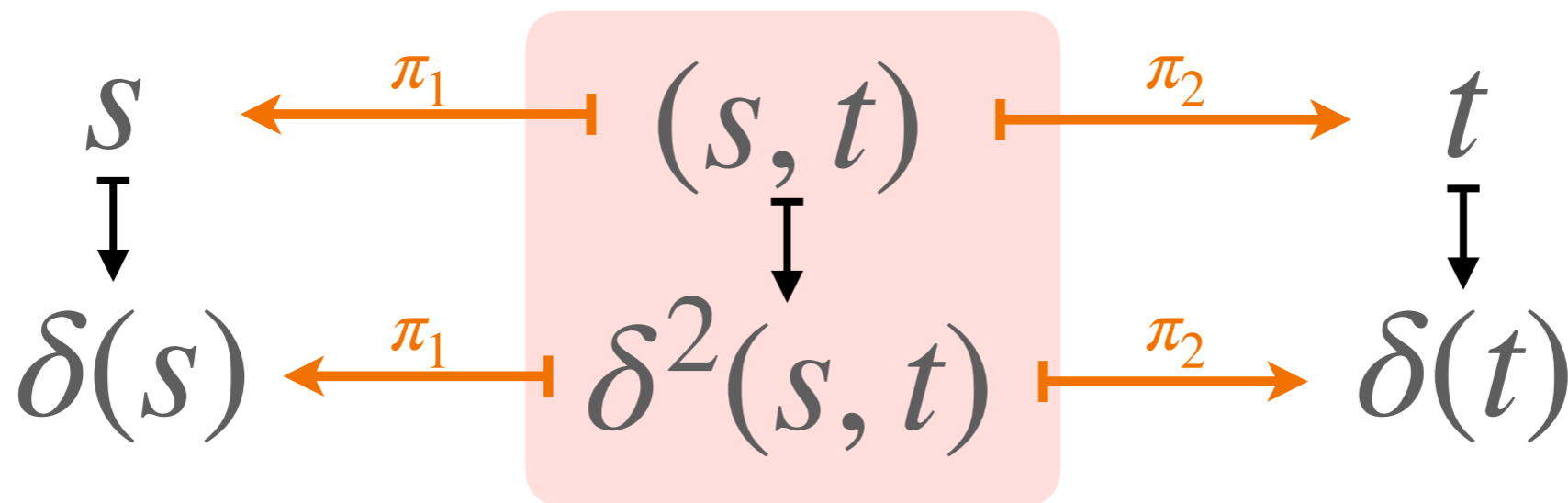
- (i) $\delta^2(s, t) \in \Gamma_S(\delta(s), \delta(t))$ for all $s, t \in S$
- (ii) $\ell^2(s, t) = eq$ if $\ell(s) = \ell(t)$; $\ell(s, t) = neq$ otherwise



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Theorem:

$s \sim t$ iff $\mathcal{T}^2, (s, t) \models \square eq$ for some coupled system \mathcal{T}^2

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$$(s, t) \longrightarrow (s_1, t_1) \longrightarrow (s_2, t_2) \longrightarrow (s_3, t_3) \longrightarrow \dots$$

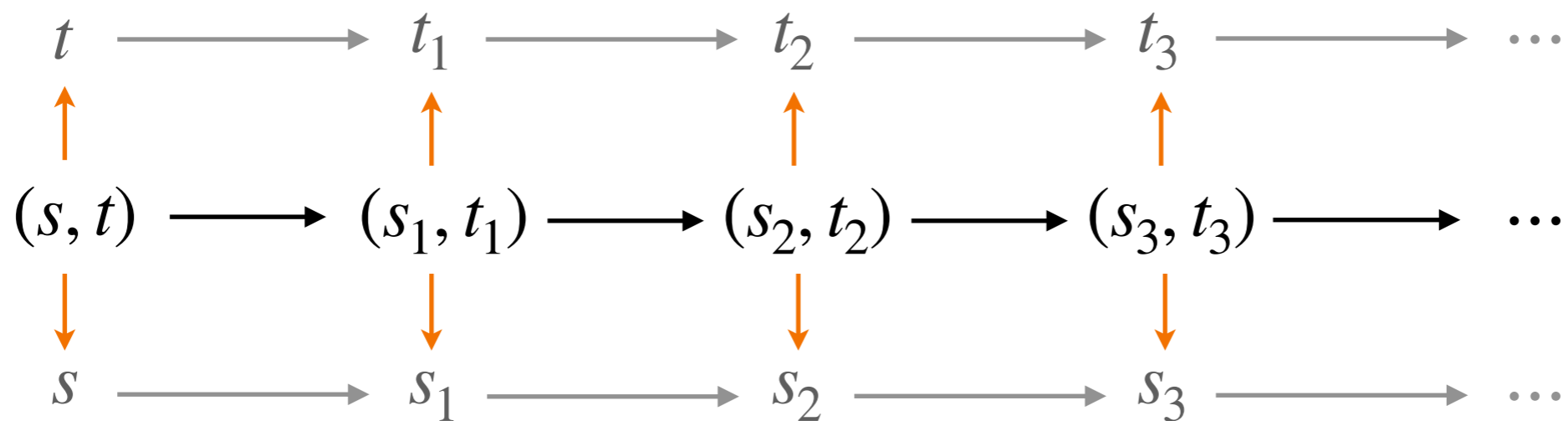
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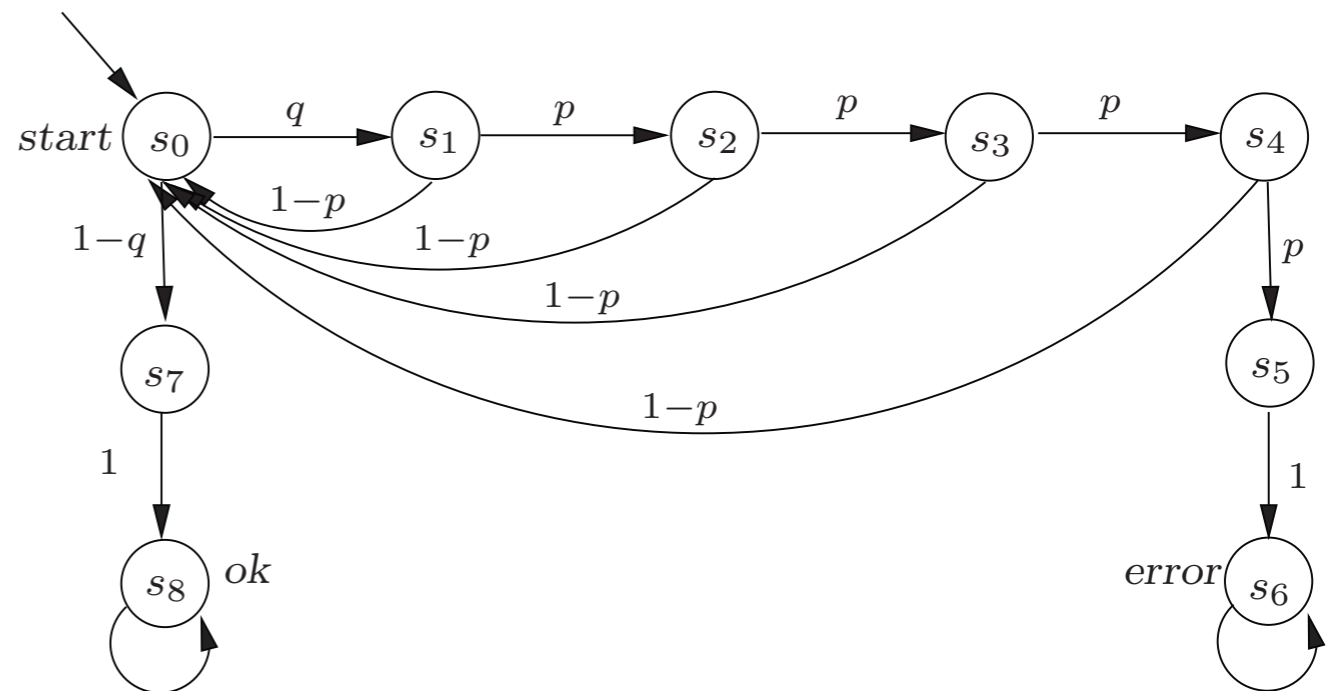
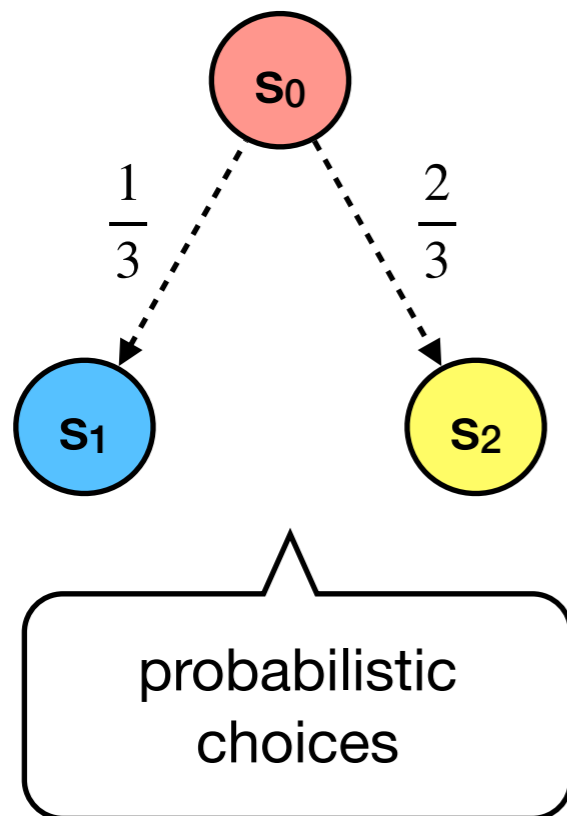
Markov chains

$$\mathcal{M} = (S, \tau, \ell)$$

States

Labelling function $\ell: S \rightarrow L$

Successor function $\tau: S \rightarrow D(S)$



Markov chain of the IPv4 zeroconf protocol (for $n=4$ probes) where $p, q \in (0,1)$. Figure from "Principles of Model Checking" by C. Baier & J-P. Katoen

Probabilistic Bisimulation

- Initially formulated by Kemeny and Snell under the name “**lumpability**”
- Larsen & Skou characterise it via “**probabilistic testability**”



Definition:

