

# Martingale-Based Methods for Reachability Probabilities

Excitements and Afterthoughts ~~about~~  
in  
Coalgebras



**Ichiro Hasuo**  
National Institute of Informatics  
Tokyo, Japan

# Overview

- \* Reachability in probabilistic programs
- \* Foundation of fixed points, in the non-probabilistic setting
  - \* Ranking functions, invariants
  - \* Foundation: Knaster-Tarski, Cousot-Cousot
- \* Known supermartingale methods
  - \* Roles of concentration lemmas
- \* Something new (from **fixed points** and **coalgebras**)
- \* Coalgebras: excitements, afterthoughts, our project

# Based on Joint Works:

- \* Natsuki Urabe, Masaki Hara and Ichiro Hasuo.  
**Categorical Liveness Checking by Corecursive Algebras.**  
LICS 2017
- \* Toru Takisaka, Yuichiro Oyabu, Natsuki Urabe and Ichiro Hasuo.  
**Ranking and Repulsing Supermartingales for Approximating Reachability in Probabilistic Programs.**  
ATVA 2018

# Probabilistic Programs

- \* Programs with
  - \* random assignment

```
x := Gaussian(0, 0.2)
```

- \* probabilistic branching

```
if prob(0.2)
```

- \* (also nondet. assignment & branching)

- \* Example: right (random walk)

- \* We disregard the Bayesian aspects
  - \* observations, conditioning, priors/posteriors, etc.
  - \* See e.g. [Gordon+, FOSE'14]

```
1  x := m
2  while x > 0 do
3    if prob(p) do
4      x := x - 1
5    else
6      x := x + 1
7    fi
8  od
```

(say,  $m = 16$  and  $p = 0.2$ )

# Reachability Probabilities in PP

- \* **Question** What is  $\Pr(\text{the program terminates})$ ?

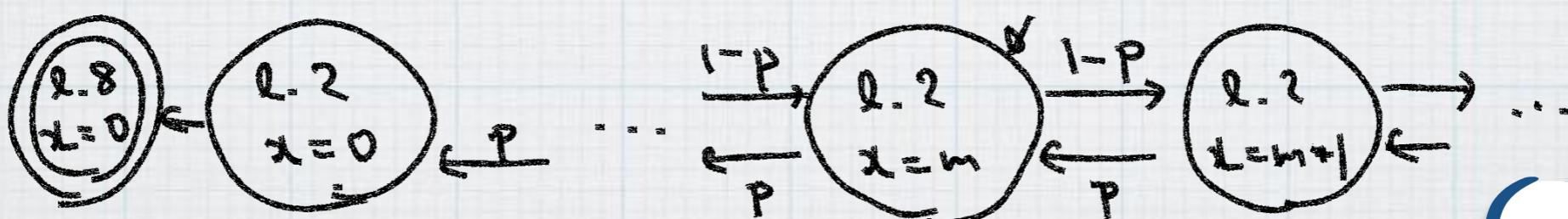
- \* How do we define it?

- \* Configuration graph

- \* A state is a pair (program location, value)

- \* Transition by small-step operations

- \* → MDP (Markov decision processes)  $M$



- \*  $\Pr(\text{Term}) = \sup_{\sigma: \text{ scheduler}} (M^\sigma \text{ reaches } \odot)$

real-valued variables  
→ infinite states  
→ not for automated analysis

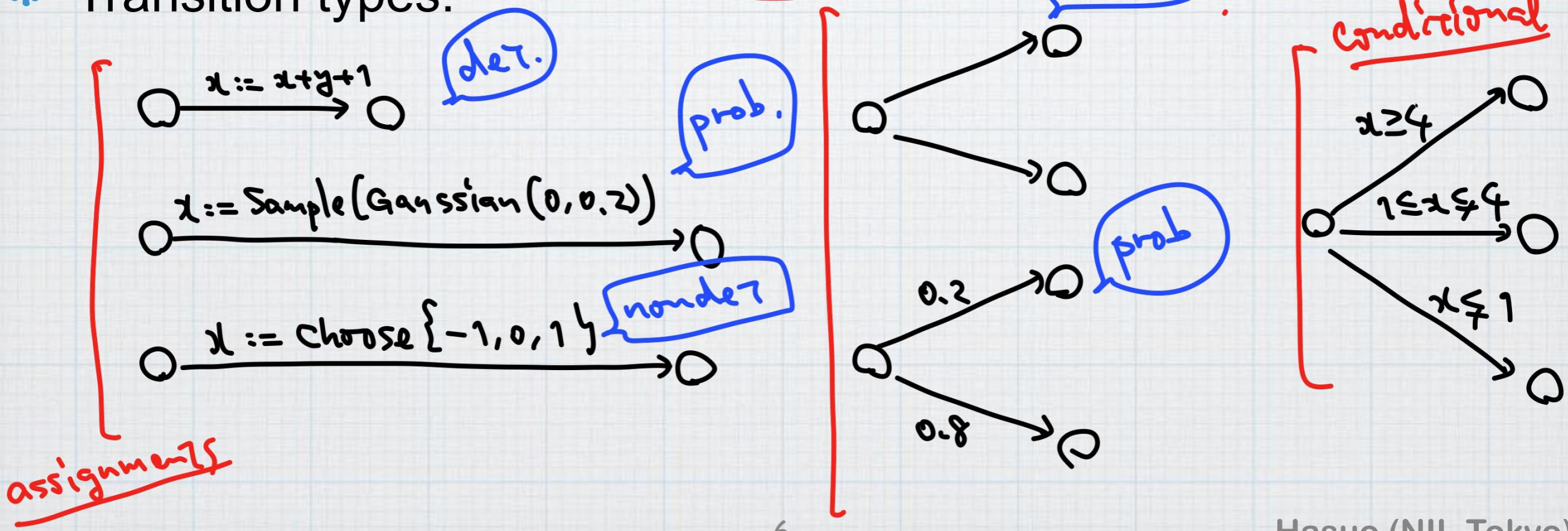
If nondet. is angelic...

# Probabilistic Control Flow Graph (pCFG) See e.g. [Chatterjee+, POPL'17]

- \* Finite graph,  
“parametric” in memory states
  - \* (... justifies my presence here!)

- \* State = (program location)

- \* Transition types:

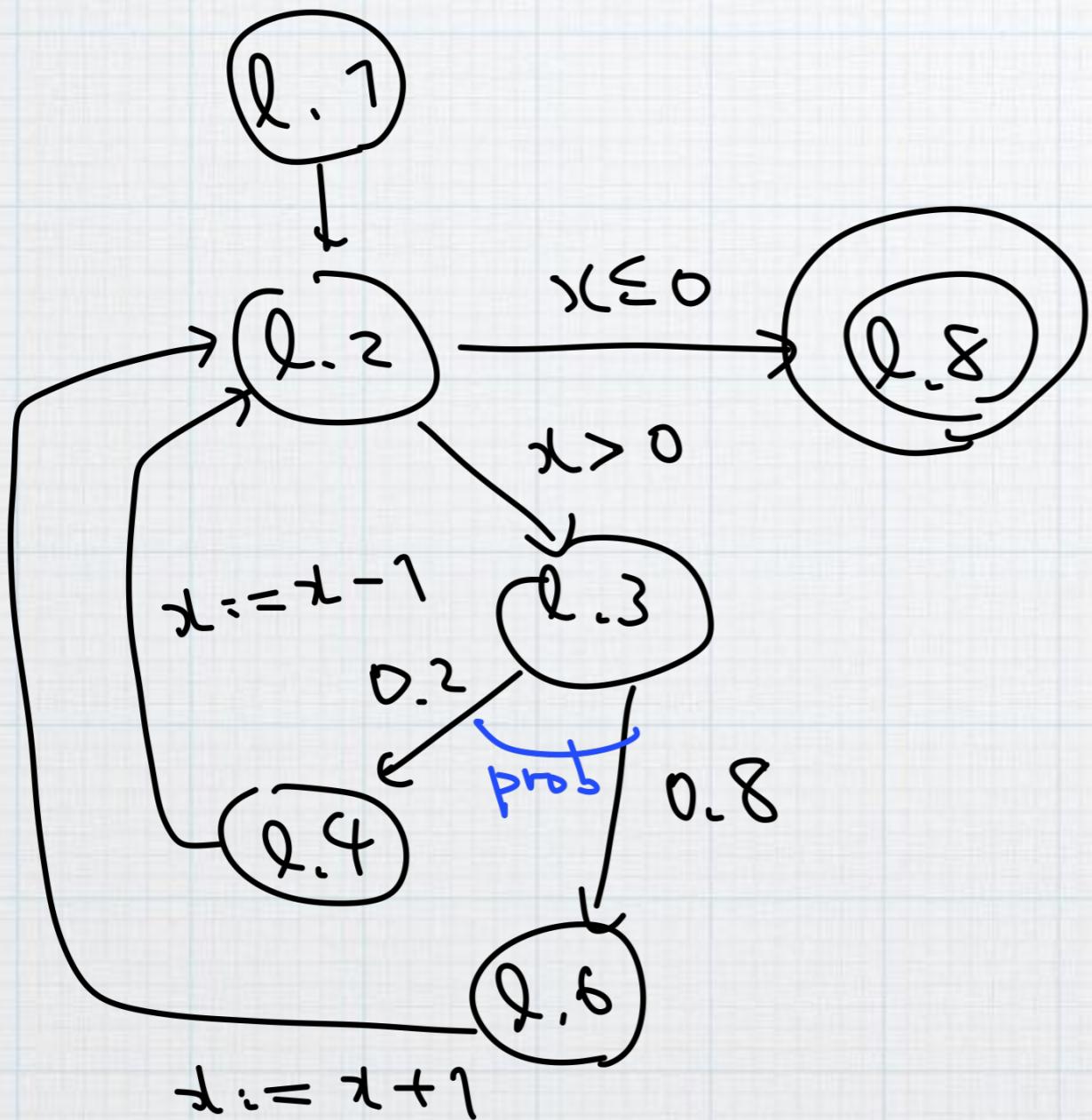


```

1  x := m
2  while x > 0 do
3    if prob(p) do
4      x := x - 1
5    else
6      x := x + 1
7    fi
8  od
(say, m = 16 and p = 0.2)

```

# Probabilistic Control Flow Graph (pCFG) See e.g. [Chatterjee+, POPL'17]



```
1   $x := m$ 
2  while  $x > 0$  do
3    if  $\text{prob}(p)$  do
4       $x := x - 1$ 
5    else
6       $x := x + 1$ 
7    fi
8  od
```

(say,  $m = 16$  and  $p = 0.2$ )

# The Problem

- \* **Given**

- \* a pCFG.  $n$  variables, state set  $L$
- \*  $C \subseteq L \times \mathbb{R}^n$   
(Lebesgue measurable) target region
- \*  $l_0 \in L, \vec{x}_0 \in \mathbb{R}^n$   
initial configuration

- \* **Answer**

$\Pr(\text{Reach}_C)$

# Approach

- \* Use **parametric certificates**, i.e. functions

$$(f_l : \mathbb{R}^n \rightarrow \mathbb{R})_{l \in L}$$

to give *approximate* answers. Template-based synthesis

- \* Qualitative questions

- \*  $\Pr(\text{Reach}_C) = ? 1$  (almost sure reachability)
- \*  $\Pr(\text{Reach}_C) \geq ? \alpha$  (threshold reachability)

- \* Quantitative questions

- \*  $\Pr(\text{Reach}_C) \geq ??$  (lowerbound, “verification”)
- \*  $\Pr(\text{Reach}_C) \leq ??$  (upperbound, “refutation”)
- \*  $\text{Exp}(\text{StepsToReach}_C)$ , upperbound, lowerbound, ...
- \* “Concentration” [Chatterjee+, POPL’16]

Find  $B$  s.t.  $(x > B \rightarrow \exists a, b. \Pr(\text{StepsToReach}_C > x) < ae^{-bx})$

# Why Overapproximation?

- \*  $\Pr(\text{Reach}_c) \leq \alpha$   
if and only if  
 $\Pr(\text{NotReach}_c) \geq 1 - \alpha$
- \* Refutation of reachability  
is  
verification of safety

