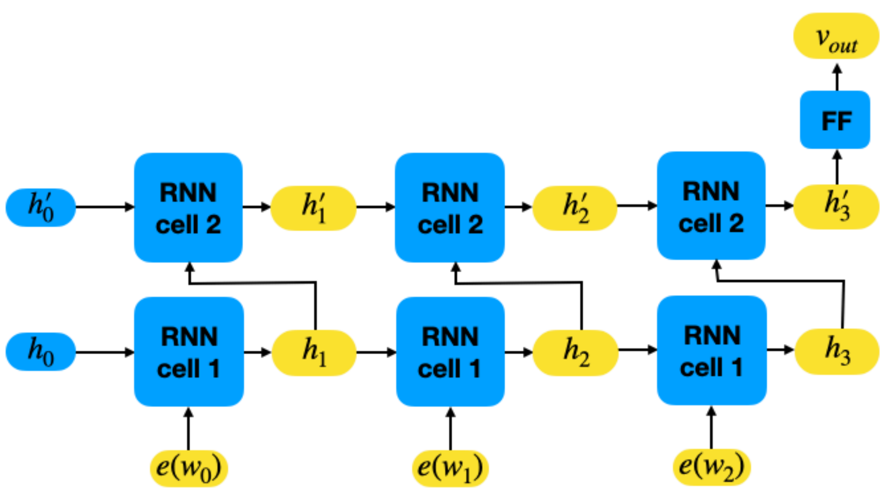
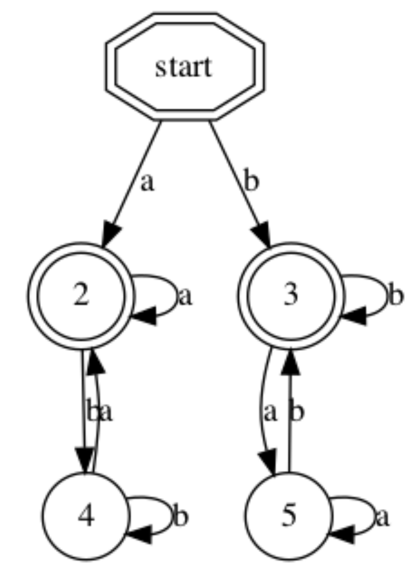
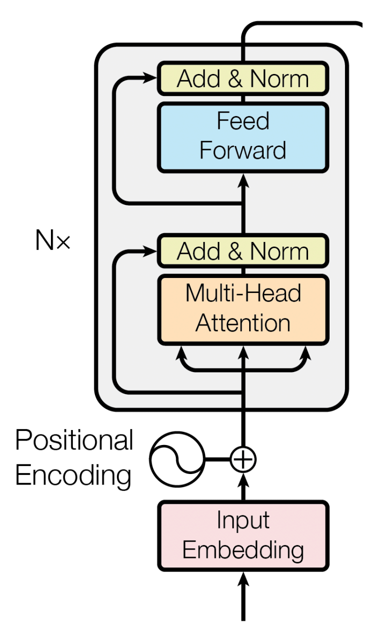
Formal Abstractions of Neural Sequence Models



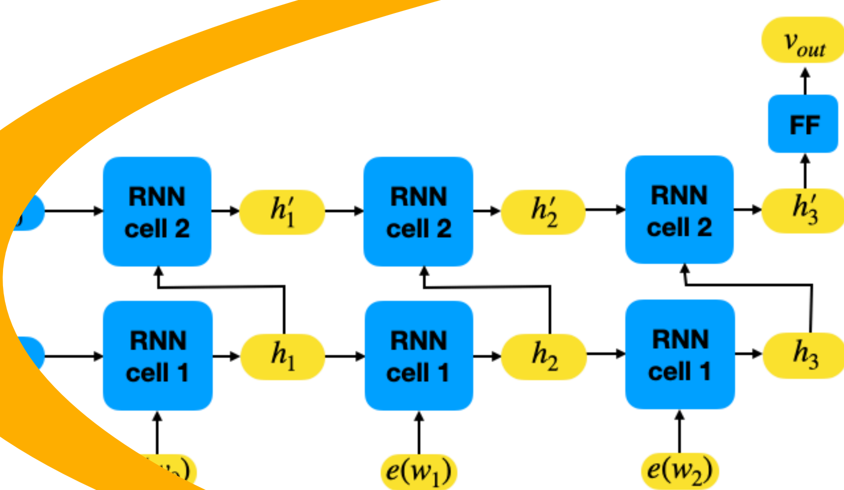


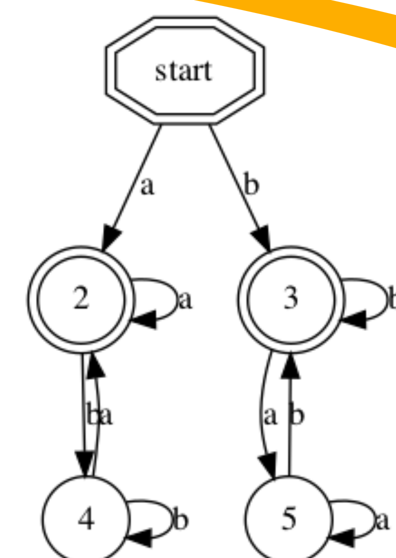


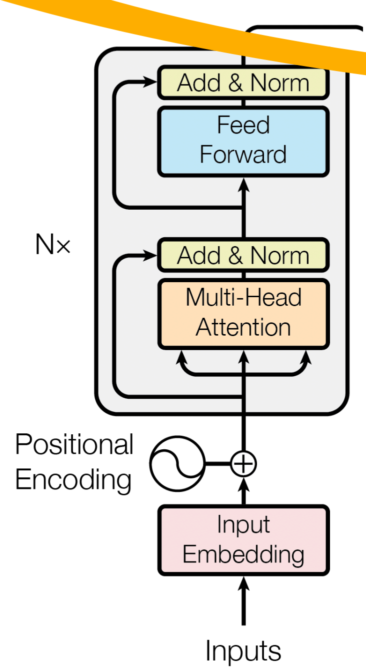
Code!?

Gail Weiss, ICGI 2021

Formal Abstractions of Neural Sequence Models







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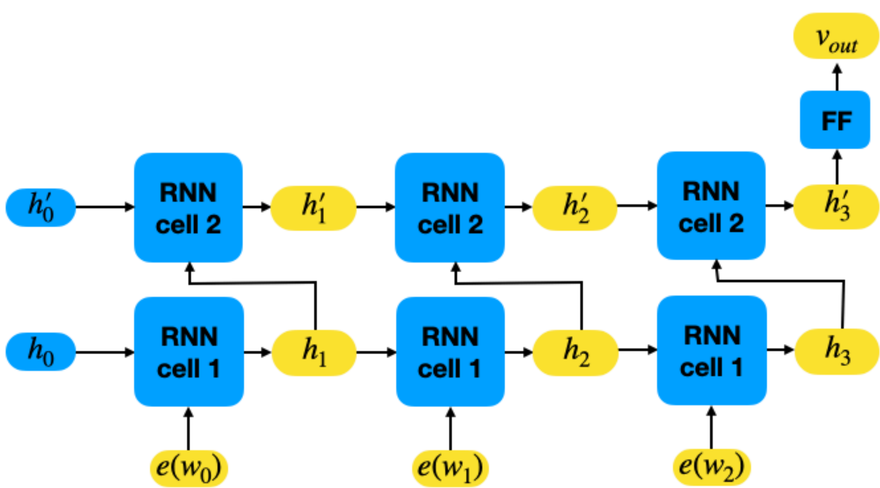

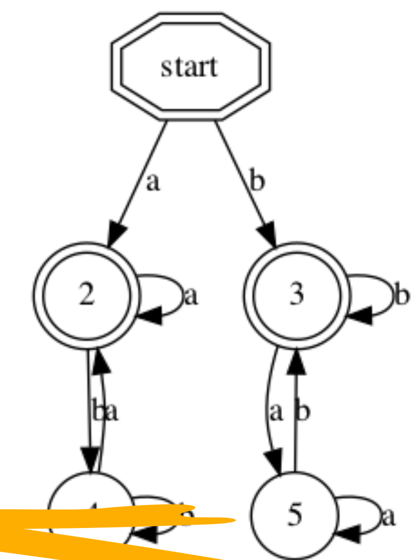

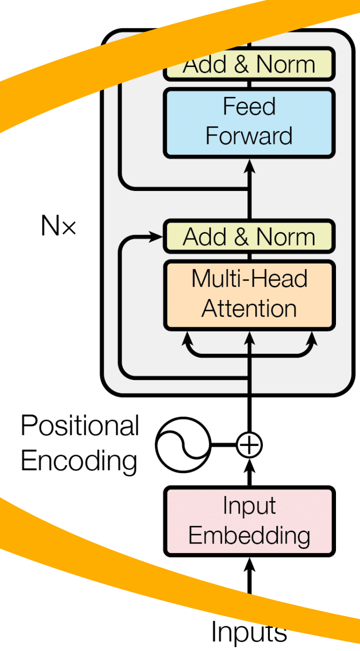

Code!?

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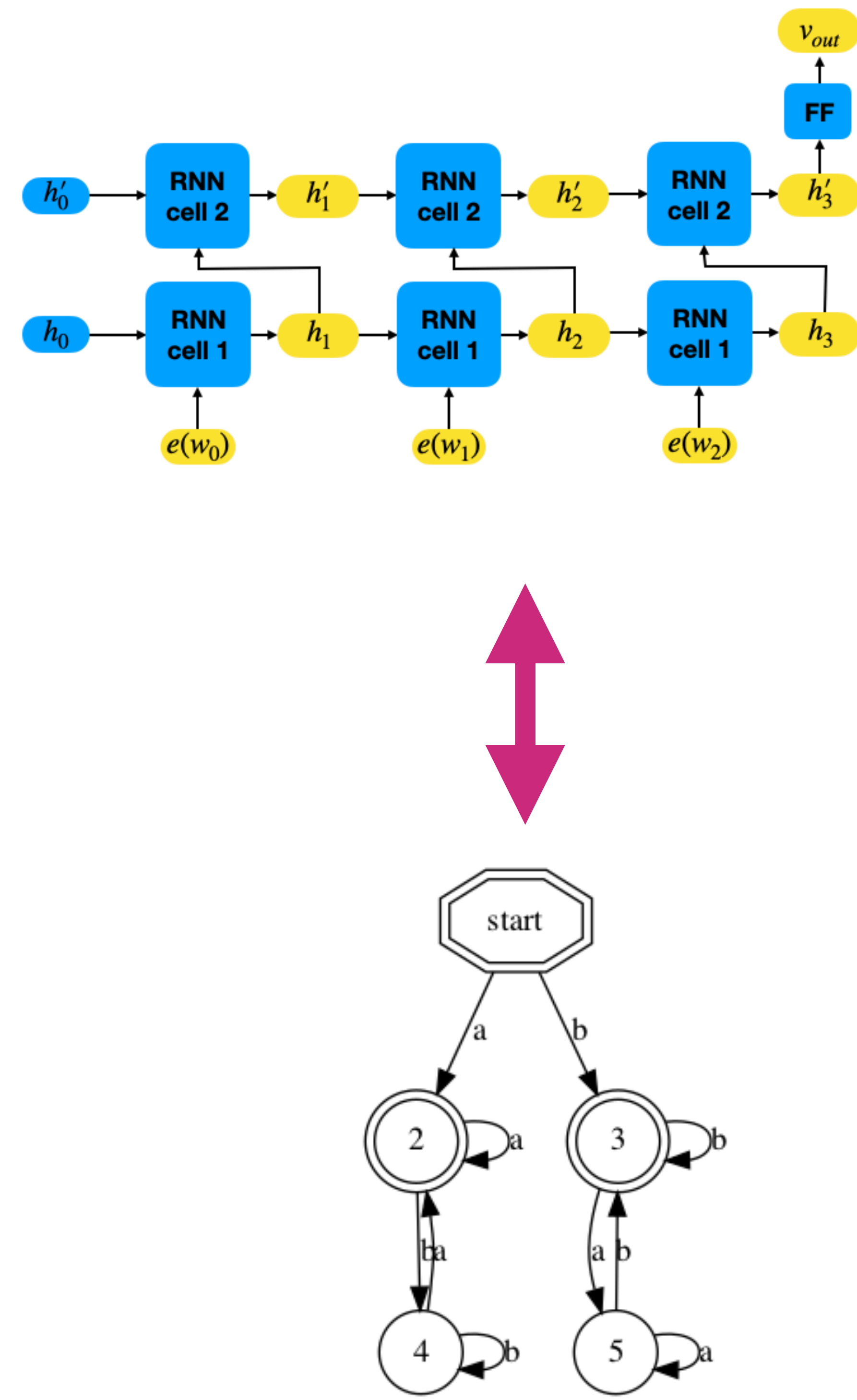
Overview

Recurrent Neural Networks (RNNs)

- Introduction
- RNN-Automata relation
- Extraction
    - DFAs
    - WFAs
    - More
- Analysis

Transformers

- Introduction
- A formal abstraction



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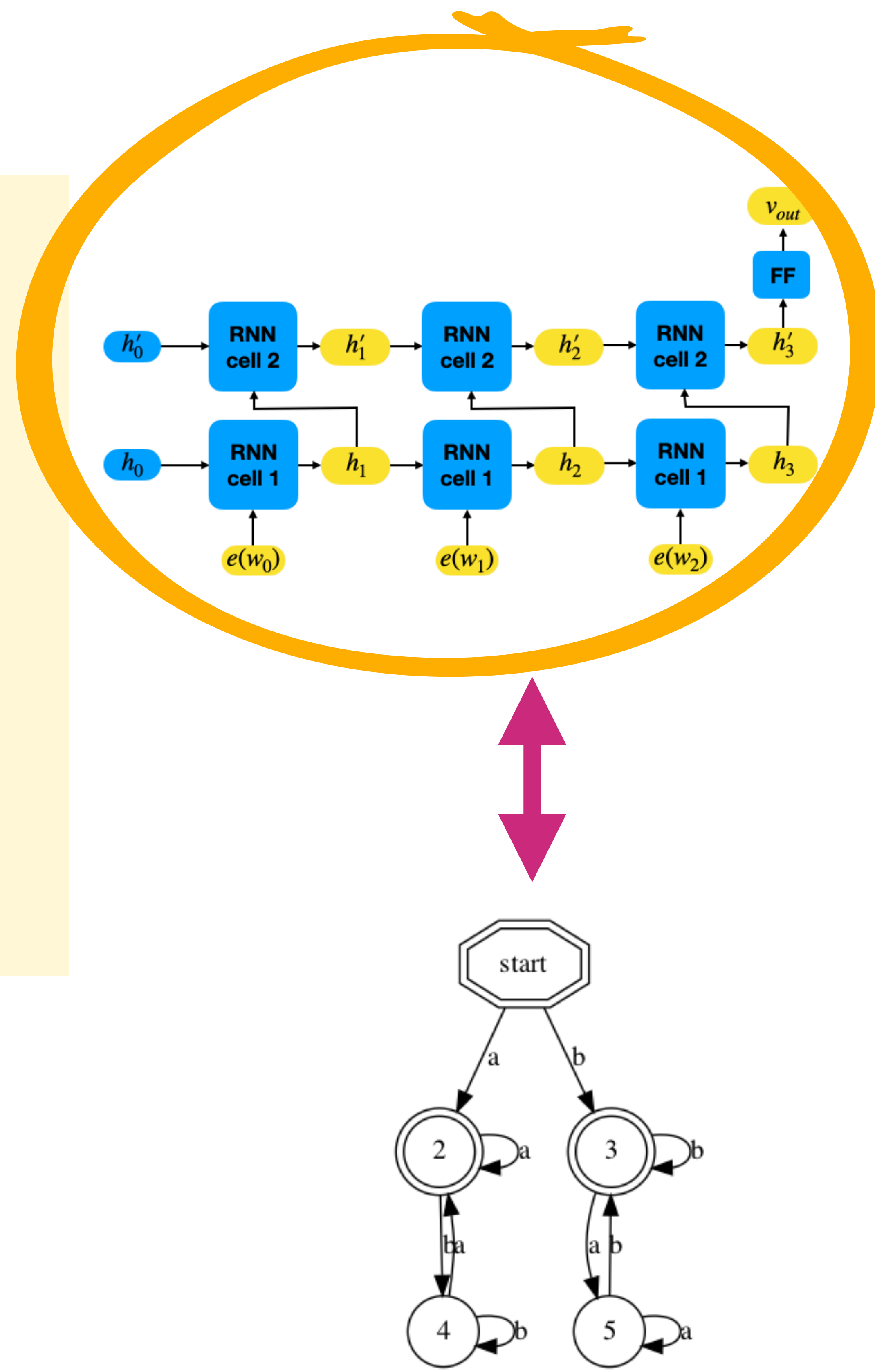
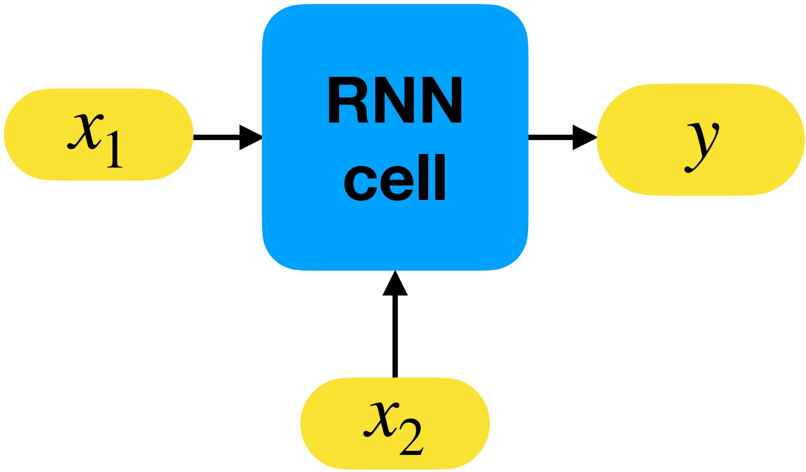


RNNs: Introduction

Finding Structure in Time
- Elman 1990



$x_1, y \in \mathbb{R}^{d_h} \qquad x_2 \in \mathbb{R}^{d_i}$

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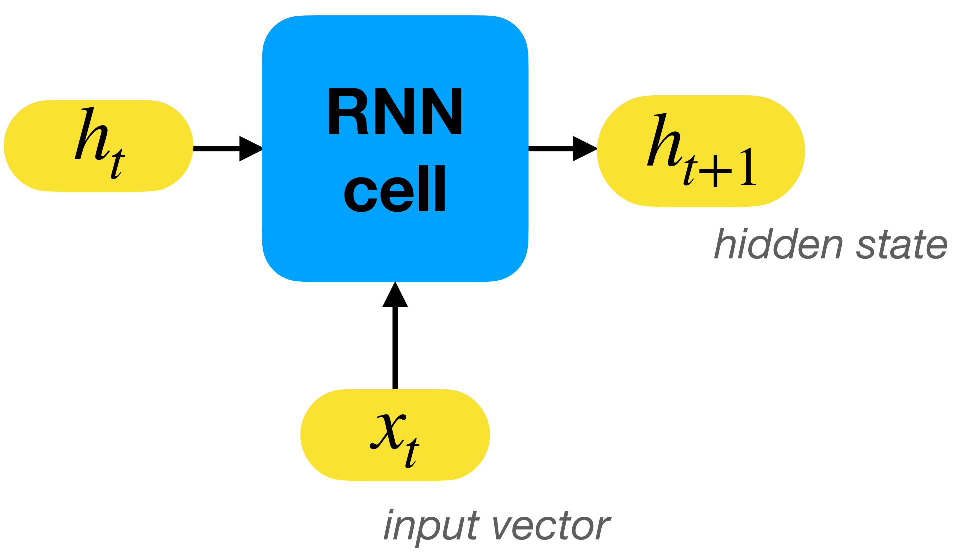

$$\forall t: \quad h_t \in \mathbb{R}^{d_h} \quad x_t \in \mathbb{R}^{d_i}$$

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Finding Structure in Time
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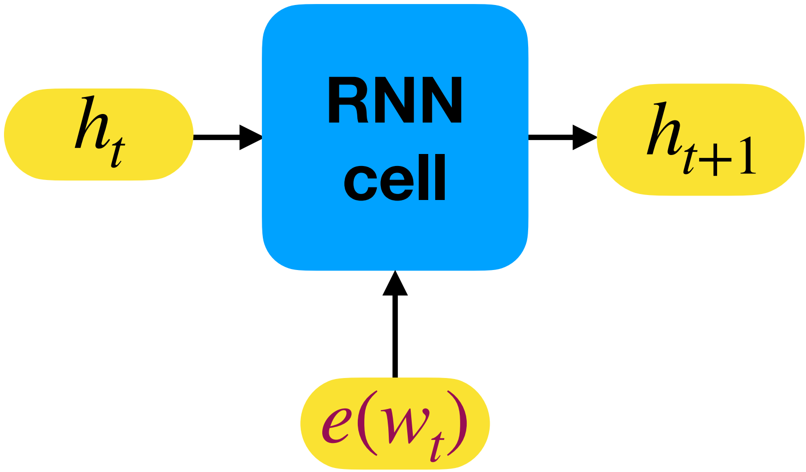
$$e : \Sigma \rightarrow \mathbb{R}^{d_i}$$

input embedding



$$x_t = e(w_t)$$

$$\forall t : \quad h_t \in \mathbb{R}^{d_h} \quad x_t \in \mathbb{R}^{d_i}$$

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Finding Structure in Time
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h_0

initial hidden state

$$e : \Sigma \rightarrow \mathbb{R}^{d_i}$$

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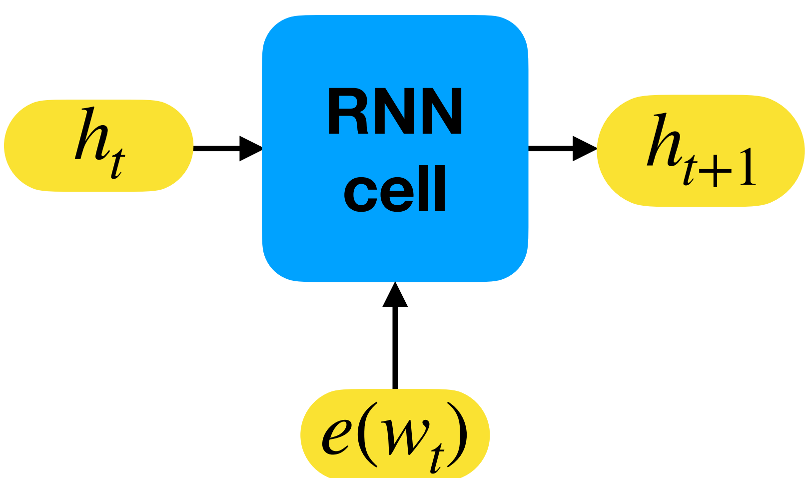

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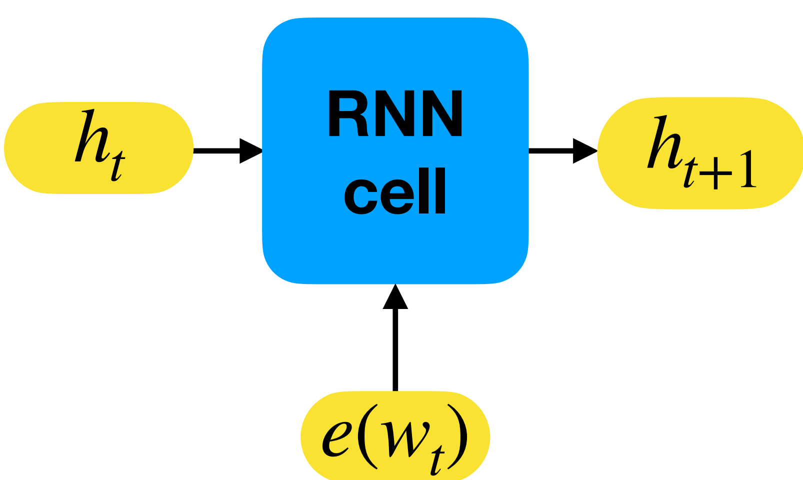

$$w = w_0 w_1 w_2 \in \Sigma^*$$

$$x_t = e(w_t)$$

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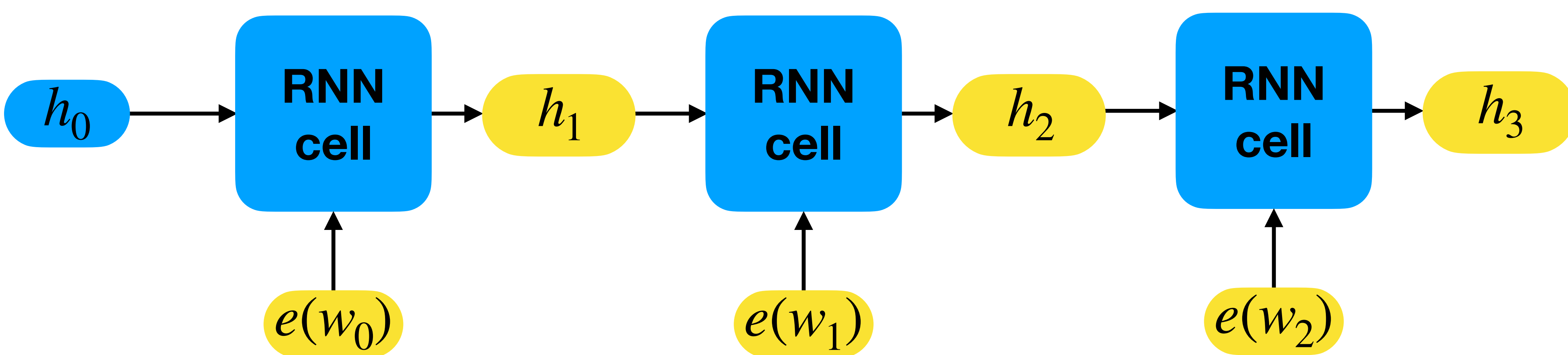

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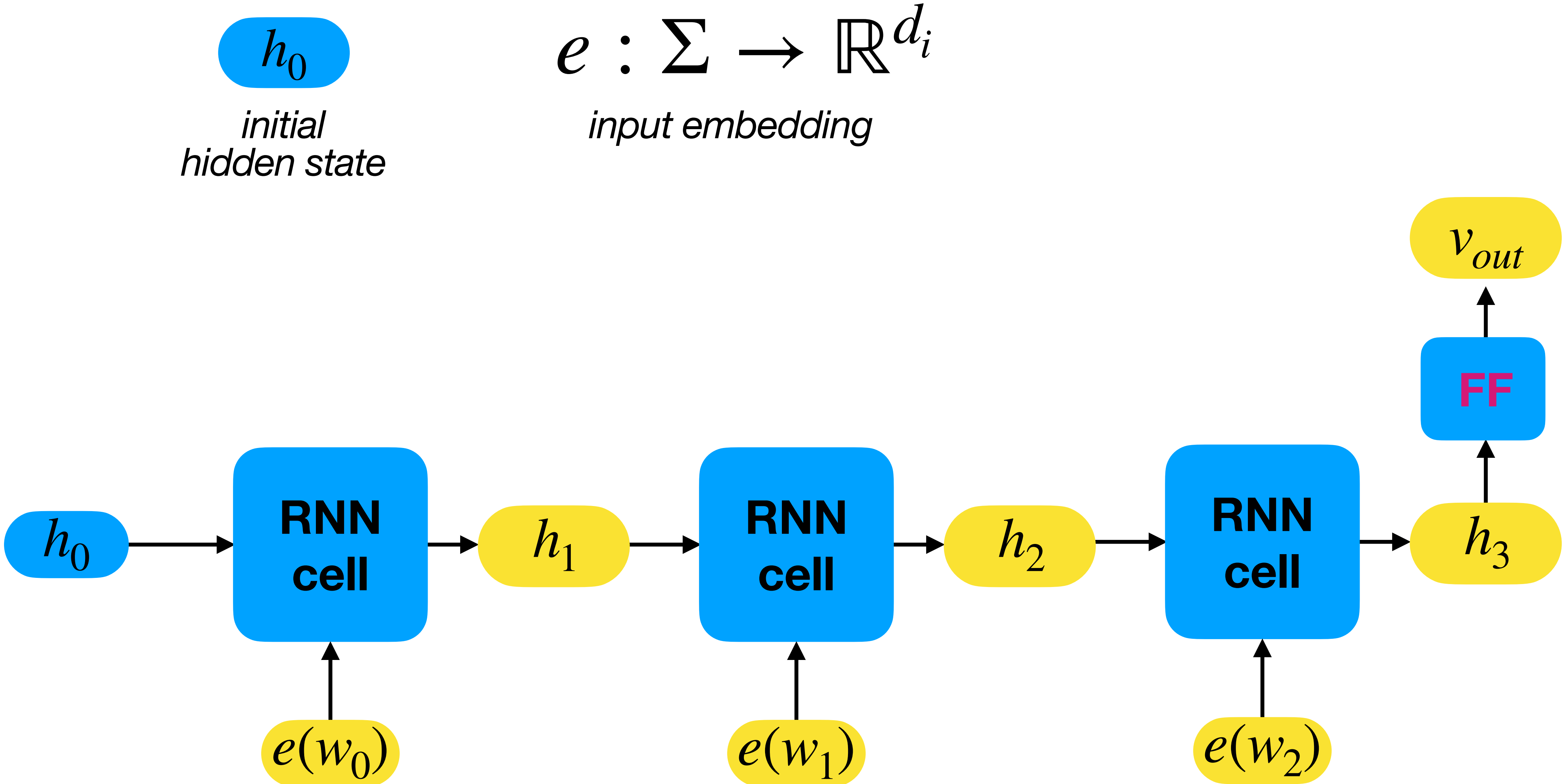