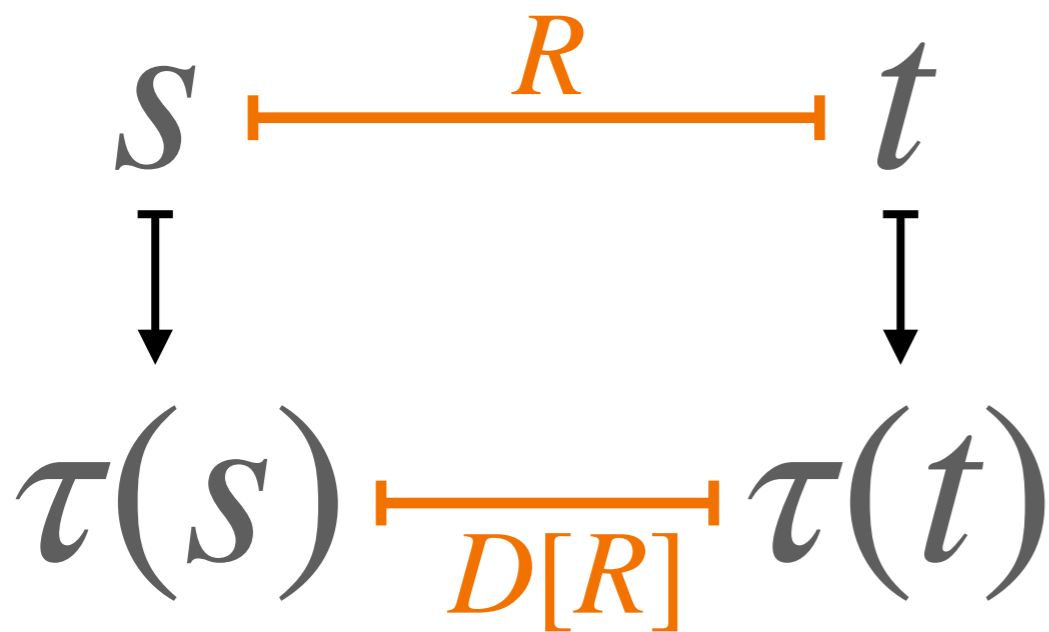
Let $R \subseteq S \times S$ be an equivalence relation, then is a *probabilistic bisimulation* if whenever $(s, t) \in R$ then

- (i) What we observe in the two states is the same, i.e., $\ell(s) = \ell(t)$
- (ii) The probability to move to R -equivalent states is the same, i.e.,
$$\forall C \in S/R \quad \sum_{c \in C} \tau(s)(c) = \sum_{c \in C} \tau(t)(c)$$

Fixed point characterisation

...just rephrasing Jonsson & Larsen'91

$$\mathcal{B}(R) = \{ (s, t) \in S \times S \mid (\tau(s), \tau(t)) \in D[R] \}$$



Theorem (Fixed point):

For any $R \subseteq S \times S$

- (1) $R \subseteq \mathcal{B}(R)$ iff R is a bisimulation
- (2) $\text{gfp}(\mathcal{B})$ coincides with bisimilarity

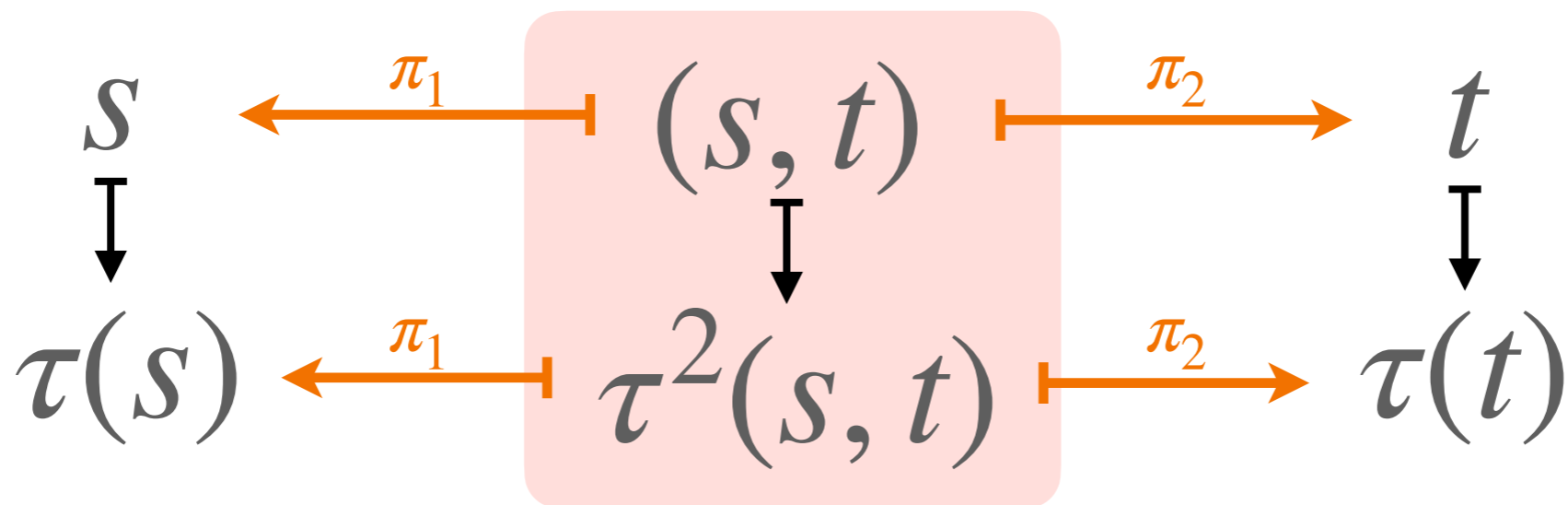
$$D[R] = \{ (\mu, \nu) : \gamma \in \Gamma_D(\mu, \nu) \text{ and } \text{supp}(\gamma) \subseteq R \}$$

Remark: Baier'96 used the above characterisation to show that probabilistic bisimulation can be computed in polynomial time

Coupled Markov chain

Given the MC \mathcal{M} , a $\mathcal{M}^2 = (S^2, \tau^2, \{eq, neq\}, \ell^2)$ is a “coupled” Markov chain for \mathcal{M} if

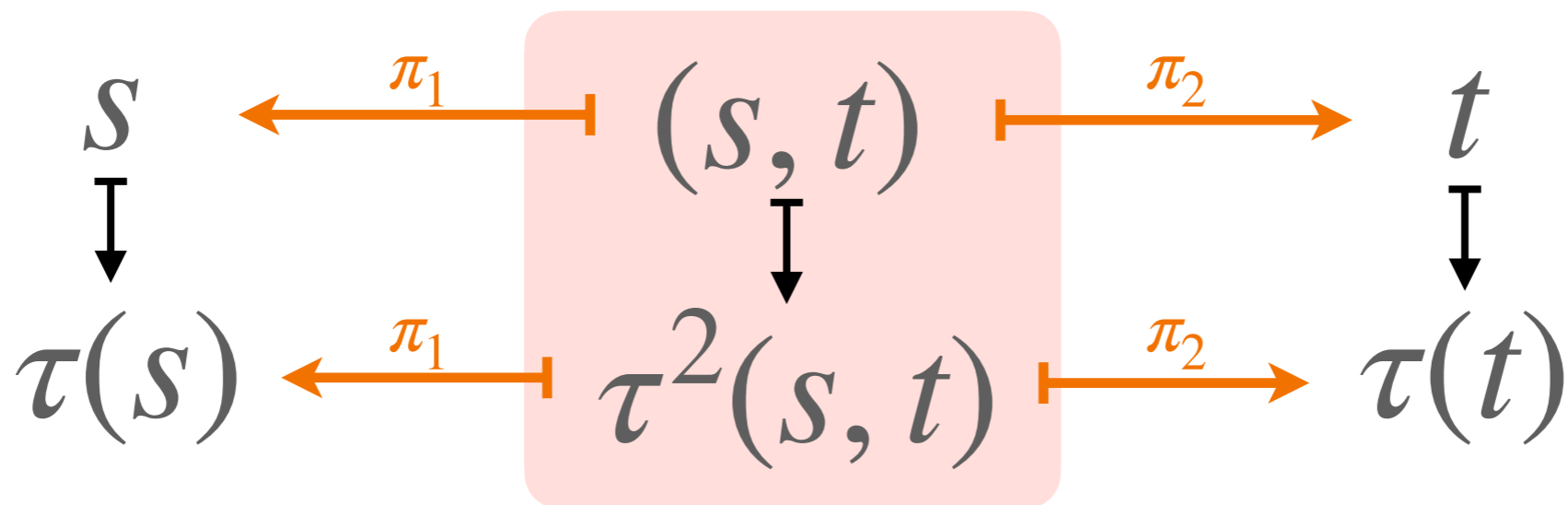
- (i) $\tau^2(s, t) \in \Gamma_D(\tau(s), \tau(t))$ for all $s, t \in S$
- (ii) $\ell^2(s, t) = eq$ if $\ell(s) = \ell(t)$; $\ell(s, t) = neq$ otherwise



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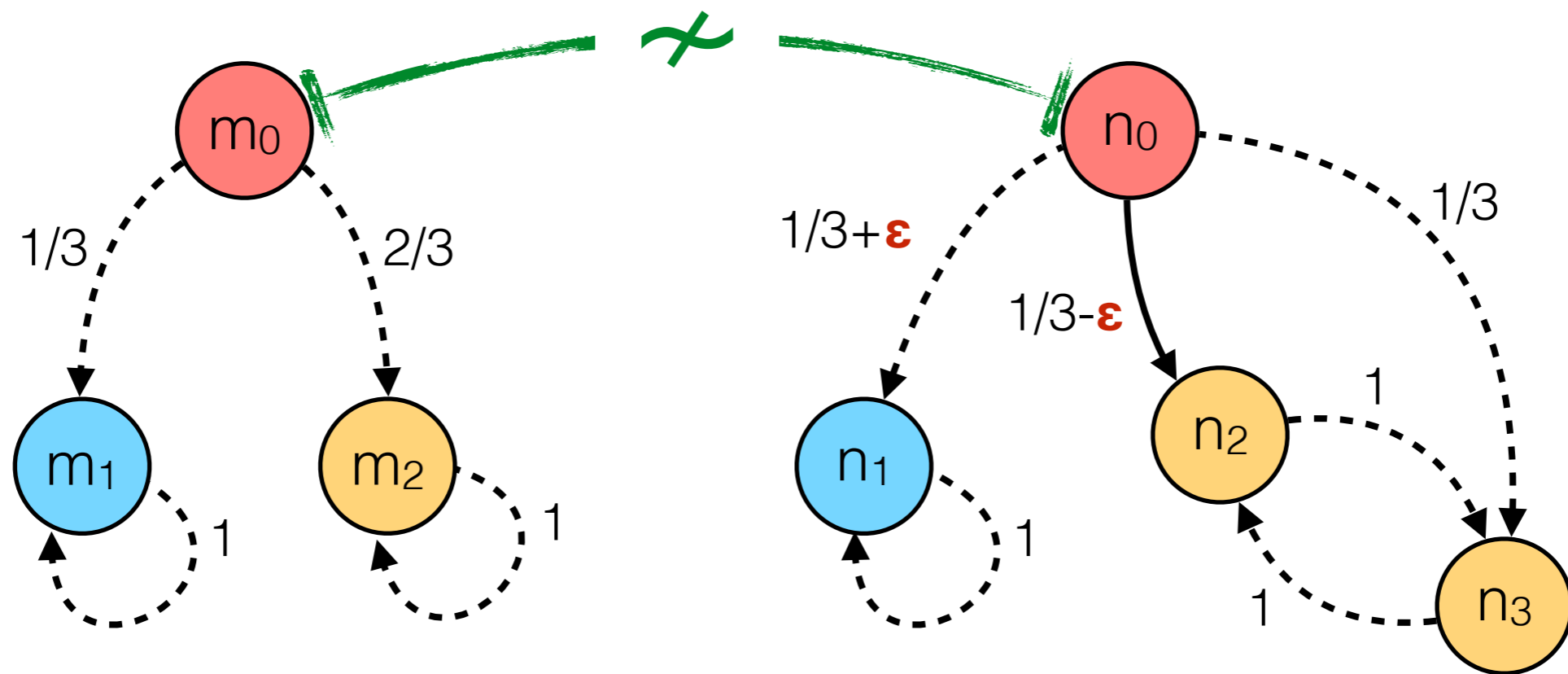