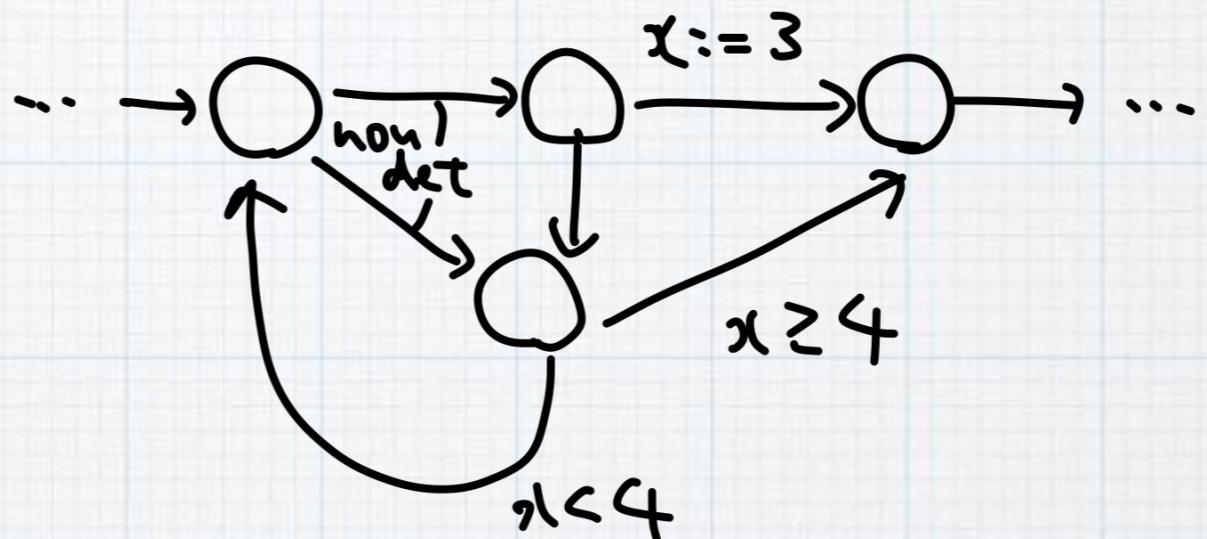
# Overview

- \* Reachability in probabilistic programs
- \* Foundation of fixed points, in the non-probabilistic setting
  - \* Ranking functions, invariants
  - \* Foundation: Knaster-Tarski, Cousot-Cousot
- \* Known supermartingale methods
  - \* Roles of concentration lemmas
- \* Something new (from **fixed points** and **coalgebras**)
- \* Coalgebras: excitements, afterthoughts, our project



# In Case of No Probabilities...

- \* ~~PCFG~~
  - \* Reachability question:  
is there a scheduler  
that leads to  $C$ ?



- \* Verify reachability by **ranking functions**, refute reachability (= verify safety) by **invariants**
  - \* From now on, our theory is not parametrized for simplicity
    - \* **Kripke frames** instead of CFGs
    - \* MDPs (or even MCs) instead of pCFGs

# Ranking Functions

$(S, \rightarrow \subseteq S \times S)$ : Kripke frame,  $C \subseteq S$ .

A *ranking function* is

$$\eta: S \rightarrow \mathbb{N} \cup \{\infty\}$$

such that

- $\forall s \in S \setminus C. \exists s' \in S.$   
 $( s \rightarrow s' \text{ and } \eta(s) \geq \eta(s') + 1 )$
- $\eta(s) = 0$  implies  $s \in C$

Thm.

$\eta(s) \neq \infty$  implies  $C$  is  
reachable from  $s$ .

- \*  $\eta$  overapproximates #(steps to  $C$ )
- \* Note:  $\mathbf{N} = \{\text{natural numbers}\}$  is well-founded
- \* Discrete analogue of (certain) **Lyapunov functions...**

# Invariants

$(S, \rightarrow \subseteq S \times S)$ : Kripke frame,  $C \subseteq S$ .

An *invariant* for  $S \setminus C$  is

$$I \subseteq S$$

such that

- $I \subseteq \square I$ , where  
 $\square I = \{s \mid \forall s' \leftarrow s. s' \in I\}$
- $I \subseteq S \setminus C$

Thm.

$s \in I$  implies  $C$  is  
not reachable from  $s$ .

\* Get trapped in  $I$

\* Discrete analogue of barrier certificates...

# Ranking Functions & Invariants

$(S, \rightarrow \subseteq S \times S)$ : Kripke frame,  $C \subseteq S$ .  
A *ranking function* is

$$\eta: S \rightarrow \mathbb{N} \cup \{\infty\}$$

such that

- $\forall s \in S \setminus C. \exists s' \in S.$   
 $( s \rightarrow s' \text{ and } \eta(s) \geq \eta(s') + 1 )$
- $\eta(s) = 0$  implies  $s \in C$

Thm.

$\eta(s) \neq \infty$  implies  $C$  is  
reachable from  $s$ .

$(S, \rightarrow \subseteq S \times S)$ : Kripke frame,  $C \subseteq S$ .  
An *invariant* for  $S \setminus C$  is

$$I \subseteq S$$

such that

- $I \subseteq \square I$ , where  
 $\square I = \{s \mid \forall s' \leftarrow s. s' \in I\}$
- $I \subseteq S \setminus C$

Thm.

$s \in I$  implies  $C$  is  
*not* reachable from  $s$ .

\* How come the difference?

$$\text{Reach}_C =_{\mu} C \cup \diamond \text{Reach}_C$$

\* NB:

$$\text{NotReach}_C =_{\nu} (S \setminus C) \cap \square \text{NotReach}_C$$

# Lattice-Theoretic Foundation

$L$ : complete lattice,  $f: L \rightarrow L$  monotone

Thm. (Knaster-Tarski)

- $\mu f = \min\{l \in L \mid f(l) \sqsubseteq l\}$

$$\Rightarrow \frac{f(l) \sqsubseteq l}{\mu f \sqsubseteq l}$$

- $\nu f = \max\{l \in L \mid l \sqsubseteq f(l)\}$

$$\Rightarrow \frac{l \sqsubseteq f(l)}{l \sqsubseteq \nu f}$$

Thm. (Cousot-Cousot)

$\perp \sqsubseteq f(\perp) \sqsubseteq \dots \sqsubseteq f^\omega(\perp) \sqsubseteq \dots$   
stabilizes, and converges to  $\mu f$

$$\Rightarrow f^\alpha(\perp) \sqsubseteq \mu f \quad (\forall \alpha \in \text{Ord})$$

$\top \sqsupseteq f(\top) \sqsupseteq \dots \sqsupseteq f^\omega(\top) \sqsupseteq \dots$   
stabilizes, and converges to  $\nu f$

$$\Rightarrow \nu f \sqsubseteq f^\alpha(\top) \quad (\forall \alpha \in \text{Ord})$$

Sound approx. from below  
Hasuo (Tokyo)

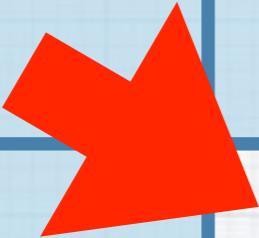
# Overview

- \* Categorically:  
initial algebra, final coalgebra,  
Lambek lemma, initial/final  
sequence, ...
- \* **Foundation of fixed points**, in the non-probabilistic setting
  - \* Ranking functions, invariants
  - \* Foundation: Knaster-Tarski, Cousot-Cousot
- \* **Known supermartingale methods**
  - \* Roles of concentration lemmas
- \* Something **new** (from our recent results)
- \* Coalgebras: excitements, afterthoughts, our project

isti

	KT	CC
Ifp	overapprox.	underapprox.
gfp	underapprox.	overapprox.

**ranking**  
martingale-like  
methods  
**(lower bd)**



**Additive**  
ranking  
supermartingale  
[McIver+ PSSE'04]  
[Chakarov+ CAV'13]

Answers what  
question?

$$\Pr(\text{Reach}_C) = ? \quad 1$$

$$\text{Exp}(\text{Step}_C) \leq ??$$

Underlying math  
(elementary)

New

**$\gamma$ -scaling**  
ranking  
submartingale  
[Urabe+ LICS'17]  
[Takisaka+, ATVA'18]

$$\Pr(\text{Reach}_C) \geq ??$$

- Coalgebra!
- (?)

**repulsing**  
martingale-like  
methods  
**(upper bd)**

**$\epsilon$ -decreasing**  
repulsing  
supermartingale  
[Chatterjee+ POPL'17]

$$\Pr(\text{Reach}_C) \leq ??$$

Azuma's  
inequality  
for martingale  
concentration

New

**Nonnegative**  
repulsing  
supermartingale  
[Steinhardt+ IJRR'12]  
[Takisaka+, ATVA'18]

$$\Pr(\text{Reach}_C) \leq ??$$

Markov's  
inequality  
for martingale  
concentration

# Disclaimer

- \* From now on:  
no nondeterminism,  
no parametrization/variables
- \* Our setting is therefore:  
A Markov chain  $(S, S \xrightarrow{\text{tr}} \mathcal{D}S)$ , and  $C \subseteq S$
- \* Variables are fine.  
Nondeterminism is fine, too, but intricate  
(measure theory). See [Takisaka+, ATVA'18]

# Additive Ranking Supermartingale

[McIver+ PSSE'04] [Chakarov+ CAV'13]

## Def.

Let  $(S, S \xrightarrow{\text{tr}} \mathcal{D}S)$  be a MC,  
 $\eta: S \rightarrow \mathbb{R}$  be a function.

$\mathbb{X}\eta: S \rightarrow \mathbb{R}$  is defined by

$$\begin{aligned} (\mathbb{X}\eta)(s) &= \sum_{s'} \text{tr}(s)(s') \cdot \eta(s') \\ &= \sum_{s'} \Pr(s \rightarrow s') \cdot \eta(s') \\ &= \text{Exp}(\eta(s') \mid s \rightarrow s'). \end{aligned}$$

\* Overapprox.  
Exp(Steps to C)

## Def.

Let  $(S, S \xrightarrow{\text{tr}} \mathcal{D}S)$  be a MC,  $C \subseteq S$ .

$\eta: S \rightarrow \mathbb{R}_{\geq 0}$  is a *ranking supermartingale* for  $C$  if

- $\forall s \in S \setminus C. \quad \eta(s) \geq (\mathbb{X}\eta)(s) + 1.$
- $\eta(s) = 0$  implies  $s \in C$

# Additive Ranking Supermartingale

[McIver+ PSSE'04] [Chakarov+ CAV'13]

## Def.

Let  $(S, S \xrightarrow{\text{tr}} \mathcal{D}S)$  be a MC,  
 $\eta: S \rightarrow \mathbb{R}$  be a function.

$\mathbb{X}\eta: S \rightarrow \mathbb{R}$  is defined by

$$\begin{aligned} (\mathbb{X}\eta)(s) &= \sum_{s'} \text{tr}(s) \\ &= \sum_{s'} \Pr(s' \\ &= \text{Exp}(\eta(s)) \end{aligned}$$

## Def.

Let  $(S, S \xrightarrow{\text{tr}} \mathcal{D}S)$  be a MC,  $C \subseteq S$ .