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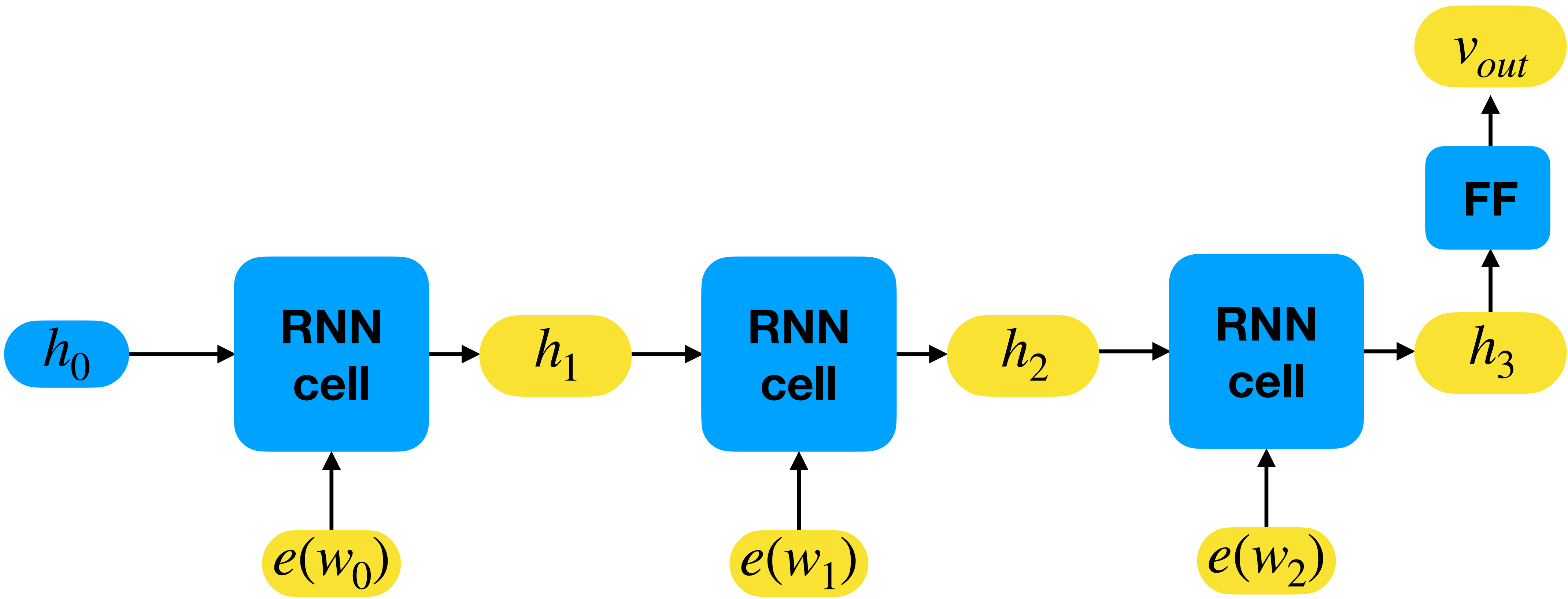

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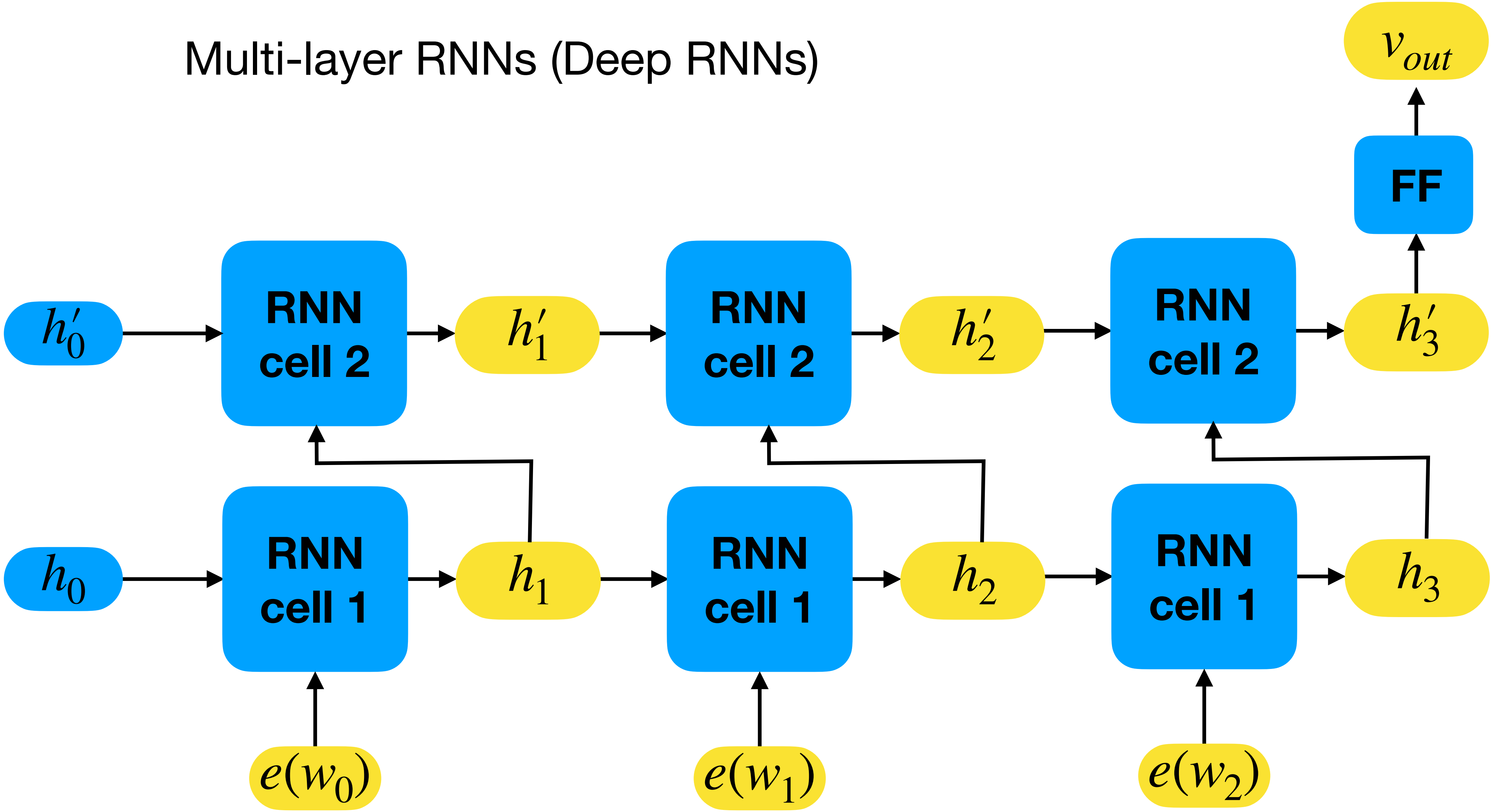
RNNs: Introduction

Multi-layer RNNs (Deep RNNs)



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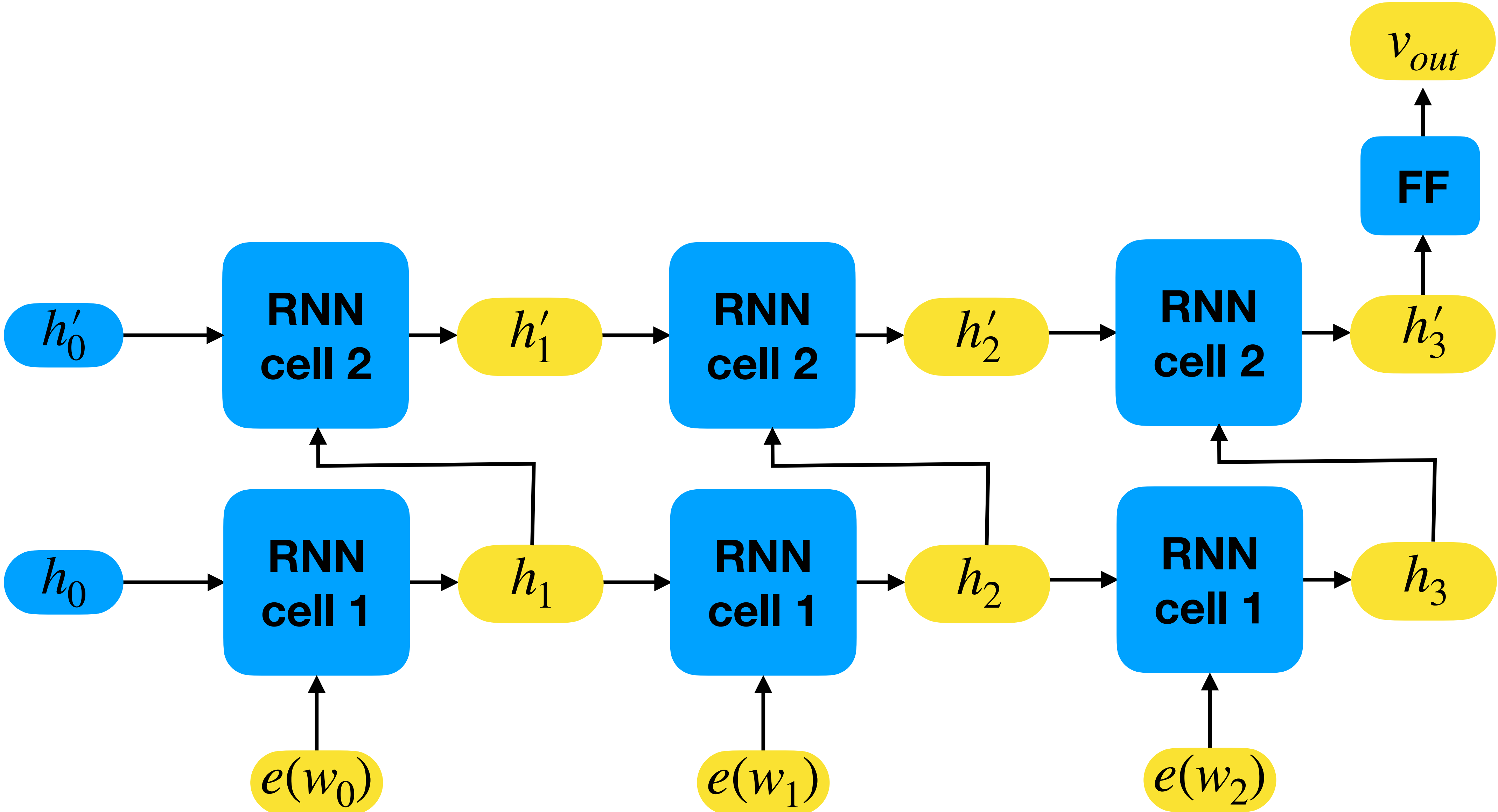

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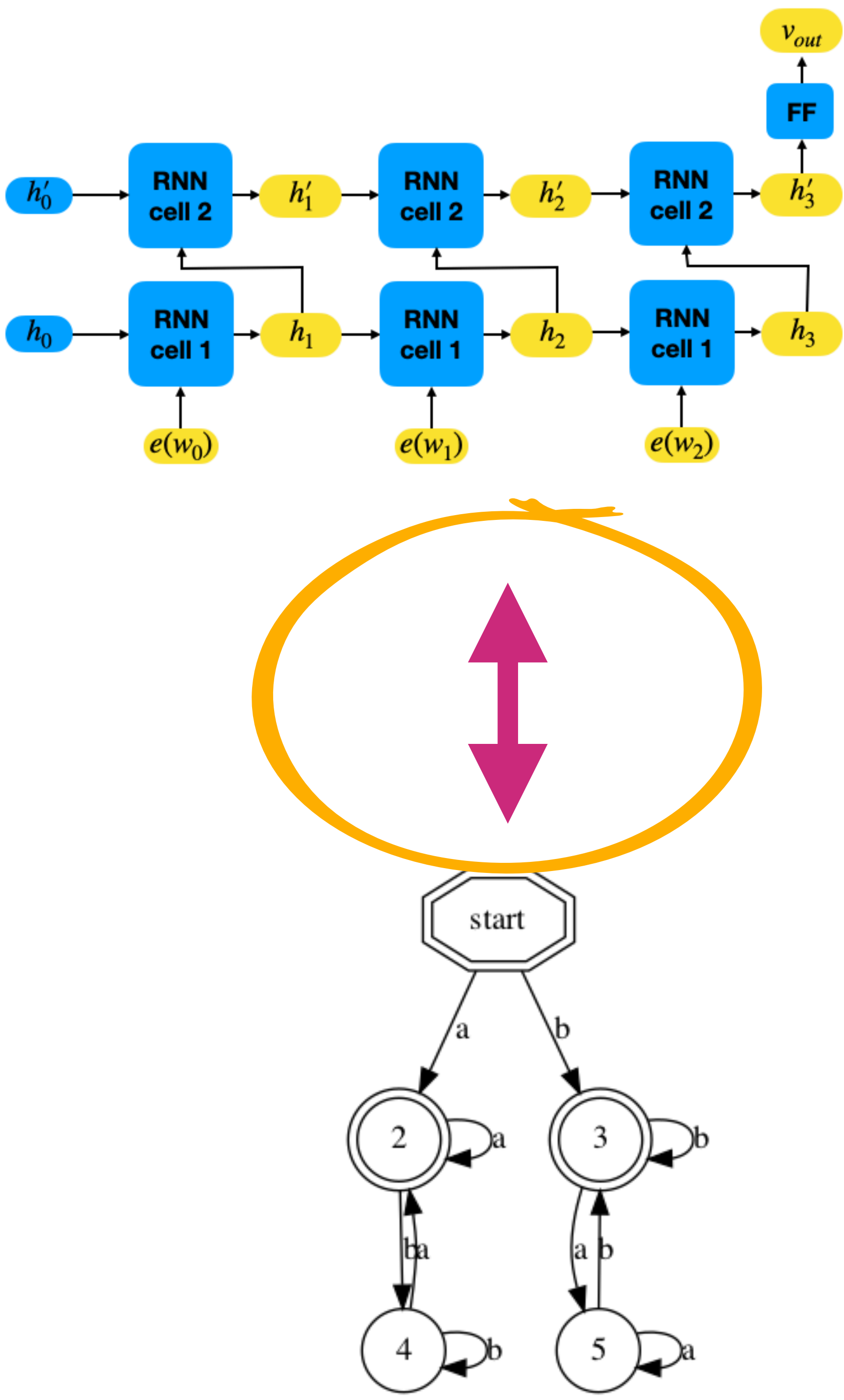
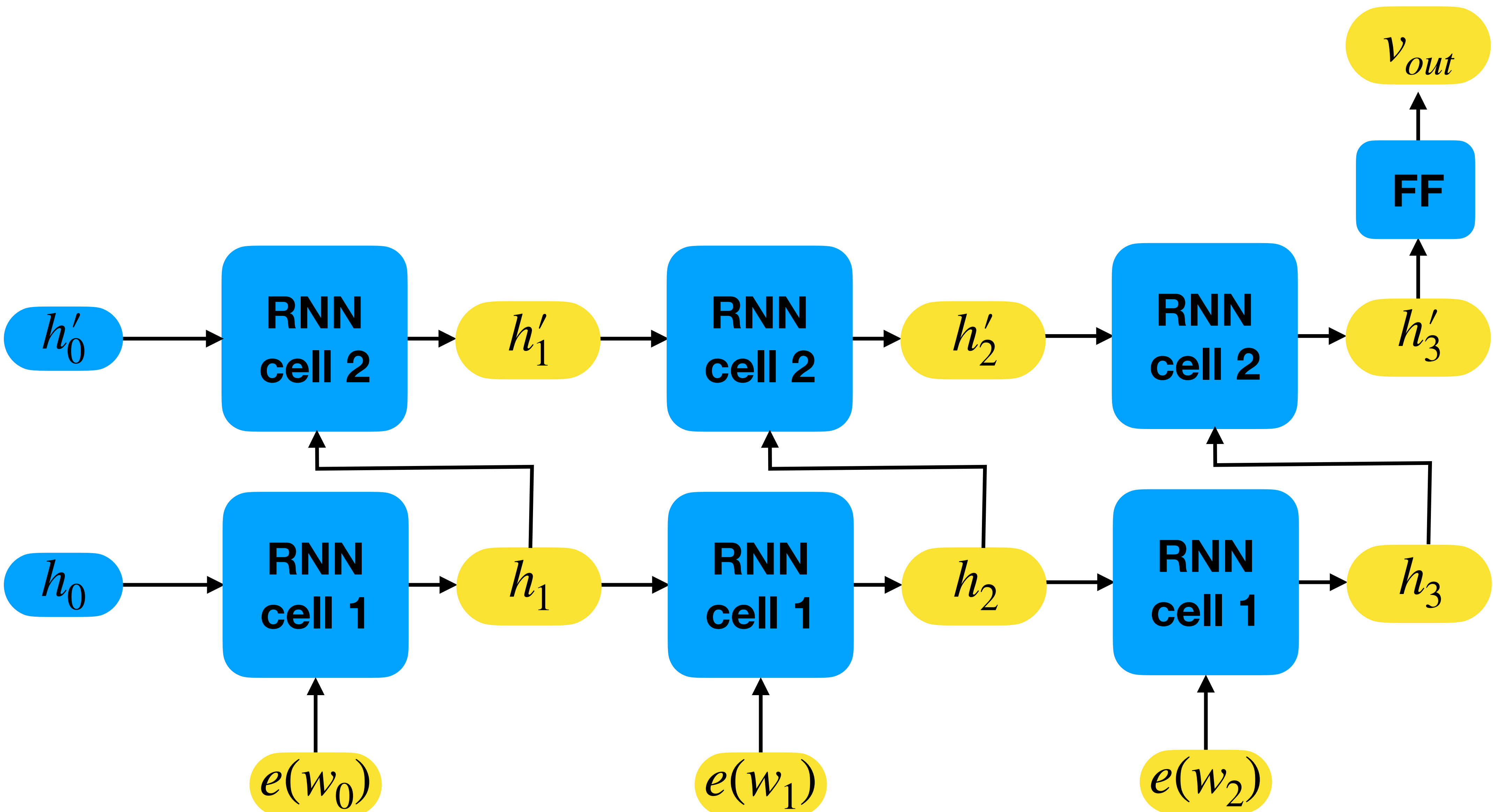


RNNs: Automata Relation



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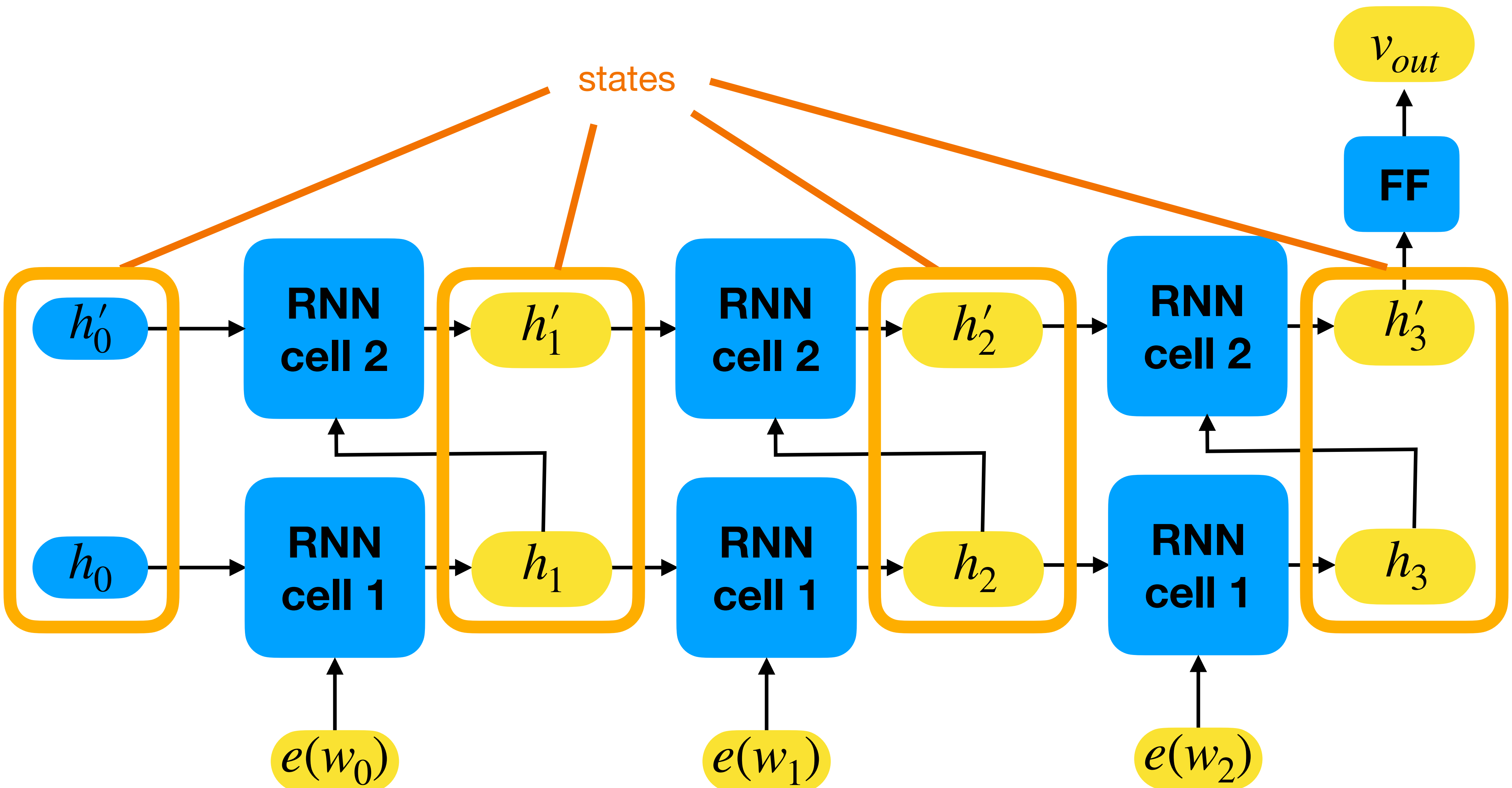

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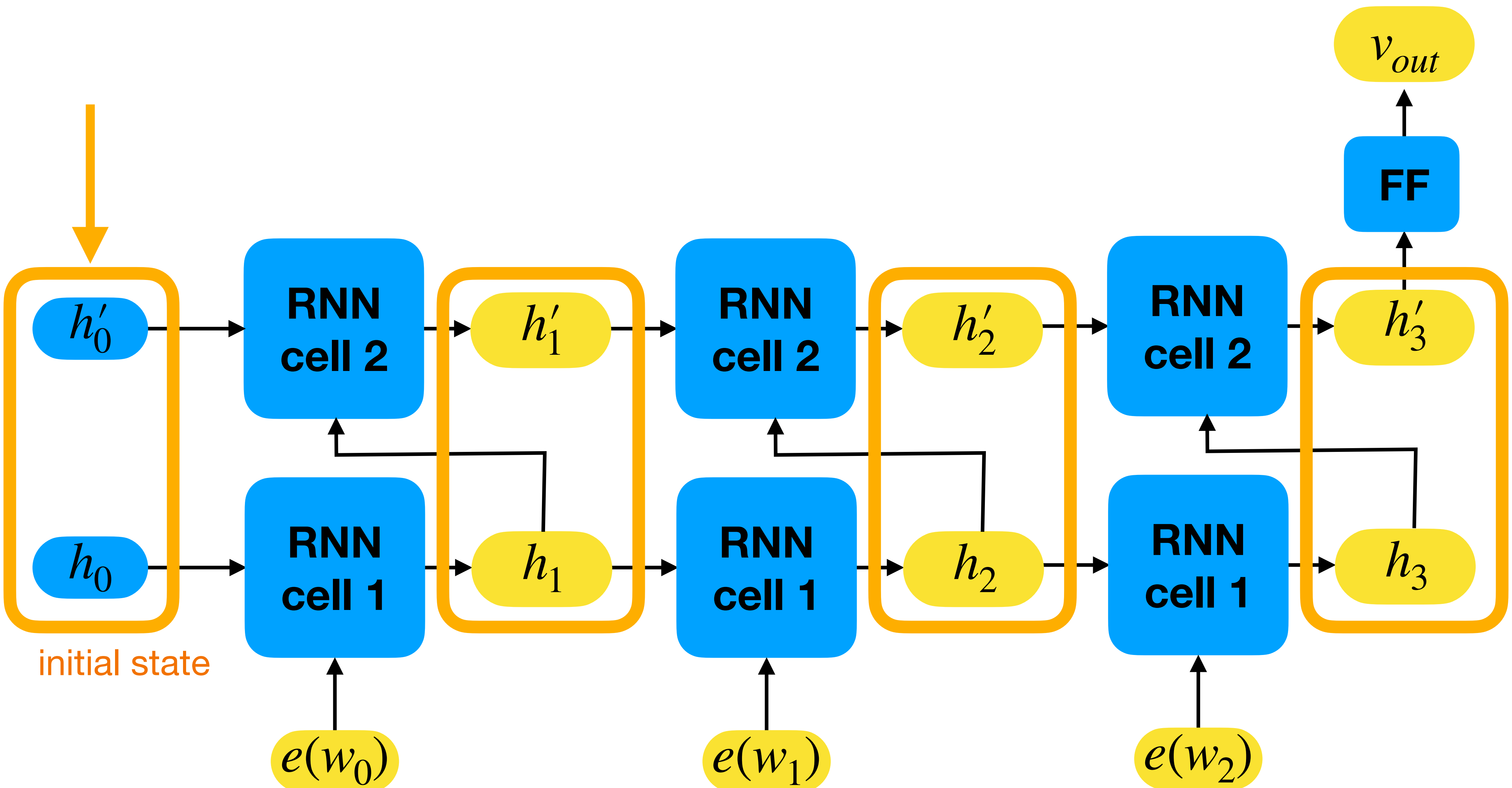

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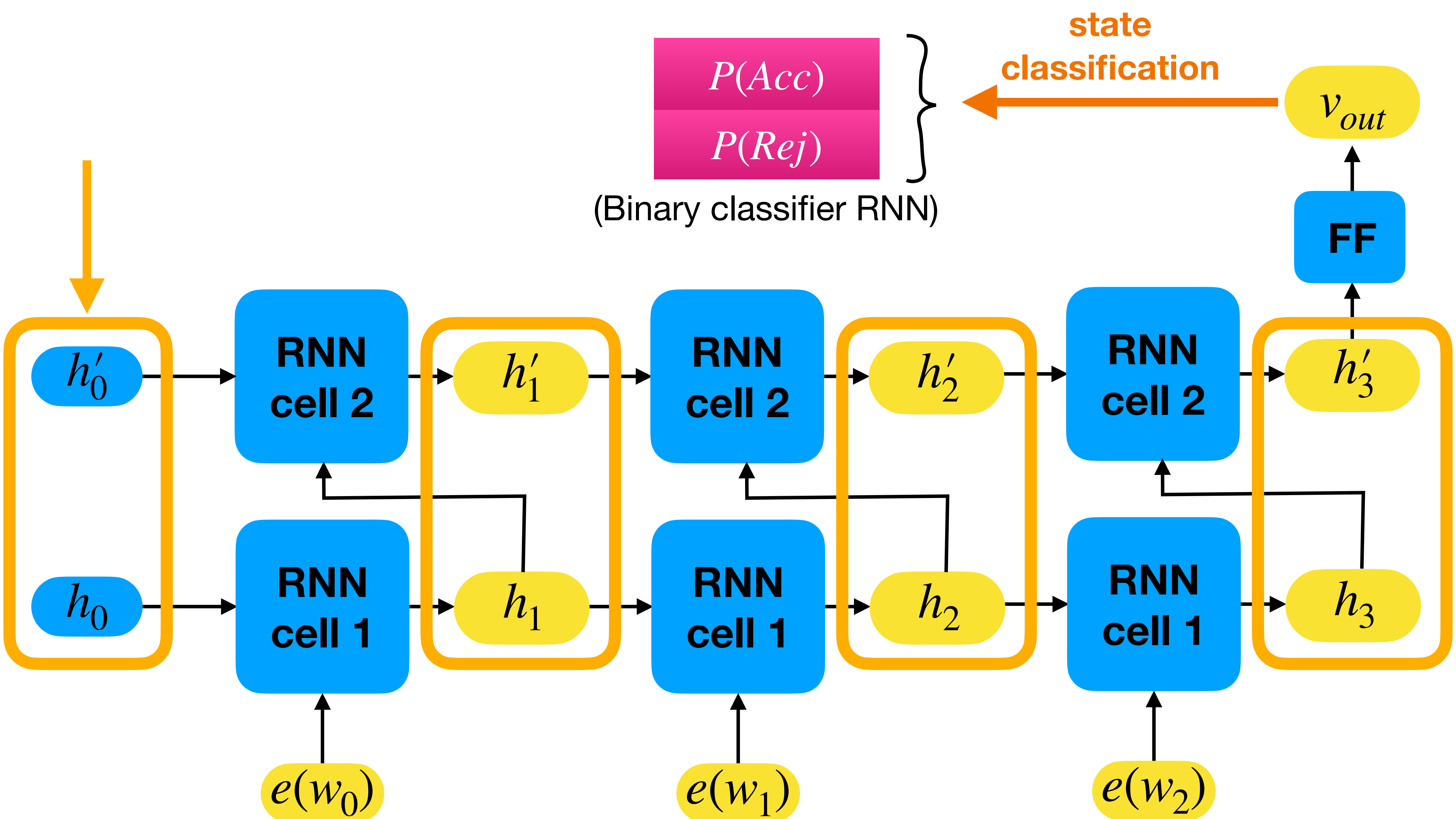

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RNNs: Automata Relation

When learning a regular language, simple RNNs (Elman RNNs) cluster their states in manner that resembles an automaton for that language

Finite State Automata and Simple Recurrent Networks

- Cleeremans et al, 1989 (references older version of Elman 1990)