Theorem [Chen, van Breugel, Worrell'12]

$s \sim t$ iff $P[\mathcal{M}^2, (s, t) \models \diamond neq] = 0$ for some coupled chain \mathcal{M}^2

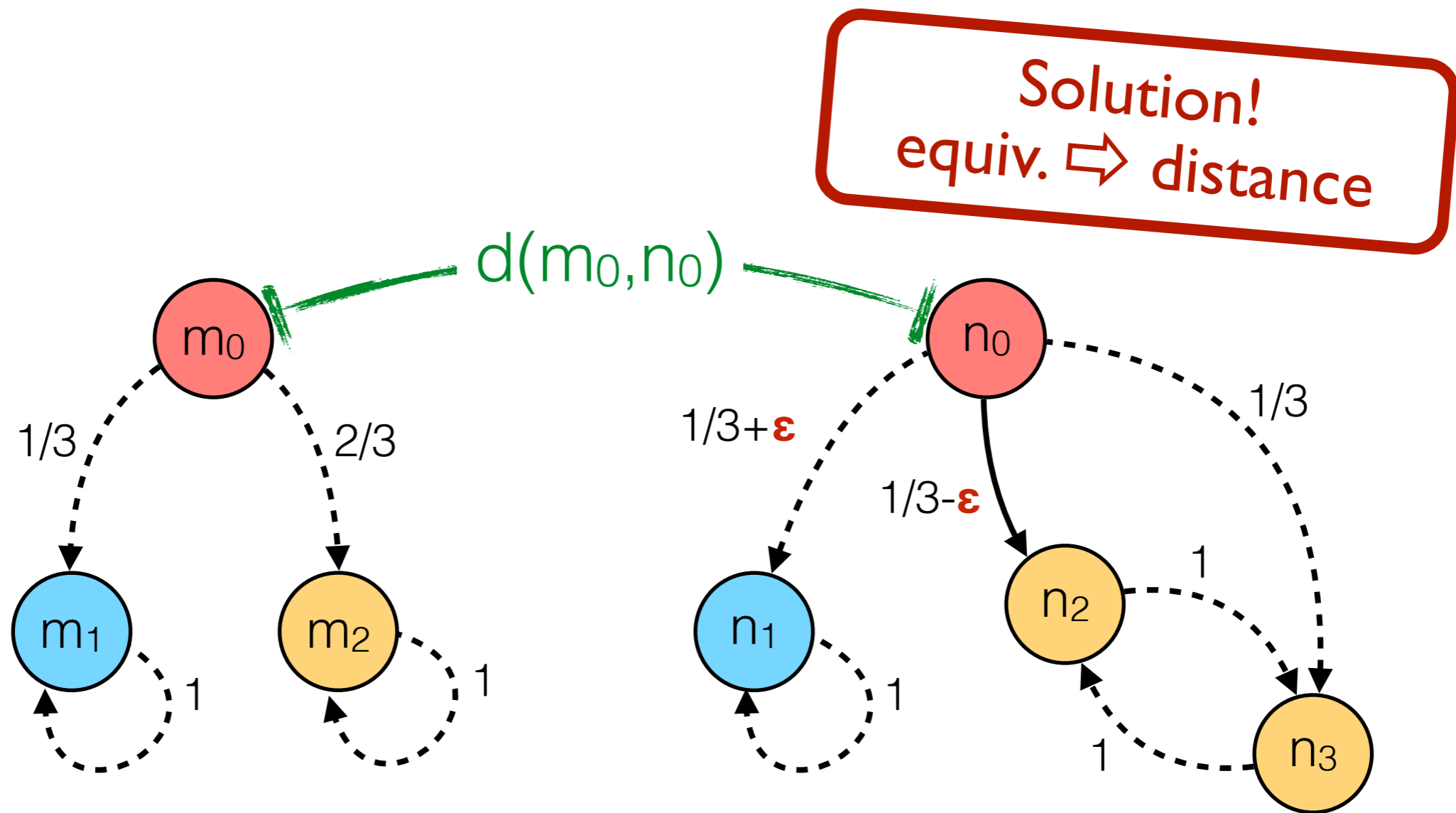
From Bisimulations to Metrics

Jou & Smolka'90 observed that behavioural equivalences are not robust for systems with real-valued data



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Probabilistic Bisimilarity Distance

- First formulated by Desharnais, Gupta, Jagadeesan, and Panangaden
- Then, van Breugel and Worrell gave a fixed point characterisation



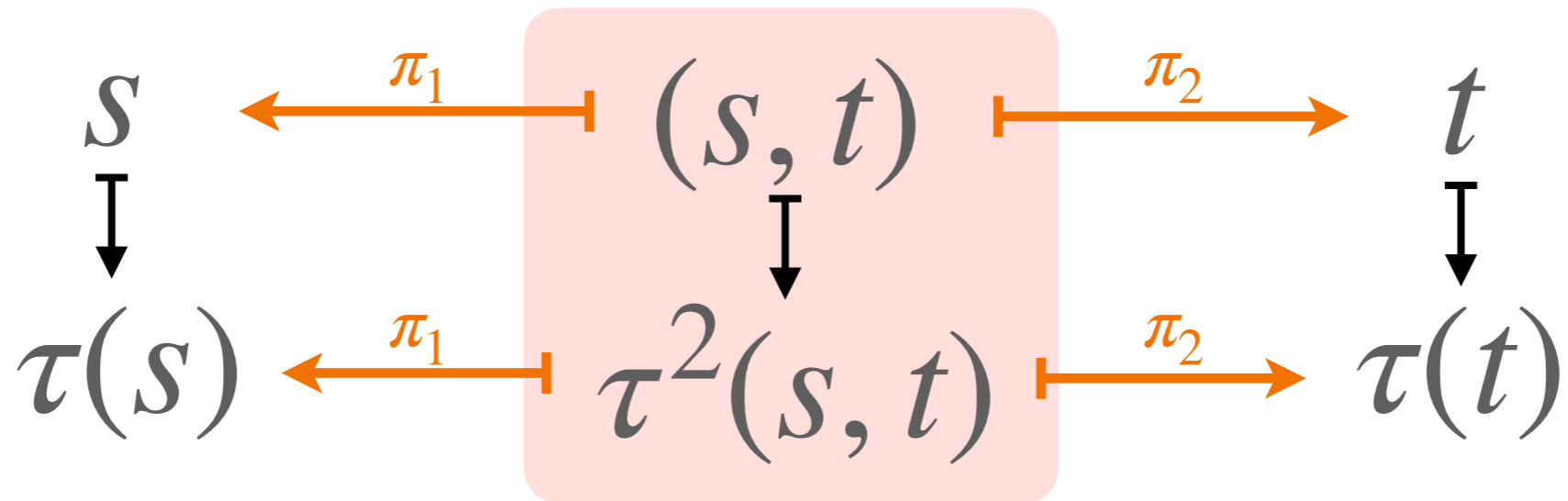
Fixed point characterisation:

The bisimilarity distance $\mathbf{d}_b : S \times S \rightarrow [0,1]$ is the least fixed point of the following (monotone) operator

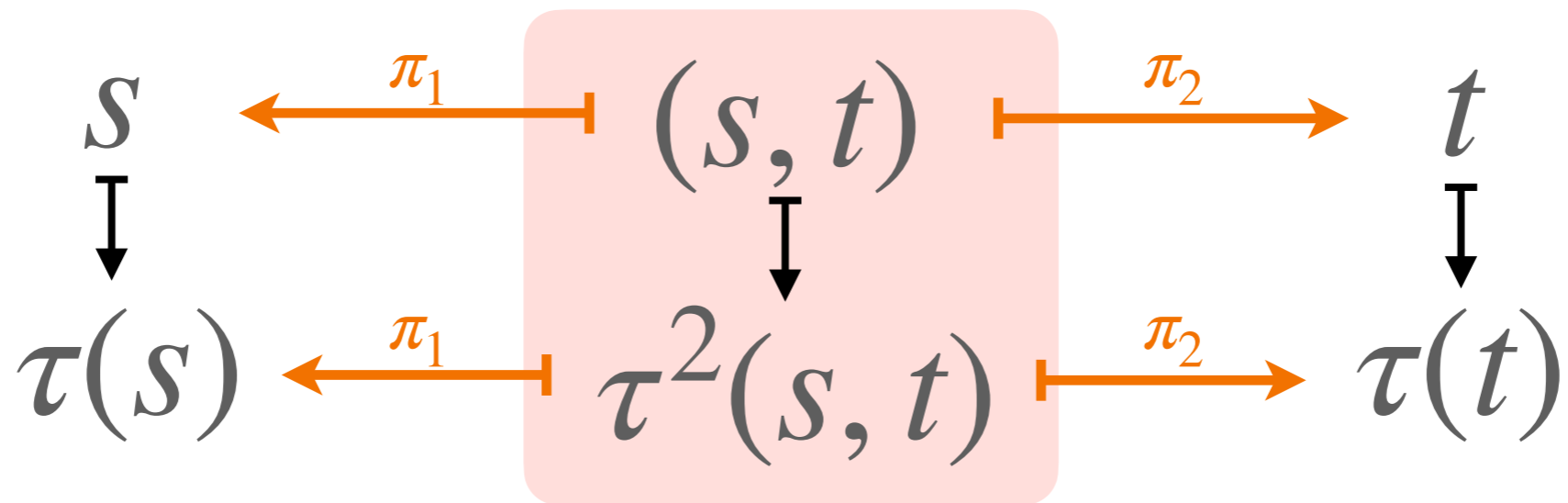
$$\Delta(d)(s, t) = \begin{cases} 1 & \text{if } \ell(s) \neq \ell(t) \\ \mathcal{K}(d)(\tau(s), \tau(t)) & \text{otherwise} \end{cases}$$

Kantorovich distance
between transition prob.