$\eta: S \rightarrow \mathbb{R}_{\geq 0}$  is a *ranking supermartingale* for  $C$  if

- $\forall s \in S \setminus C. \quad \eta(s) \geq (\mathbb{X}\eta)(s) + 1.$
- $\eta(s) = 0$  implies  $s \in C$

## Thm.

Let  $\eta$  be a ranking supermartingale for  $C$ . Then:

- $\Pr(\text{Reach}_C) = 1$  (almost sure reachability)
- $\text{Exp}(\text{Steps from } s \text{ to } C) \leq \eta(s)$

**ranking**  
martingale-like  
methods  
**(lower bd)**



**repulsing**  
martingale-like  
methods  
**(upper bd)**

**Additive**  
ranking  
supermartingale  
[McIver+ PSSE'04]  
[Chakarov+ CAV'13]

**$\gamma$ -scaling**  
ranking  
submartingale  
[Urabe+ LICS'17]  
[Takisaka+, ATVA'18]

**$\epsilon$ -decreasing**  
repulsing  
supermartingale  
[Chatterjee+ POPL'17]

**Nonnegative**  
repulsing  
supermartingale  
[Steinhardt+ IJRR'12]  
[Takisaka+, ATVA'18]

Answers what  
question?

$$\Pr(\text{Reach}_C) = ? \quad 1$$
$$\text{Exp}(\text{Step}_C) \leq ??$$

$$\Pr(\text{Reach}_C) \geq ??$$

$$\Pr(\text{Reach}_C) \leq ??$$

$$\Pr(\text{Reach}_C) \leq ??$$

Underlying math  
(elementary)

**New**

- Coalgebra!
- (?)

Azuma's  
inequality  
for martingale  
concentration

**New**

Markov's  
inequality  
for martingale  
concentration

# $\varepsilon$ -Decreasing Repulsing Supermartingale

[Chatterjee+ POPL'17]

## Def.

Let  $(S, S \xrightarrow{\text{tr}} \mathcal{D}S)$  be a MC,  $C \subseteq S$ ,  $\varepsilon > 0$ ,  $\kappa > 0$ .

$\eta: S \rightarrow \mathbb{R}$  is an  $\varepsilon$ -decreasing repulsing supermartingale for  $C$  with  $\kappa$ -bdd difference if

- $\forall s \in S \setminus C. \quad \eta(s) \geq (\mathbb{X}\eta)(s) + \varepsilon.$
- $\forall c \in C. \quad \eta(c) \geq 0.$
- $\forall s \in S. \forall s' \in \text{supp}(\text{tr}(s)).$   
 $|\eta(s) - \eta(s')| \leq \kappa.$

## Thm.

Let  $\eta$  be such a repulsing supermartingale for  $C$ . Assume  $\eta(s) < 0$ . Then

$$\Pr(\text{Reach}_{s,C}) \leq \alpha \frac{\gamma^{\lceil |\eta s|/\kappa \rceil}}{1 - \gamma}$$

$$\text{where } \alpha = e^{\frac{\varepsilon \cdot \eta(s)}{(\kappa + \varepsilon)^2}}, \gamma = e^{-\frac{\varepsilon^2}{2(\kappa + \varepsilon)^2}}.$$

# $\varepsilon$ -Decreasing Repulsing Supermartingale

[Chatterjee+ POPL'17]

## Def.

Let  $(S, S \xrightarrow{\text{tr}} \mathcal{D}S)$  be a MC,  $C \subseteq S$ ,  $\varepsilon > 0$ ,  $\kappa > 0$ .

$\eta: S \rightarrow \mathbb{R}$  is an  $\varepsilon$ -decreasing repulsing supermartingale for  $C$  with  $\kappa$ -bdd difference if

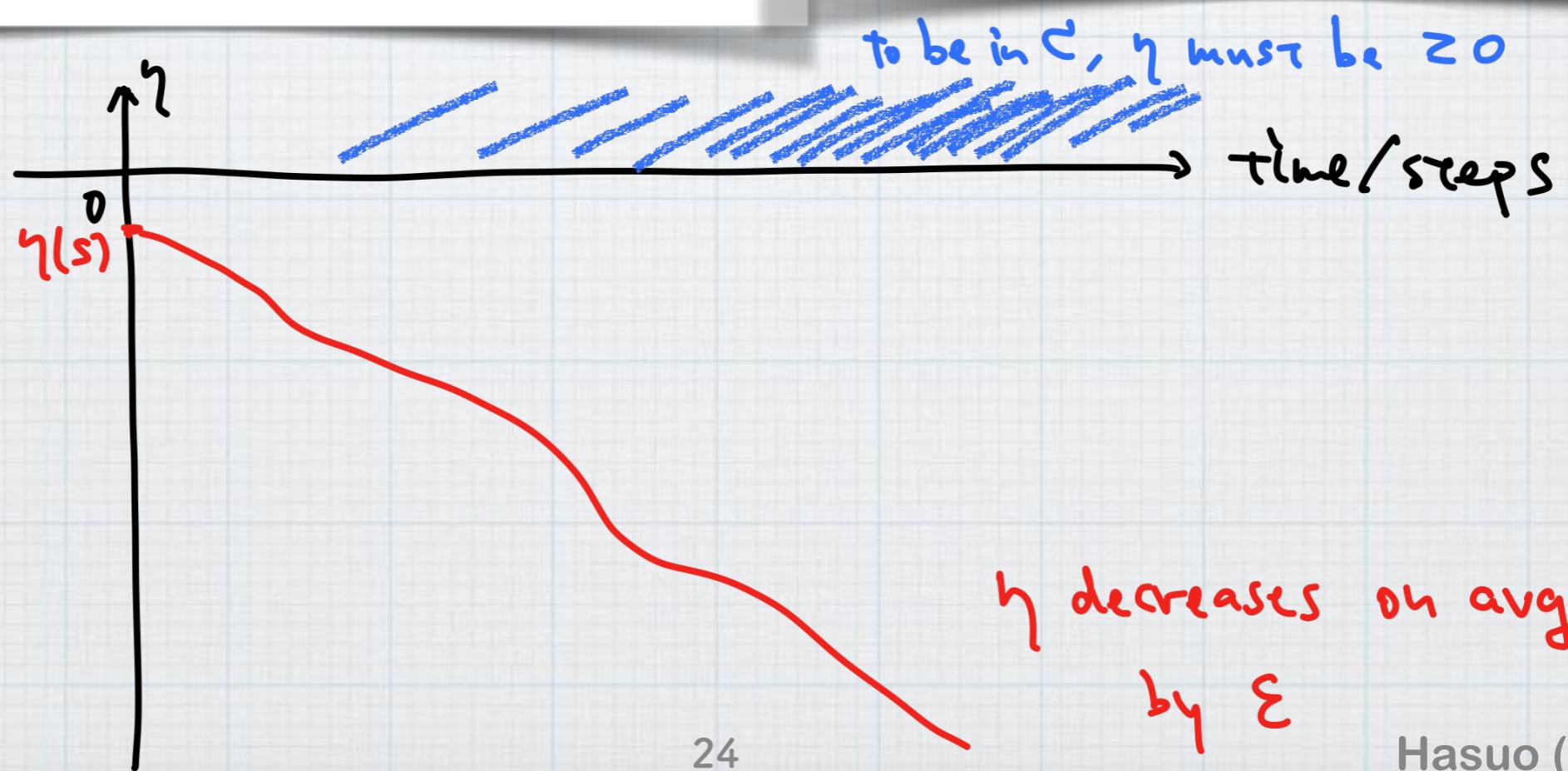
- $\forall s \in S \setminus C$ .  $\eta(s) \geq (\mathbb{X}\eta)(s) + \varepsilon$ .
- $\forall c \in C$ .  $\eta(c) \geq 0$ .
- $\forall s \in S$ .  $\forall s' \in \text{supp}(\text{tr}(s))$ .  
 $|\eta(s) - \eta(s')| \leq \kappa$ .

## Thm.

Let  $\eta$  be such a repulsing supermartingale for  $C$ . Assume  $\eta(s) < 0$ . Then

$$\Pr(\text{Reach}_{s,C}) \leq \alpha \frac{\gamma^{\lceil |\eta s|/\kappa \rceil}}{1 - \gamma}$$

where  $\alpha = e^{\frac{\varepsilon \cdot \eta(s)}{(\kappa + \varepsilon)^2}}$ ,  $\gamma = e^{-\frac{\varepsilon^2}{2(\kappa + \varepsilon)^2}}$ .



# $\varepsilon$ -Decreasing Repulsing Supermartingale

[Chatterjee+ POPL'17]

## Def.

Let  $(S, S \xrightarrow{\text{tr}} \mathcal{D}S)$  be a MC,  $C \subseteq S$ ,  $\varepsilon > 0$ ,  $\kappa > 0$ .

$\eta: S \rightarrow \mathbb{R}$  is an  $\varepsilon$ -decreasing repulsing supermartingale for  $C$  with  $\kappa$ -bdd difference if

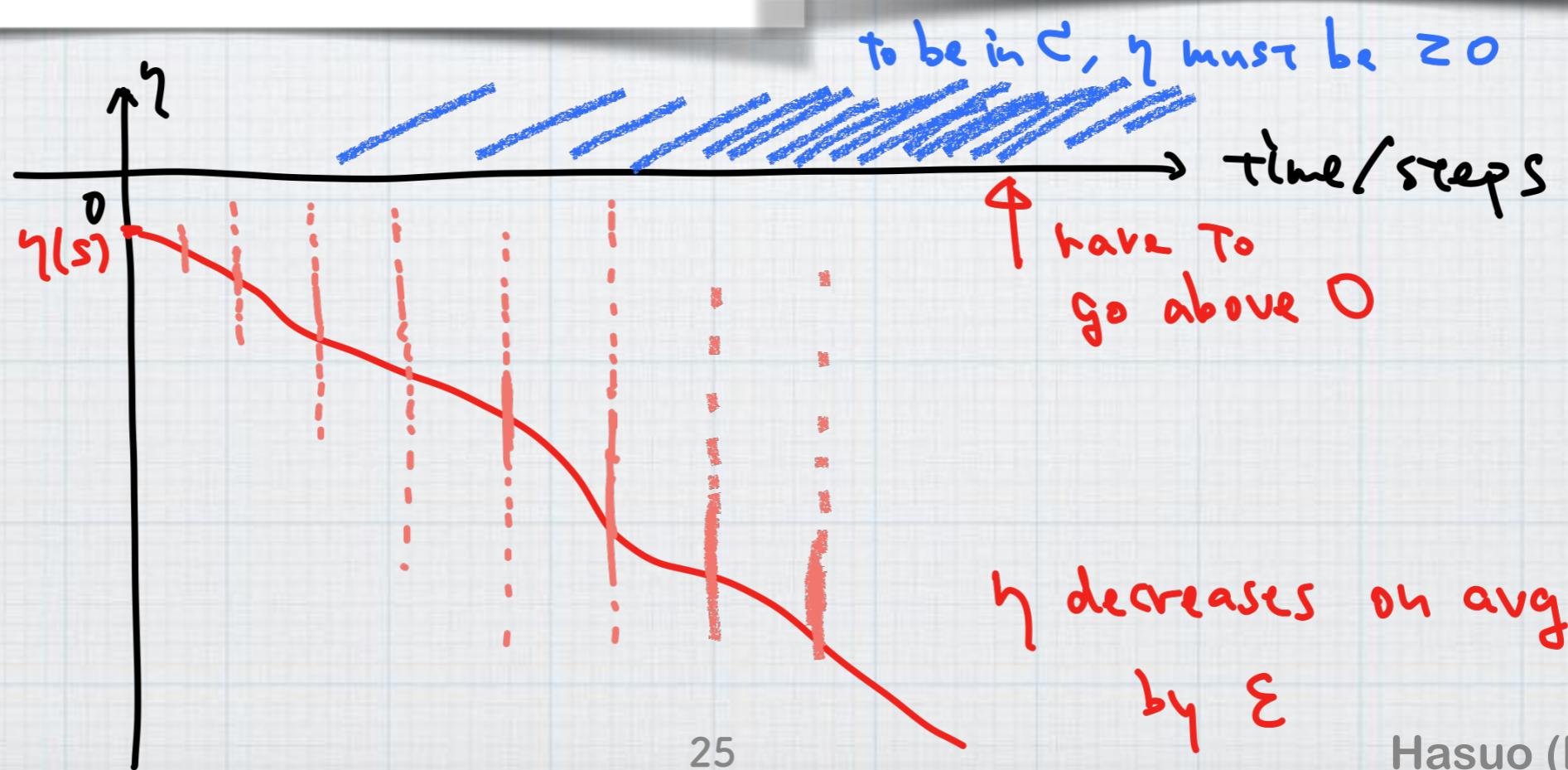
- $\forall s \in S \setminus C$ .  $\eta(s) \geq (\mathbb{X}\eta)(s) + \varepsilon$ .
- $\forall c \in C$ .  $\eta(c) \geq 0$ .
- $\forall s \in S$ .  $\forall s' \in \text{supp}(\text{tr}(s))$ .  
 $|\eta(s) - \eta(s')| \leq \kappa$ .