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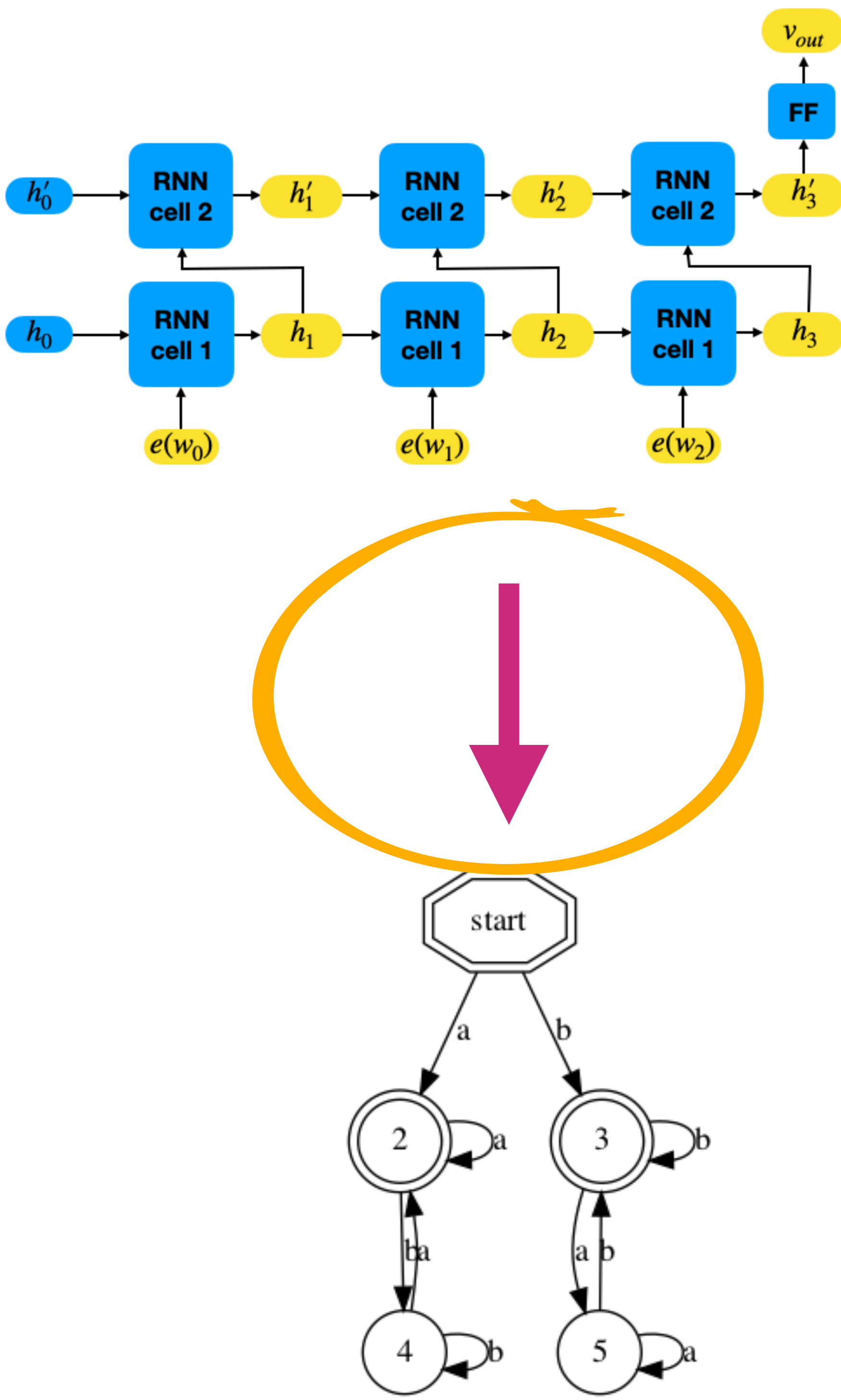

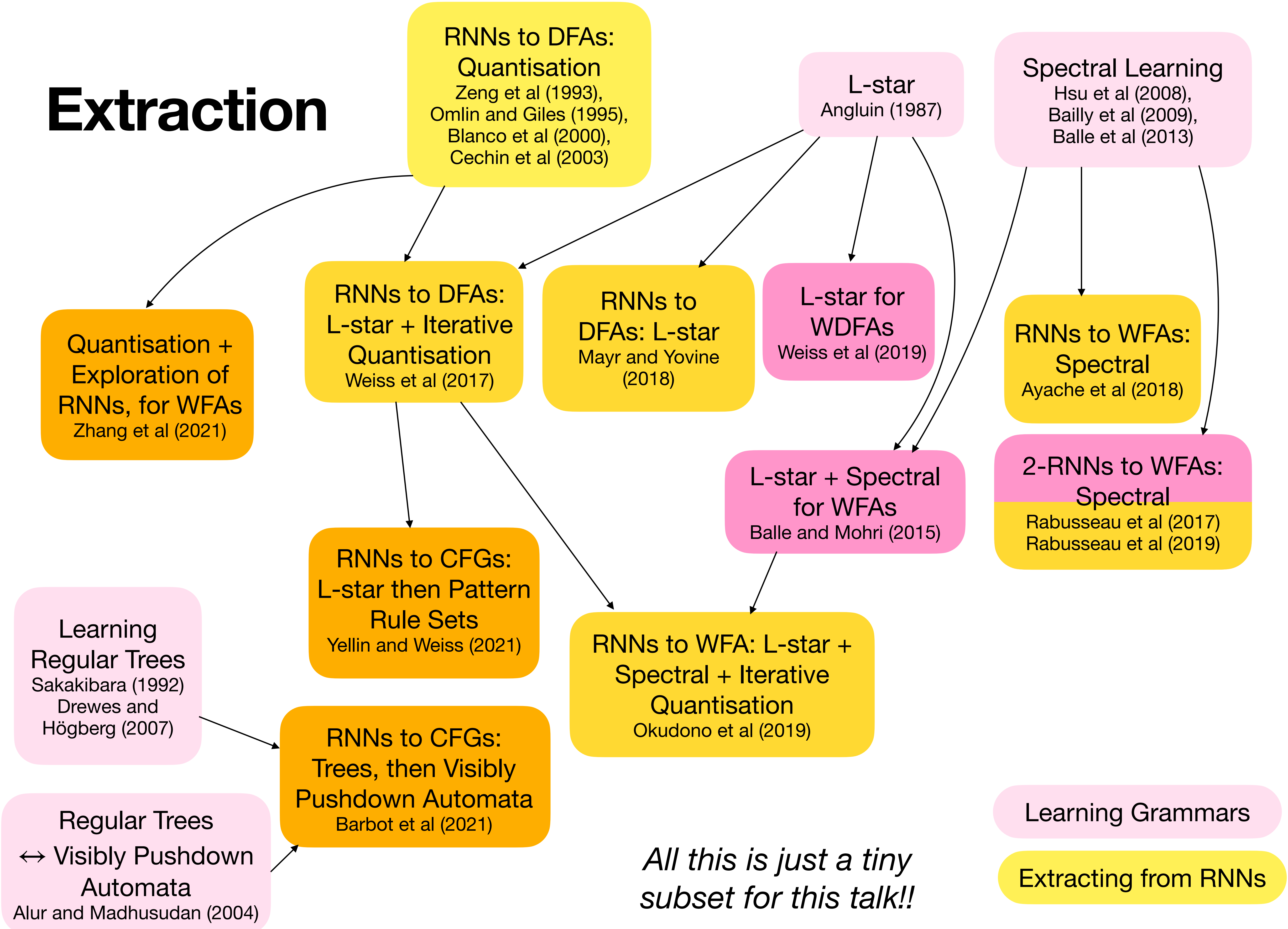

Extraction
RNNs to DFAs: Quantisation
Zeng et al (1993), Omlin and Giles (1995), Blanco et al (2000), Cechin et al (2003)
L-star
Angluin (1987)
Spectral Learning
Hsu et al (2008), Bailly et al (2009), Balle et al (2013)
Quantisation + Exploration of RNNs, for WFAs
Zhang et al (2021)
RNNs to DFAs: L-star + Iterative Quantisation
Weiss et al (2017)
RNNs to DFAs: L-star
Mayr and Yovine (2018)
L-star for WDFAs
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RNNs to WFAs: Spectral
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L-star + Spectral for WFAs
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Rabusseau et al (2017)
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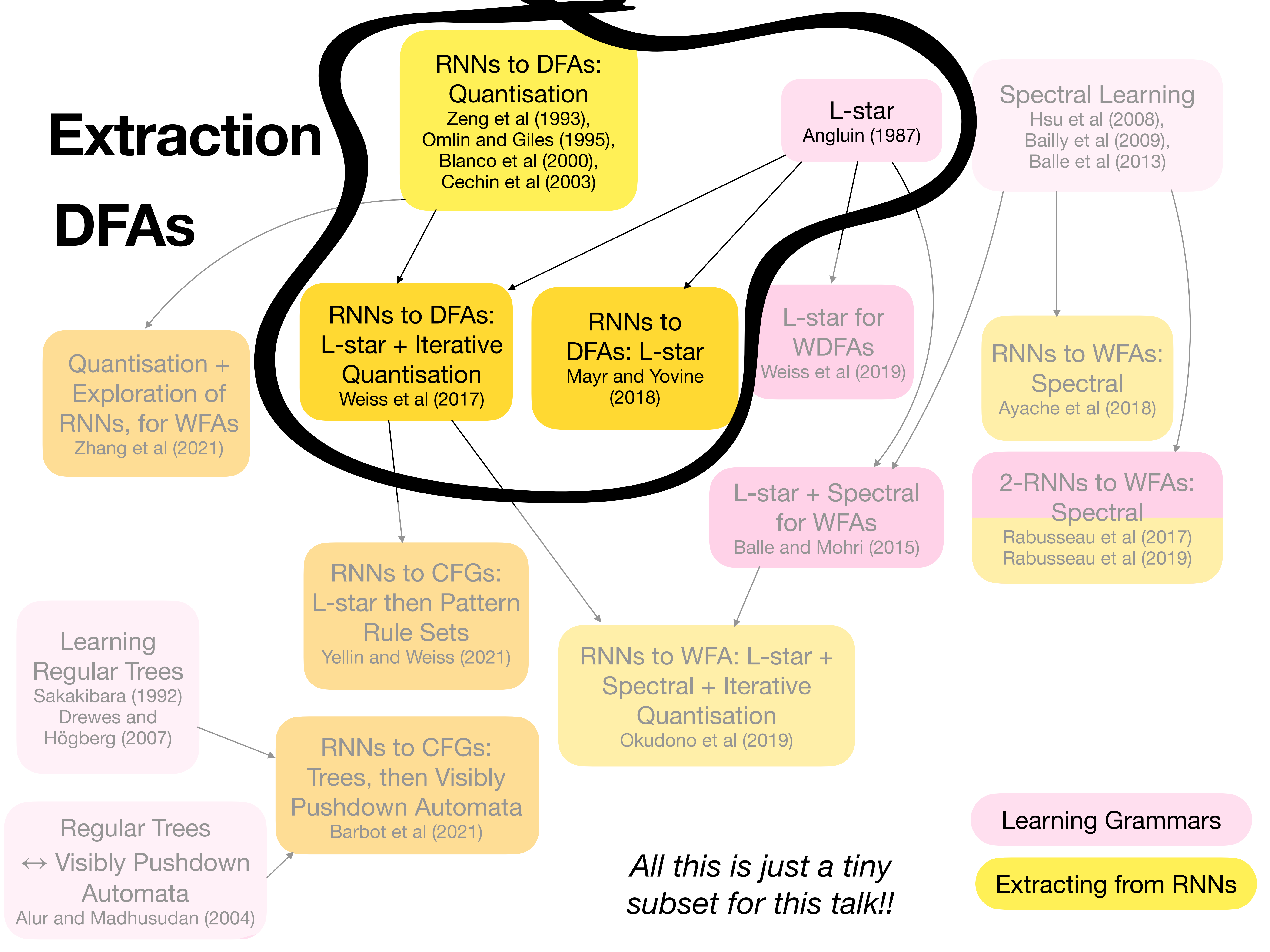
RNNs to CFGs: L-star then Pattern Rule Sets
Yellin and Weiss (2021)
Learning Regular Trees
Sakakibara (1992)
Drewes and Högberg (2007)
RNNs to WFA: L-star + Spectral + Iterative Quantisation
Okudono et al (2019)
RNNs to CFGs: Trees, then Visibly Pushdown Automata
Barbot et al (2021)
Regular Trees ↔ Visibly Pushdown Automata
Alur and Madhusudan (2004)
All this is just a tiny subset for this talk!!
Learning Grammars
Extracting from RNNs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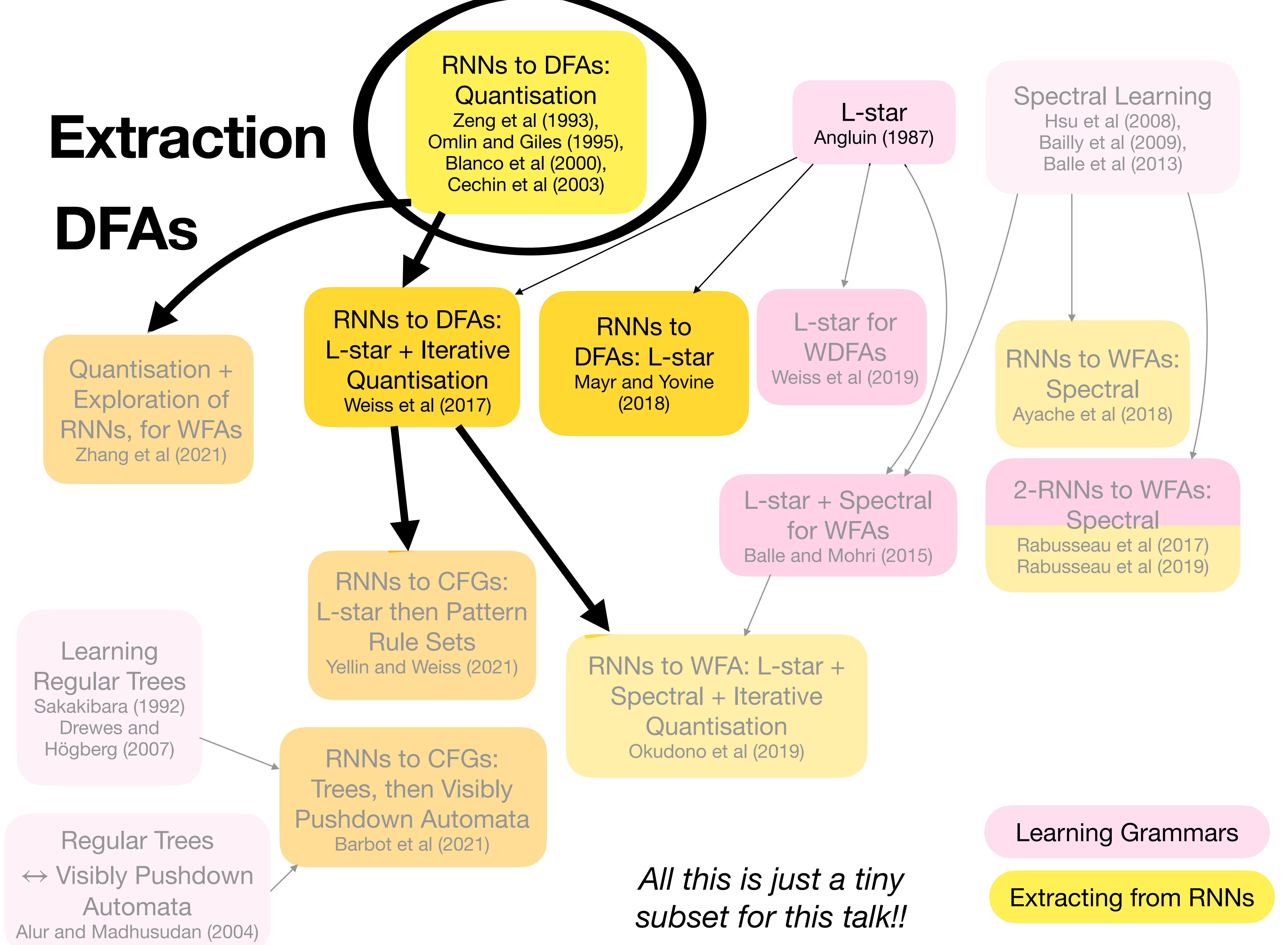
Extraction DFAs



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RNNs: Extracting DFAs: Clustering

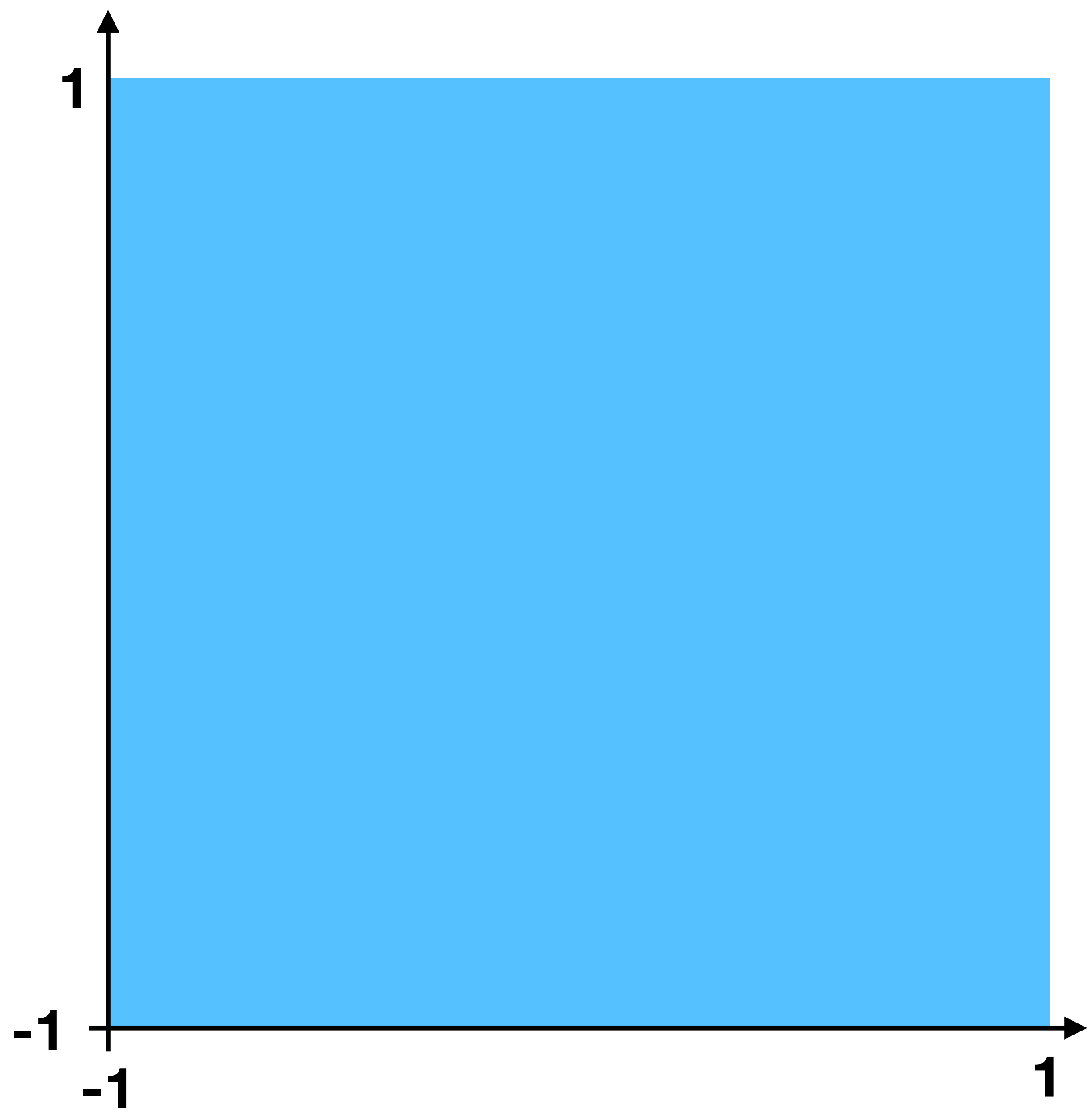
Omlin and Giles, 1996

Partition the RNN state space by dividing each dimension into q equal portions. Explore the partitions, marking transitions between them according to first-visited state in each partition

Extraction of Rules from Discrete-time Recurrent Neural Networks

RNNs: Extracting DFAs: Clustering

Quantisation, example (on RNN with total hidden state dimension 2)



Input alphabet: {a,b}

Extraction of Rules from Discrete-time Recurrent Neural Networks
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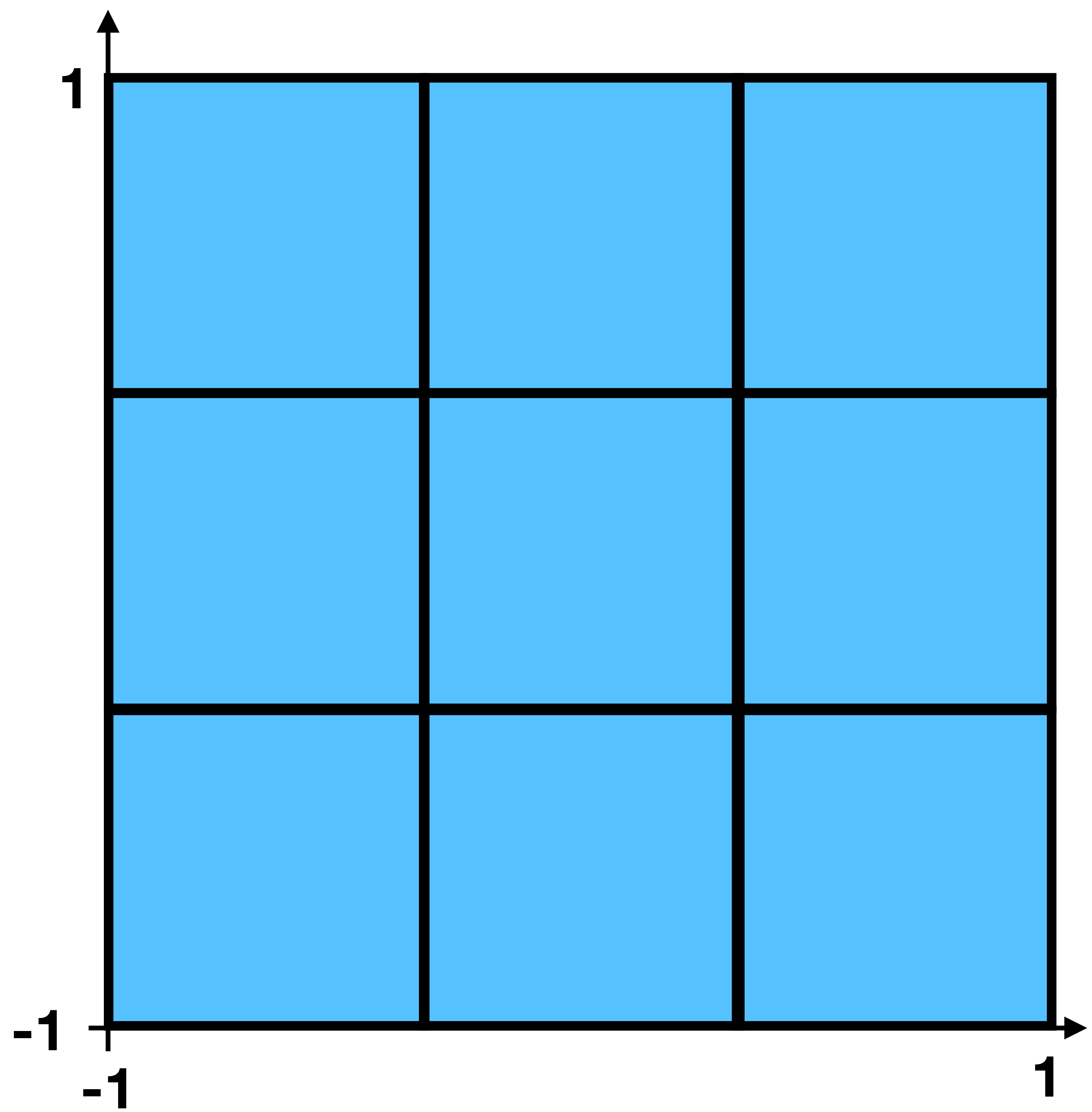

Input alphabet: {a,b}

quantisation level: $q = 3$

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RNNs: Extracting DFAs: Clustering

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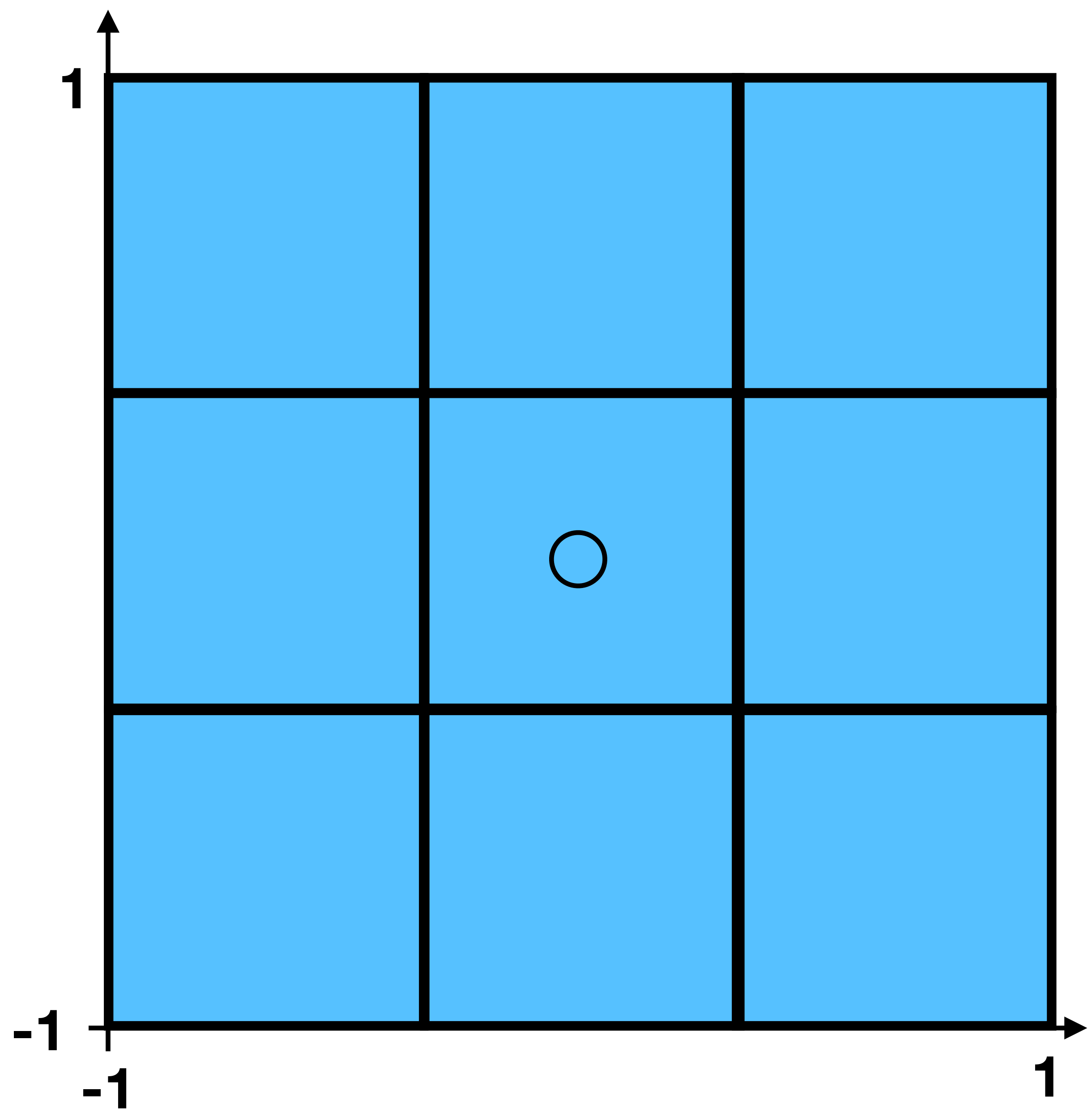

Input alphabet: {a,b}

○ Initial state: (0,0)

quantisation level: $q = 3$

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RNNs: Extracting DFAs: Clustering

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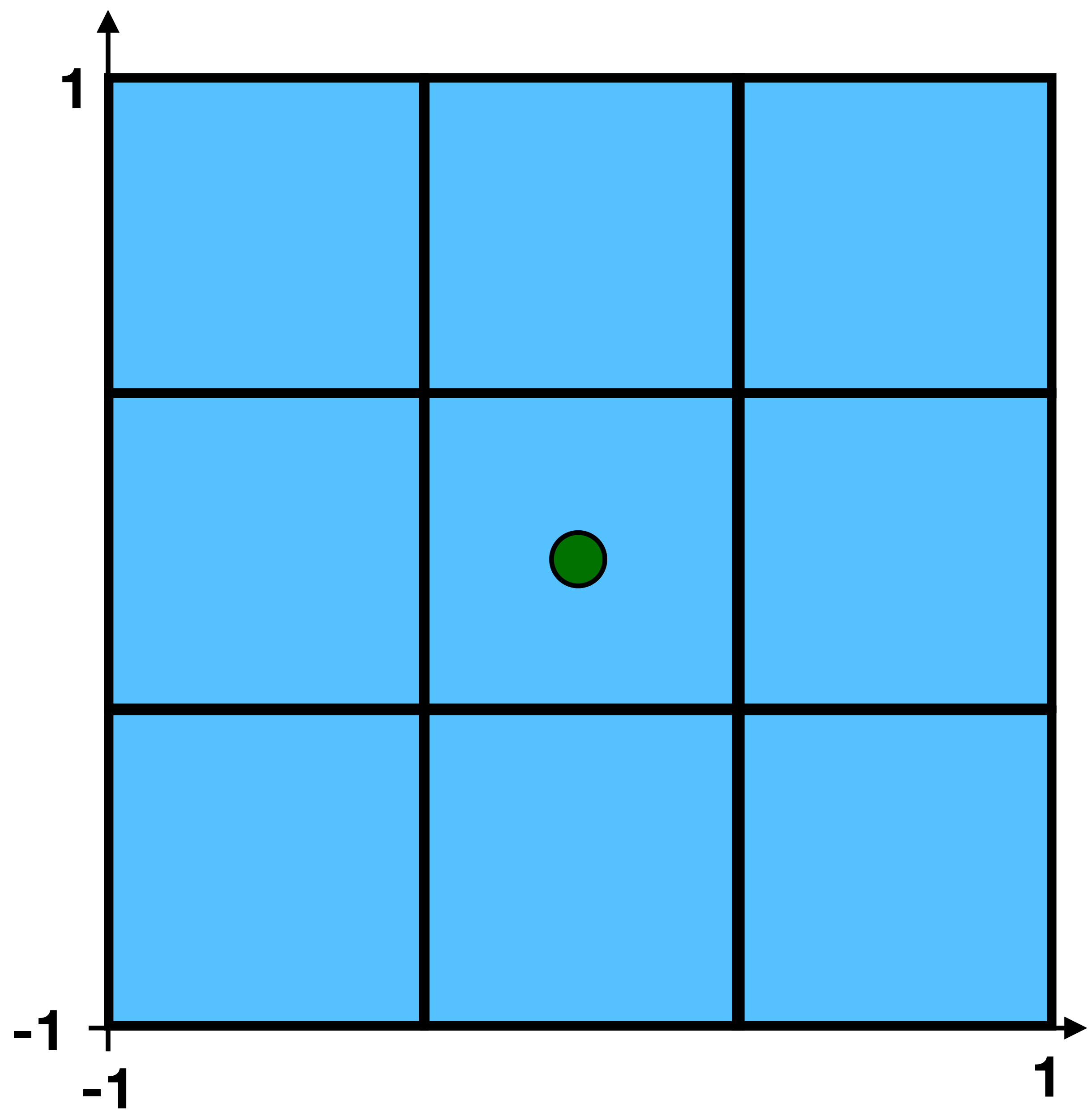