Coupled Markov chain (part 2)



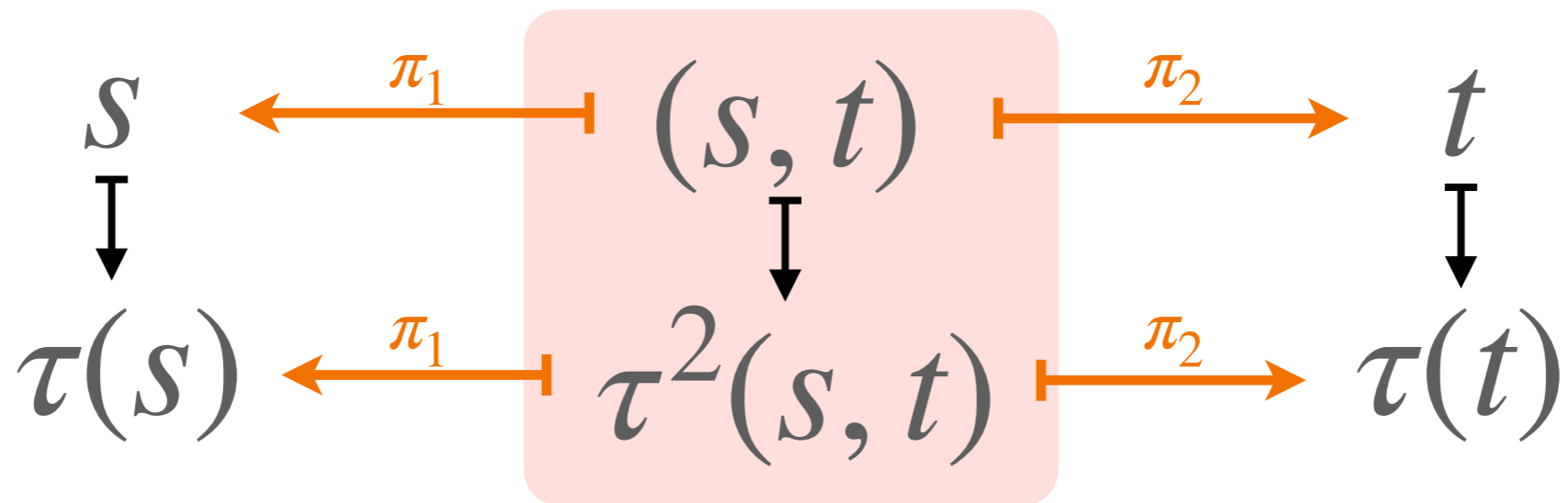
Coupled Markov chain (part 2)



Coupling Theorem [Chen, van Breugel, Worrell'12]

- (i) $\mathbf{d}_b(s, t) \leq P[\mathcal{M}^2, (s, t) \vDash \diamond neq]$ for all coupled chain \mathcal{M}^2
- (ii) $\mathbf{d}_b(s, t) = P[\mathcal{M}^2, (s, t) \vDash \diamond neq]$ for some coupled chain \mathcal{M}^2

Coupled Markov chain (part 2)



Coupling Theorem [Chen, van Breugel, Worrell'12]

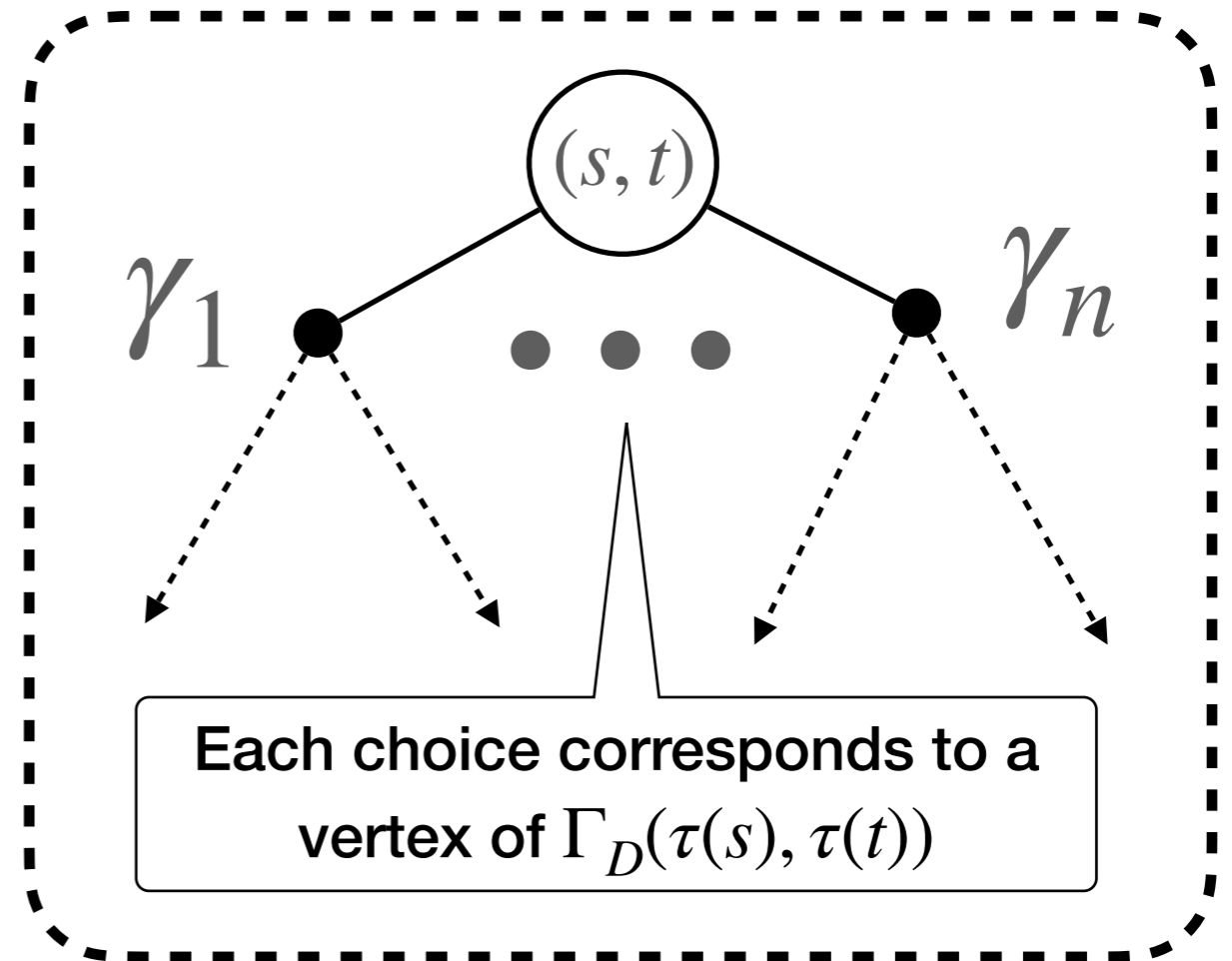
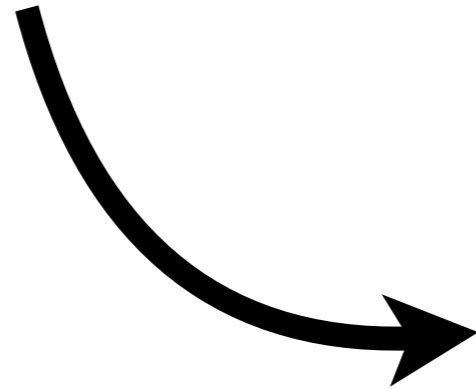
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Nice behavioural properties:

- (i) $\mathbf{d}_b(s, t) = 0$ iff $s \sim t$
- (ii) $\sup_{\phi \in LTL} |P[\mathcal{M}, s \vDash \phi] - P[\mathcal{M}, t \vDash \phi]| \leq \mathbf{d}_b(s, t)$

Bisim. Distance & Optimal value

Define a (coupled) Markov decision process \mathcal{C} as follows



Theorem [Bacci², Larsen, Mardare'13]

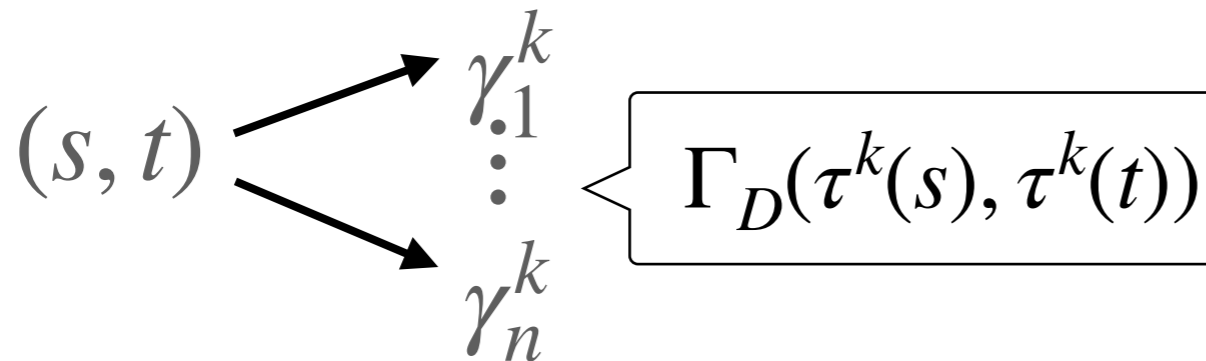
$$\mathbf{d}_b(s, t) = \inf_{\pi \in \Pi} P^\pi[\mathcal{C}, (s, t) \models \diamond neq]$$

We proposed an on-the-fly policy iteration procedure to compute $\mathbf{d}_b(s, t)$ (see Bacci et al. TACAS'13)