## Thm.

Let  $\eta$  be such a repulsing supermartingale for  $C$ . Assume  $\eta(s) < 0$ . Then

$$\Pr(\text{Reach}_{s,C}) \leq \alpha \frac{\gamma^{\lceil |\eta s|/\kappa \rceil}}{1 - \gamma}$$

where  $\alpha = e^{\frac{\varepsilon \cdot \eta(s)}{(\kappa + \varepsilon)^2}}$ ,  $\gamma = e^{-\frac{\varepsilon^2}{2(\kappa + \varepsilon)^2}}$ .



# $\varepsilon$ -Decreasing Repulsing Supermartingale

[Chatterjee+ POPL'17]

## Def.

Let  $(S, S \xrightarrow{\text{tr}} \mathcal{D}S)$  be a MC,  $C \subseteq S$ ,  $\varepsilon > 0$ ,  $\kappa > 0$ .

$\eta: S \rightarrow \mathbb{R}$  is an  $\varepsilon$ -decreasing repulsing supermartingale for  $C$  with  $\kappa$ -b'dd difference if

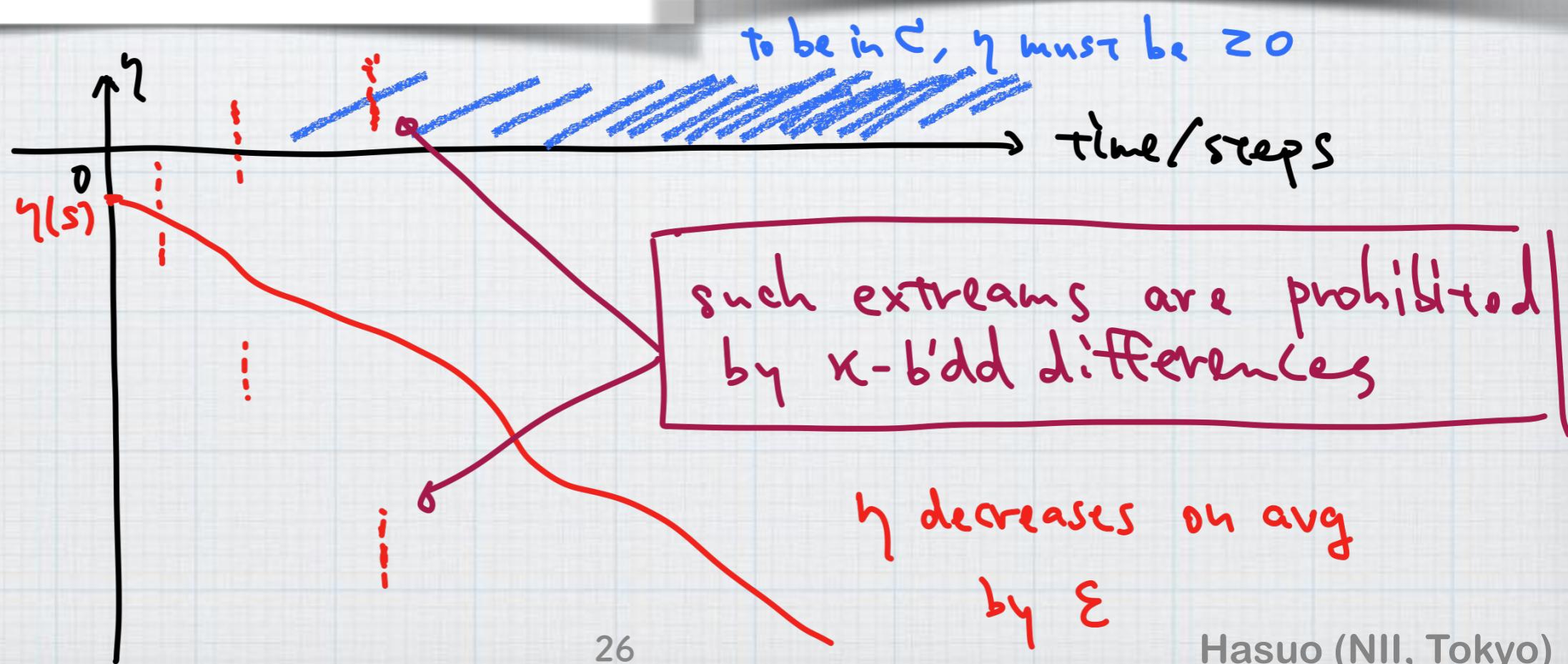
- $\forall s \in S \setminus C$ .  $\eta(s) \geq (\mathbb{X}\eta)(s) + \varepsilon$ .
- $\forall c \in C$ .  $\eta(c) \geq 0$ .
- $\forall s \in S$ .  $\forall s' \in \text{supp}(\text{tr}(s))$ .  
 $|\eta(s) - \eta(s')| \leq \kappa$ .

## Thm.

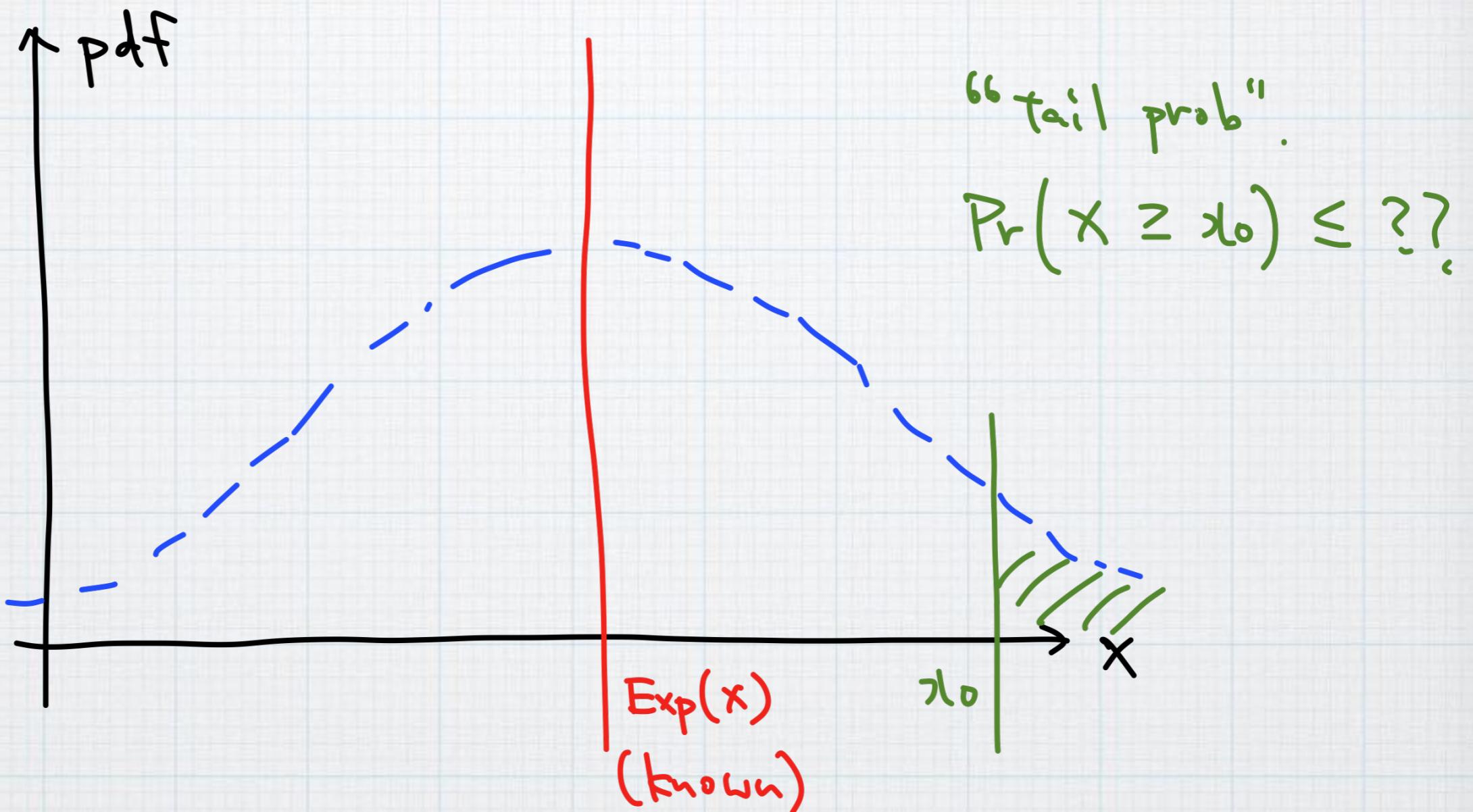
Let  $\eta$  be such a repulsing supermartingale for  $C$ . Assume  $\eta(s) < 0$ . Then

$$\Pr(\text{Reach}_{s,C}) \leq \alpha \frac{\gamma^{\lceil |\eta_s|/\kappa \rceil}}{1 - \gamma}$$

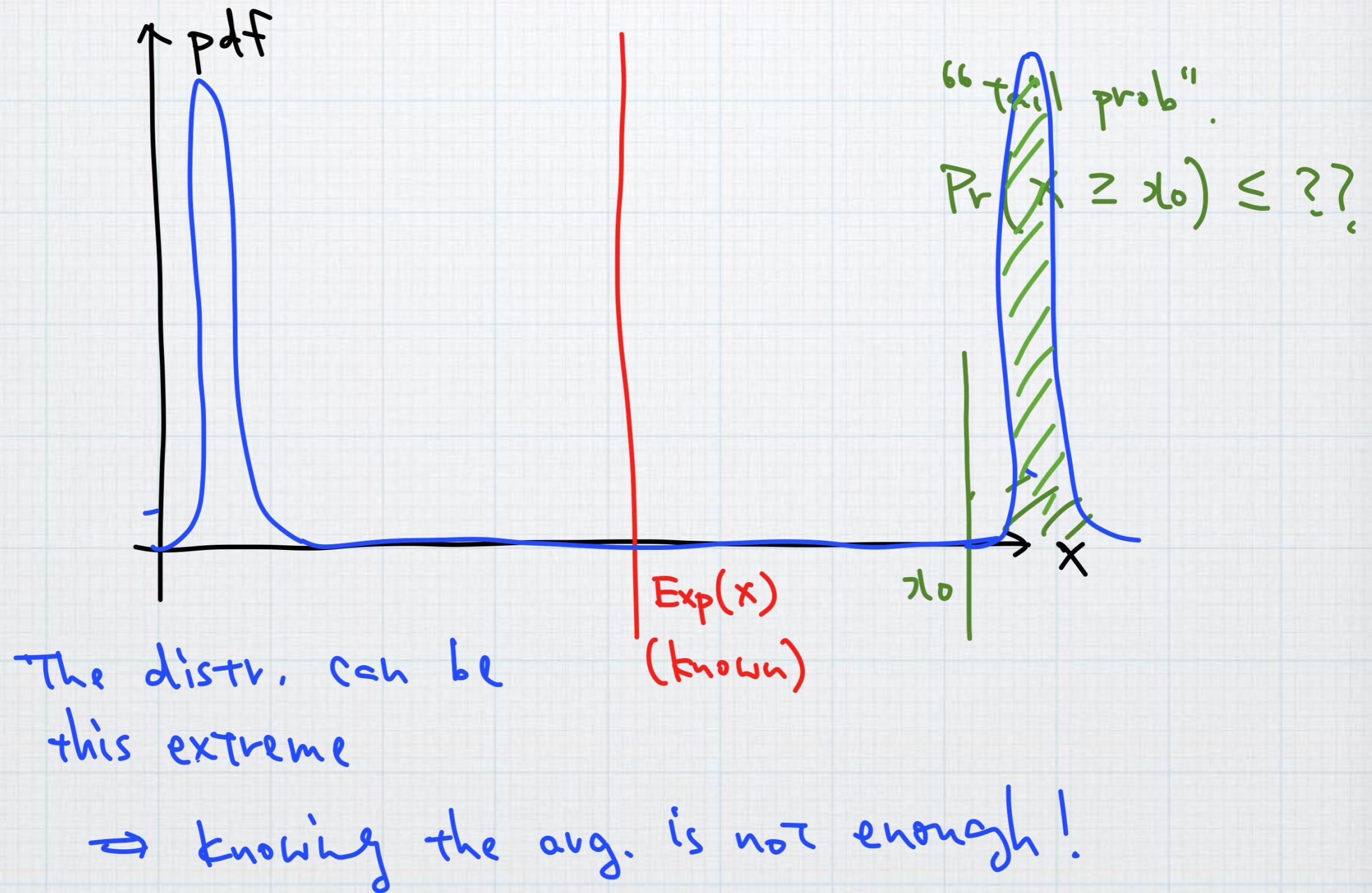
where  $\alpha = e^{\frac{\varepsilon \cdot \eta(s)}{(\kappa + \varepsilon)^2}}$ ,  $\gamma = e^{-\frac{\varepsilon^2}{2(\kappa + \varepsilon)^2}}$ .