Input alphabet: {a,b}

Initial state: (0,0)

Accepting state

Rejecting state

quantisation level: $q = 3$

Extraction of Rules from Discrete-time Recurrent Neural Networks
- Omlin and Giles, 1996

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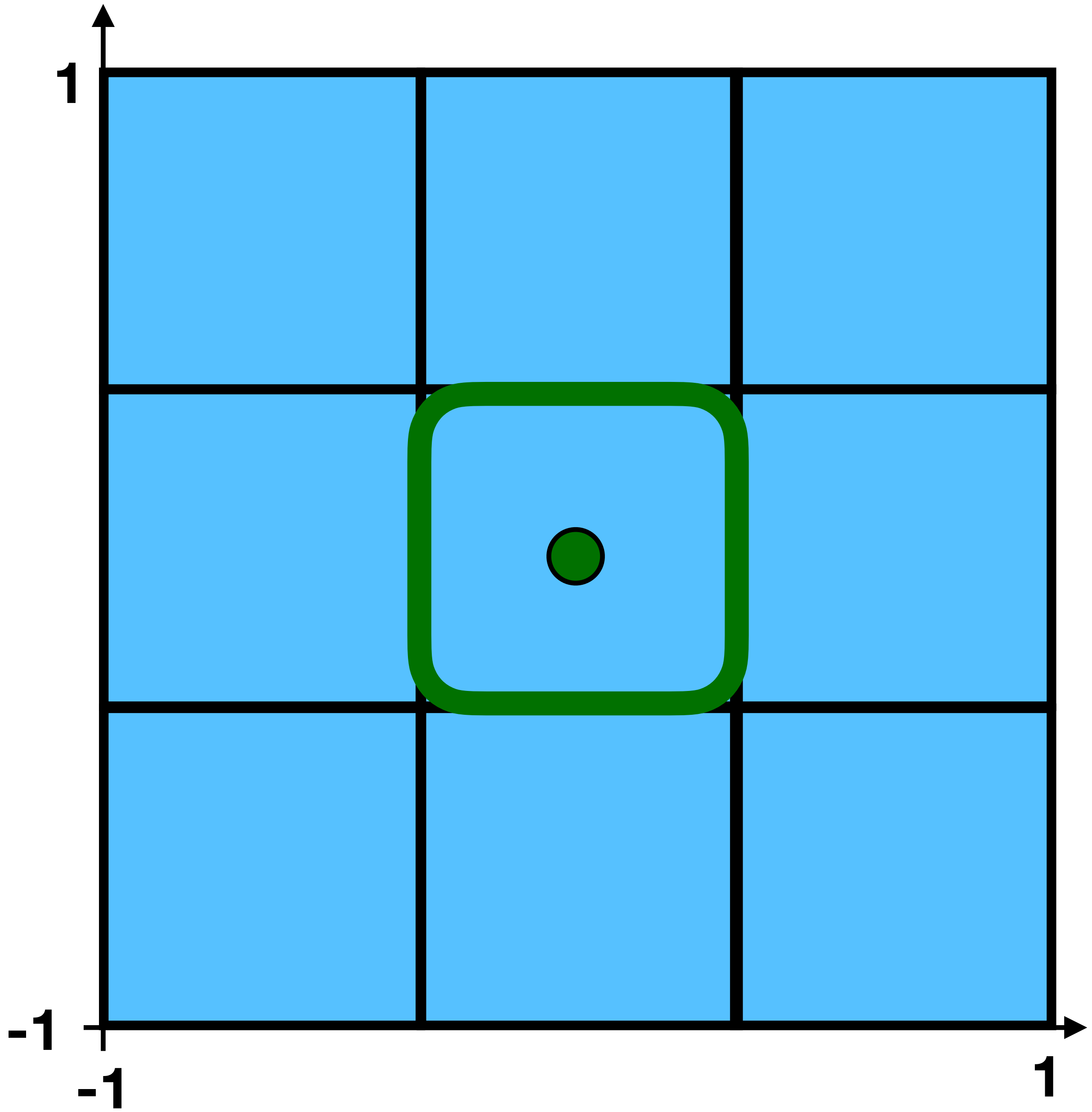

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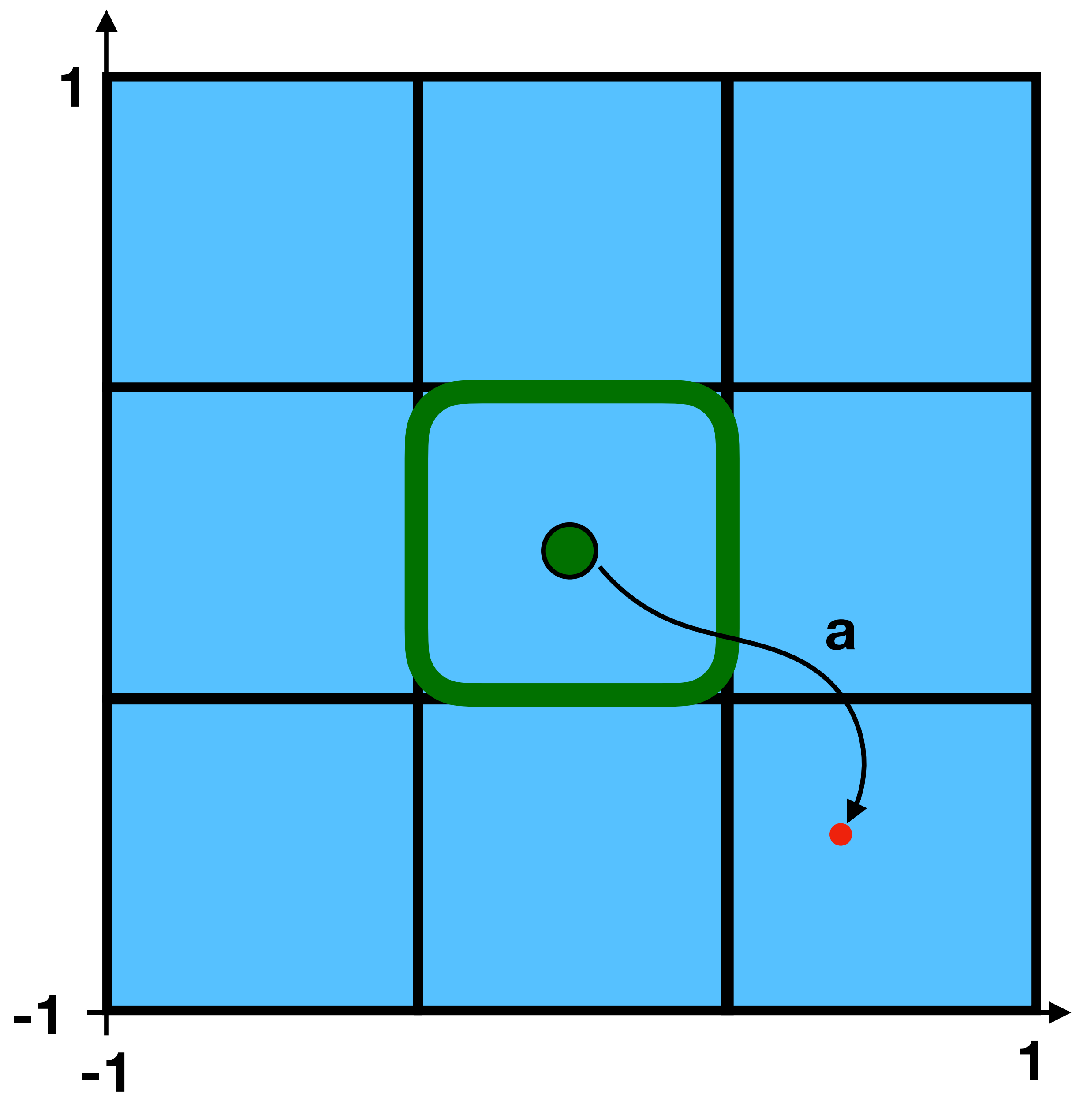

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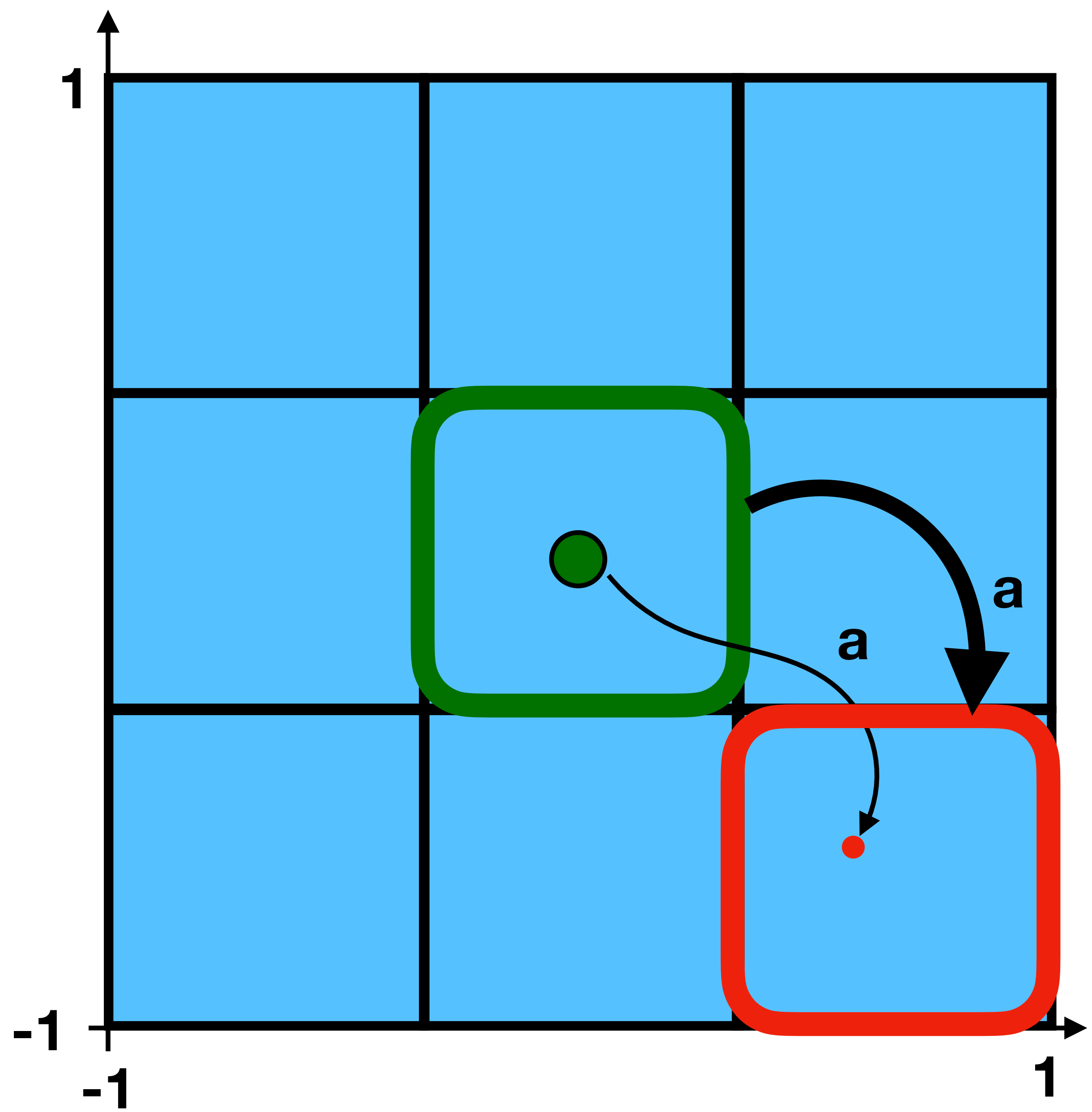

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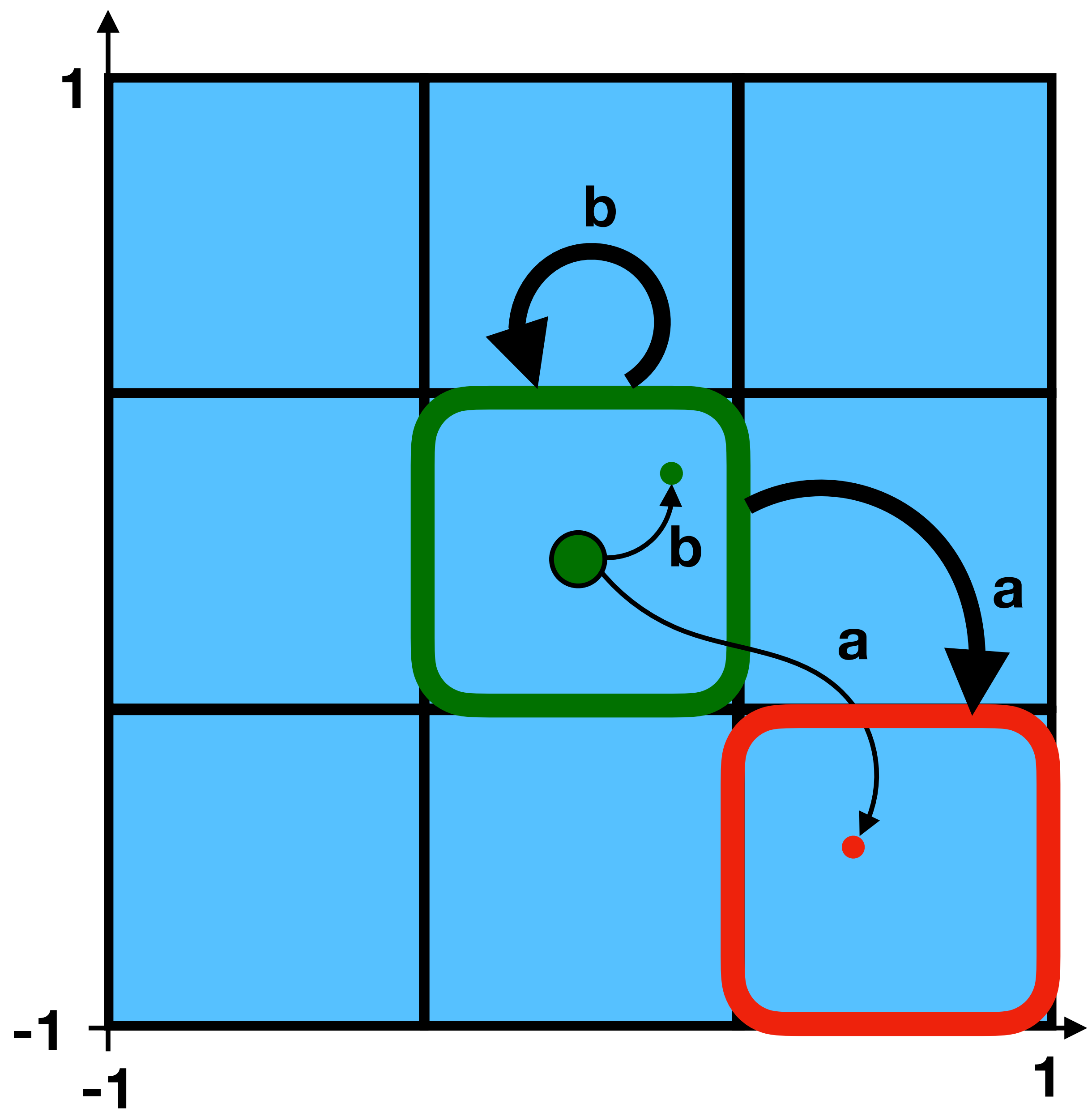

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Initial state: (0,0)

Accepting state

Rejecting state

quantisation level: $q = 3$

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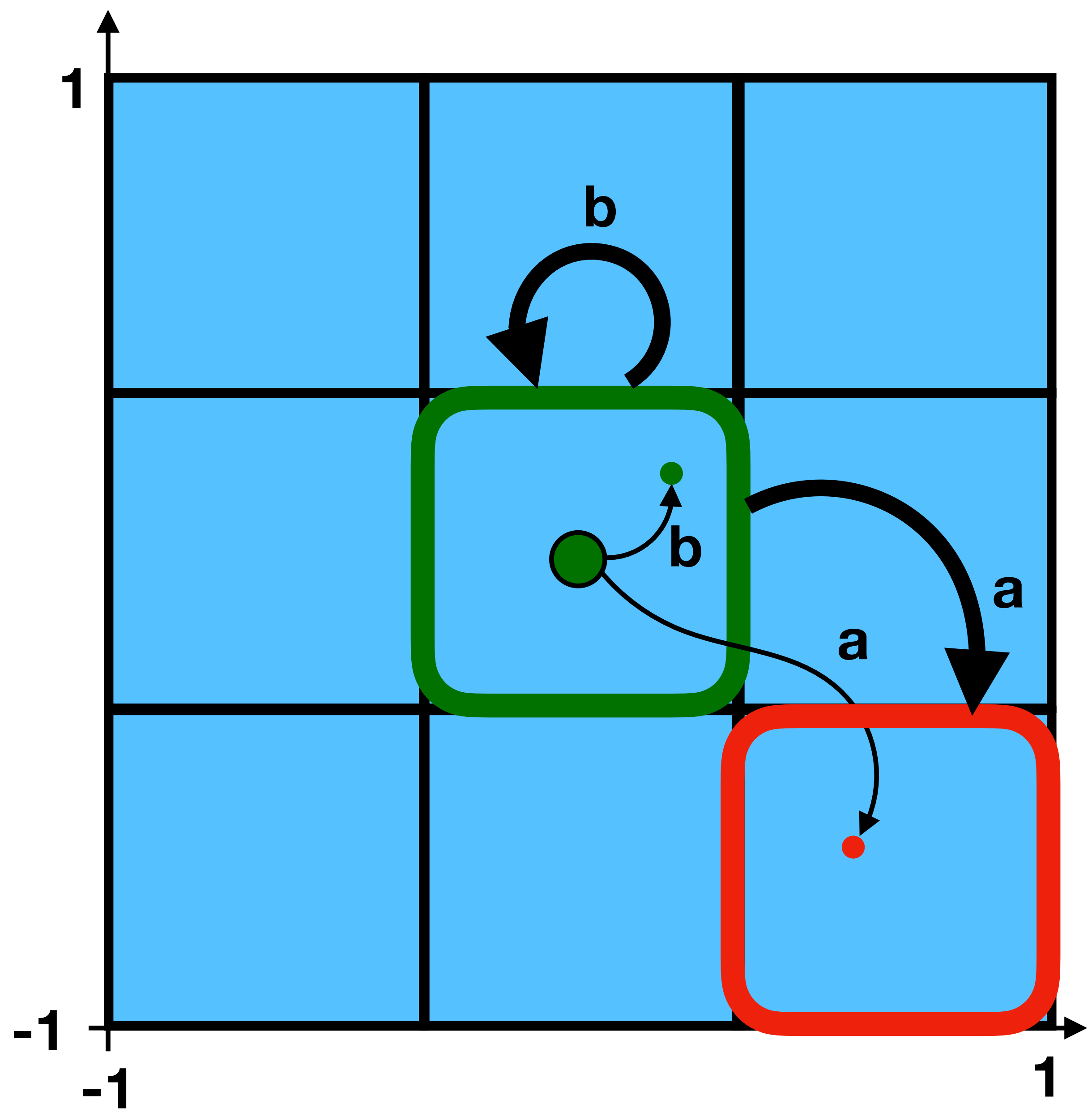

Input alphabet: {a,b}

Initial state: (0,0)

Accepting state

Rejecting state

etc…

quantisation level: $q = 3$

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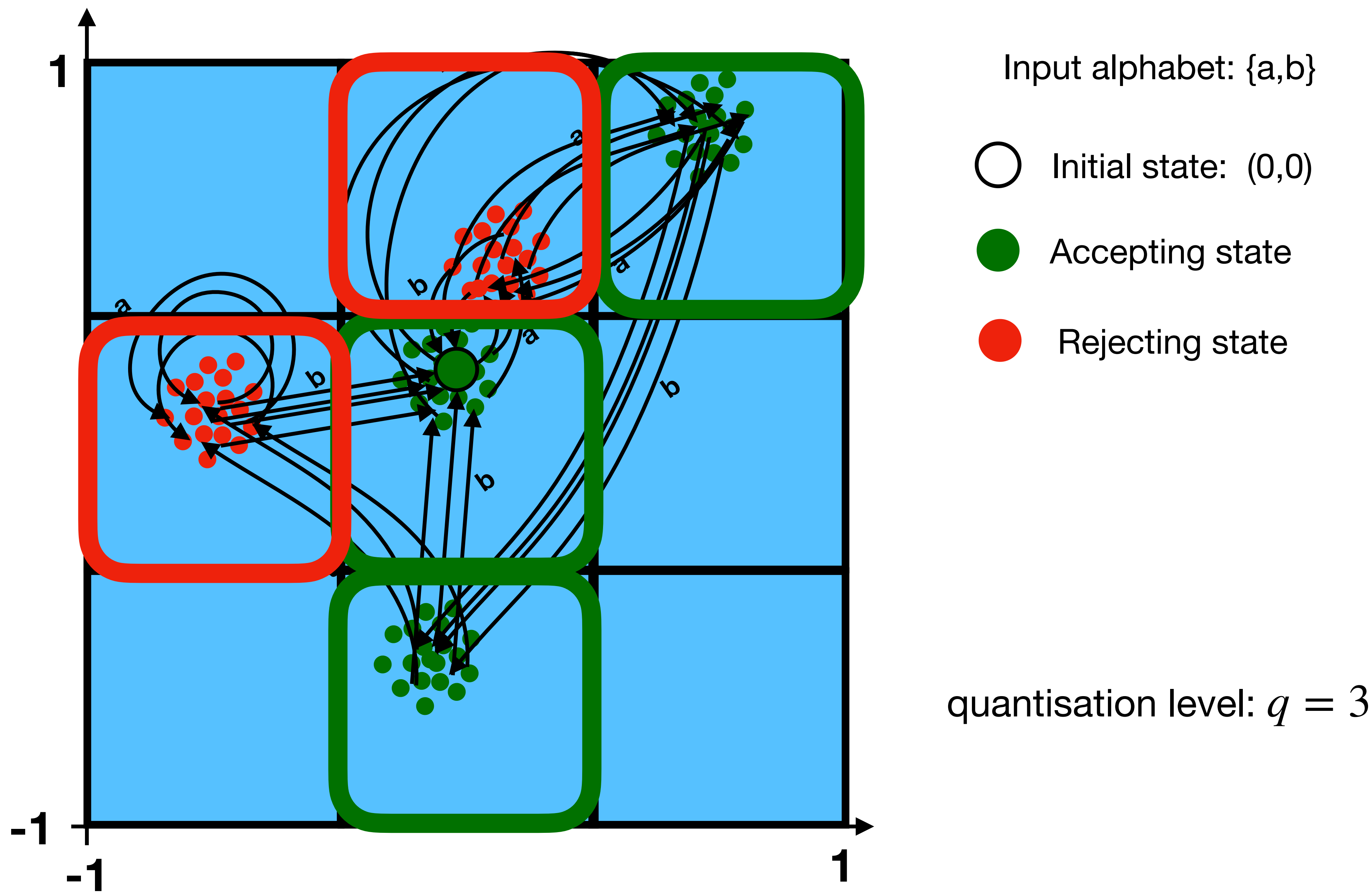

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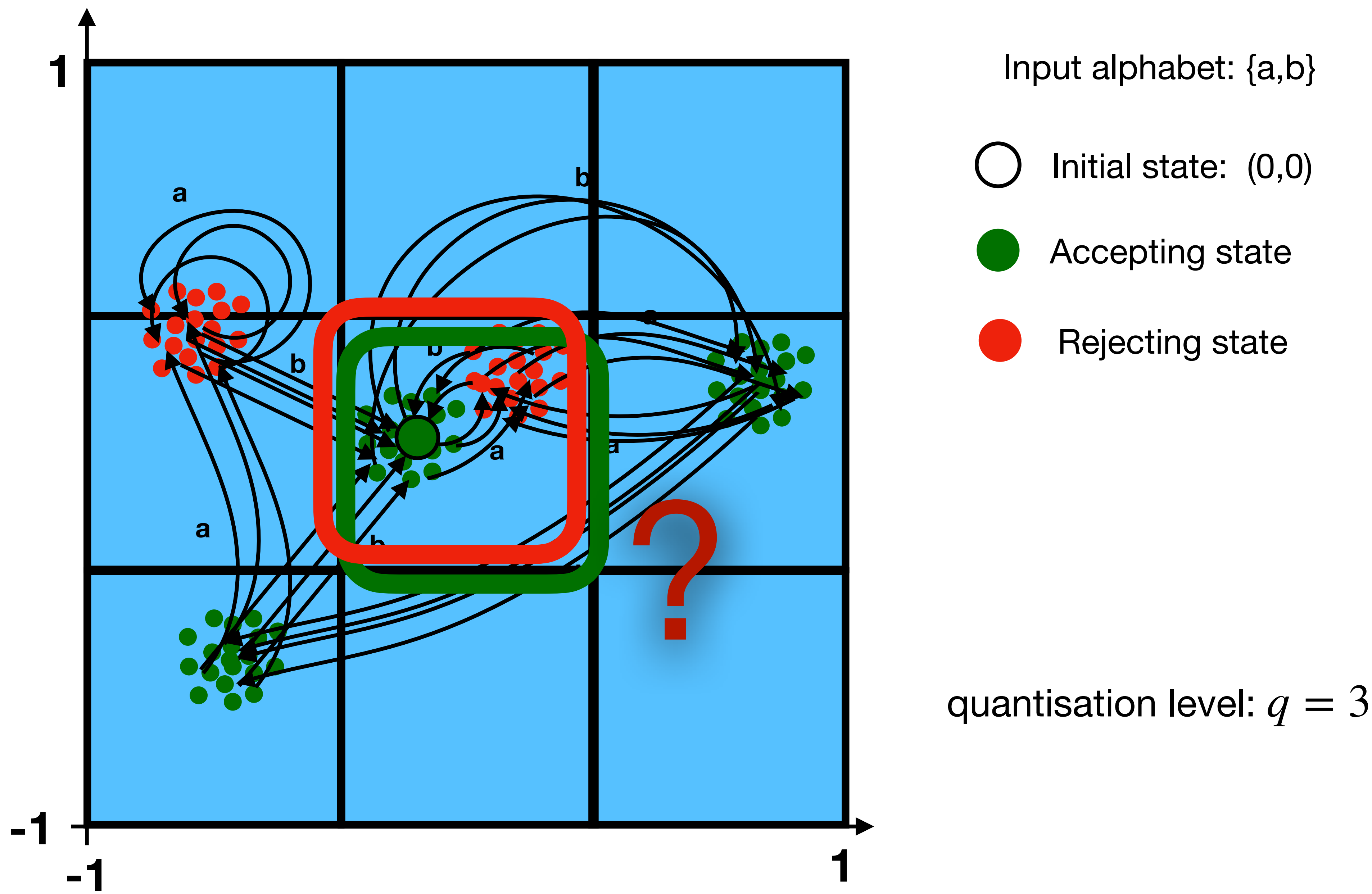