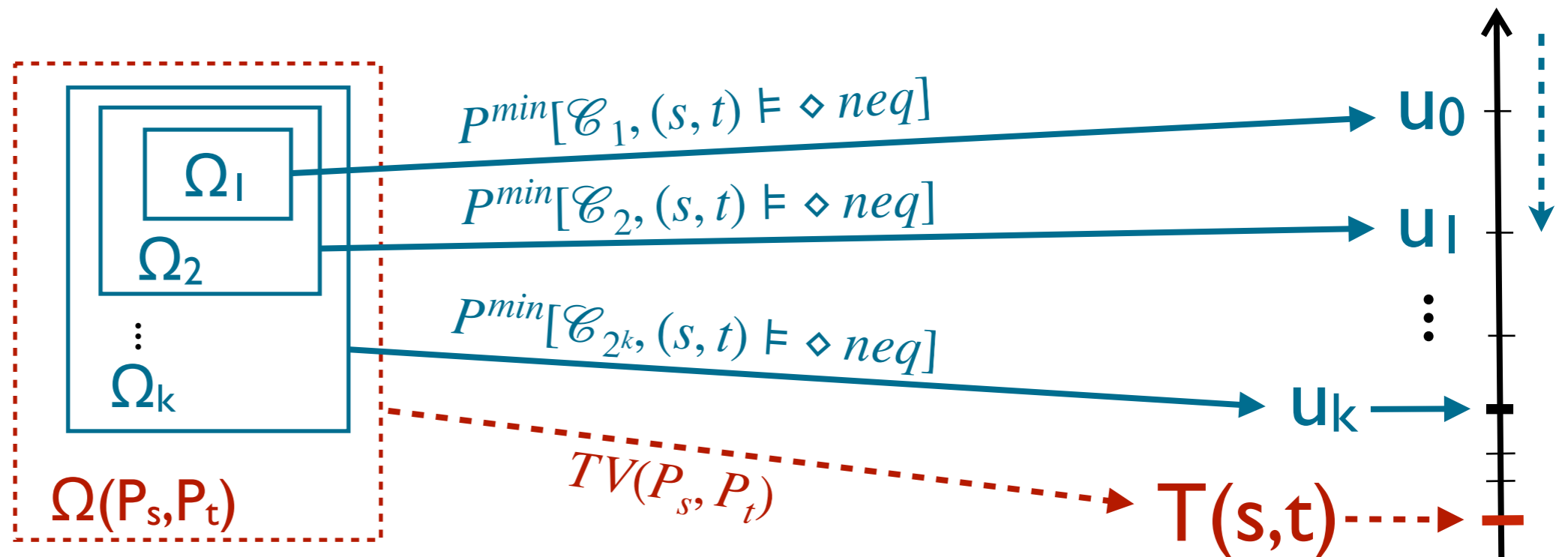
Approximating Total Variation

[Bacci², Larsen, Mardare ICTAC'15]

Coupled MDP of rank k



MDP emitting pairs of **k successive steps** at each time interval



$$u_k = P^{min}[\mathcal{C}_{2^k}, (s, t) \models \diamond neq]$$

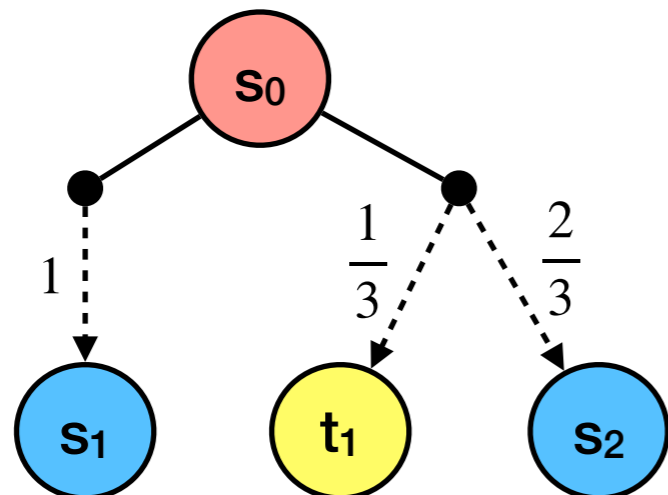
Probabilistic Automata

$$\mathcal{A} = (S, \delta, \ell)$$

States

Labelling function $\ell: S \rightarrow L$

Successor function $\tau: S \rightarrow 2^{D(S)}$



nondeterministic choice

+

probabilistic choices

Remark: similar to MDPs but here the nondeterministic choice is taken internally by the system

Probabilistic Bisimilarity Distance

- Generalises bisimilarity distance by Segala and Lynch
- Introduced by Deng, Chothia, Palamidessi, and Pang



Definition:

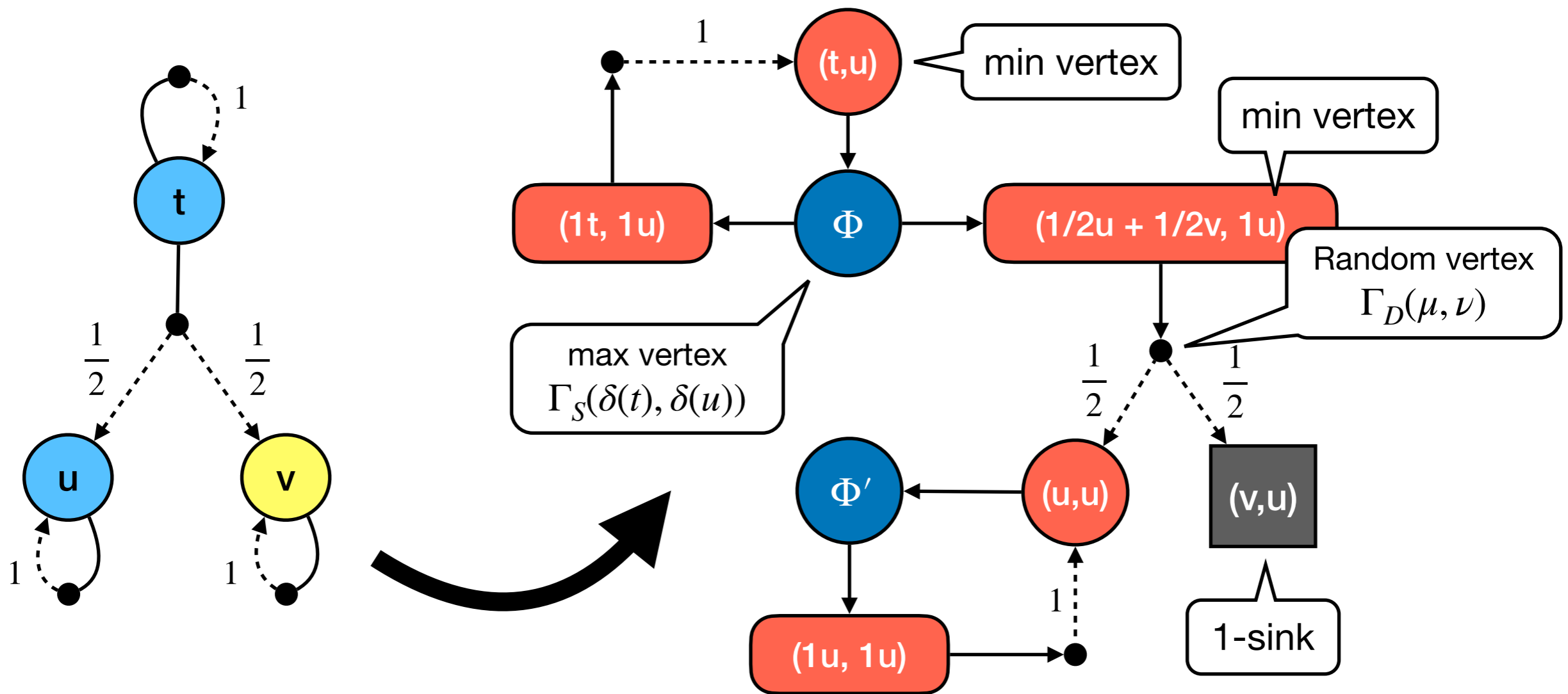
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$$\Delta(d)(s, t) = \begin{cases} 1 & \text{if } \ell(s) \neq \ell(t) \\ \mathcal{H}(\mathcal{K}(d))(\delta(s), \delta(t)) & \text{otherwise} \end{cases}$$

Compose Hausdorff and Kantorovich lifting

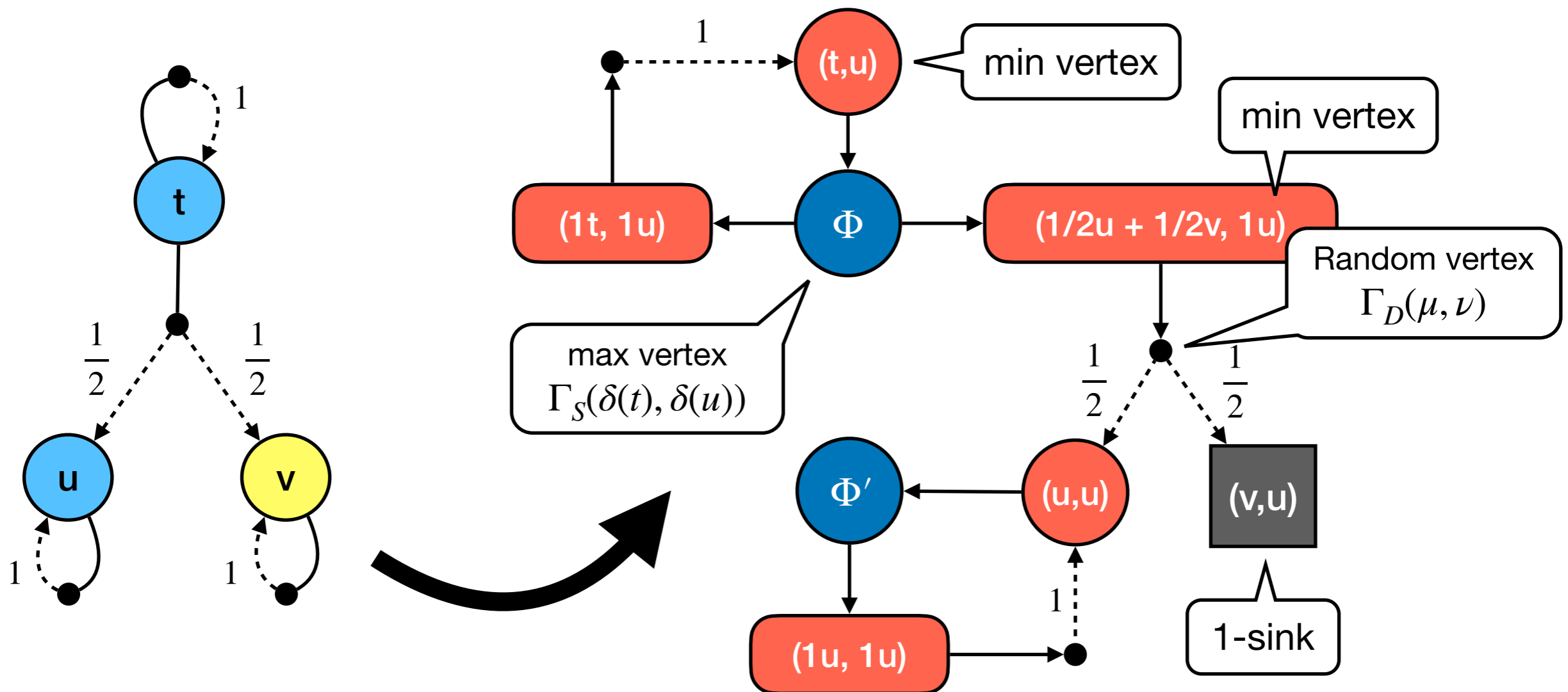
Prob. Bisimilarity Game

[Bacci², Larsen, Mardare, Tang, van Breugel'19]