# Concentration of Measure Inequalities



# Concentration of Measure Inequalities



# Concentration of Measure I: Azuma's Inequality Used in [Chatterjee+ POPL'17]

Def. Let  $(S, S \xrightarrow{\text{tr}} \mathcal{D}S)$  be a MC.

A *supermartingale* is  $\eta: S \rightarrow \mathbb{R}$  such that

$$\forall s \in S. \quad \eta(s) \geq (\mathbb{X}\eta)(s)$$

When one-step  
difference is  
bounded...

Rem. Let  $s_0 \rightarrow s_1 \rightarrow \dots$  be a run of the MC, with  $s_0$  fixed. Then  $s_n$  is a rand. var. in  $S$  for each  $n$ , and  $\eta(s_n)$  is a rand. var. in  $\mathbb{R}$ .

Thm. (Azuma) Let  $\eta$  have  $\kappa$ -bdd difference. For each  $\lambda > 0$  and  $n \in \mathbb{N}$ ,

$$\Pr(\eta(s_n) - \eta(s_0) \geq \lambda) \leq e^{-\frac{\lambda^2}{2n\kappa^2}}$$

# Concentration of Measure II: The Chebyshev-Cantelli Inequality

Used e.g.in [Bouissou+ TACAS'16]

Thm. (Chebyshev–Cantelli) Let  $X$  be a random variable with mean  $\mu$  and variance  $\sigma^2$ . Then for each  $k > 0$ ,

$$\Pr(X - \mu \geq k\sigma) \leq \frac{1}{1 + k^2}$$

If variance is known...

# Concentration of Measure III: Bernstein's Inequality

Used e.g.in [Bouissou+ TACAS'16]

Thm. (Bernstein) Let  $\eta$  be a supermartingale, where

- conditional variance is bounded:  $\exists \sigma$  such that

$$\text{Var}(\eta(s') \mid s \rightarrow s') \leq \sigma^2$$

- deviation from the mean is bounded:  
 $\exists M$  such that,  $\forall i \in [0, n]$ ,

$$|\eta(s_i) - \text{Exp}(\eta(s_i))| \leq M$$

Then

$$\Pr(\eta(s_n) - \eta(s_0) \geq \lambda) \leq \exp\left(\frac{-\lambda^2}{2n\sigma^2 + \frac{2}{3}M\lambda}\right)$$

		Answers what question?	Underlying math
<b>ranking</b> martingale-like methods ( <b>lower</b> bd)	<b>Additive</b> ranking supermartingale <small>[McIver+ PSSE'04] [Chakarov+ CAV'13]</small>	$\Pr(\text{Reach}_C) = ?$ 1 $\text{Exp}(\text{Step}_C) \leq ??$	(elementary)  <b>New</b>
 <b>repulsing</b> martingale methods ( <b>upper</b> bd)	<b><math>\gamma</math>-scaling</b> ranking submartingale <small>[Urabe+ LICS'17] [Takisaka+, ATVA'18]</small>	$\Pr(\text{Reach}_C) \geq ??$	<ul style="list-style-type: none"> <li>• Coalgebra!</li> <li>• (?)</li> </ul>
 <b><math>\epsilon</math>-decreasing</b> repulsing supermartingale <small>[Chatterjee+ POPL'17]</small>		$\Pr(\text{Reach}_C) \leq ??$	Azuma's inequality for martingale concentration  <b>New</b>
	<b>Nonnegative</b> repulsing supermartingale <small>[Steinhardt+ IJRR'12] [Takisaka+, ATVA'18]</small>	$\Pr(\text{Reach}_C) \leq ??$	Markov's inequality for martingale concentration

# Overview

- \* Reachability in probabilistic programs
- \* Foundation of fixed points, in the non-probabilistic setting
  - \* Ranking functions, invariants
  - \* Foundation: Knaster-Tarski, Cousot-Cousot
- \* Known supermartingale methods
  - \* Roles of concentration lemmas
- \* Something new (from **fixed points** and **coalgebras**)
- \* Coalgebras: excitements, afterthoughts, our project



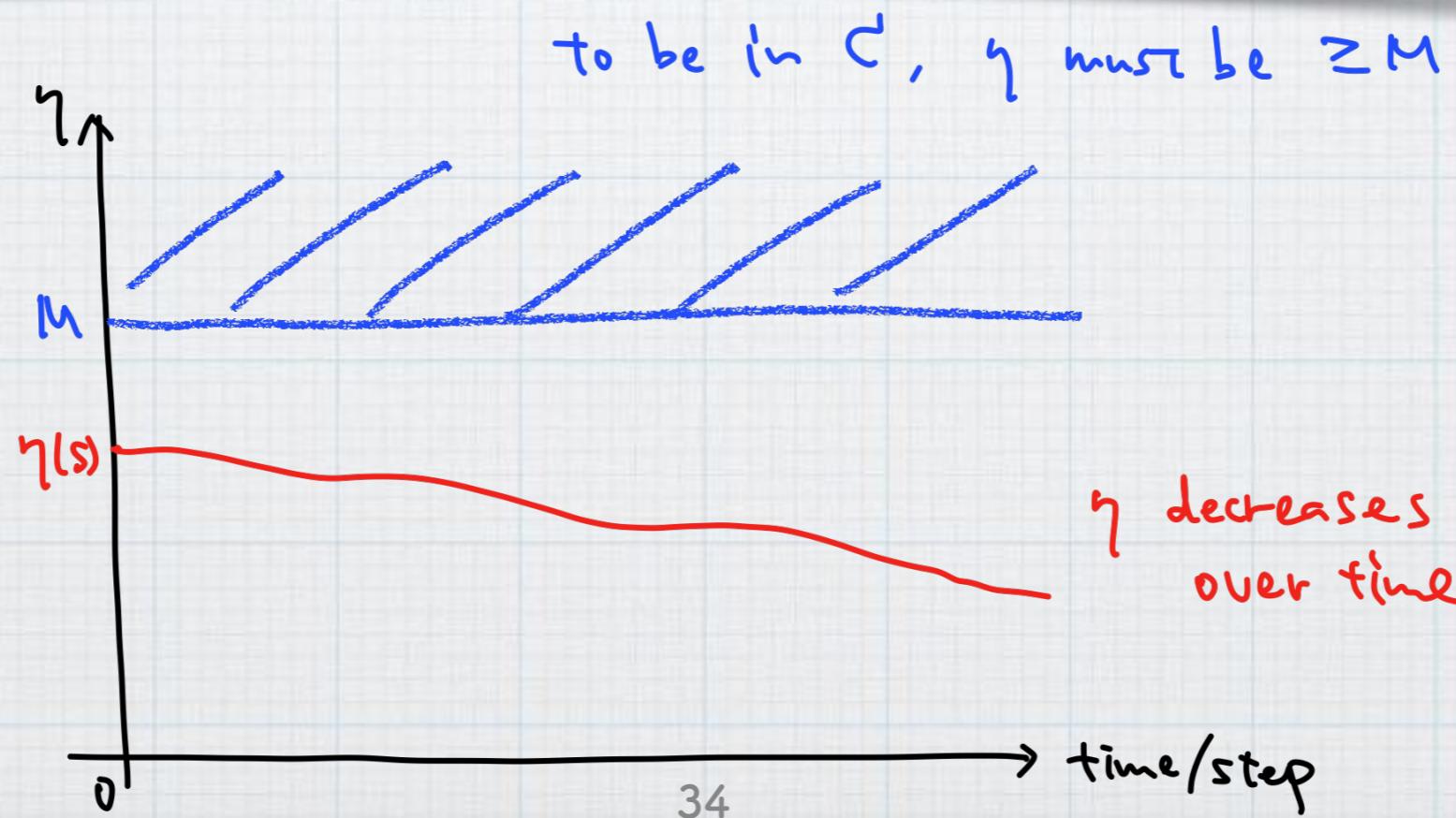
# Nonnegative Repulsing Supermartingale

[Steinhardt+ IJRR'12] [Takisaka, Oyabu, Urabe, IH, in preparation]

Def. Let  $(S, S \xrightarrow{\text{tr}} \mathcal{D}S)$  be a MC,  $C \subseteq S$  and  $M > 0$ .

$\eta: S \rightarrow \mathbb{R}$  is a *nonnegative repulsing supermartingale* for  $C$  at  $M$  if

- $\forall s \in S. \quad \eta(s) \geq 0$
- $\forall s \in S \setminus C. \quad \eta(s) \geq (\mathbb{X}\eta)(s)$
- $\forall c \in C. \quad \eta(c) \geq M$



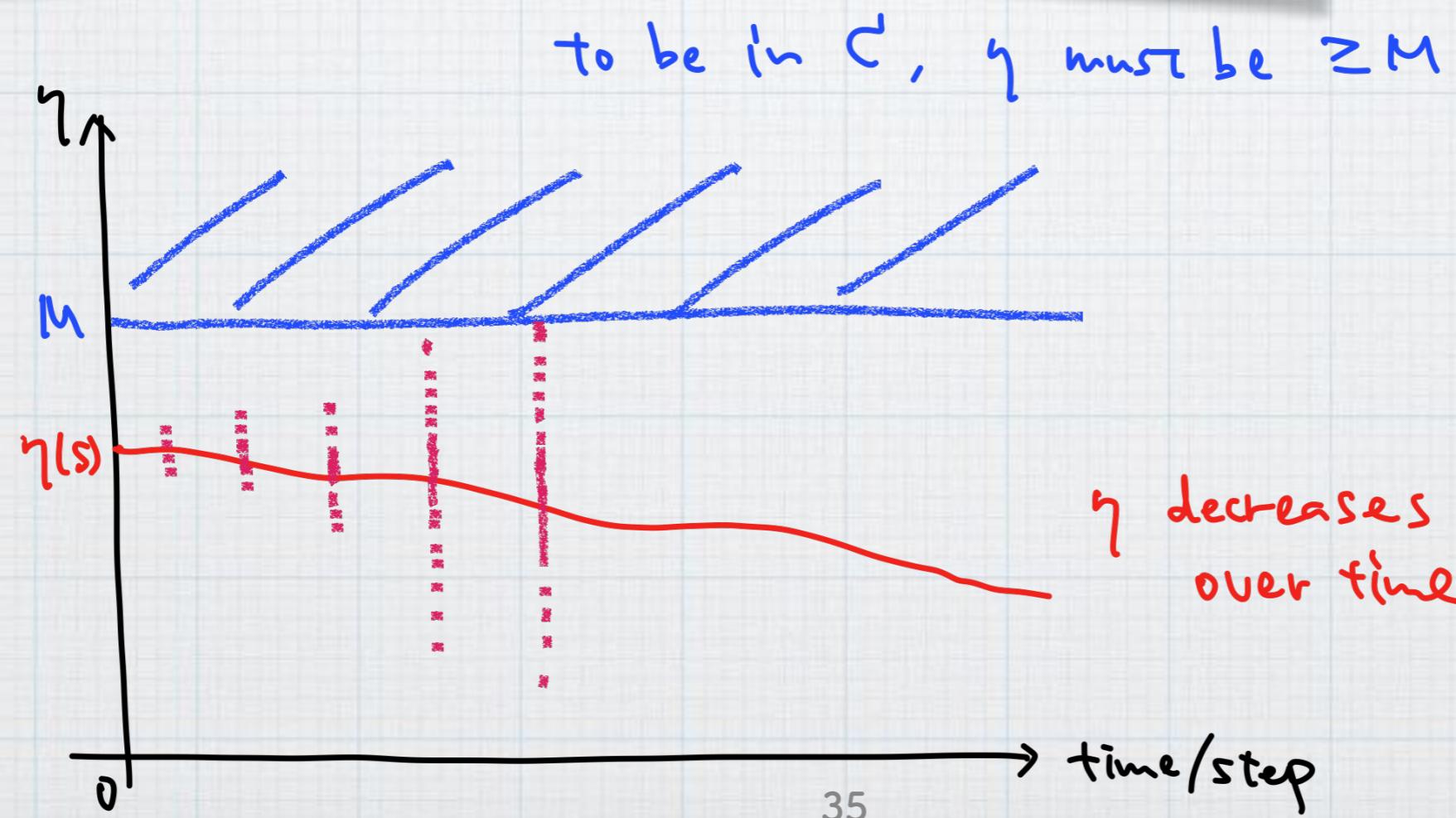
# Nonnegative Repulsing Supermartingale

[Steinhardt+ IJRR'12] [Takisaka, Oyabu, Urabe, IH, in preparation]