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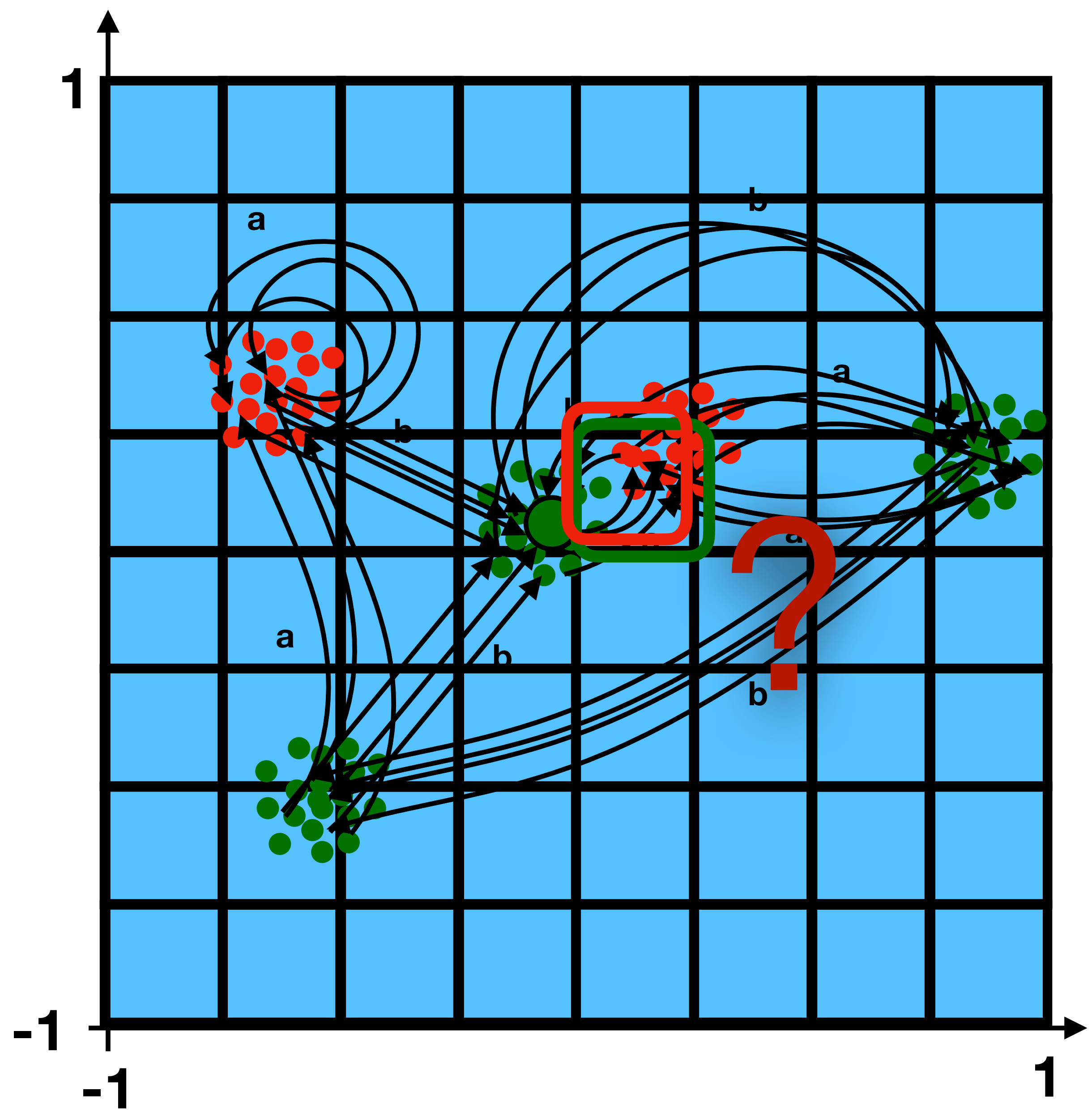


Input alphabet: {a,b}

Initial state: (0,0)

Accepting state

Rejecting state

quantisation level: $q = 8$

Extraction of Rules from Discrete-time Recurrent Neural Networks

- Omlin and Giles, 1996

RNNs: Extracting DFAs: Clustering

Other approaches to clustering

Learning Finite State Machines With Self-clustering Recurrent Networks

Zeng et al, 1993

Extracting Rules from a (Fuzzy / Crisp) Recurrent Neural Network using a Self-Organizing Map

Blanco et al, 2000

State automata extraction from recurrent neural nets using k-means and fuzzy clustering

Cechin et al, 2003

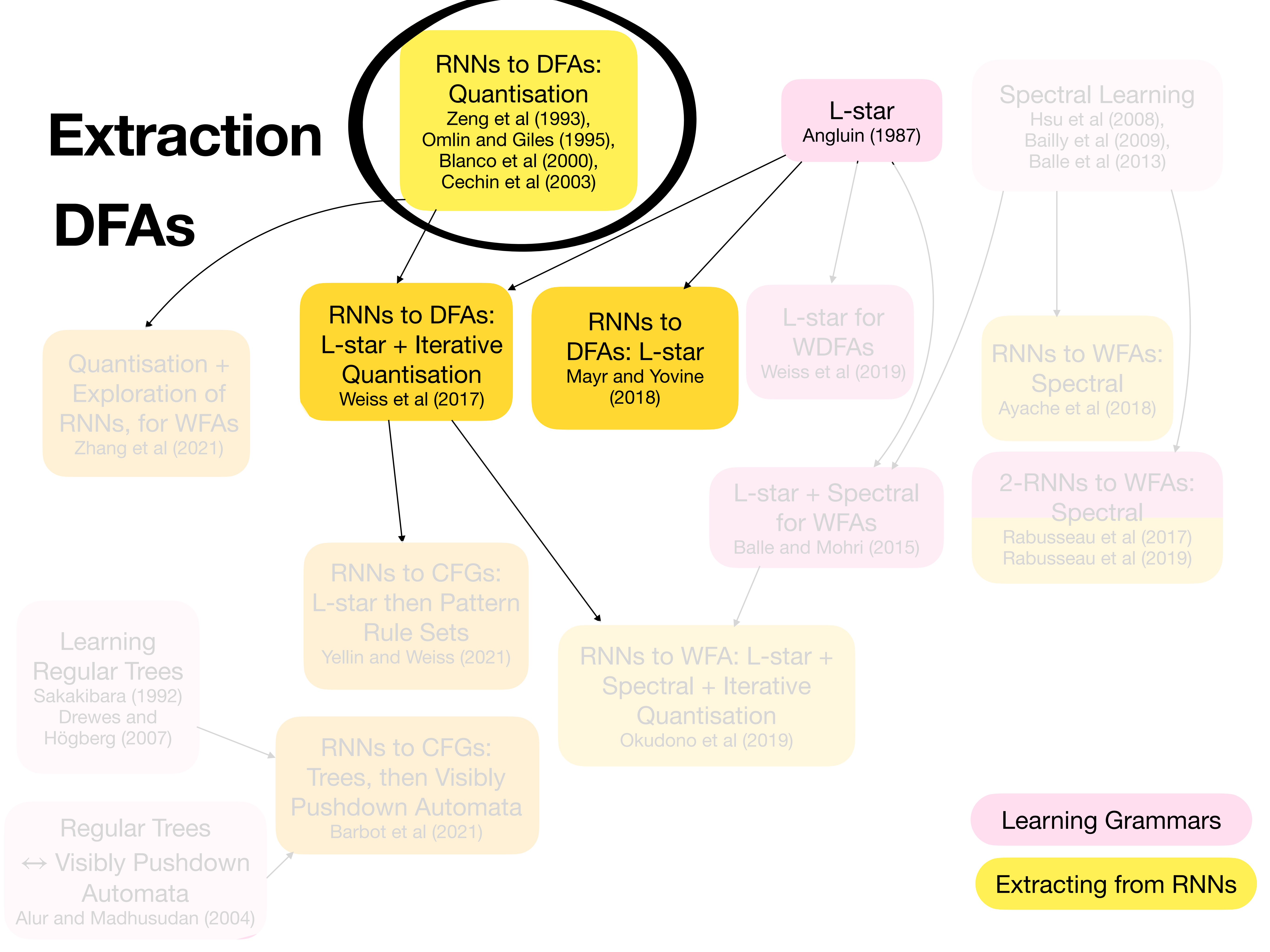
Surveys:

Rule Extraction from Recurrent Neural Networks: A Taxonomy and Review

Jacobsson, 2005

An Empirical Evaluation of Rule Extraction from Recurrent Neural Networks

Wang et al, 2017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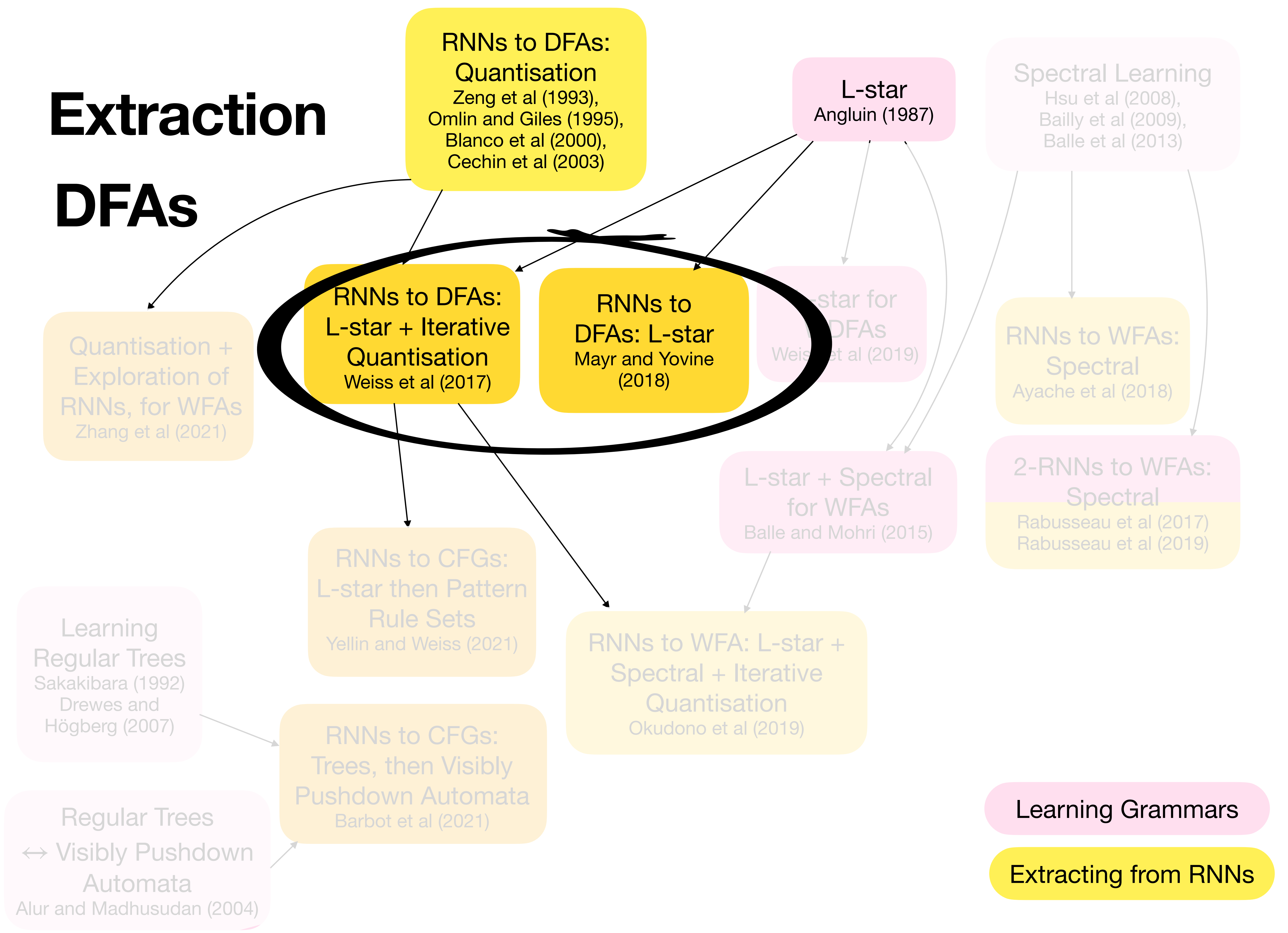
RNNs to WFA: L-star + Spectral + Iterative Quantisation
Okudono et al (2019)
RNNs to CFGs: Trees, then Visibly Pushdown Automata
Barbot et al (2021)
Regular Trees ↔ Visibly Pushdown Automata
Alur and Madhusudan (2004)
Learning Grammars
Extracting from RNNs


Extraction
DFAs
RNNs to DFAs: Quantisation
Zeng et al (1993), Omlin and Giles (1995), Blanco et al (2000), Cechin et al (2003)
L-star
Angluin (1987)
Spectral Learning
Hsu et al (2008), Bailly et al (2009), Balle et al (2013)
Quantisation + Exploration of RNNs, for WFAs
Zhang et al (2021)
RNNs to DFAs: L-star + Iterative Quantisation
Weiss et al (2017)
RNNs to DFAs: L-star
Mayr and Yovine (2018)
star for
DFAs
Weis
et al (2019)
RNNs to WFAs: Spectral
Ayache et al (2018)
2-RNNs to WFAs: Spectral
Rabusseau et al (2017)
Rabusseau et al (2019)
L-star + Spectral for WFAs
Balle and Mohri (2015)
RNNs to CFGs: L-star then Pattern Rule Sets
Yellin and Weiss (2021)
Learning Regular Trees
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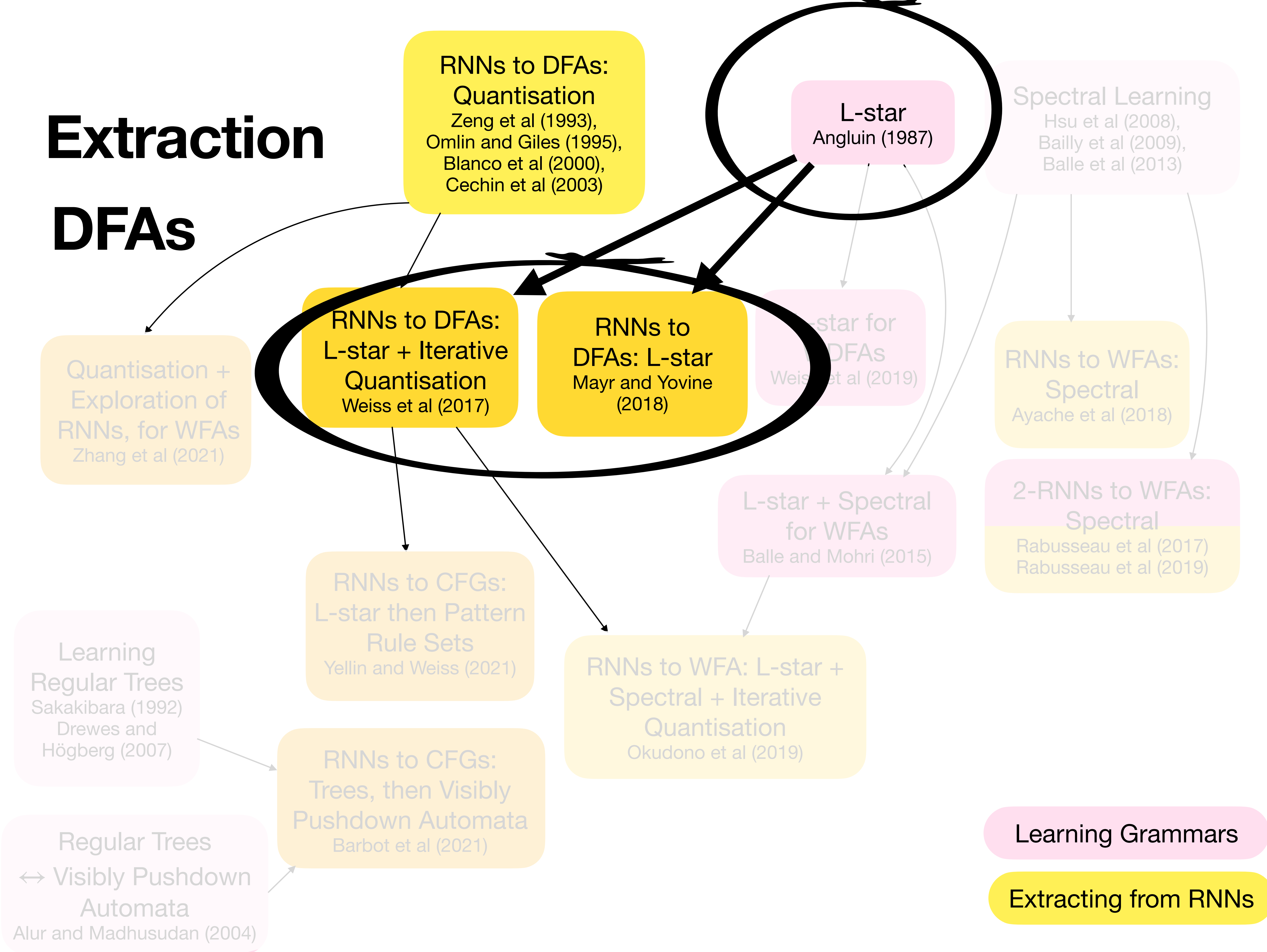
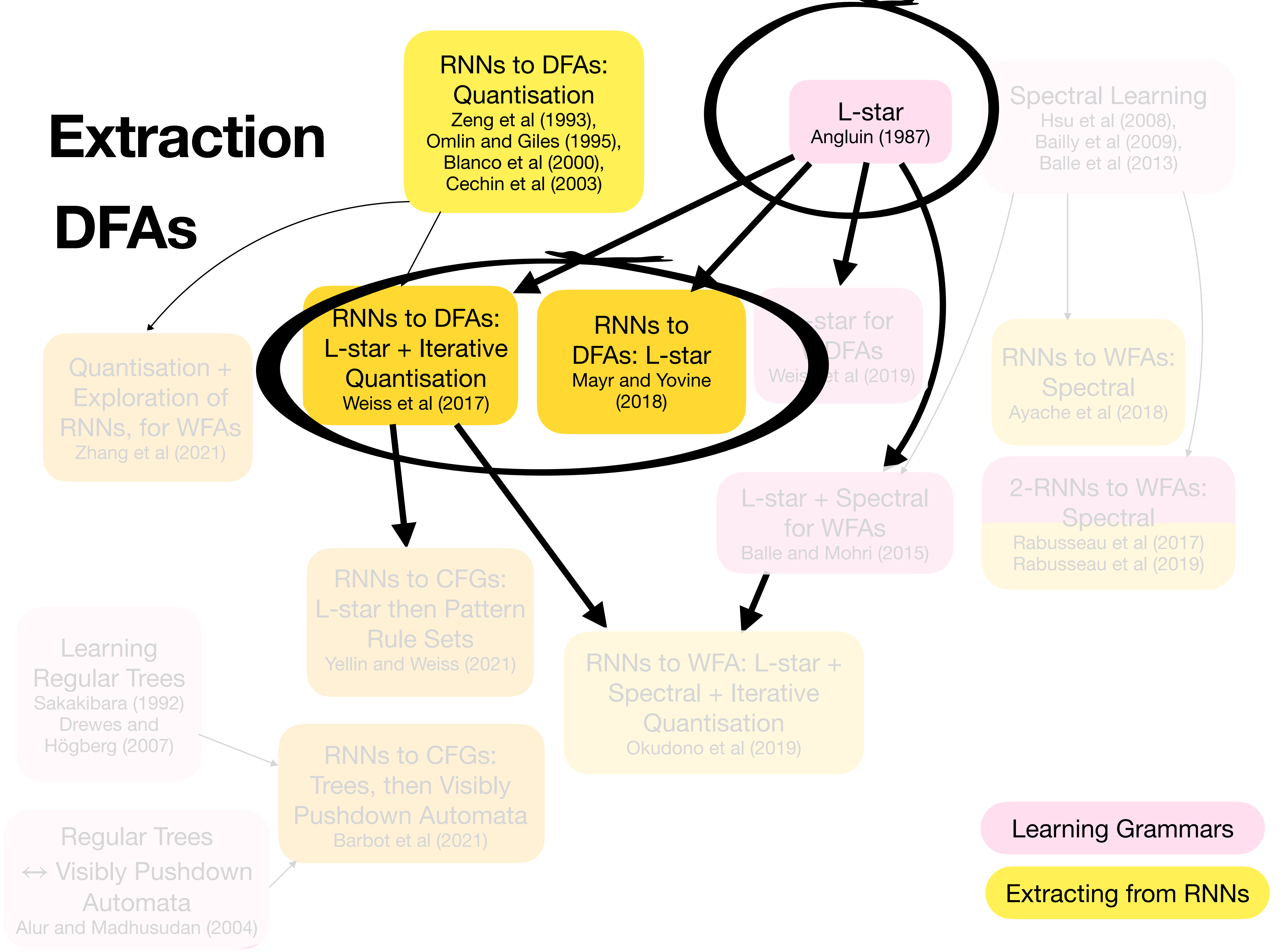
Extraction DFAs



Extraction DFAs



RNNs: Extracting DFAs: L-star

The L-star algorithm

$\varepsilon?$

$a?$

$b?$

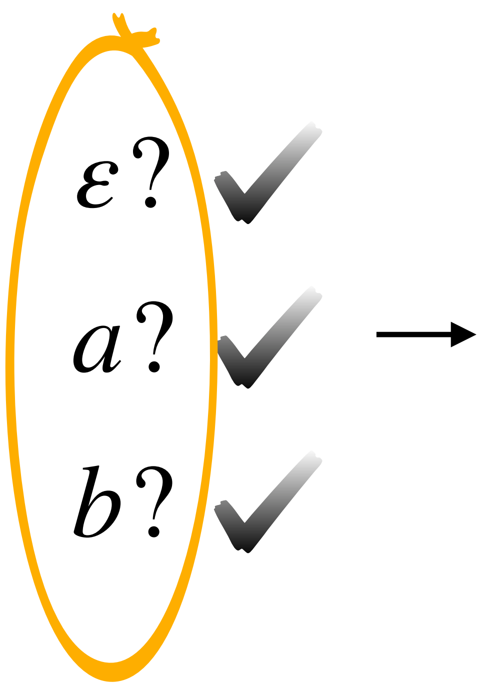
Membership Queries

Learning Regular Sets from Queries and Counterexamples

Angluin 1987

RNNs: Extracting DFAs: L-star

The L-star algorithm



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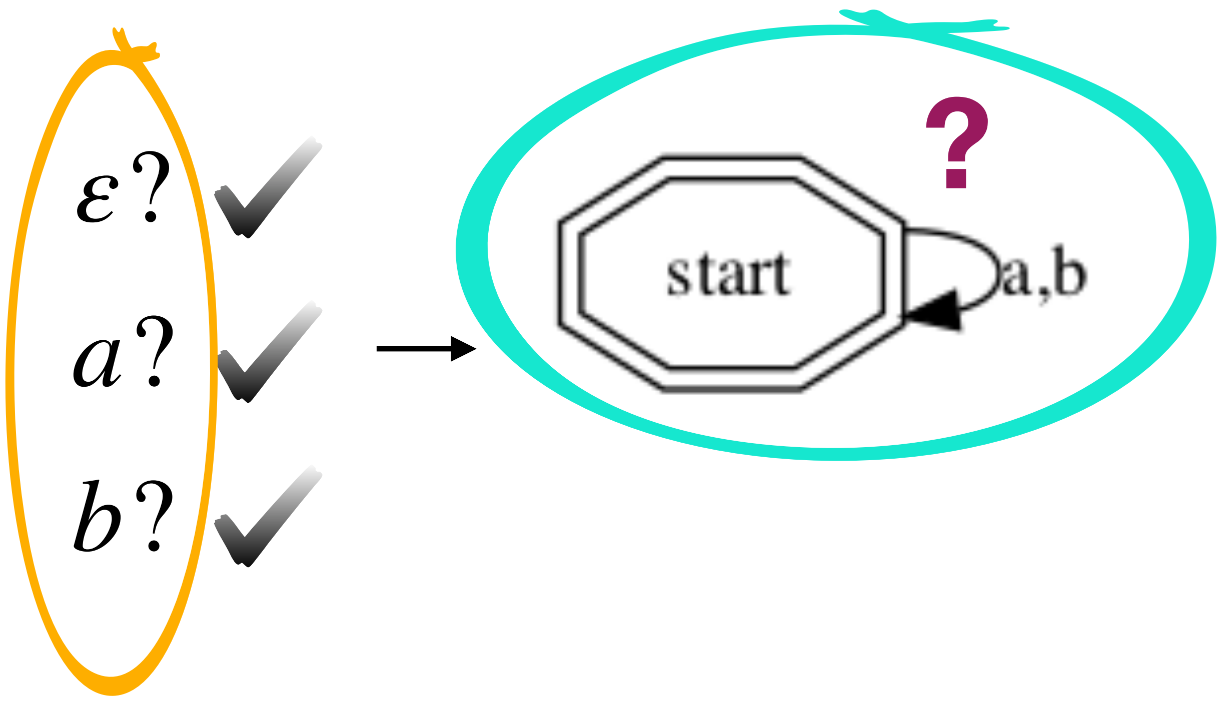

Learning Regular Sets from Queries and Counterexamples

Angluin 1987

Membership Queries

Equivalence Queries

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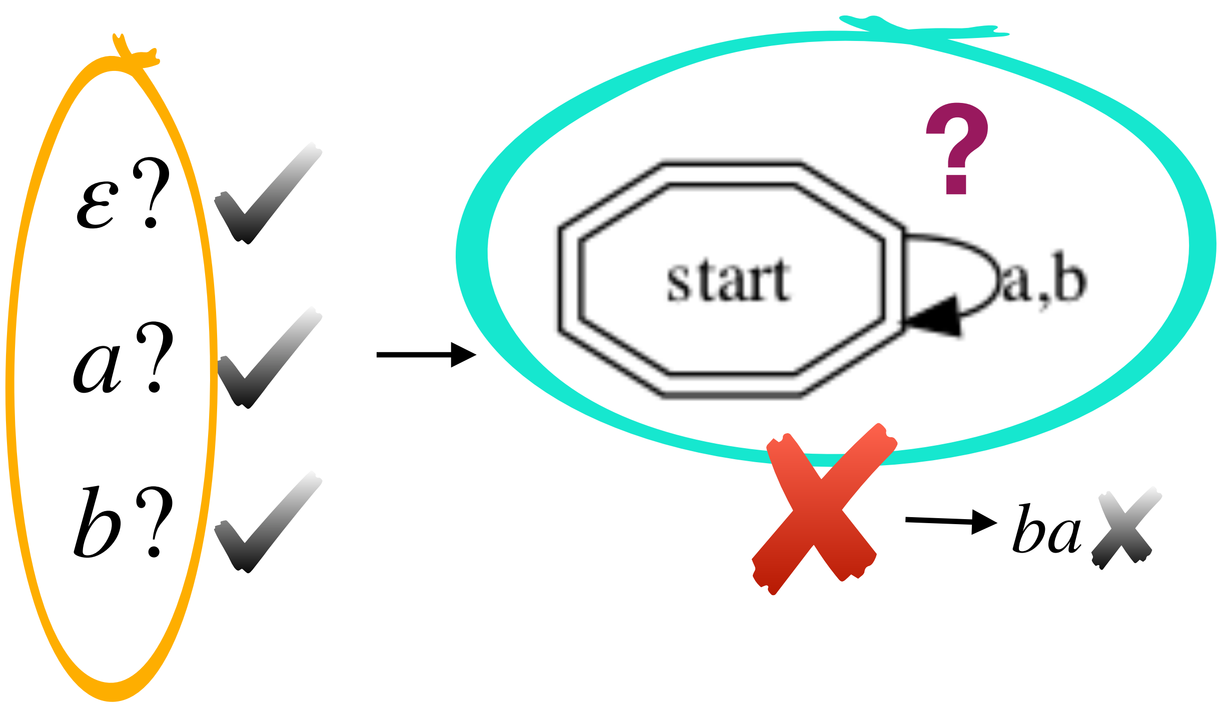

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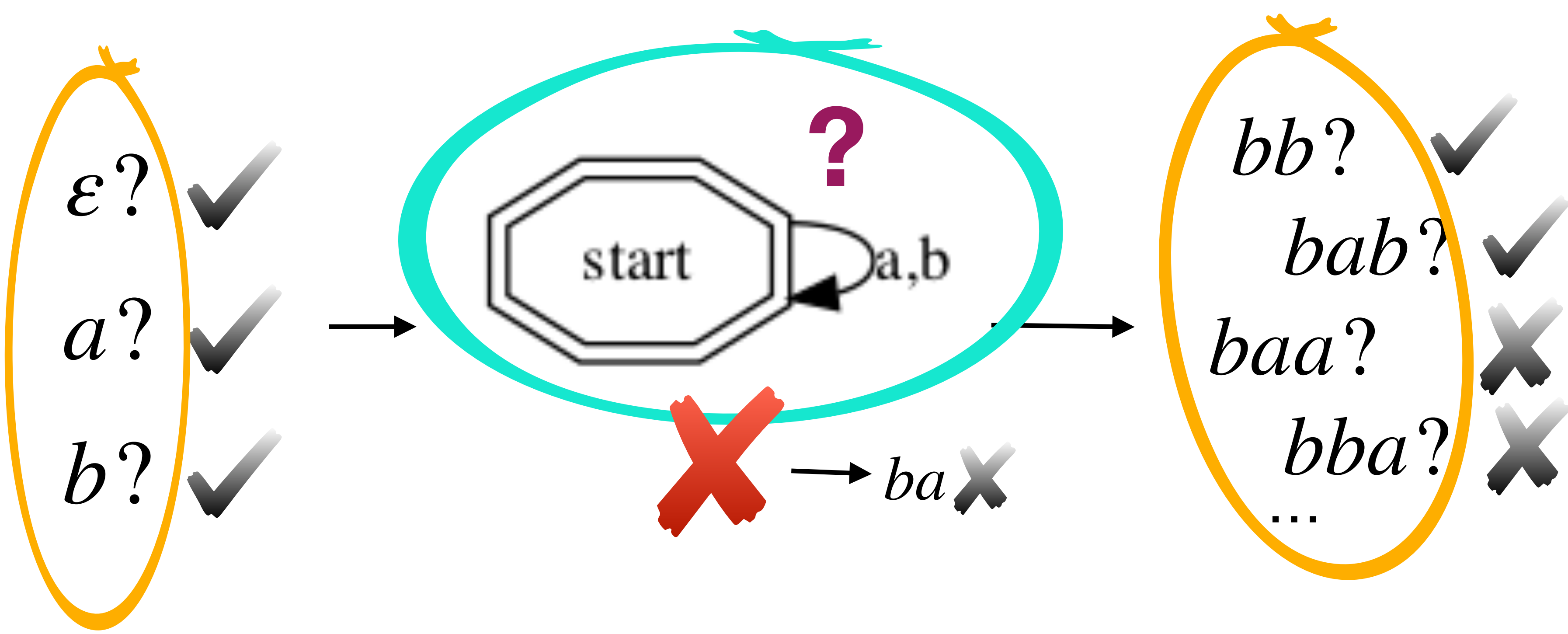