Prob. Bisimilarity Game

[Bacci², Larsen, Mardare, Tang, van Breugel'19]



Theorem [Bacci², Larsen, Mardare, Tang, van Breugel'19]

Let G be the SSGs induced by \mathcal{A} . Then, the optimal value of the equals \mathbf{d}_b

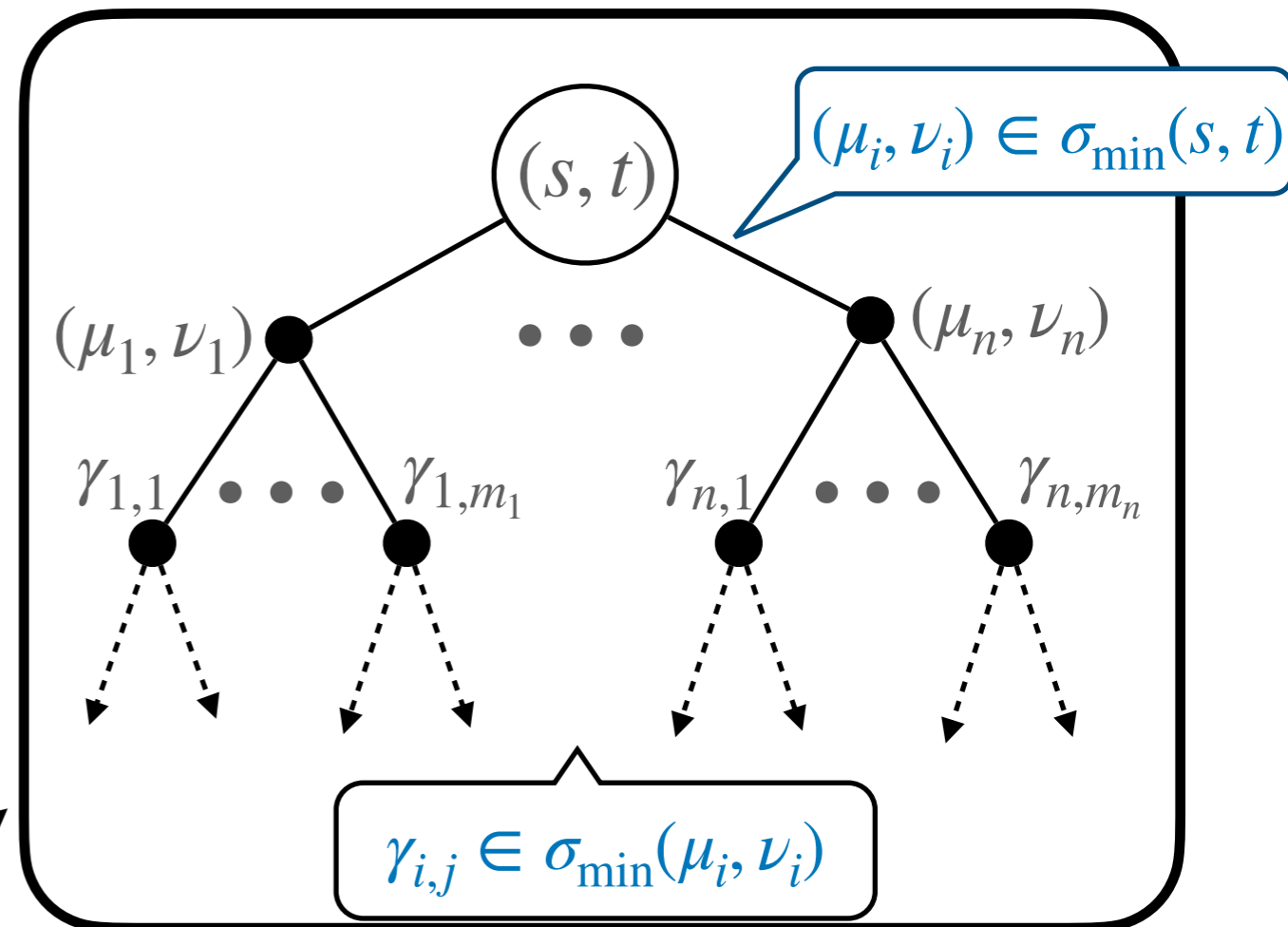
Coupled Probabilistic Automata

[Bacci², Larsen, Mardare, Tang, van Breugel'19]

A strategy for the min-player

- $\sigma_{\min}(s, t) \in \Gamma_S(\delta(s), \delta(t))$
- $\sigma_{\min}(\mu, \nu) \in \Gamma_D(\mu, \nu)$

...induces a coupled probabilistic automaton \mathcal{A}^2



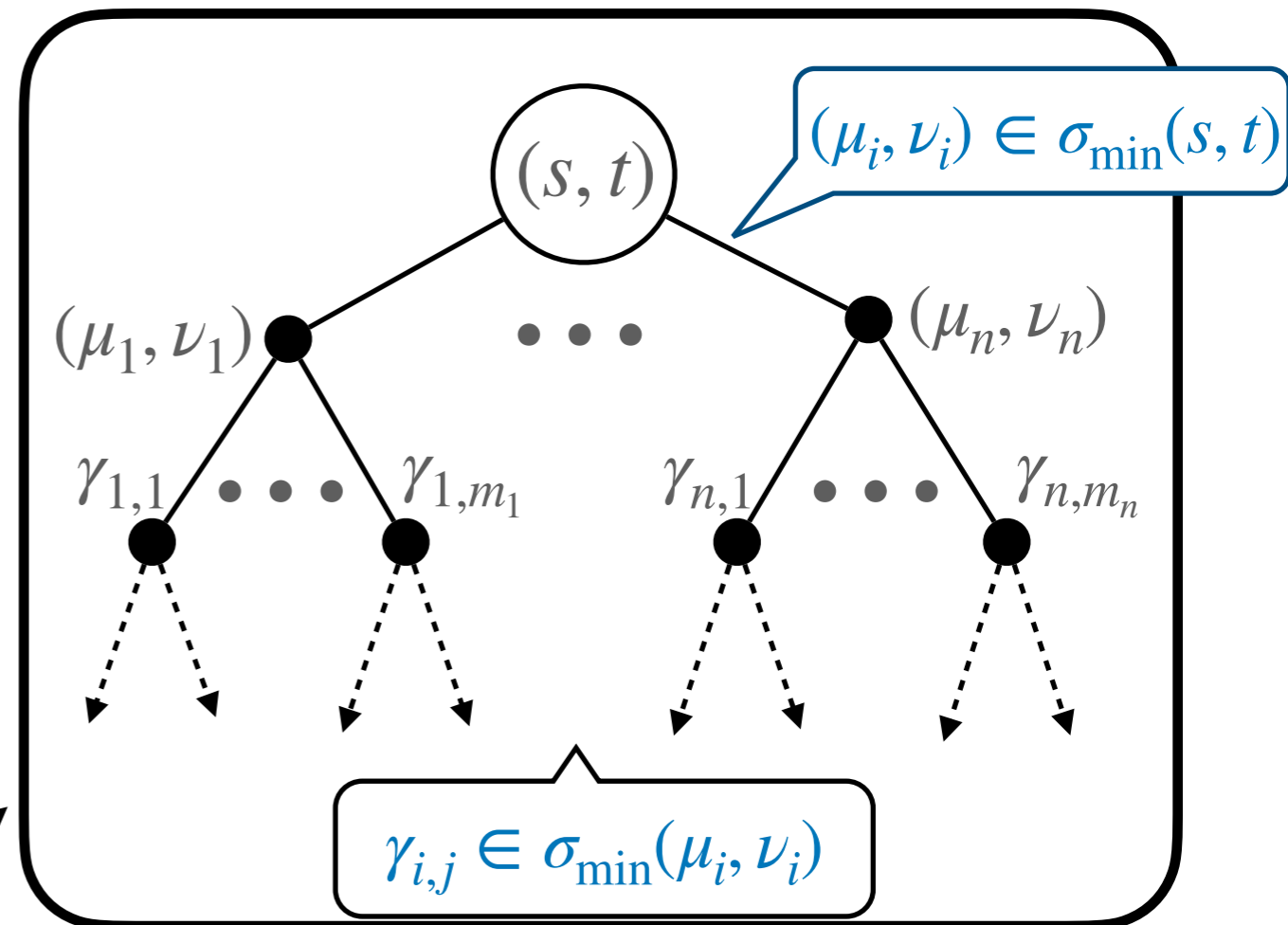
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Theorem [Bacci², Larsen, Mardare, Tang, van Breugel'21]

- $\mathbf{d}_b(s, t) \leq \sup_{\pi \in \Pi} P^\pi[\mathcal{A}^2, (s, t) \models \diamond neq]$ for all coupled automata \mathcal{A}^2
- $\mathbf{d}_b(s, t) = \sup_{\pi \in \Pi} P^\pi[\mathcal{A}^2, (s, t) \models \diamond neq]$ for some coupled automaton \mathcal{A}^2

Relation with Model Checking

[Bacci², Larsen, Mardare, Tang, van Breugel'21]

Some useful upper-bounds w.r.t. linear-time model checking

Theorem: For any LTL formula φ ,

$$|Max_s(\varphi) - Max_t(\varphi)| \leq \mathbf{d}_b(s, t) \quad \text{and} \quad |Min_s(\varphi) - Min_t(\varphi)| \leq \mathbf{d}_b(s, t)$$

where $Max_s(\varphi) = \sup_{\pi \in \Pi} P^\pi[\mathcal{A}, s \models \varphi]$ and $Min_s(\varphi) = \inf_{\pi \in \Pi} P^\pi[\mathcal{A}, s \models \varphi]$