Def. Let  $(S, S \xrightarrow{\text{tr}} \mathcal{D}S)$  be a MC,  $C \subseteq S$  and  $M > 0$ .

$\eta: S \rightarrow \mathbb{R}$  is a *nonnegative repulsing supermartingale* for  $C$  at  $M$  if

- $\forall s \in S. \quad \eta(s) \geq 0$
- $\forall s \in S \setminus C. \quad \eta(s) \geq (\mathbb{X}\eta)(s)$
- $\forall c \in C. \quad \eta(c) \geq M$



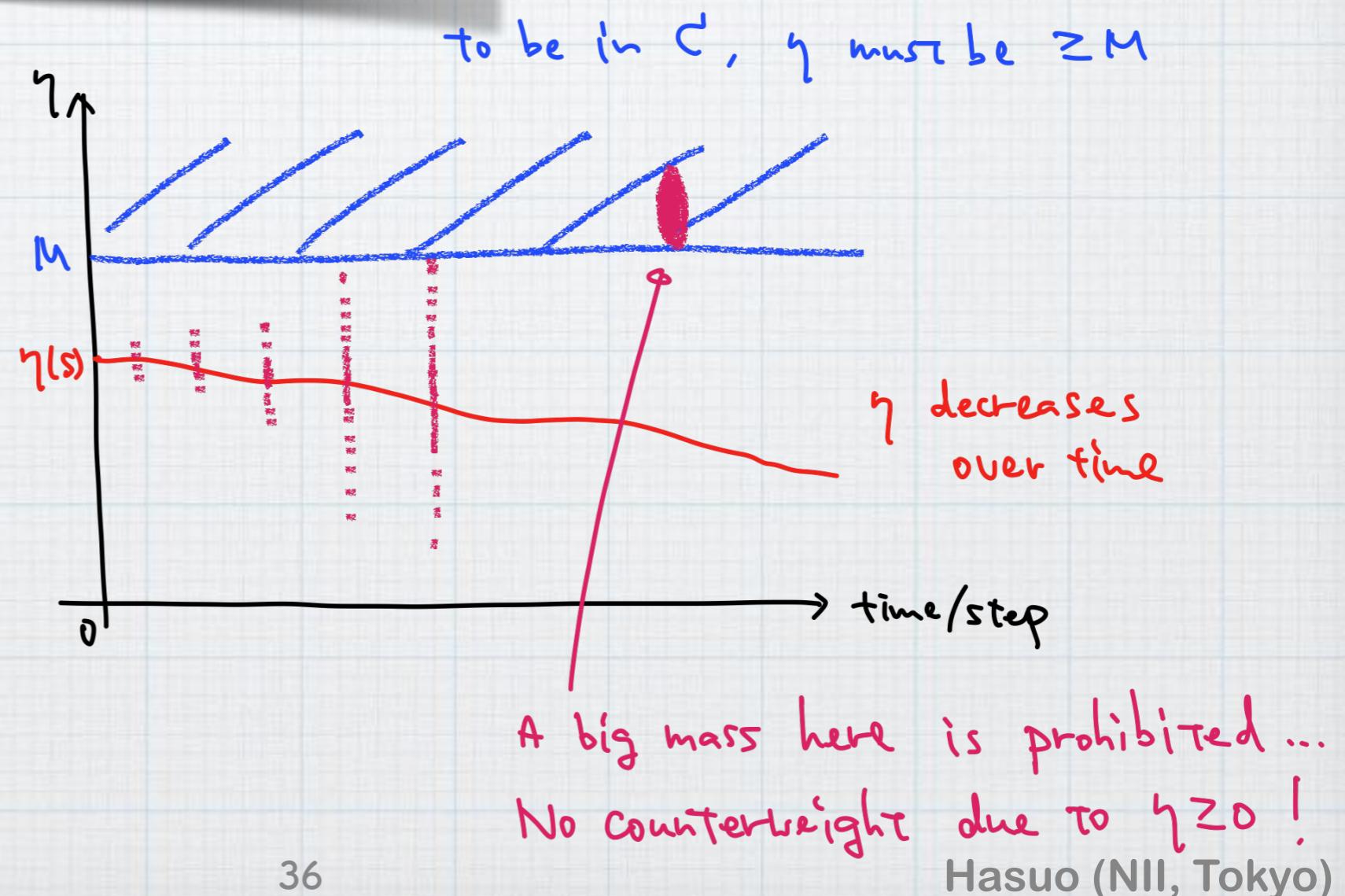
# Nonnegative Repulsing Supermartingale

[Steinhardt+ IJRR'12] [Takisaka, Oyabu, Urabe, IH, in preparation]

Def. Let  $(S, S \xrightarrow{\text{tr}} \mathcal{D}S)$  be a MC,  $C \subseteq S$  and  $M > 0$ .

$\eta: S \rightarrow \mathbb{R}$  is a *nonnegative repulsing supermartingale* for  $C$  at  $M$  if

- $\forall s \in S. \quad \eta(s) \geq 0$
- $\forall s \in S \setminus C. \quad \eta(s) \geq (\mathbb{X}\eta)(s)$
- $\forall c \in C. \quad \eta(c) \geq M$



# Nonnegative Repulsing Supermartingale

[Steinhardt+ IJRR'12]. With nondeterminism: [Takisaka, Oyabu, Urabe, IH, ATVA'18]

Def. Let  $(S, S \xrightarrow{\text{tr}} \mathcal{D}S)$  be a MC,  $C \subseteq S$  and  $M > 0$ .

$\eta: S \rightarrow \mathbb{R}$  is a *nonnegative repulsing supermartingale* for  $C$  at  $M$  if

- $\forall s \in S. \quad \eta(s) \geq 0$
- $\forall s \in S \setminus C. \quad \eta(s) \geq (\mathbb{X}\eta)(s)$
- $\forall c \in C. \quad \eta(c) \geq M$

Thm. (upper bound)

$$\Pr(\text{Reach}_{s,C}) \leq \frac{1}{M} \eta_s$$

Thm. (completeness) There exists a nonnegative repulsing supermartingale  $\eta$  for  $C$  at  $M$  such that

$$\Pr(\text{Reach}_{s,C}) = \frac{1}{M} \eta_s$$

*Proof.* Take  $M = 1$ ,  $\eta(s) = \Pr(\text{Reach}_{s,C})$ .

		Answers what question?	Underlying math
ranking martingale-like methods <b>(lower bd)</b>	<b>Additive</b> ranking supermartingale [McIver+ PSSE'04] [Chakarov+ CAV'13]	$\Pr(\text{Reach}_C) = ?$ 1 $\text{Exp}(\text{Step}_C) \leq ??$	(elementary) <b>New</b>
<b>repulsing</b> martingale methods <b>(upper bd)</b>	<b><math>\gamma</math>-scaling</b> ranking submartingale [Urabe+ LICS'17] [Takisaka+, ATVA'18]	$\Pr(\text{Reach}_C) \geq ??$	<ul style="list-style-type: none"> <li>• Coalgebra!</li> <li>• (?)</li> </ul>
	<b><math>\epsilon</math>-decreasing</b> repulsing supermartingale [Chatterjee+ POPL'17]	$\Pr(\text{Reach}_C) \leq ??$	Azuma's inequality for martingale concentration <b>New</b>
	<b>Nonnegative</b> repulsing supermartingale [Steinhardt+ IJRR'12] [Takisaka+, ATVA'18]	$\Pr(\text{Reach}_C) \leq ??$	<b>Knaster-Tarski!</b>

# Concentration of Measure: No Need!

Def. Let  $(S, S \xrightarrow{\text{tr}} \mathcal{D}S)$  be a MC,  $C \subseteq S$ .

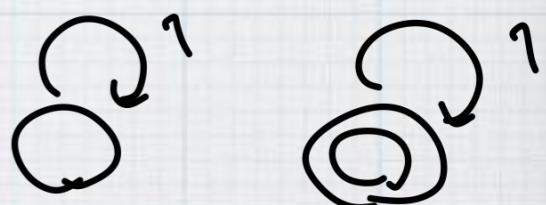
Let  $\mathbb{X}_C: [0, 1]^S \longrightarrow [0, 1]^S$  be defined by

$$\left( \eta: S \rightarrow [0, 1] \right) \xrightarrow{\mathbb{X}_C} \left( \begin{array}{lll} \mathbb{X}_C\eta: & S & \longrightarrow [0, 1] \\ & s & \longmapsto \begin{cases} 1 & \text{if } s \in C \\ (\mathbb{X}\eta)(s) & \text{if } s \notin C \end{cases} \end{array} \right)$$

Thm. (upper bound)

$$\Pr(\text{Reach}_C) =_{\mu} \mathbb{X}_C \Pr(\text{Reach}_C)$$

(Easy from the Cousot-Cousot characterization of lfp)



Rem.