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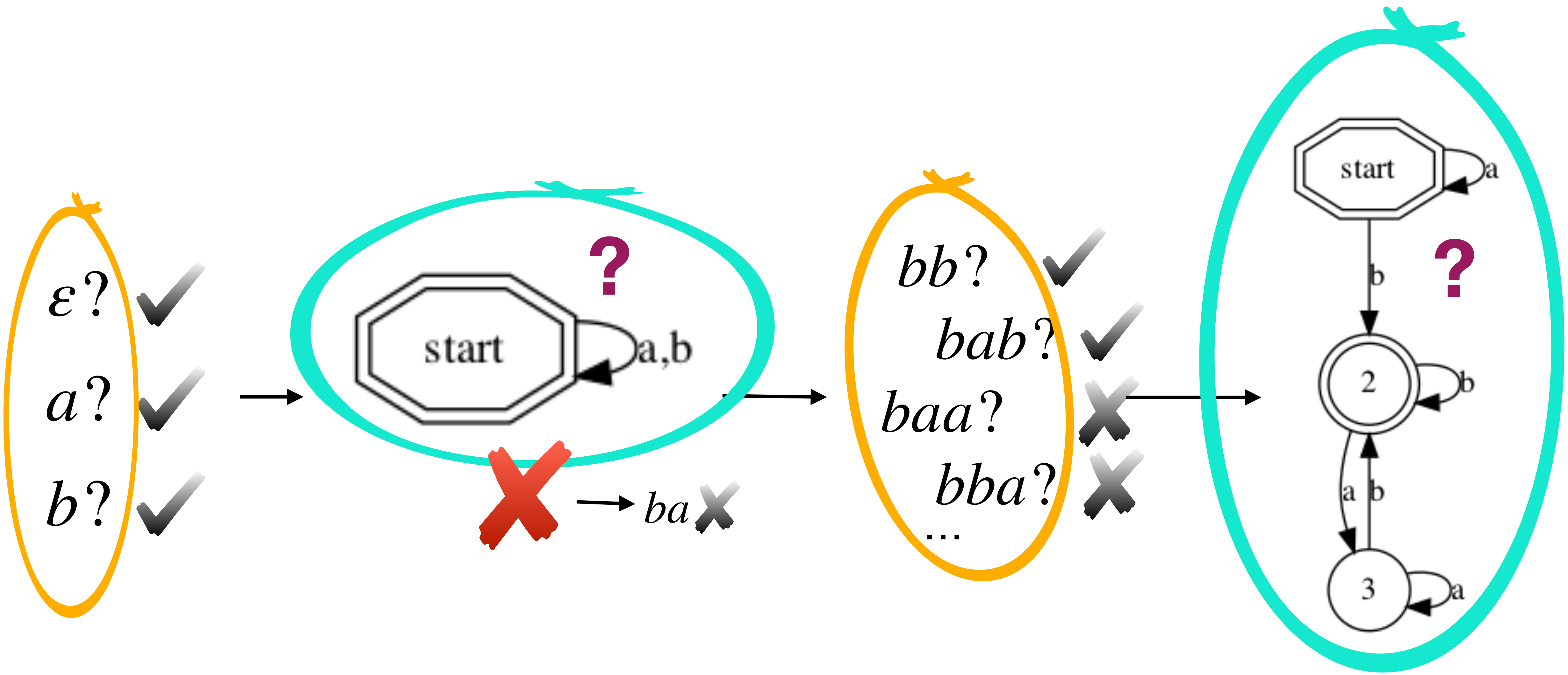

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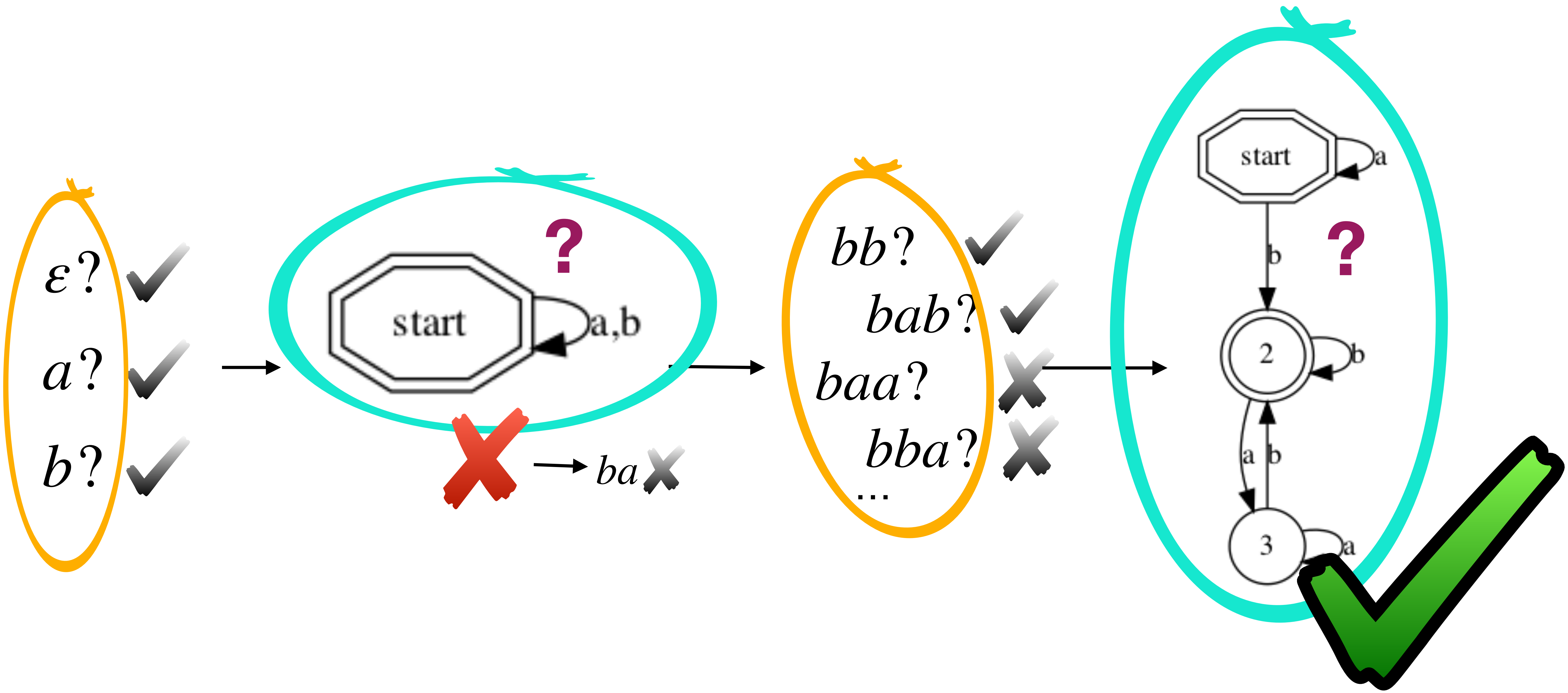

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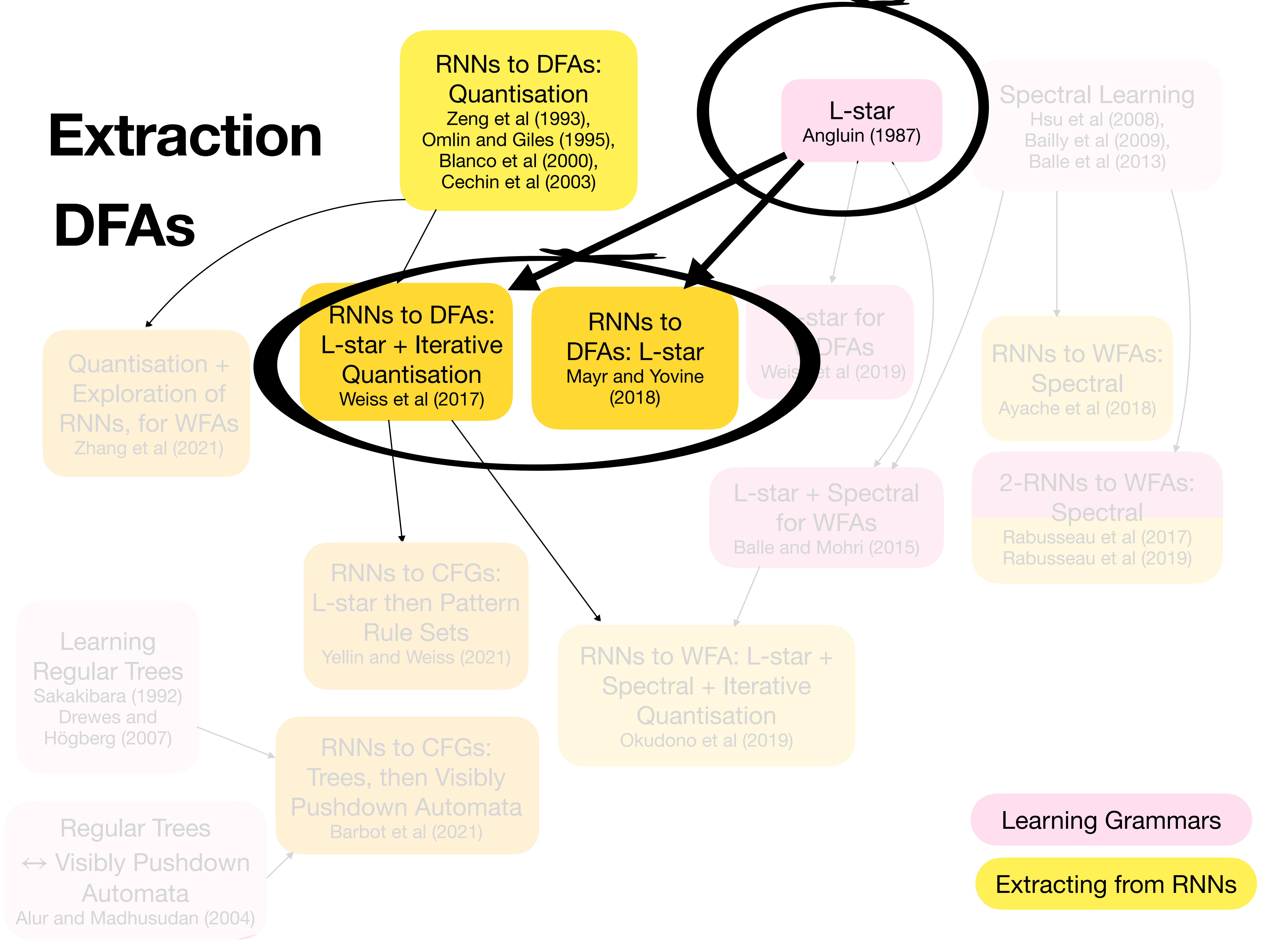
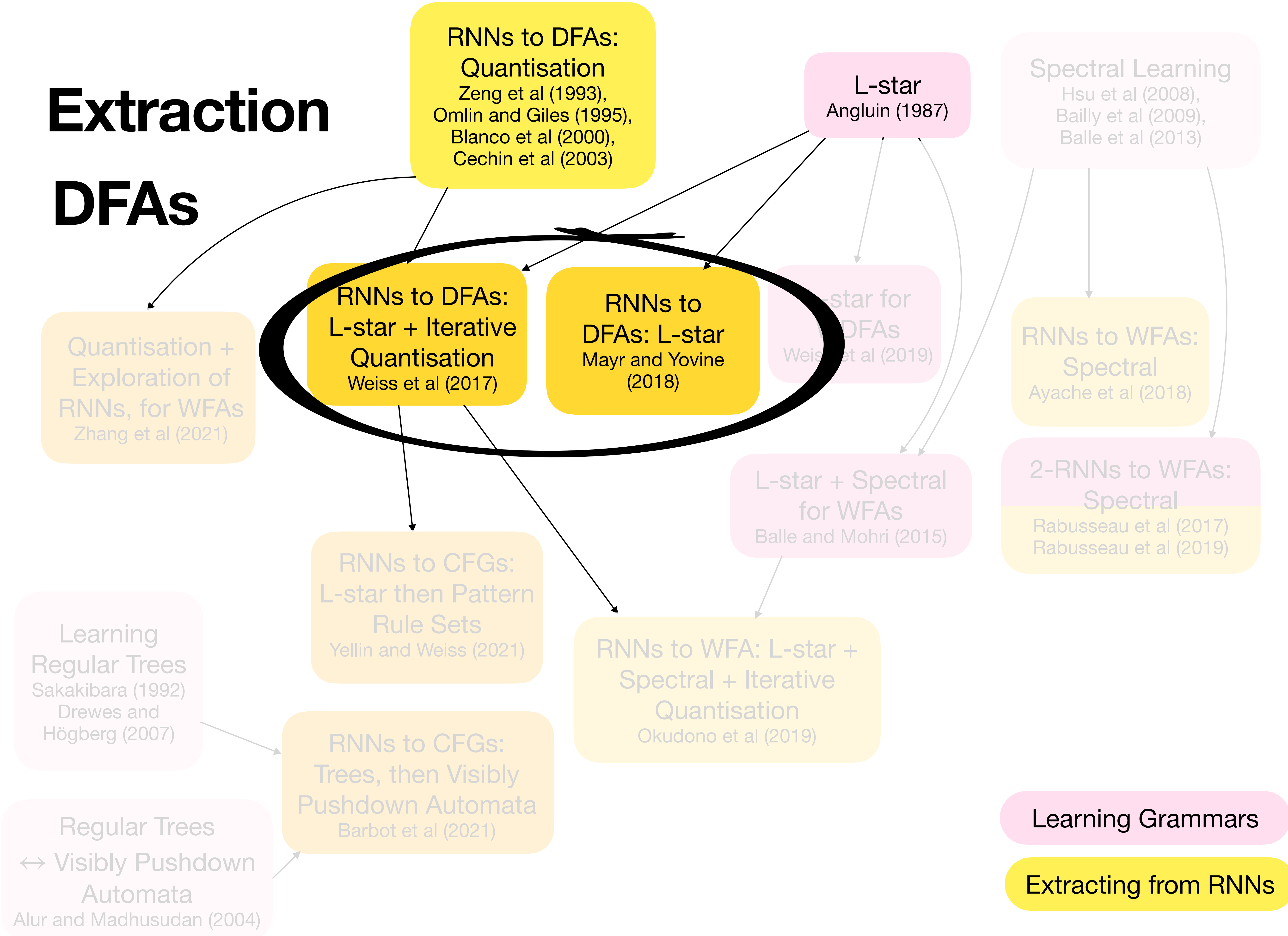


Extraction DFAs



RNNs: Extracting DFAs: L-star

Apply L-star to an RNN, to learn a DFA representing/approximating it

Extracting Automata from Recurrent Neural Networks using Queries and Counterexamples
Weiss et al, 2017

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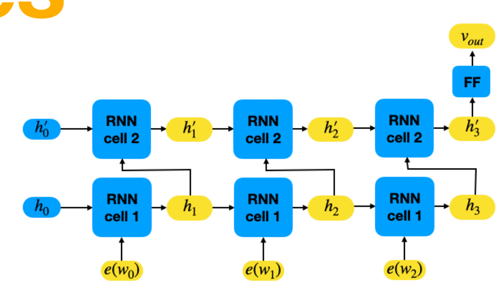
Membership Queries

bab?



✓ or ✗

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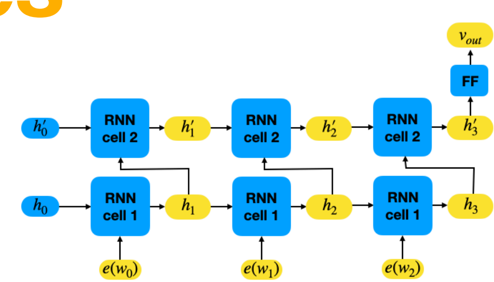
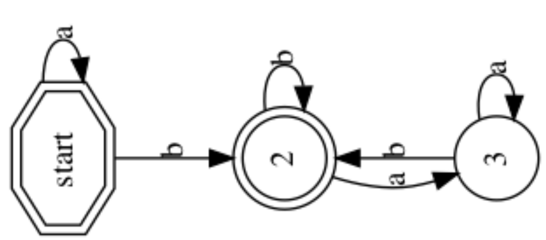
Membership Queries

bab? →



→ ✓ or ✗

Equivalence Queries



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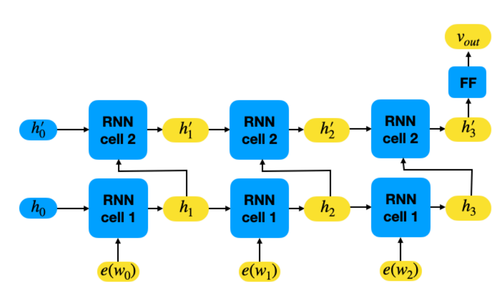
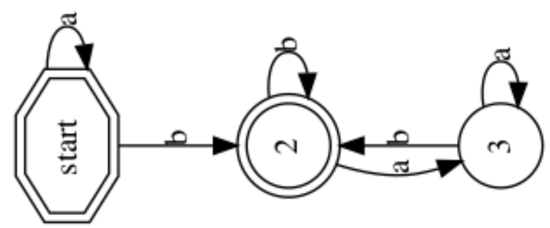


RNNs: Extracting DFAs: L-star

Equivalence Queries



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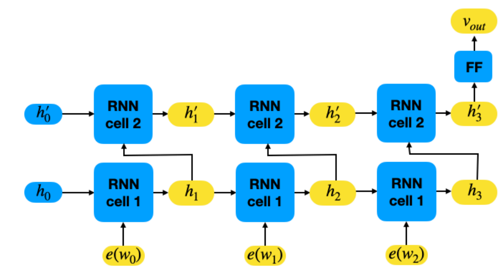

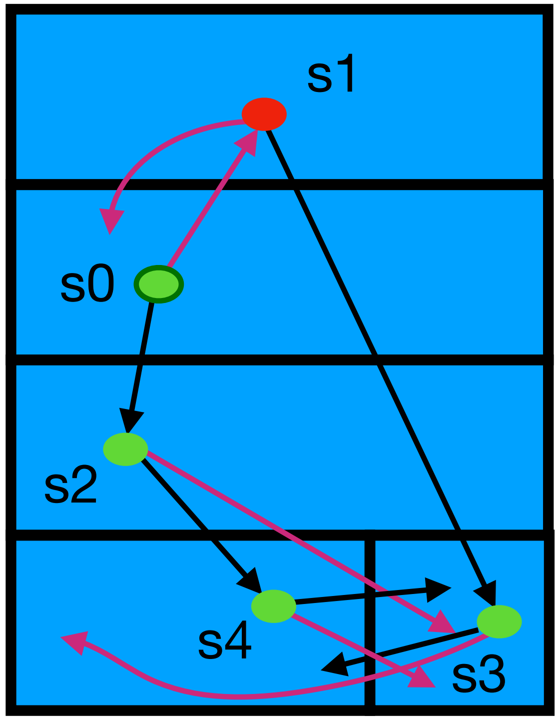

Extracting Automata from Recurrent Neural Networks using Queries and Counterexamples

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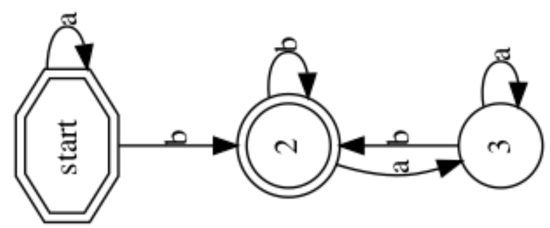
RNNs: Extracting DFAs: L-star

Equivalence Queries 

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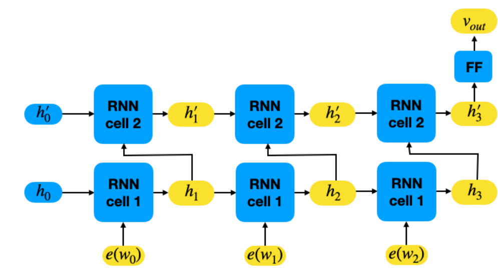

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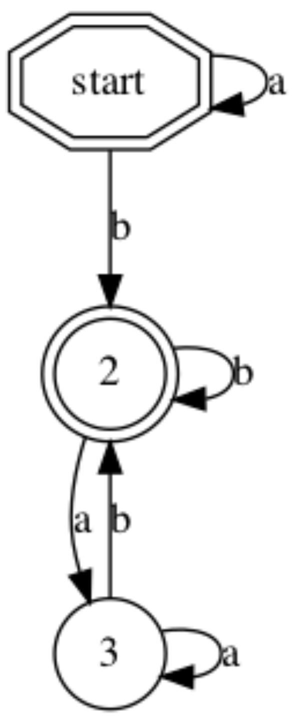

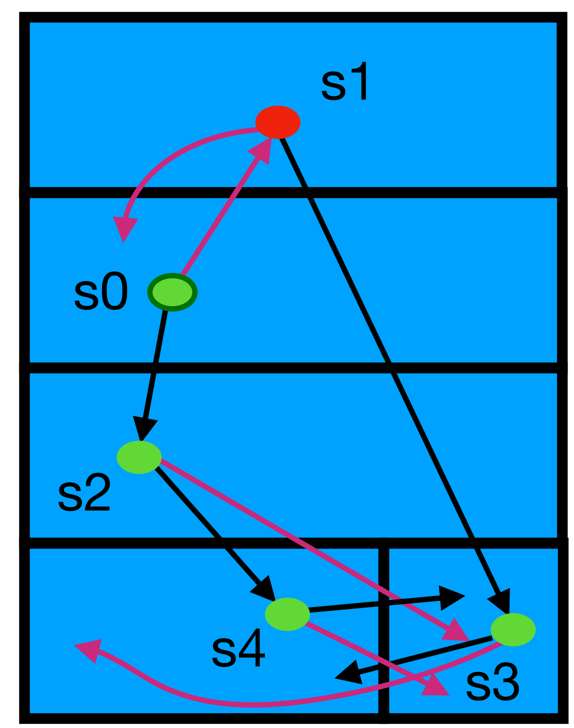

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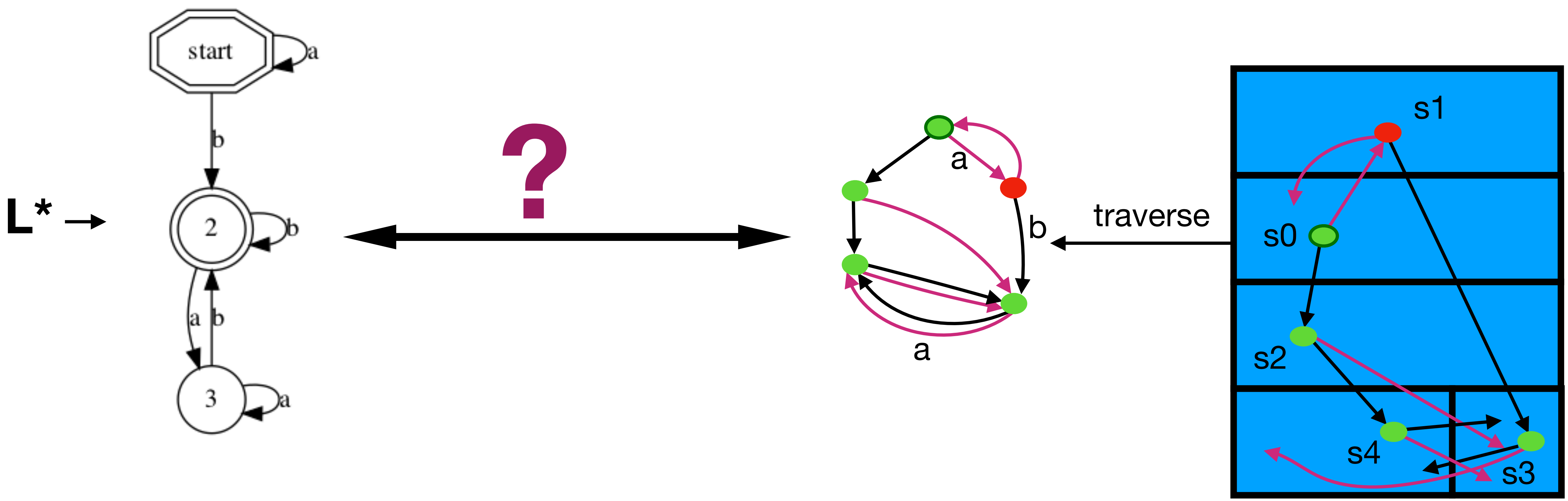

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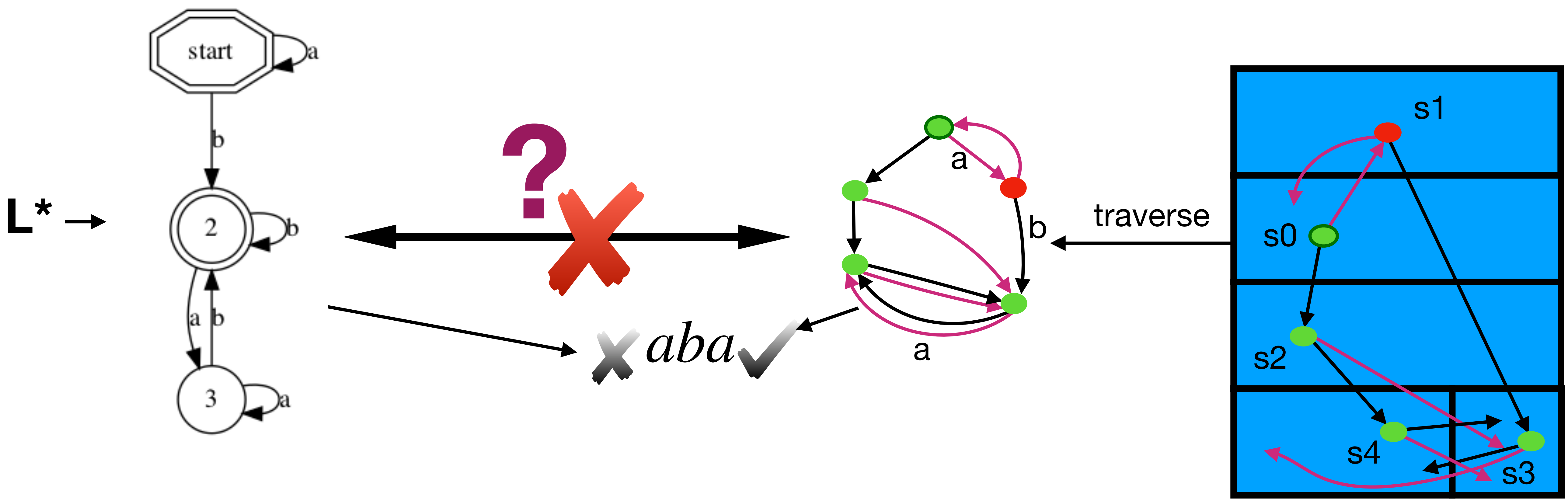

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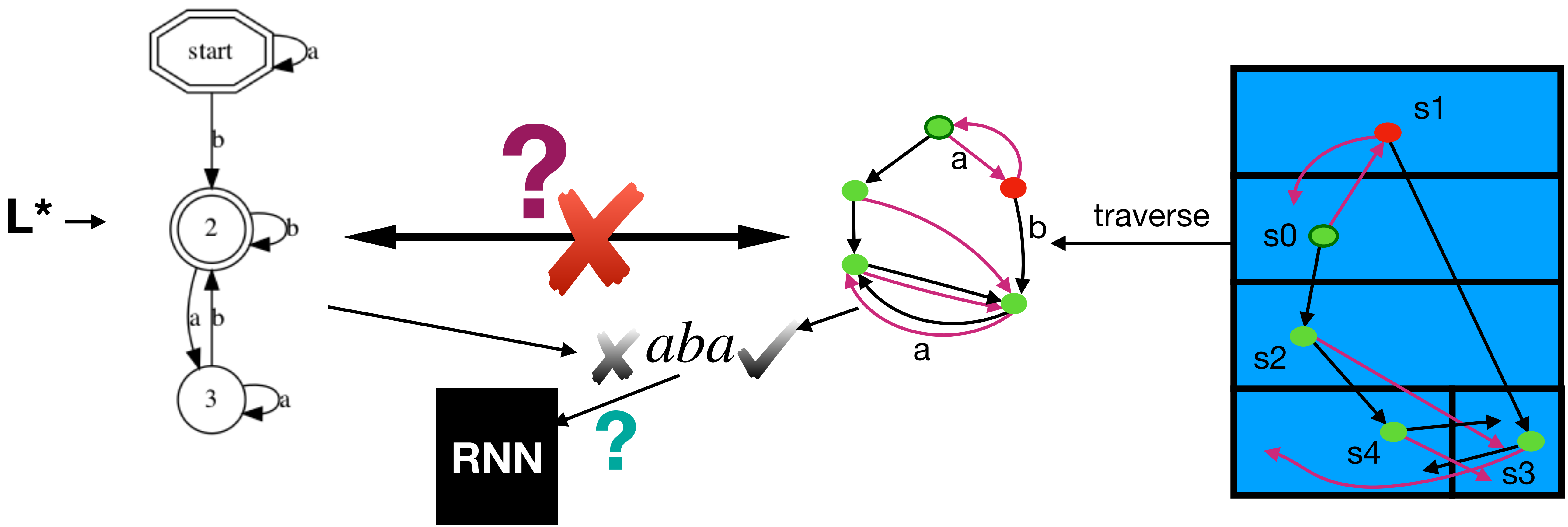