Theorem:

$$\mathcal{H}(\mathbb{T}\mathbb{V})\left(\{P_s^\pi \mid \pi \in \Pi\}, \{P_t^\pi \mid \pi \in \Pi\}\right) \leq \mathbf{d}_b(s, t)$$

where $\mathbb{T}\mathbb{V}(\mu, \nu) = \sup_{\varphi \in LTL} |\mu(\varphi) - \nu(\varphi)|$

$$\forall \pi \in \Pi. \exists \pi' \in \Pi. |P^\pi[\mathcal{A}, s \models \varphi] - P^{\pi'}[\mathcal{A}, t \models \varphi]| \leq \mathbf{d}_b(s, t)$$

Bonus Material

...if someone is still awake

Bisimulations for ODEs

[Cardelli, Tribastone, Tschaikowski, Vandin'16]

$$\begin{aligned}\dot{x}_1 &= f_{x_1}(x_1, \dots, x_n) \\ \dot{x}_2 &= f_{x_2}(x_1, \dots, x_n) \\ &\vdots \\ \dot{x}_n &= f_{x_n}(x_1, \dots, x_n)\end{aligned}$$

ODE system induced
by a polynomial vector
field $f: \mathbb{R}^X \rightarrow \mathbb{R}^X$

Backward Differential Equivalence (BDE)

Definition 1 (Backward differential equivalence). *Let f be a vector field over X . An equivalence relation $R \subseteq X \times X$ is a BDE for f if the implication*

$$\left(\bigwedge_{(x,y) \in R} v_x = v_y \right) \Rightarrow \left(\bigwedge_{(x,y) \in R} f_x(v) = f_y(v) \right)$$

is true for all $v \in \mathbb{R}^X$.

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Relates variables with
identical ODE solutions
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⋮

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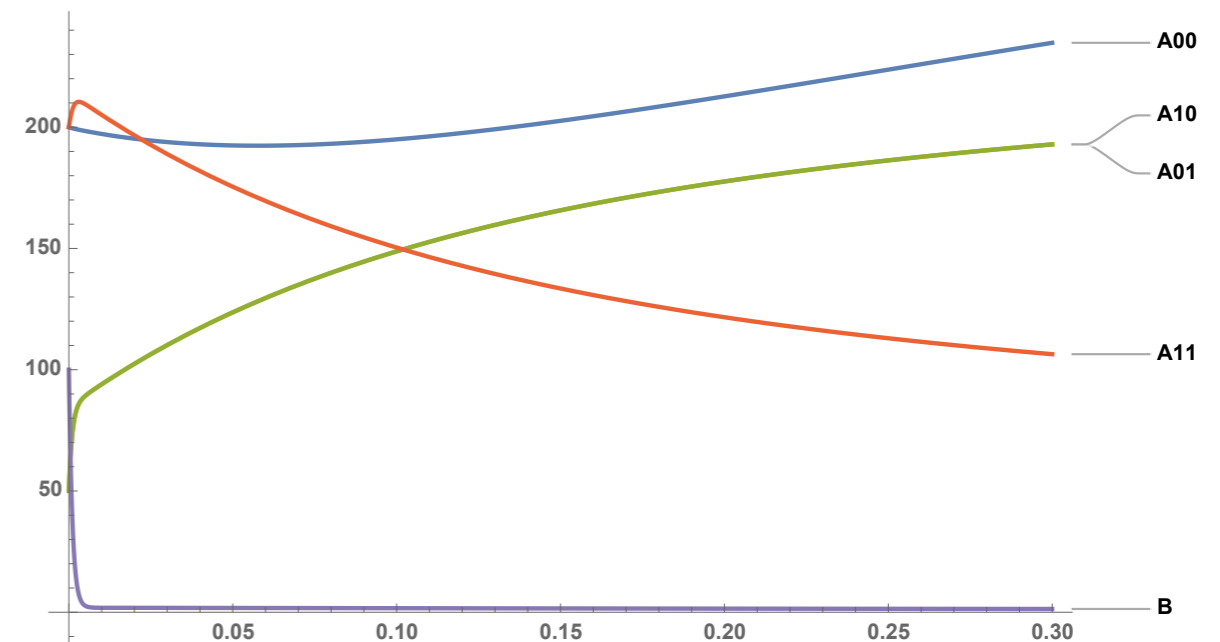
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$$\dot{A}_{00} = -4A_{00}B + 3A_{10} + 3A_{01}$$

$$\dot{A}_{01} = 2A_{00}B - 3A_{01} - A_{01}B + 3A_{11}$$

$$\dot{A}_{10} = 2A_{00}B - 3A_{10} - A_{10}B + 3A_{11}$$

$$\dot{A}_{11} = A_{10}B + A_{01}B - 6A_{11}$$

$$\dot{B} = -4A_{00}B + 3A_{10} + 3A_{01} - A_{10}B - A_{01}B + 6A_{11}$$

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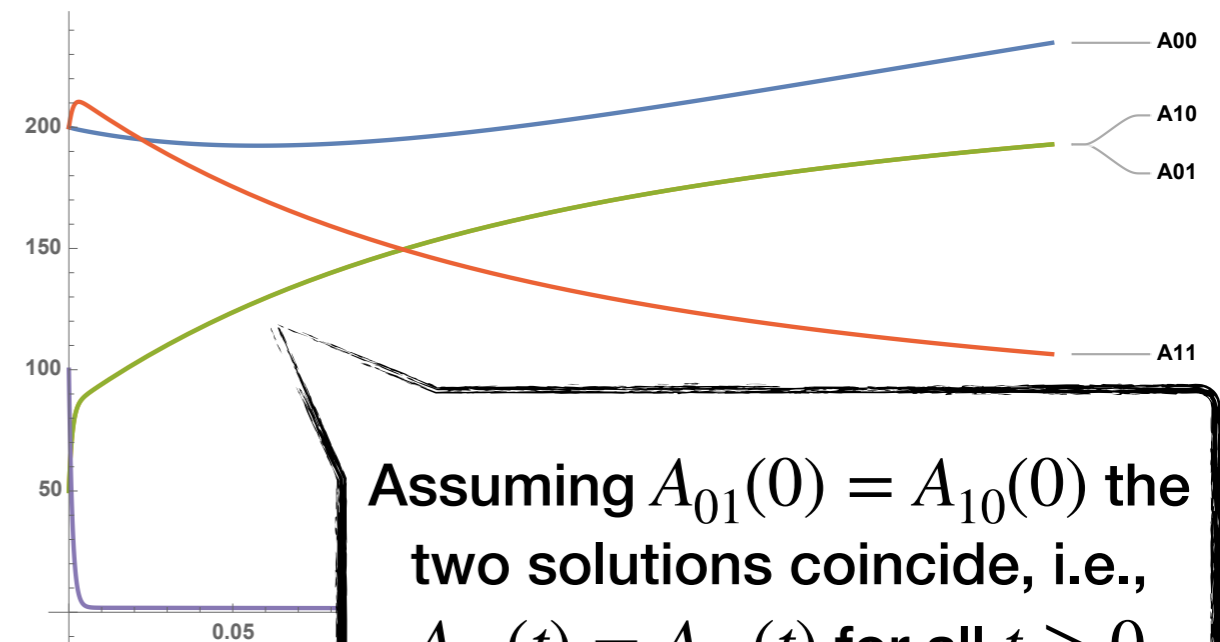
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is true for all $v \in \mathbb{R}^X$.



Assuming $A_{01}(0) = A_{10}(0)$ the
two solutions coincide, i.e.,
 $A_{01}(t) = A_{10}(t)$ for all $t \geq 0$

$$\dot{A}_{00} = -4A_{00}B + 3A_{10} + 3A_{01}$$

$$\dot{A}_{01} = 2A_{00}B - 3A_{01} - A_{01}B + 3A_{11}$$

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Proving Backward Equivalence

[Bacci², Larsen, Tribastone, Tschaikowski, Vandin'21]

We want to find some $R \subseteq X \times X$ satisfying

$$\forall v \in \mathbb{R}^X. \bigwedge_{(x,y) \in R} v_x = v_y \implies p(v) = q(v)$$

....and **explain why the implication holds**

Our solution

- We introduce a variant of **Strassen's theorem** for proving dominance between polynomial functions
- A witness of the implication is given via two type of couplings:
 - (1) **Monomials couplings**: lift equivalence among variables to equivalence among monomials
 - (2) **Linear couplings**: lift equivalence among variables to equivalence among linear functions

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Lift equivalence over variables to
equivalences over polynomials

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Monomial & Linear couplings

Monomial Coupling

$\rho \in \Gamma_{\mathbf{M}}(m, n)$ iff $\rho: X \times X \rightarrow \mathbb{N}$ such that

- $\sum_{y \in X} \rho(x, y) = m(x)$ for all $x \in X$
- $\sum_{x \in X} \rho(x, y) = n(y)$ for all $y \in X$
- $\rho(x, y) \geq 0$ for all $x, y \in X$

$$m = v^4 w^4$$

$$n = x^2 y^3 z^3$$

	v^4	w^4
x^2		2
y^3	3	
z^3	1	2

Linear Coupling

$\omega \in \Gamma_{\mathbf{L}}(g, h)$ iff $\omega: X \times X \rightarrow \mathbb{R}$ such that

- $\sum_{y \in X} \omega(x, y) = (g^+ + h^-)(x)$ for all $x \in X$
- $\sum_{x \in X} \omega(x, y) = (h^+ + g^-)(y)$ for all $y \in X$
- $\omega(x, y) \geq 0$ for all $x, y \in X$

$$g = 4v + 4w - 2x$$

$$h = 3y + 3z$$

	$4v$	$4w$
$2x$		2
$3y$	3	
$3z$	1	2

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$$m = v^4 w^4$$

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$$M[R] = \{(m, n) \mid \rho \in \Gamma_M(m, n), \text{supp}(\rho) \subseteq R\}$$

Linear Coupling

$$g = 4v + 4w - 2x$$

$$h = 3y \quad 3z$$

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$3y$	3	
$3z$	1	2

$$L[R] = \{(g, h) \mid \omega \in \Gamma_L(g, h), \text{supp}(\omega) \subseteq R\}$$

Future work

Future work

Lifting Relations

Lifting Metrics

Monomial & Linear couplings

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Future work

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Lifting Relations

Lifting Metrics

Lifting Equality to Monomials

Consider the monomials m and n

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$$n = v^4 w^4$$

	v^4	w^4	
x^2			
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Lifting Equality to Monomials