- The *least* fixed point
- In the complete lattice  $[0, 1]$ , so that a sink state gets **0**

# Lattice-Theoretic Foundation

$L$ : complete lattice,  $f: L \rightarrow L$  monotone

**Thm.** (Knaster-Tarski)

- $\mu f = \min\{l \in L \mid f(l) \sqsubseteq l\}$

$$\Rightarrow \frac{f(l) \sqsubseteq l}{\mu f \sqsubseteq l}$$

- $\nu f = \max\{l \in L \mid l \sqsubseteq f(l)\}$

$$\Rightarrow \frac{l \sqsubseteq f(l)}{l \sqsubseteq \nu f}$$

**Thm.** (Cousot-Cousot)

$$\perp \sqsubseteq f(\perp) \sqsubseteq \cdots \sqsubseteq f^\omega(\perp) \sqsubseteq \cdots$$

stabilizes, and converges to  $\mu f$

$$\Rightarrow f^\alpha(\perp) \sqsubseteq \mu f \quad (\forall \alpha \in \text{Ord})$$

$$\top \sqsupseteq f(\top) \sqsupseteq \cdots \sqsupseteq f^\omega(\top) \sqsupseteq \cdots$$

stabilizes, and converges to  $\nu f$

$$\Rightarrow \nu f \sqsubseteq f^\alpha(\top) \quad (\forall \alpha \in \text{Ord})$$

# Concentration of Measure: No Need!

**Thm.** Let  $\eta: S \rightarrow [0, 1]$  be such that

$$\mathbb{X}_C(\eta) \leq \eta ,$$

that is,

- $\forall s \in S \setminus C. \quad \eta(s) \geq (\mathbb{X}\eta)(s)$
- $\forall c \in C. \quad \eta(c) \geq 1$

Then, for each  $s \in S$ ,

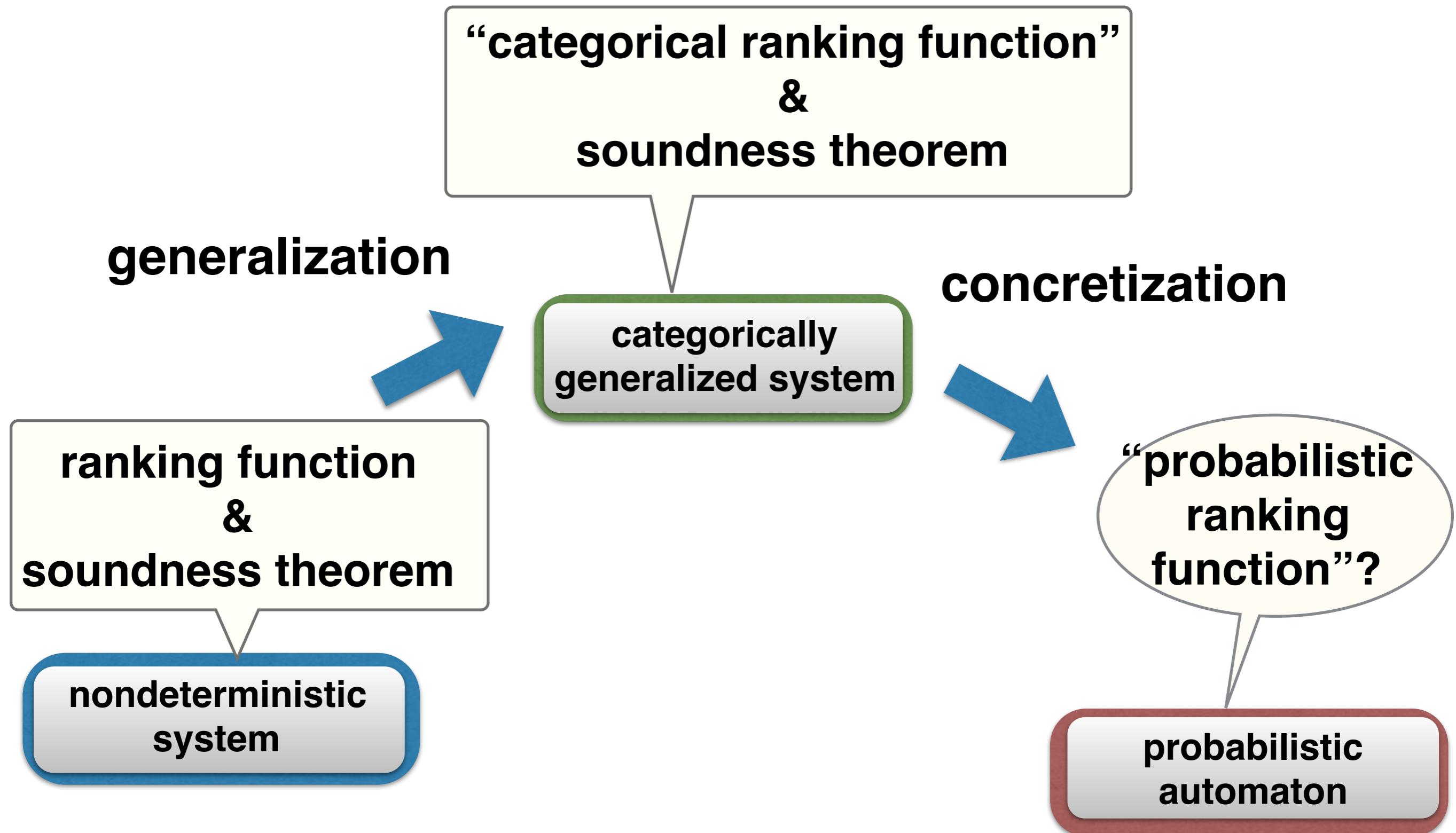
$$\Pr(\text{Reach}_{s,C}) \leq \eta(s)$$

$$\begin{array}{ccc} \mathbb{X}_C \text{ Reach}_{s,C} & \dashrightarrow & \mathbb{X}_C \eta \\ \text{init} \downarrow \cong & & \downarrow \\ \text{Reach}_{s,C} & \dashrightarrow & \eta \end{array} \quad \text{in the poset } [0, 1]^S$$

- \* Very simple, but not previously known
- \* Soundness and completeness follow easily
- \* Template-based synthesis:  
experimentally outperforms the known method [Chatterjee+ POPL'17]

		Answers what question?	Underlying math
<p>ranking martingale methods <b>(lower bd)</b></p> 	<p><b>Additive</b> ranking supermartingale [McIver+ PSSE'04] [Chakarov+ CAV'13]</p>	$\Pr(\text{Reach}_C) = ?$ $\text{Exp}(\text{Step}_C) \leq ??$	(elementary) <span style="color: red;">New</span>
<p>repulsing martingale-like methods <b>(upper bd)</b></p>	<p><b><math>\gamma</math>-scaling</b> ranking submartingale [Urabe+ LICS'17] [Takisaka+, ATVA'18]</p>	$\Pr(\text{Reach}_C) \geq ??$	<ul style="list-style-type: none"> <li>LFP characterization</li> <li>(Categorical consideration)</li> </ul>
	<p><b><math>\epsilon</math>-decreasing</b> repulsing supermartingale [Chatterjee+ POPL'17]</p>	$\Pr(\text{Reach}_C) \leq ??$	Azuma's inequality for martingale concentration <span style="color: red;">New</span>
	<p><b>Nonnegative</b> repulsing supermartingale [Steinhardt+ IJRR'12] [Takisaka+, ATVA'18]</p>	$\Pr(\text{Reach}_C) \leq ??$	Knaster-Tarski!

# Methodology [UrabeHH, LICS'17]



# Categorical Ranking Function

Def:

A *ranking domain* wrt.  $\sigma : F\Omega \rightarrow \Omega$  is a triple

$(r : FR \rightarrow R, q : R \rightarrow \Omega, \sqsubseteq_R)$  s.t.

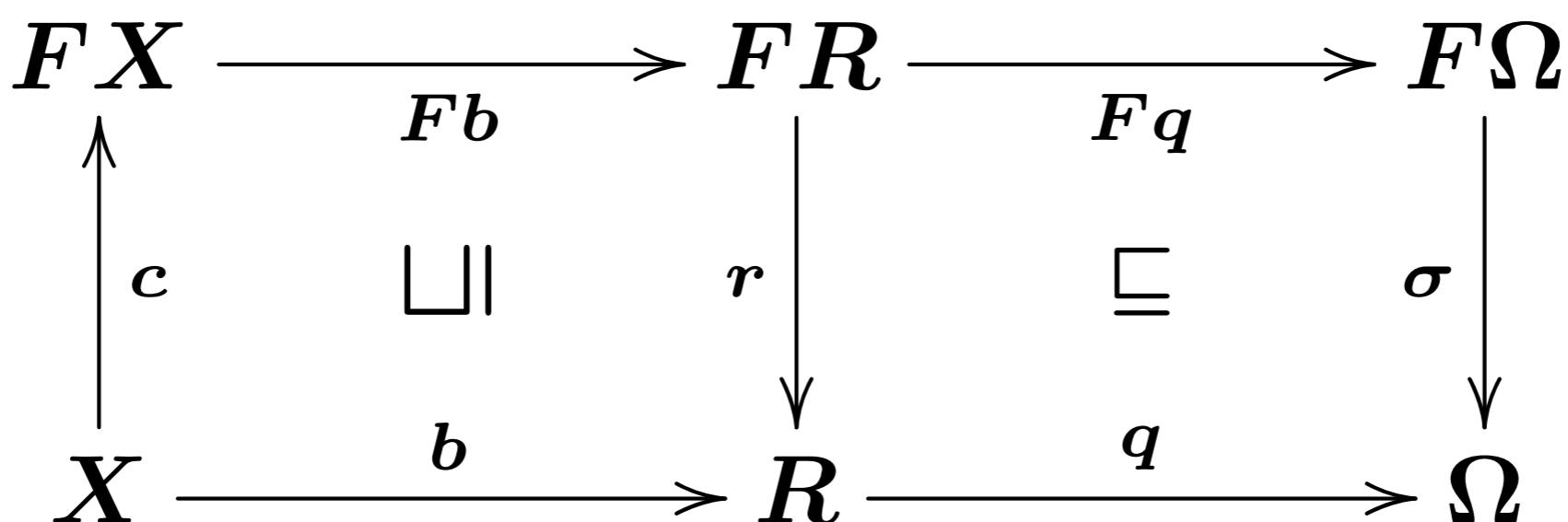
1.  $R$  is a complete lattice and  $\Phi_{c,r}$  is monotone
2.  $q$  is monotone,  $\perp$ -preserving and continuous
3.  $q \circ r \sqsubseteq \sigma \circ Fq$
4.  $r$  is corecursive

Def:

An arrow  $b : X \rightarrow R$  is a *ranking arrow* wrt.  $(r, q, \sqsubseteq_R)$  if:

$$b \sqsubseteq_R r \circ Fr \circ c$$

44



# Corecursive Algebra

Def:

An algebra  $r : FR \rightarrow R$  is **corecursive** if for all coalgebra  $c : X \rightarrow FX$ , a coalgebra-algebra homomorphism from  $\mathcal{C}$  to  $r$  uniquely exists.

$$\begin{array}{ccc} FX & \xrightarrow{\quad F(r)_c \quad} & FR \\ \uparrow c & = & \downarrow r \\ X & \xrightarrow{\quad (r)_c \quad} & R \end{array}$$

- It has been used to ensure **productivity** of general structured corecursion [Capretta et al., SBMF '09]
- We use it to ensure **termination**

# Scaled Multiplicative Ranking Submartingale

Def:

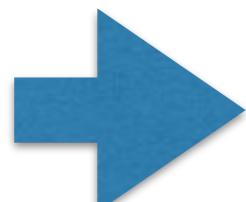
For  $\gamma \in (0, 1)$ , a function  $b : X \rightarrow [0, 1]$  is a  $\gamma$ -scaled multiplicative ranking submartingale if:

$$\gamma \cdot \sum_{x' \in X} \Pr(x \rightarrow x') \cdot b(x') \geq b(x)$$

By soundness of (categorical) ranking arrows,

Thm:

$$b(x) \leq \Pr \left( \begin{array}{l} \text{an accepting state} \\ \text{is reached from } x \end{array} \right)$$



Quantitative reasoning



# Abstract Technique

$$A ::= \text{true} \mid \text{false} \mid A_1 \wedge A_2 \mid \neg A \mid a_1 < a_2 \mid \forall x \in {}^*\mathbb{N}. A \mid \forall x \in {}^*\mathbb{R}. A$$

# Identify “mathematical essense”

# Choose parameter $e_1$

# Choose parameter $e_2$

# Existing Technique

$$T_1 = T[e_1]$$

```
    'replace_interests' => false,  
    'send_welcome'      => false,  
);  
  
return $result;  
}  
else {  
    $result = array ('response'=>'error', 'message'  
    => "User '$username' does not exist");  
  
    return $result;  
}
```

- \* Formal methods,  
from software  
to cyber-physical systems.  
“Metatheoretical transfer”
- \* Real-world application,  
exploiting abstraction and  
generality

# $T[e_2]$



# Some Afterthoughts...

- \* LP characterization of reachability probabilities  
(e.g. [Baier & Katoen])
  - \* Minimize  $\mathbf{x}$
  - \* subject to  $\mathbf{x} = \mathbf{Ax} + \mathbf{b}$
  - \* Here  $\mathbf{A}$  is the transition matrix, and  $\mathbf{b}$  is the membership of  $\mathbf{C}$
- \* Our scaled multiplicative ranking supermartingale
  - \* Scale the constraint to  $\mathbf{x} = \gamma(\mathbf{Ax} + \mathbf{b})$  with  $0 < \gamma < 1$   
→ Makes the solution  $\mathbf{x}_0$  **unique**. It is an lfp and a gfp
  - \* Once we find  $\mathbf{x}$  such that  $\mathbf{x} \leq \gamma(\mathbf{Ax} + \mathbf{b})$ , we have  $\mathbf{x} \leq \mathbf{x}_0$  by Knaster-Tarski
- \* (Still the categorical axiomatics gives a nice clue, I believe)

# ERATO 蓮尾メタ数理システムデザインプロジェクト ERATO Metamathematics for Systems Design Project

国立情報学研究所 & 科学技術振興機構

National Institute of Informatics & Japan Science and Technology Agency



- \* Our goal:  
**Formal methods for cyber-physical systems (CPS)**
  - \* Pursued by many...  
e.g. NSF's CPS initiative (computer science + control theory)
  
- \* Our uniqueness position paper [Hasuo, New Gener. Comp. '17]
  - \* Theory: **foundation and diversity**
    - \* Algebraic, logical and categorical **metatheory**  
→  
“**Mathematical transfer**” from software to CPS
    - \* Logic/automata, control  
+ category theory, software engineering,  
machine learning, probability theory, ...
  