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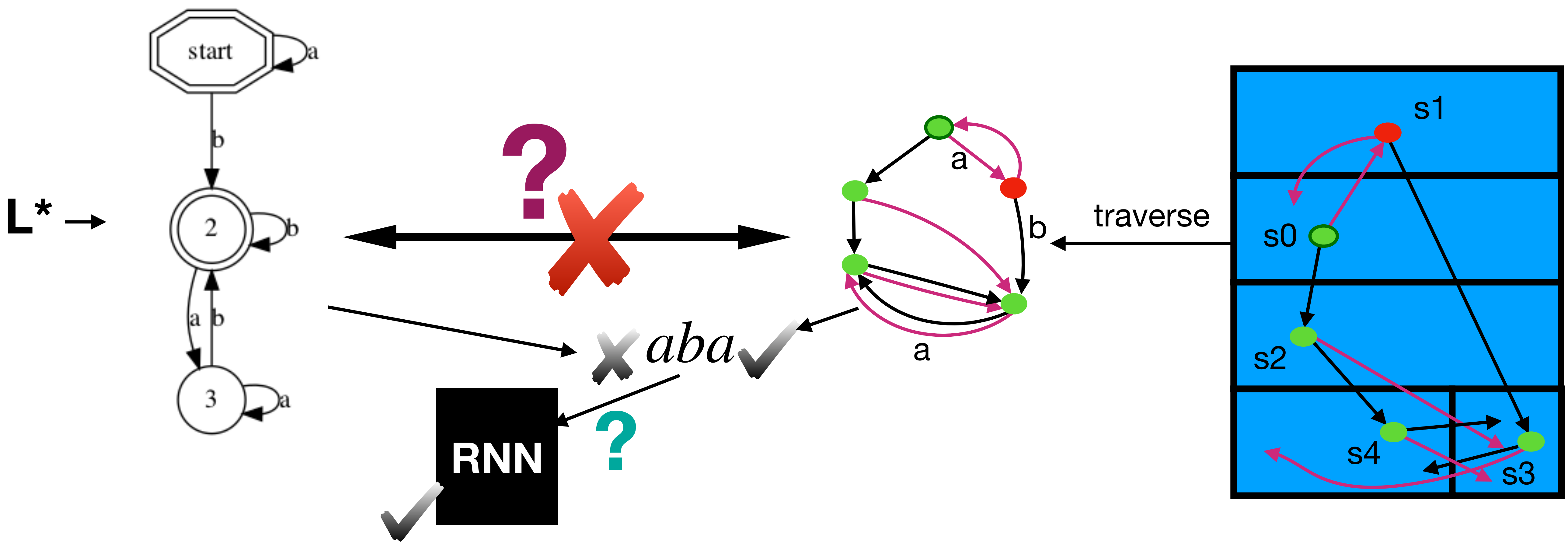

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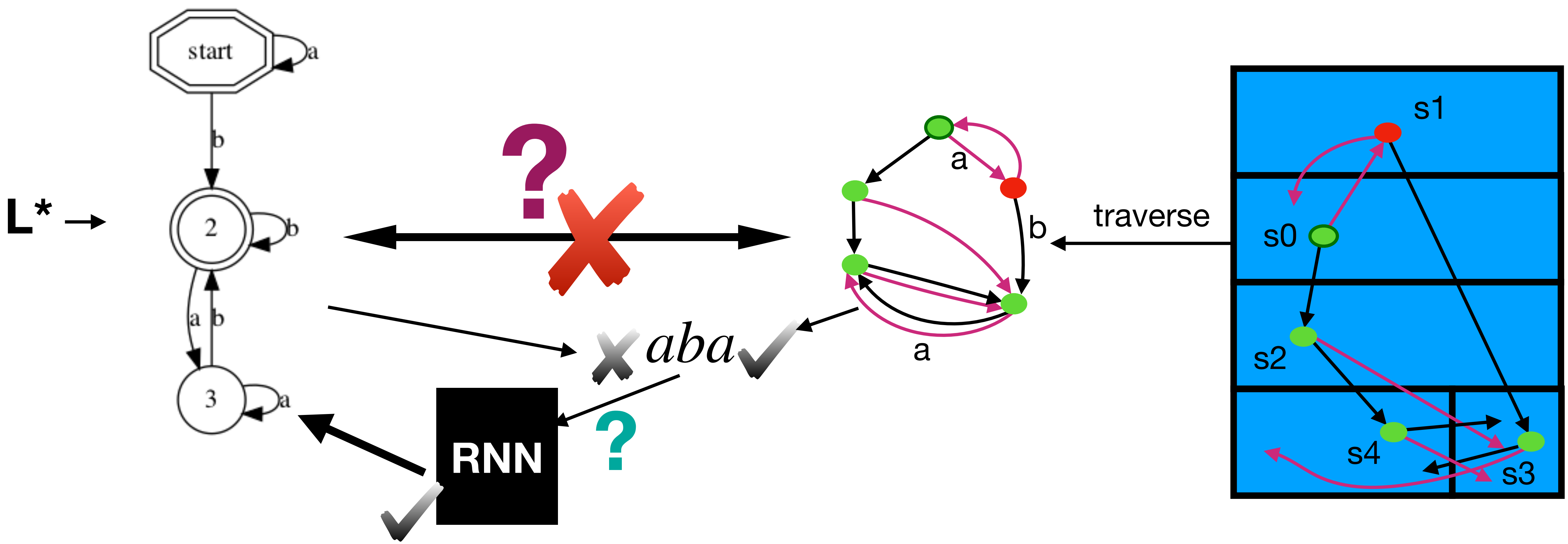

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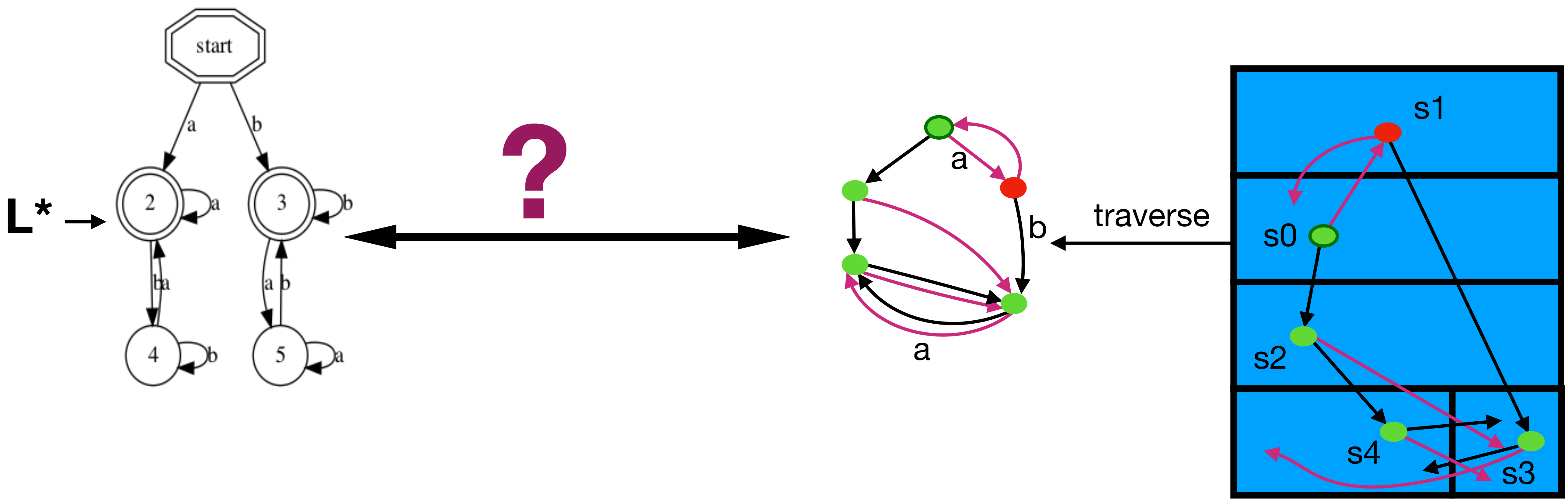

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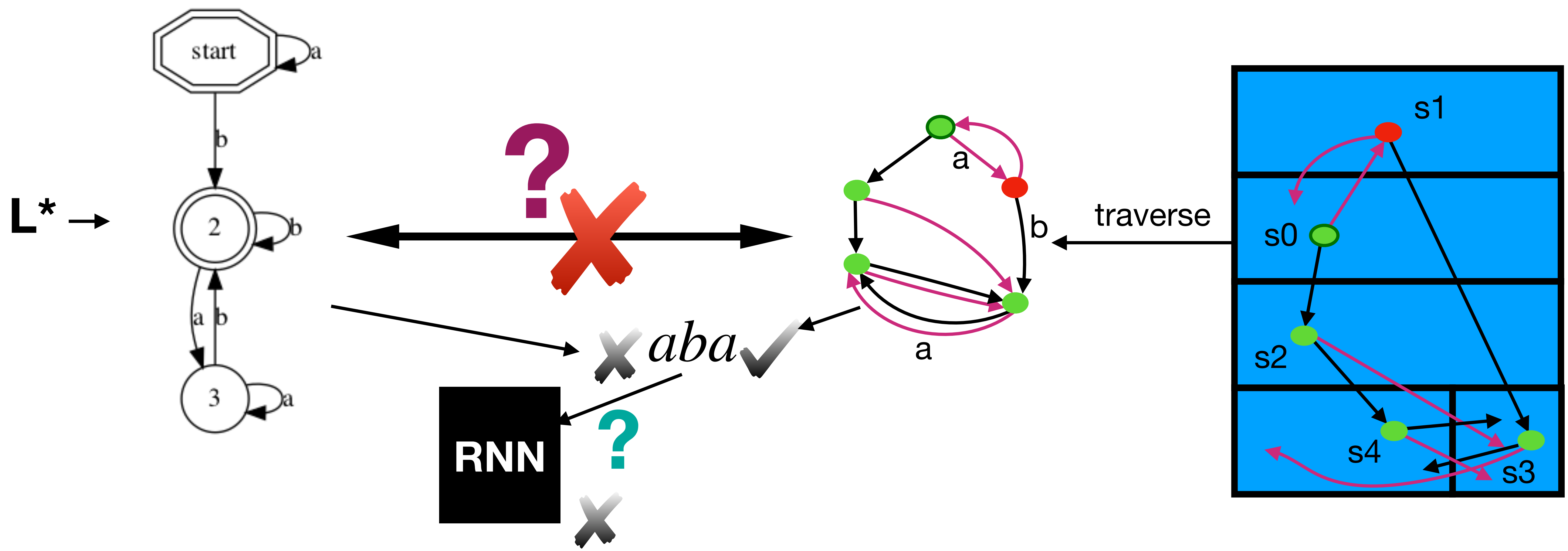

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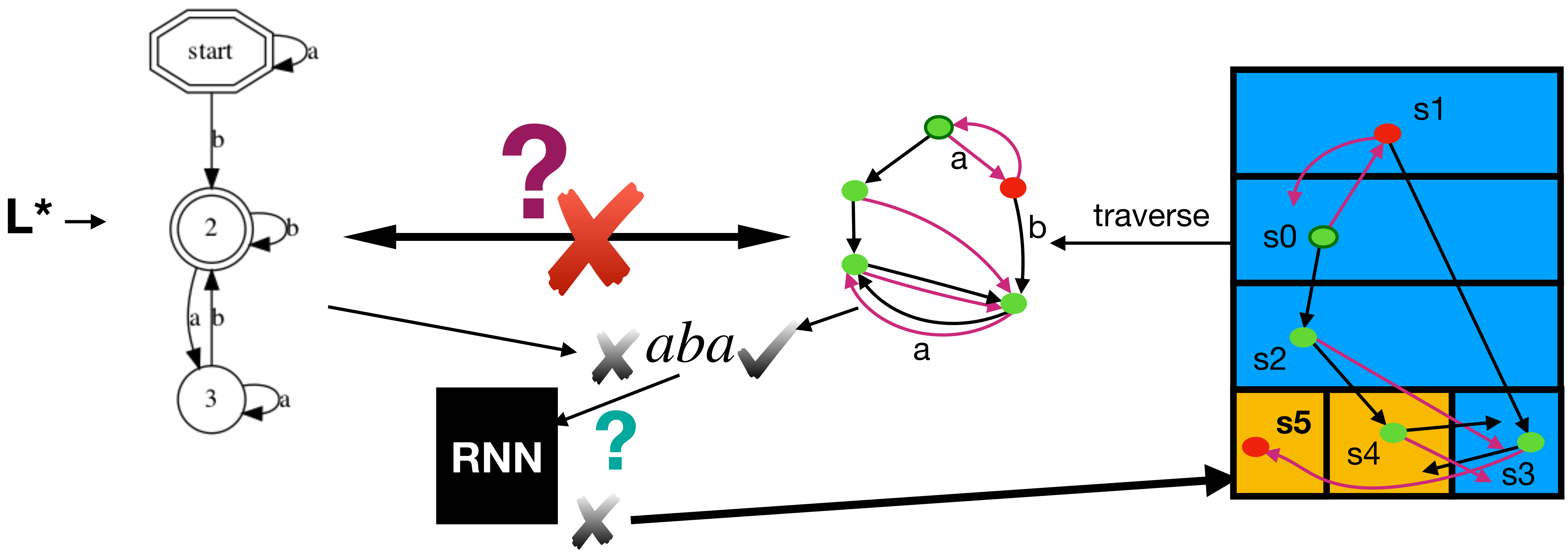

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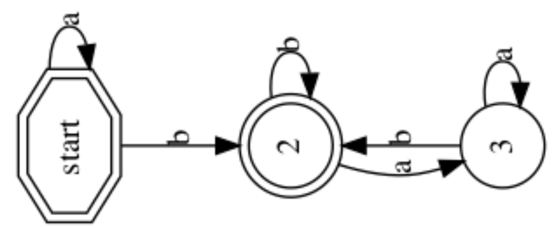

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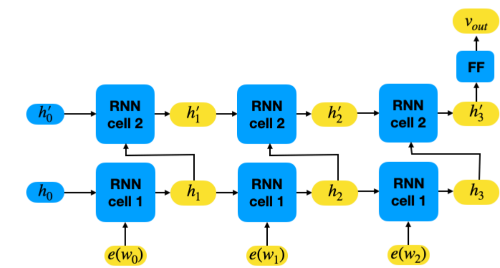

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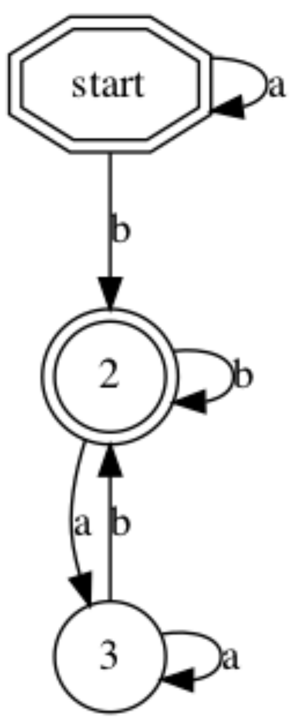

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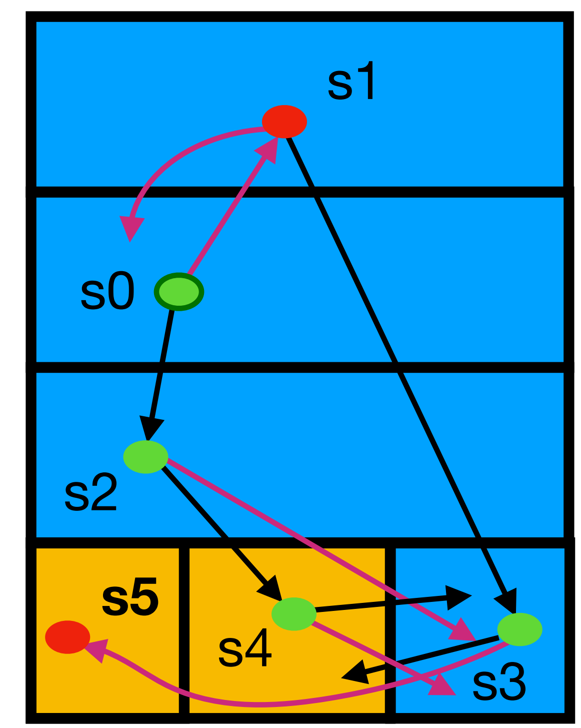

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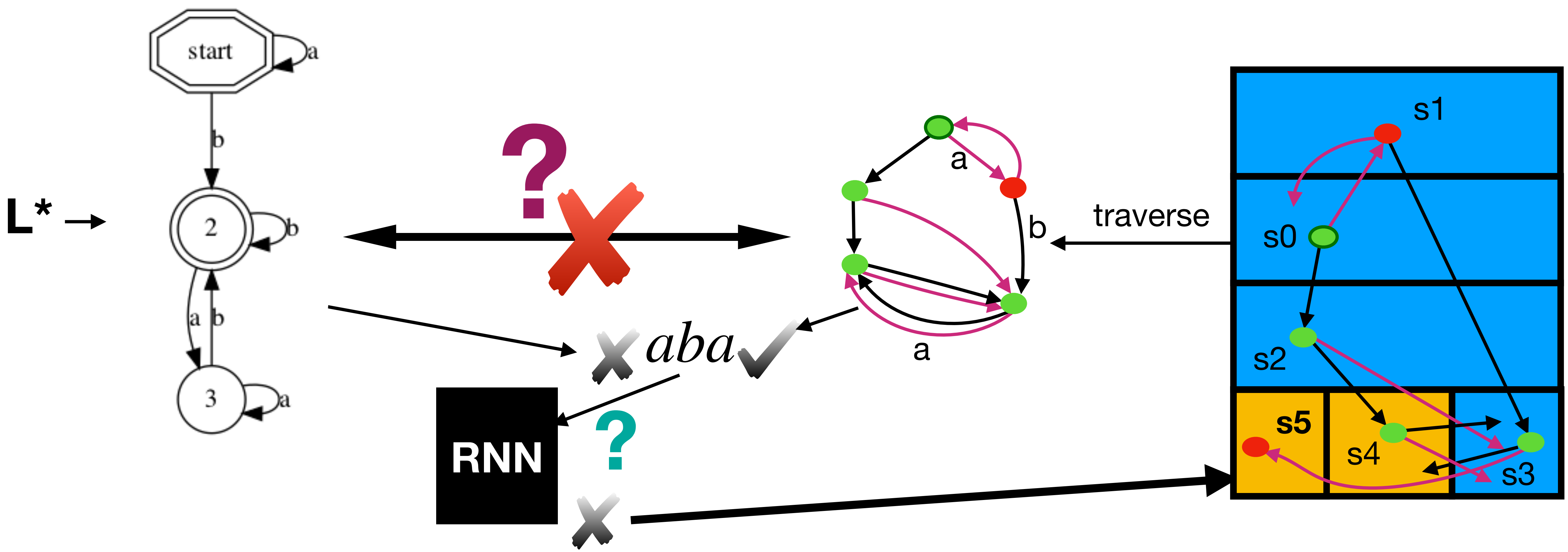

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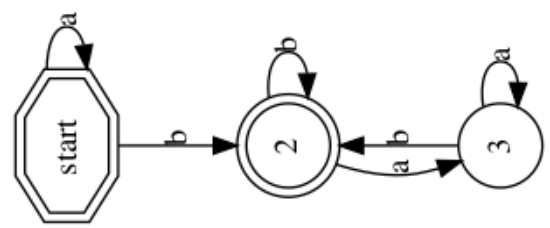

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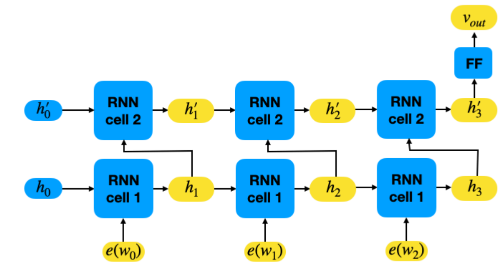

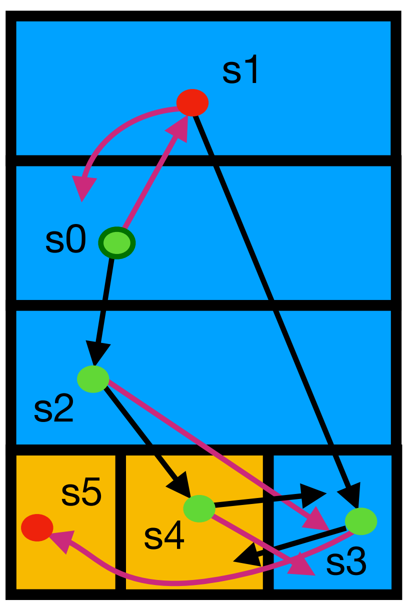

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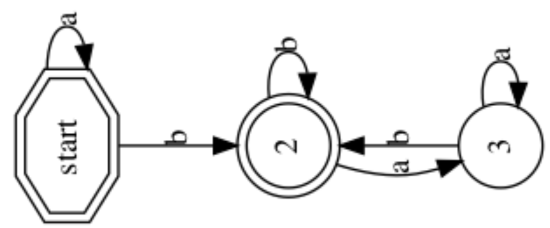

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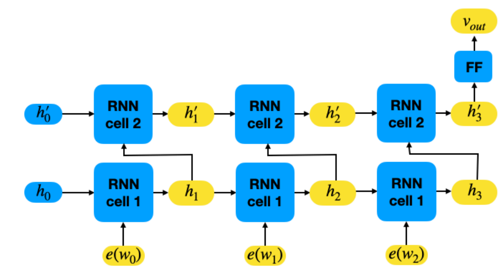

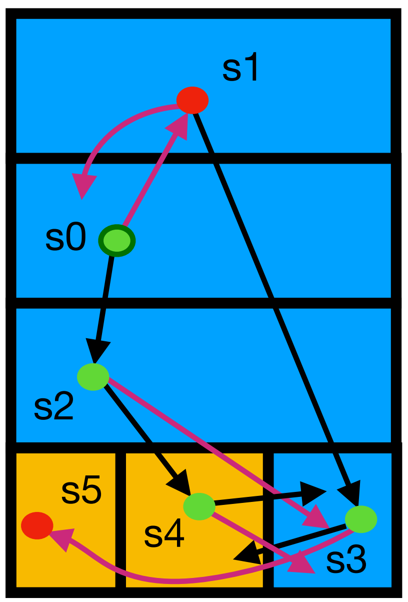

Randomly Sample for Counterexamples

(Paper provides PAC analysis of this approach for equivalence queries)

Extracting Automata from Recurrent Neural Networks using Queries and Counterexamples

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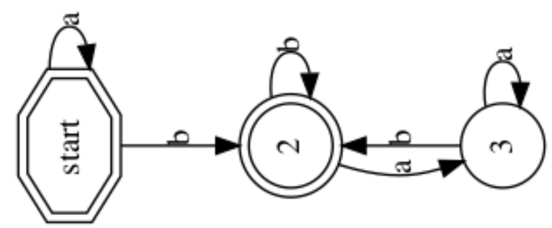

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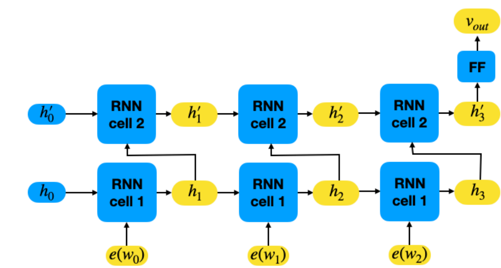

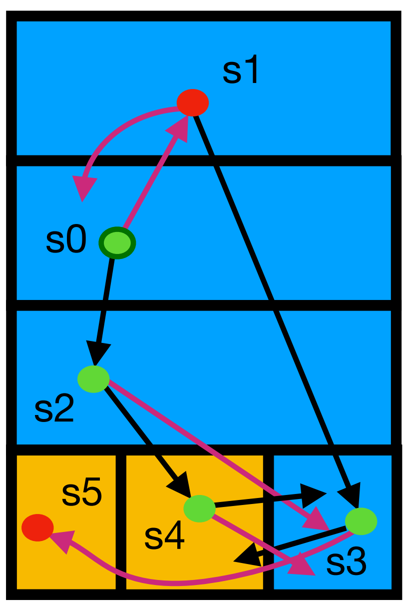

Randomly Sample for Counterexamples

(Paper provides PAC analysis of this approach for equivalence queries)

Faster	**Slower**
Assumes white-box RNN	**Assumes black-box NN**
Complicated	**Simple**

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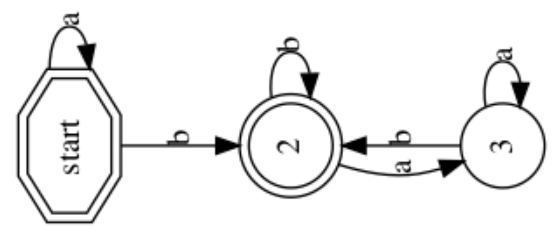

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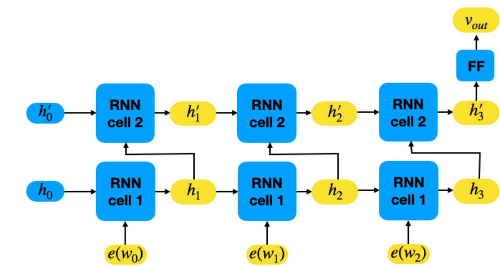

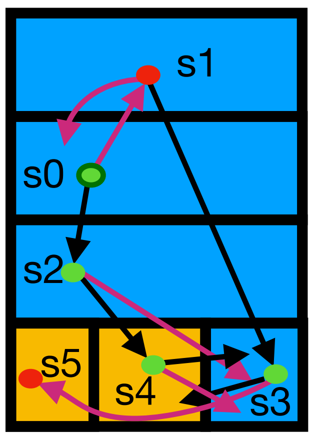

Randomly Sample for Counterexamples

Faster

Slower

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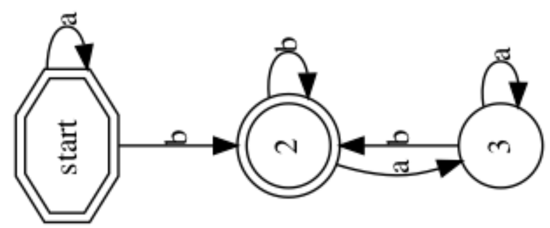

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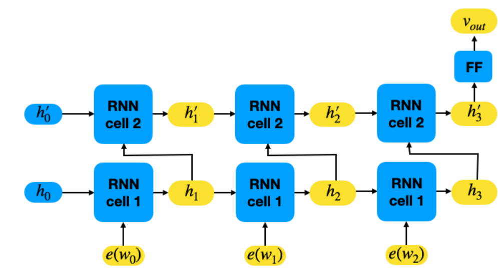
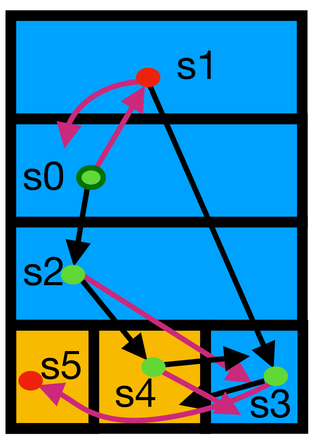




Randomly Sample for Counterexamples

Faster

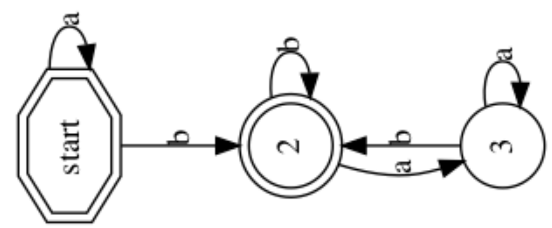
Slower

Learning Balanced Parentheses over $\Sigma = \{(,), a - z\}$

e.g. $()$, $()a()b$, $abc(()(a))$, etc

RNNs: Extracting DFAs: L-star

Equivalence Queries



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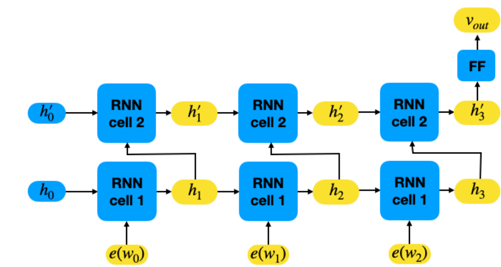
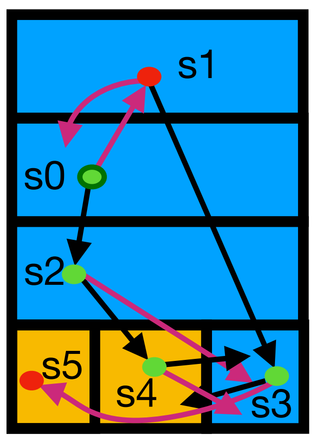
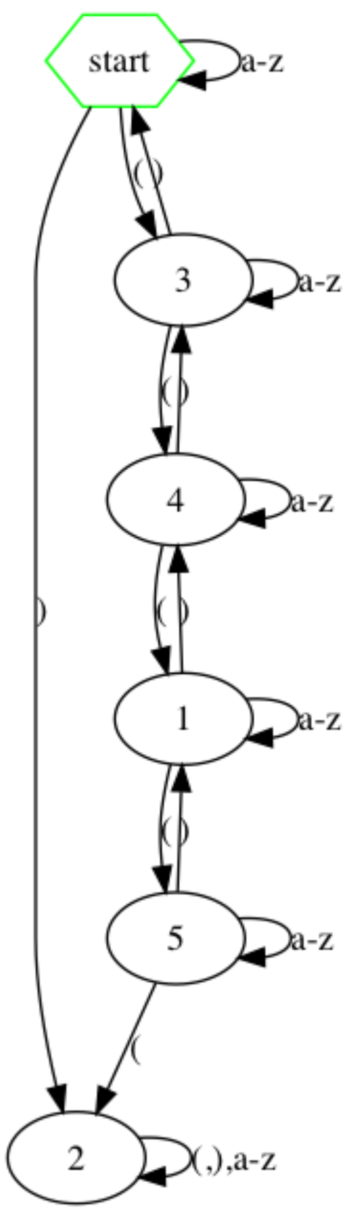




Randomly Sample for Counterexamples

Faster **Slower**



Learning Balanced Parentheses over $\Sigma = \{(,),a-z\}$

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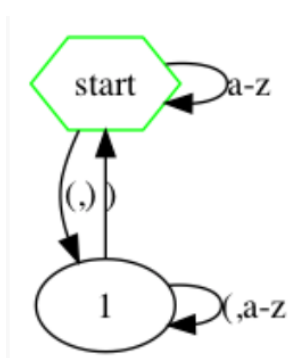