Consider the monomials m and n

$$m = x^2 y^3 z^3$$

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...assume that $x = w$,
 $y = v$, and $z = v = w$

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...assume that $x = w$,
 $y = v$, and $z = v = w$

	v^4	w^4
x^2	0	2
y^3	3	0
z^3	1	2

$$m = x^2 y^3 z^3$$

$$= (x^0 x^2)(y^3 y^0)(z^1 z^2)$$

$$= (v^0 v^3 v^1)(w^2 w^0 w^2)$$

$$n = v^4 w^4$$

Coupling Method for Polynomials

Linear Couplings

Theorem: Let $R \subseteq X \times X$ be an equivalence relation. The following are equivalent

- (1) $(g, h) \in \mathbf{L}[R]$
- (2) For all $v \in \mathbb{R}^X$, $\bigwedge_{(x,y) \in R} v_x \leq v_y \Rightarrow g(v) \leq h(v)$
- (3) For all $v \in \mathbb{R}^X$, $\bigwedge_{(x,y) \in R} v_x = v_y \Rightarrow g(v) = h(v)$

Moreover (1) \Rightarrow (2) \wedge (3) **hold for any relation** R

Monomial Couplings

Theorem: Let $R \subseteq X \times X$ be an equivalence relation. The following are equivalent

- (1) $(m, n) \in \mathbf{M}[R]$
- (2) For all $v \in \mathbb{R}_{>0}^X$, $\bigwedge_{(x,y) \in R} v_x \leq v_y \Rightarrow m(v) \leq n(v)$
- (3) For all $v \in \mathbb{R}^X$, $\bigwedge_{(x,y) \in R} v_x = v_y \Rightarrow m(v) = n(v)$

Moreover (1) \Rightarrow (2) \wedge (3) **holds for any relation** R

$$P[R] := L[M[R]]$$

Corollary: $(p, q) \in P[R]$ implies $\left(\bigwedge_{(x,y) \in R} v_x = v_y \Rightarrow p(v) = q(v) \right)$ for all $v \in \mathbb{R}^X$.

Backward Differential Bisimulation

We define **BDB** as a **post-fixed point** of the following operator.

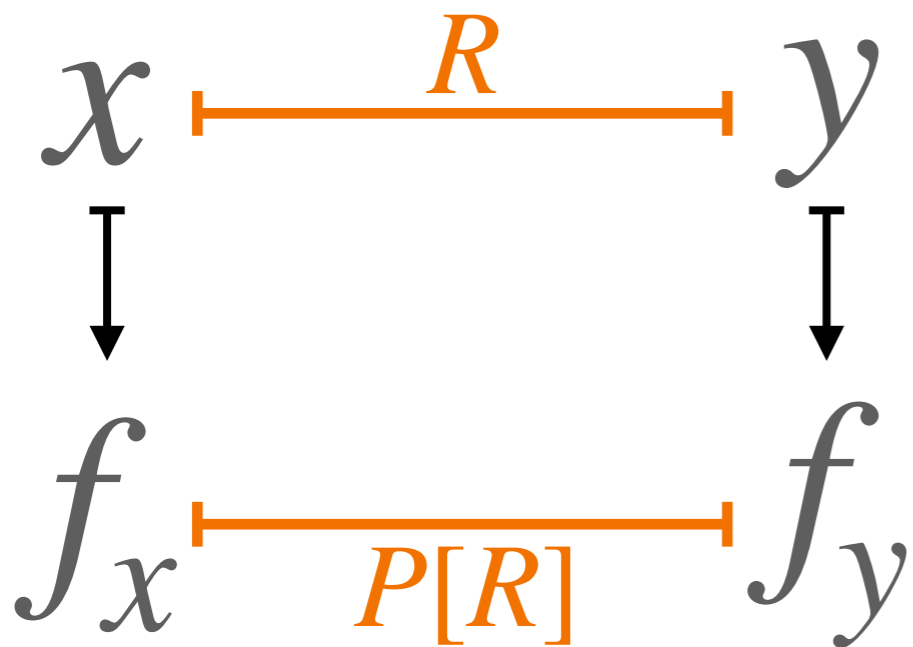
$$\mathcal{B}(R) = \{ (x, y) \mid (f_x, f_y) \in P[R] \}$$

From here we provided an on-the-fly procedure to test BDE which exploits up-to techniques (see Bacci et al. LICS'21])

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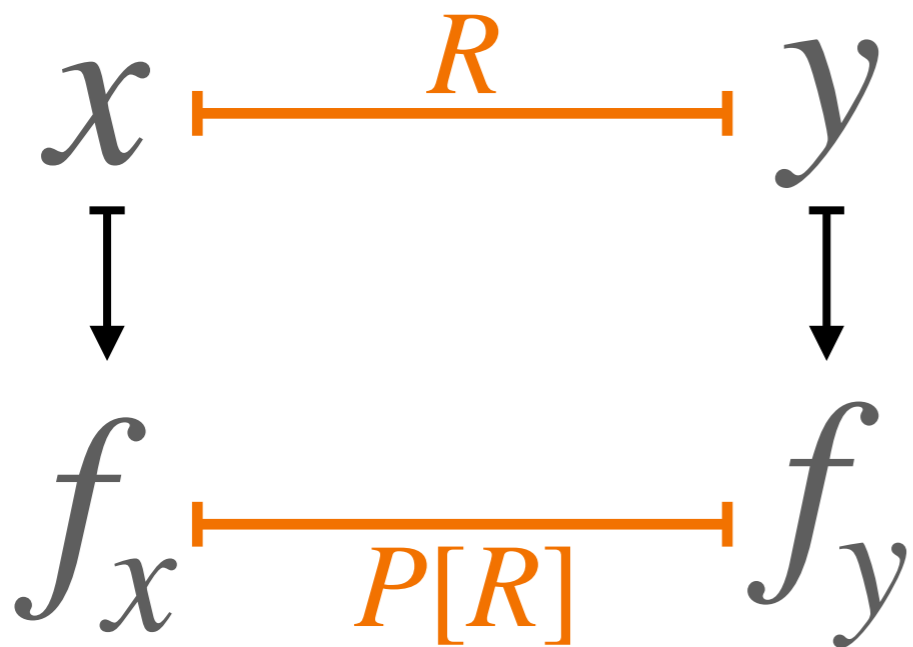


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Theorem:

For any $R \subseteq X \times X$

- (1) If R is a BDB, then R^* is a BDE
- (2) If R is a BDE, then R is a BDB
- (3) $\text{gfp}(\mathcal{B})$ is the greatest BDE

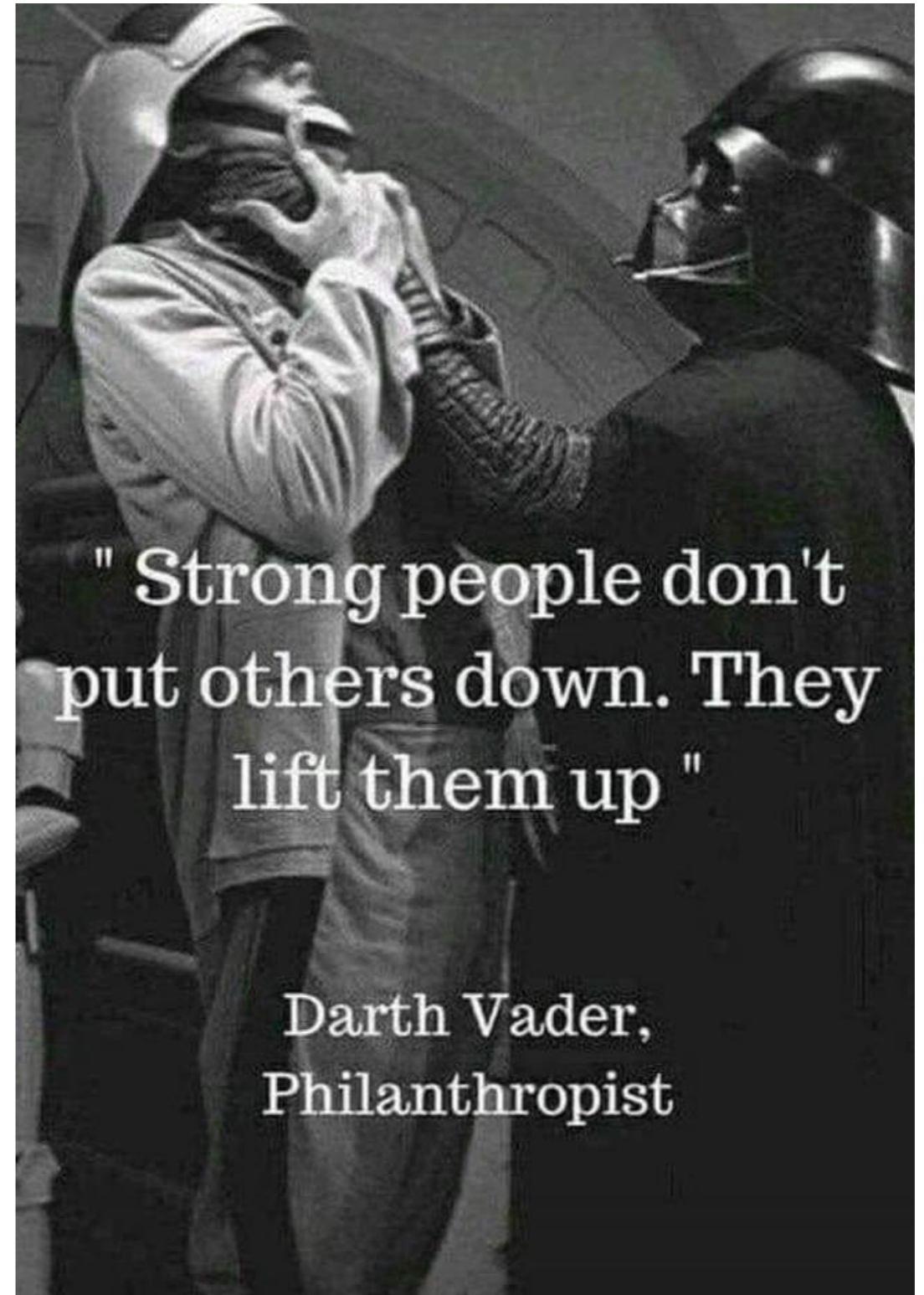
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Almost done

...stay awake a few more seconds

Conclusion

- Comparing the behaviours reduces to **lifting relations/distances from states to other structures**
- Coupling is a powerful technique to
 - Define new behavioural equivalences & metrics
 - Define algorithms to compute them
 - Prove useful properties
 - Approximate minimisation
 - LTL dissimilarity upper-bounds



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