- \* Application:  
tackle **real systems** ( $\Leftarrow$  real automated driving cars)
  - \* Industrial collaboration
  - \* The **autonomoose** project at U. Waterloo
  - \* Cars  $\leftarrow$  efficient testing  $\leftarrow$  formal reasoning  
 $\leftarrow$  **categories!**



# Overview

- \* Reachability in **probabilistic programs**
- \* **Foundation of fixed points**, in the non-probabilistic setting
  - \* Ranking functions, invariants
  - \* Foundation: Knaster-Tarski, Cousot-Cousot
- \* **Known supermartingale** methods
  - \* Roles of concentration lemmas
- \* Something **new** (from our recent results)
- \* Coalgebras: excitements, afterthoughts, our project



# Summary

- \* **Coalgebras:** excitements, afterthoughts, ... Still I love them!
  - \* Buechi and parity conditions  
[Urabe, Shimizu & IH, CONCUR'16] [Urabe & IH, CMCS'18]  
→ Tutorial at CONCUR'18
- \* Real-world application of categorical methods. Our approach
  - \* As a **metatheory**
  - \* for deriving object-level (accessible and automated) techniques
- \* Reachability in probabilistic programs is **rich**
  - \* **Martingale** methods for (over-/under-) approximations
    - \* Role of **concentration lemmas**
    - \* Knaster-Tarski foundation is still useful

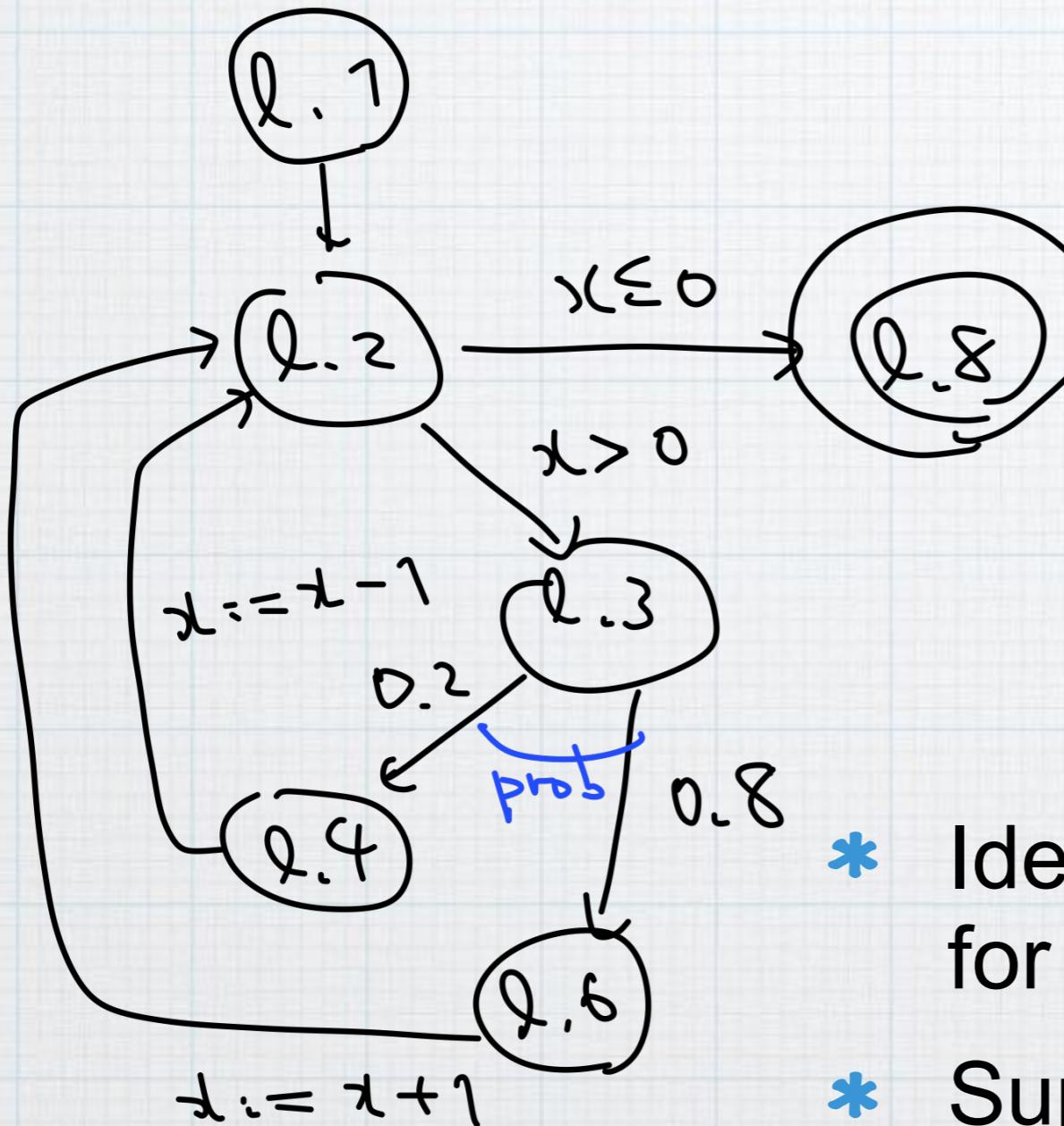
We're hiring!

Max 3.5 yrs, PD & senior researchers  
logic + automata + categories + machine  
learning + software engineering  
→ CPS, automated driving

Thank you for your attention!  
Ichiro Hasuo (NII, Tokyo)  
<http://group-mmm.org/~ichiro/>

# Appendix

# Probabilistic Control Flow Graph (pCFG) See e.g. [Chatterjee+, POPL'17]



```

1  x := m
2  while x > 0 do
3      if prob(p) do
4          x := x - 1
5      else
6          x := x + 1
7      fi
8  od
  
```

(say,  $m = 16$  and  $p = 0.2$ )

- \* Idea: a state  $l$  in pCFG stands for  $\{ (l, [x \mapsto r]) \mid r \in \mathbb{R} \}$
- \* Supermartingales are given by  $\eta_l: \mathbb{R}^{\{x\}} \rightarrow \mathbb{R}, \quad i = 1, \dots, 8$

# Template-Based Synthesis

- \* Let's use linear templates, for example
- \* Meaning:  $\eta_l : \mathbb{R}^{\{x\}} \rightarrow \mathbb{R}, \quad i = 1, \dots, 8$

$$\eta_l(r) \equiv a_l r + b_l$$

- \*  $a_l, b_l$ : undetermined parameters
- \* They are determined so that supermartingale constraints are satisfied, e.g.

- \* Constraint solving by LP, SDP, QE,  
...

## Def.

Let  $(S, S \xrightarrow{\text{tr}} \mathcal{D}S)$  be a MC,  $C \subseteq S$ .

$\eta: S \rightarrow \mathbb{R}_{\geq 0}$  is a *ranking supermartingale* for  $C$  if

- $\forall s \in S \setminus C. \quad \eta(s) \geq (\mathbb{X}\eta)(s) + 1.$
- $\eta(s) = 0$  implies  $s \in C$

		Answers what question?	Underlying math
ranking supermartingale <b>(lower bd)</b>	<b>Additive</b> ranking supermartingale [McIver+ PSSE'04] [Chakarov+ CAV'13]	$\Pr(\text{Reach}_C) = ?$ 1 $\text{Exp}(\text{Step}_C) \leq ??$	(elementary)
repulsing supermartingale <b>(upper bd)</b>	<b>Multiplicative</b> ranking supermartingale [Urabe+ LICS'17]	$\Pr(\text{Reach}_C) \geq ??$	<ul style="list-style-type: none"> <li>• LP characterization</li> <li>• (Categorical consideration)</li> </ul>
repulsing supermartingale <b>(upper bd)</b>	<b><math>\epsilon</math>-decreasing</b> repulsing supermartingale [Chatterjee+ POPL'17]	$\Pr(\text{Reach}_C) \leq ??$	Azuma's inequality for martingale concentration
repulsing supermartingale <b>(upper bd)</b>	<b>Nonnegative</b> repulsing supermartingale [Steinhardt+ IJRR'12] [Takisaka+, in preparation]	$\Pr(\text{Reach}_C) \leq ??$	Markov's inequality for martingale concentration

# Preliminary Experimental Results

```
1  x := m
2  while x > 0 do
3    if x < N do
4      if prob(p) do
5        x := x - 1
6      else
7        x := x + 1
8    fi
9  else
10   x := x + 1
11 fi
12 od
```

Fig. 1. APP corresponding to Example 1

```
1  x := Geometric(0.5)
2  while x ≥ 1 do
3    x := x - 1
4  od
5  if prob(0.5) do
6    while x ≤ 0 do
7      x := x - 1
8    od
9  else
10   skip
11 od
```

Fig. 2. APP corresponding to Example 2

```
1  x := Uniform[0, 1]
2  while x < 1 do
3    if prob(p) do
4      x := 2 * x
5    else
6      x := 0.5 * x
7    fi
8 od
```

Fig. 3. APP corresponding to Example 3

```
1  x := m
2  while x > 0 do
3    if prob(p) do
4      x := x - 1
5    else
6      x := x + 1
7    fi
8 od
```

Fig. 4. APP corresponding to Example 4

# Preliminary Experimental Results

```

1  x := m
2  while x > 0 do
3    if x < N do
4      if prob(p) do
5        x := x - 1
6      else
7        x := x + 1
8    fi
9  else
10   x := x + 1
11 fi
12 od

```

**Fig. 1.** APP corresponding to Example 1

```

1  x := Geometric(0.5)
2  while x ≥ 1 do
3    x := x - 1
4  od
5  if prob(0.5) do
6    while x ≤ 0 do
7      x := x - 1
8    od
9  else
10   skip
11 od

```

**Fig. 2.** APP corresponding to Example 2

```

1  x := Uniform[0, 1]
2  while x < 1 do
3    if prob(p) do
4      x := 2 * x
5    else
6      x := 0.5 * x
7    fi
8 od

```

**Fig. 3.** APP corresponding to Example 3

```

1  x := m
2  while x > 0 do
3    if prob(p) do
4      x := x - 1
5    else
6      x := x + 1
7    fi
8 od

```

**Fig. 4.** APP corresponding to Example 4

example	true reachability probability	Nonnegative (ours)	ε-decreasing
1	$\frac{(0.4/0.6)^5 - (0.4/0.6)^{10}}{1 - (0.4/0.6)^{10}} \approx 0.116364$	0.5054945055	< 1
2	0.5	0.5	—
2a	0.5	0.5	—
2b	0.5	0.5	—
3	$\int_0^1 \left(\frac{0.25}{0.75}\right)^{\lceil \log_2(1/x) \rceil} dx \approx 0.2$	0.5	—
4	$\left(\frac{0.25}{0.75}\right)^1 \approx 0.333333$	—	< 1