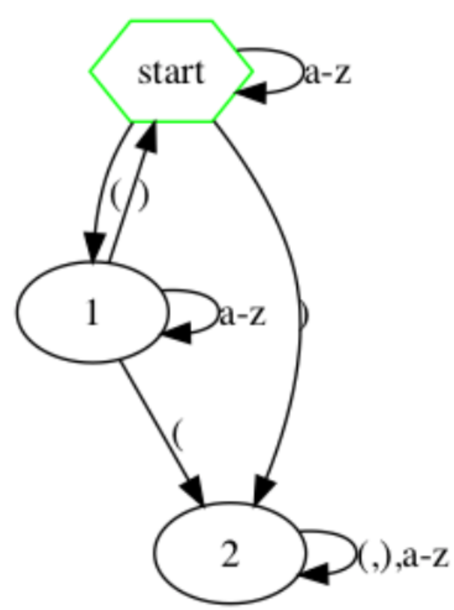

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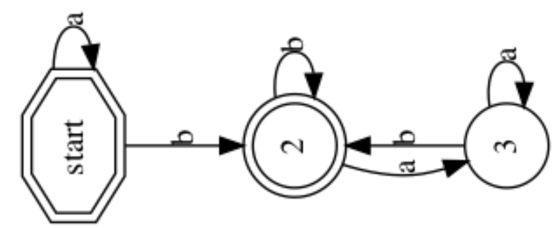
RNNs: Extracting DFAs: L-star

Equivalence Queries



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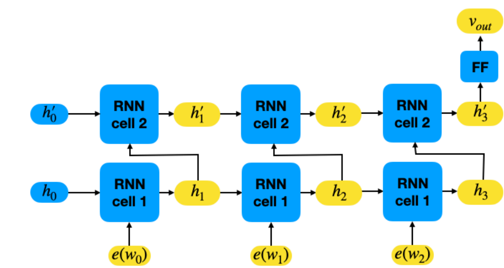
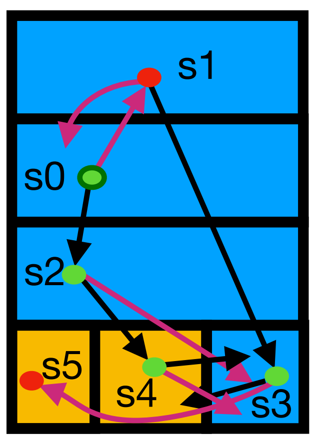




Randomly Sample for Counterexamples

Faster **Slower**

Learning Balanced Parentheses over $\Sigma = \{(,), a - z\}$

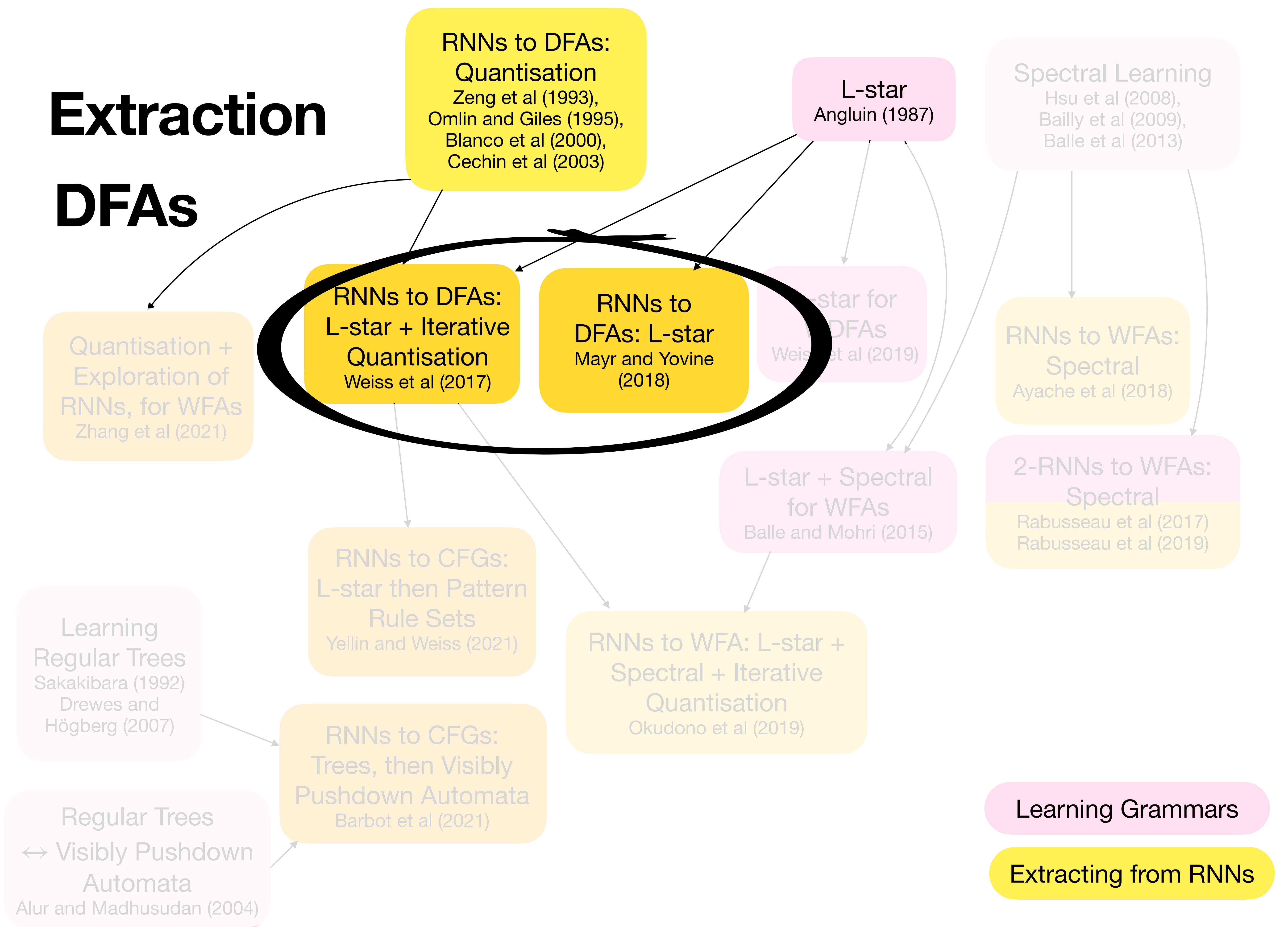
e.g. $()$, $()a()b$, $abc(()(a))$, etc

Random sampling counterexamples:

))	(1.5s)
tg(gu()uh)	(57.5s)
((wviw(iac)r)mrsnqqb)iew	(231.5s)

Abstraction based counterexamples:

))	(1.4s)
(())	(1.6s)
((()))	(3.1s)
(((())))	(3.1s)
((((()))))	(3.4s)
(((((())))))	(4.7s)
((((((()))))))	(6.3s)
(((((((())))))))	(9.2s)
((((((((()))))))))	(14.0s)



Extraction
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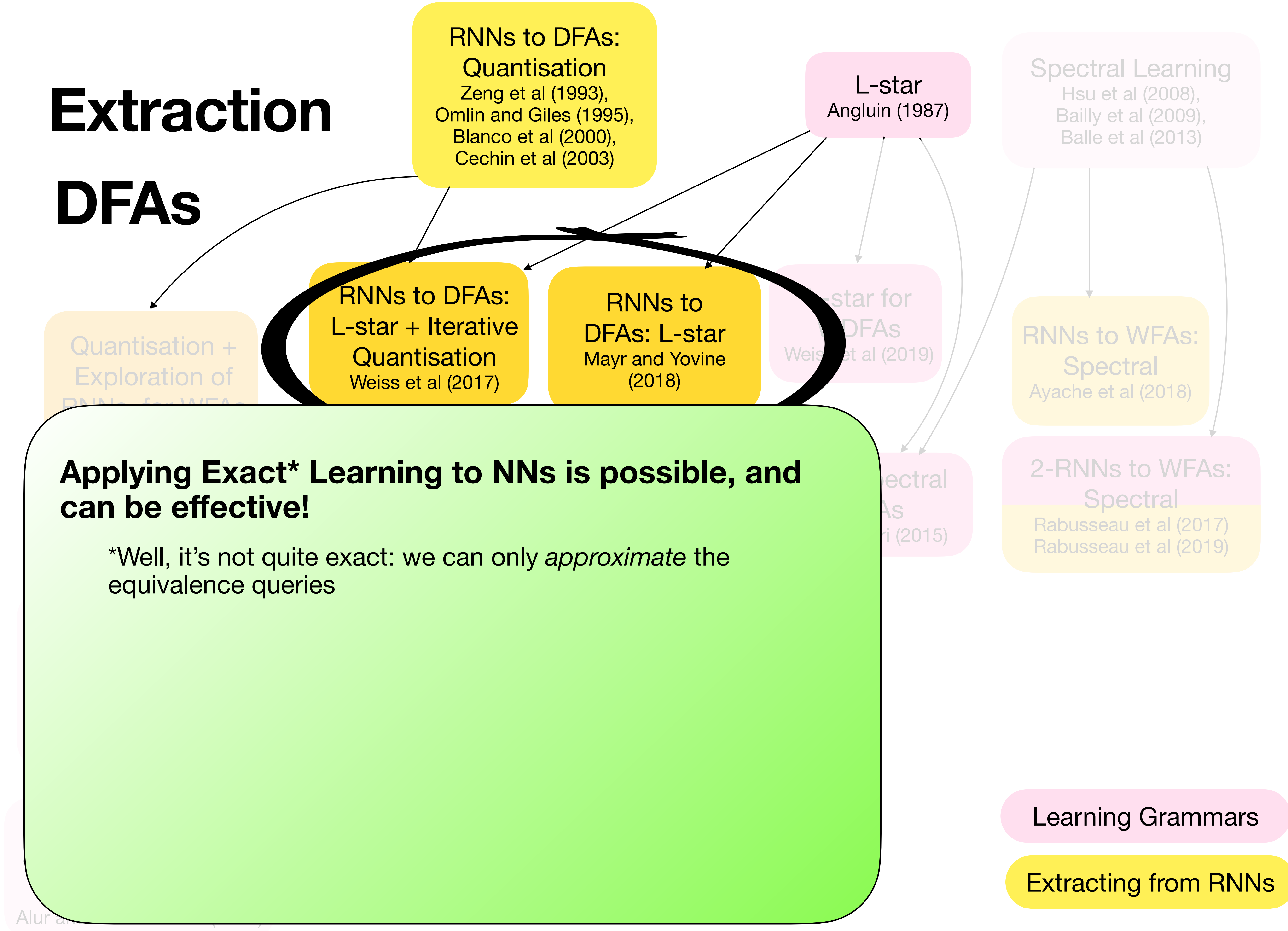
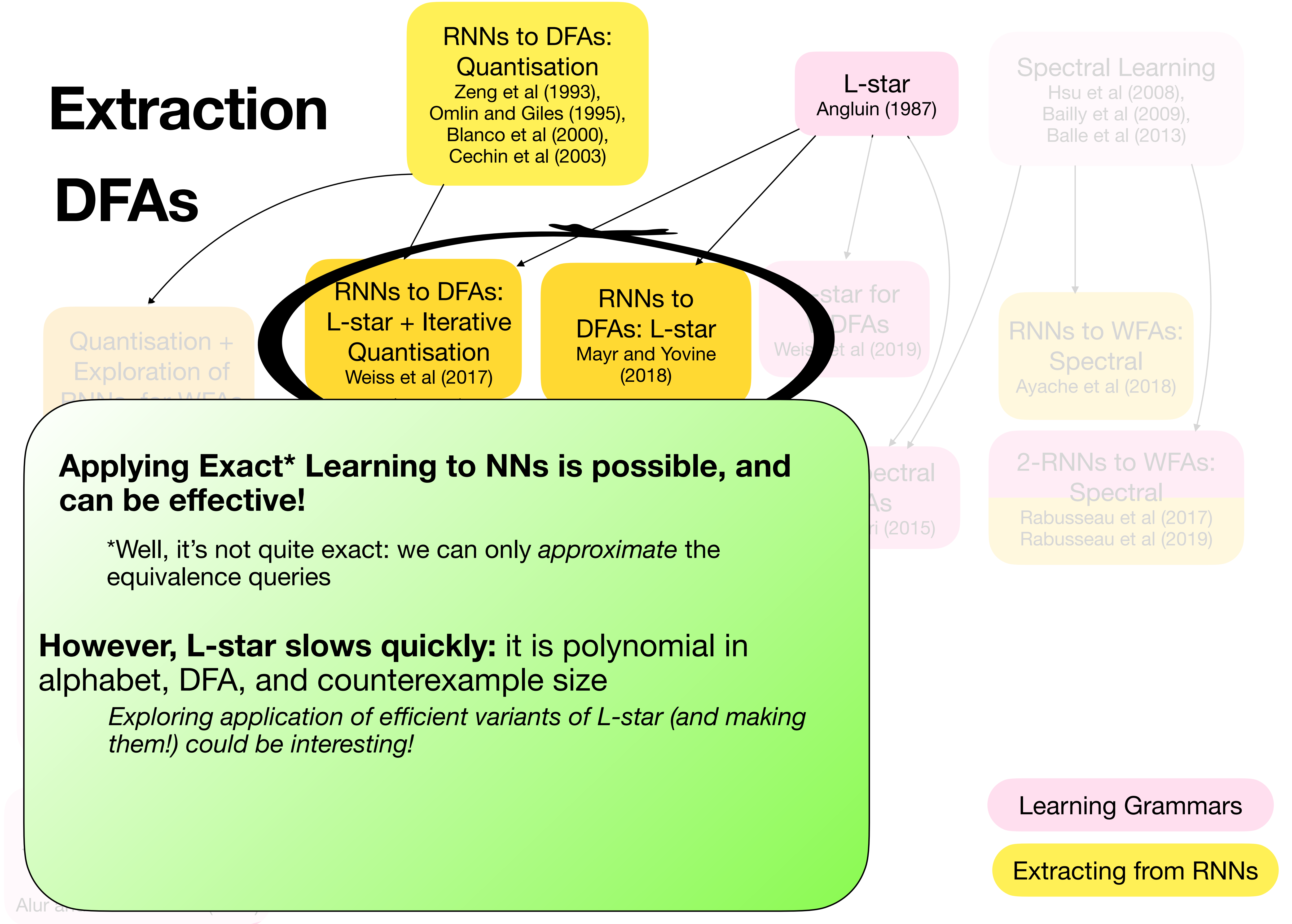


Applying Exact* Learning to NNs is possible, and can be effective!

*Well, it's not quite exact: we can only *approximate* the equivalence queries

Extraction

DFAs



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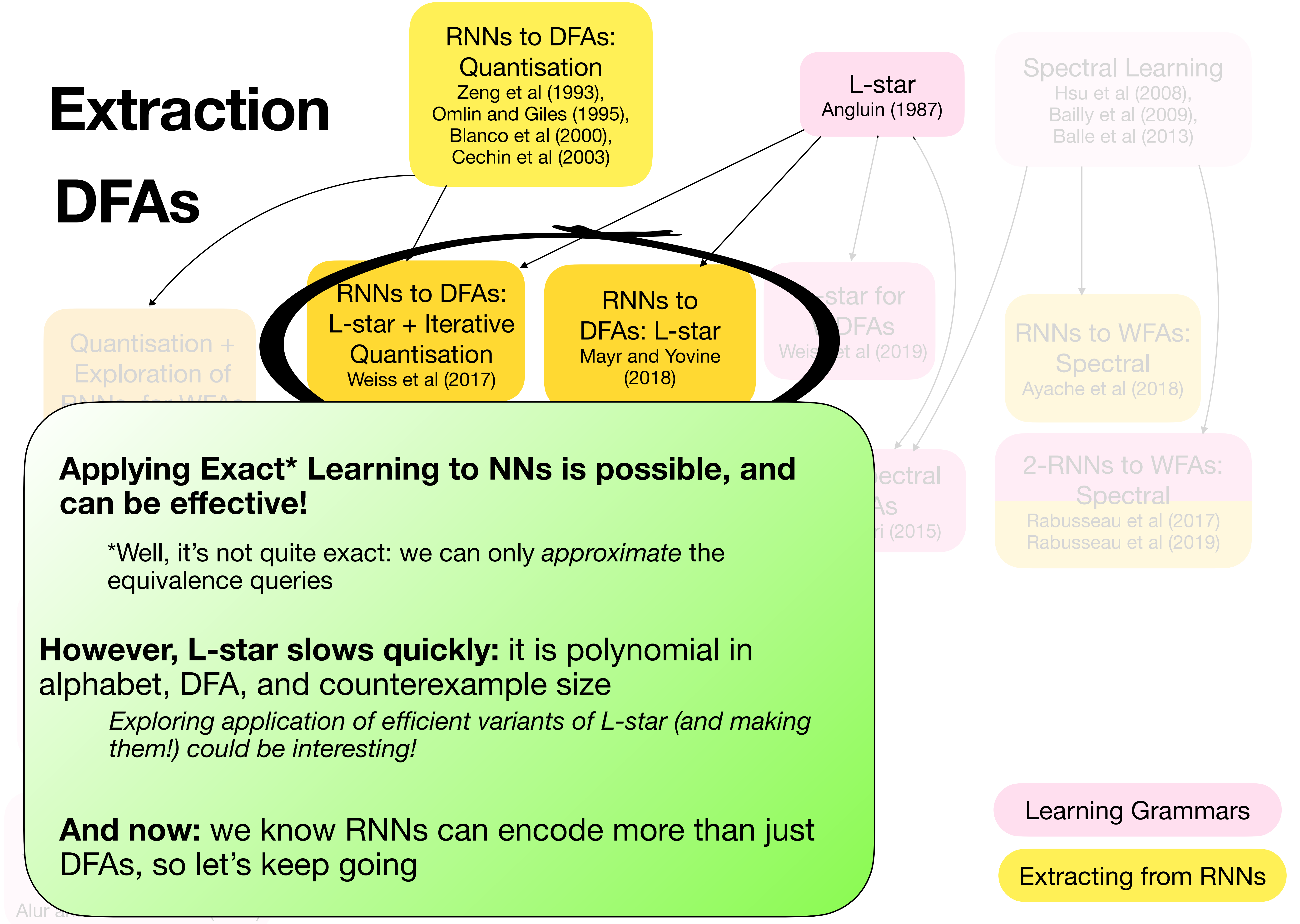
However, L-star slows quickly: it is polynomial in alphabet, DFA, and counterexample size

Exploring application of efficient variants of L-star (and making them!) could be interesting!

Extraction DFAs



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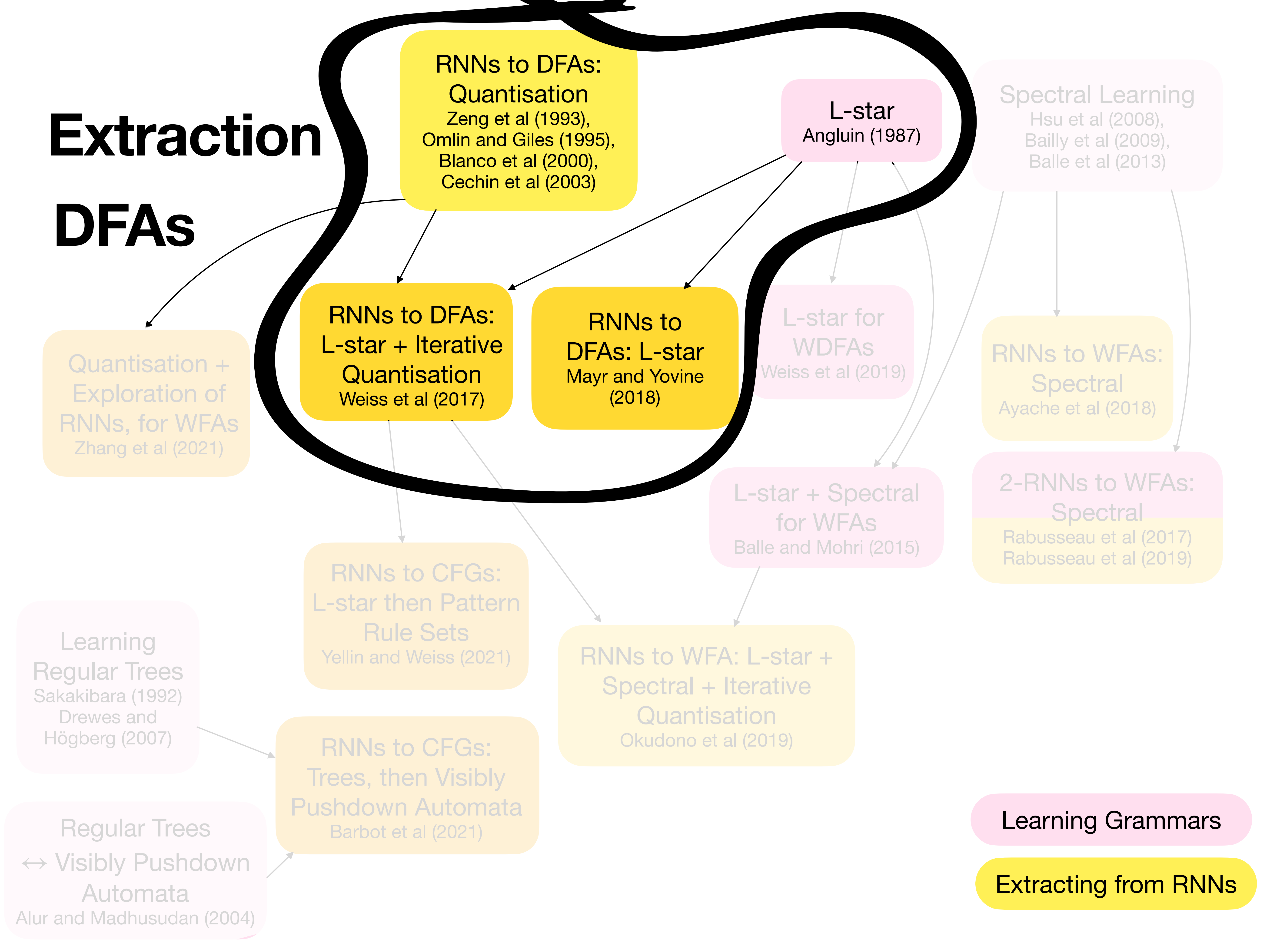
And now: we know RNNs can encode more than just DFAs, so let's keep going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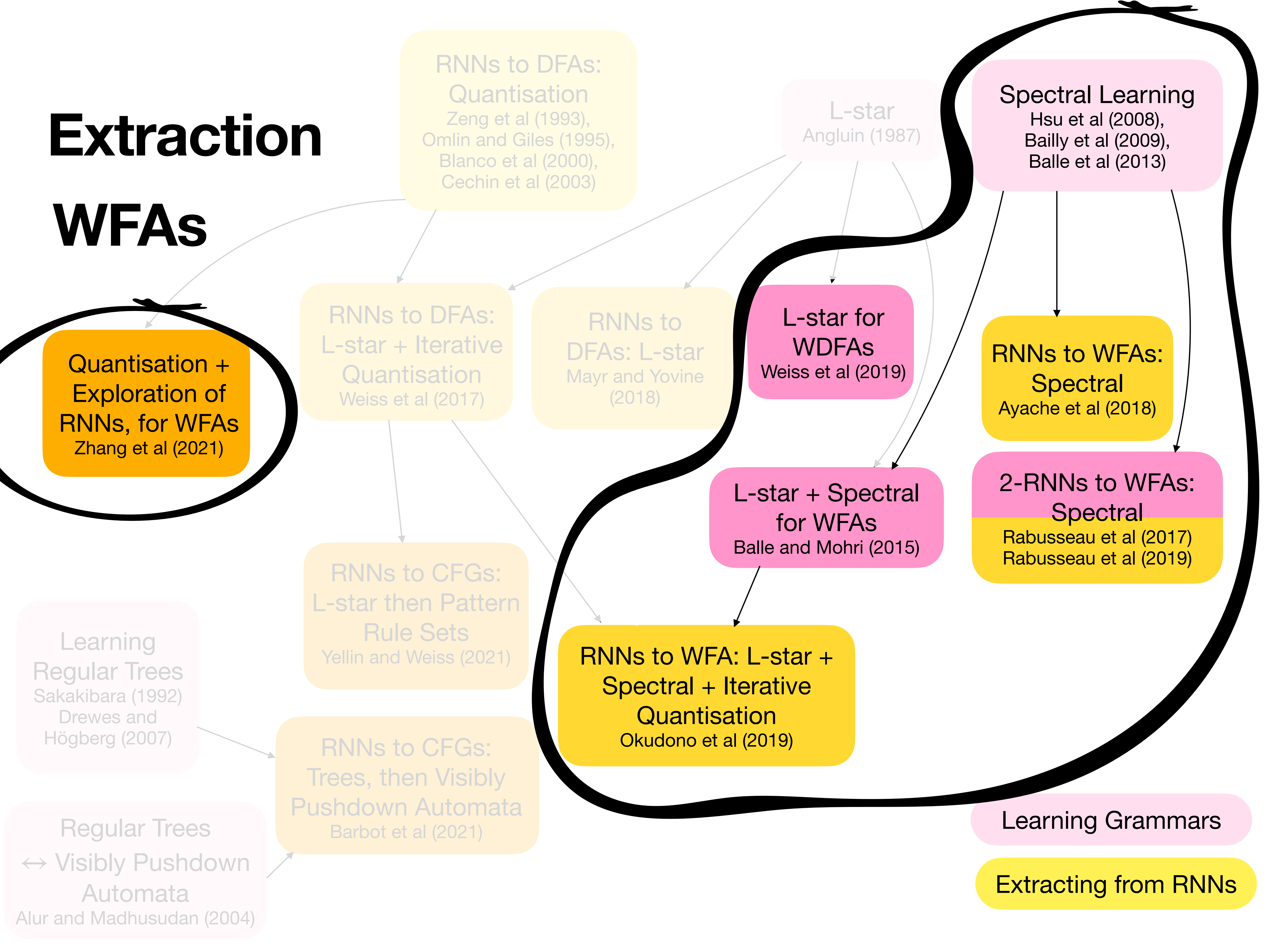

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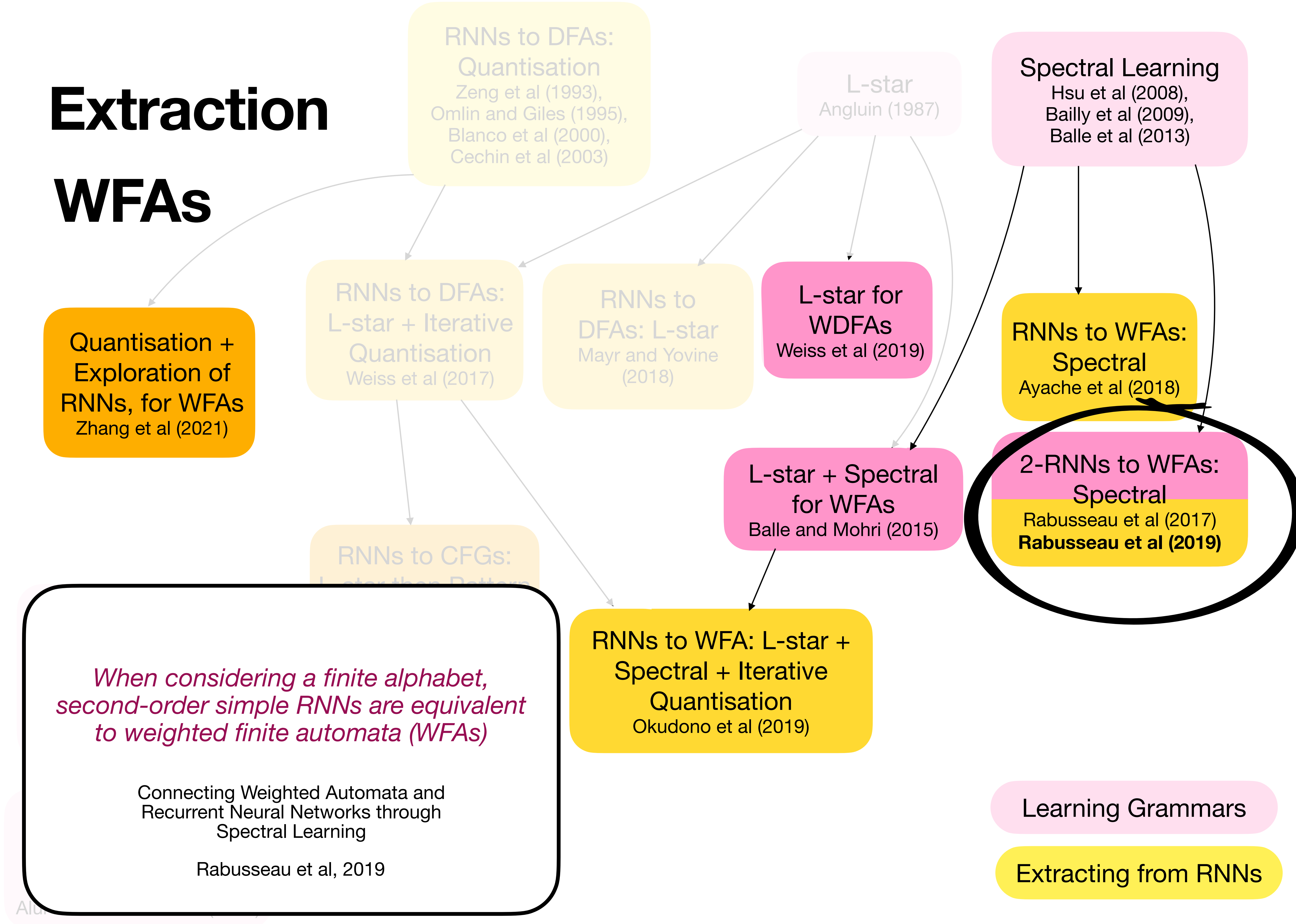
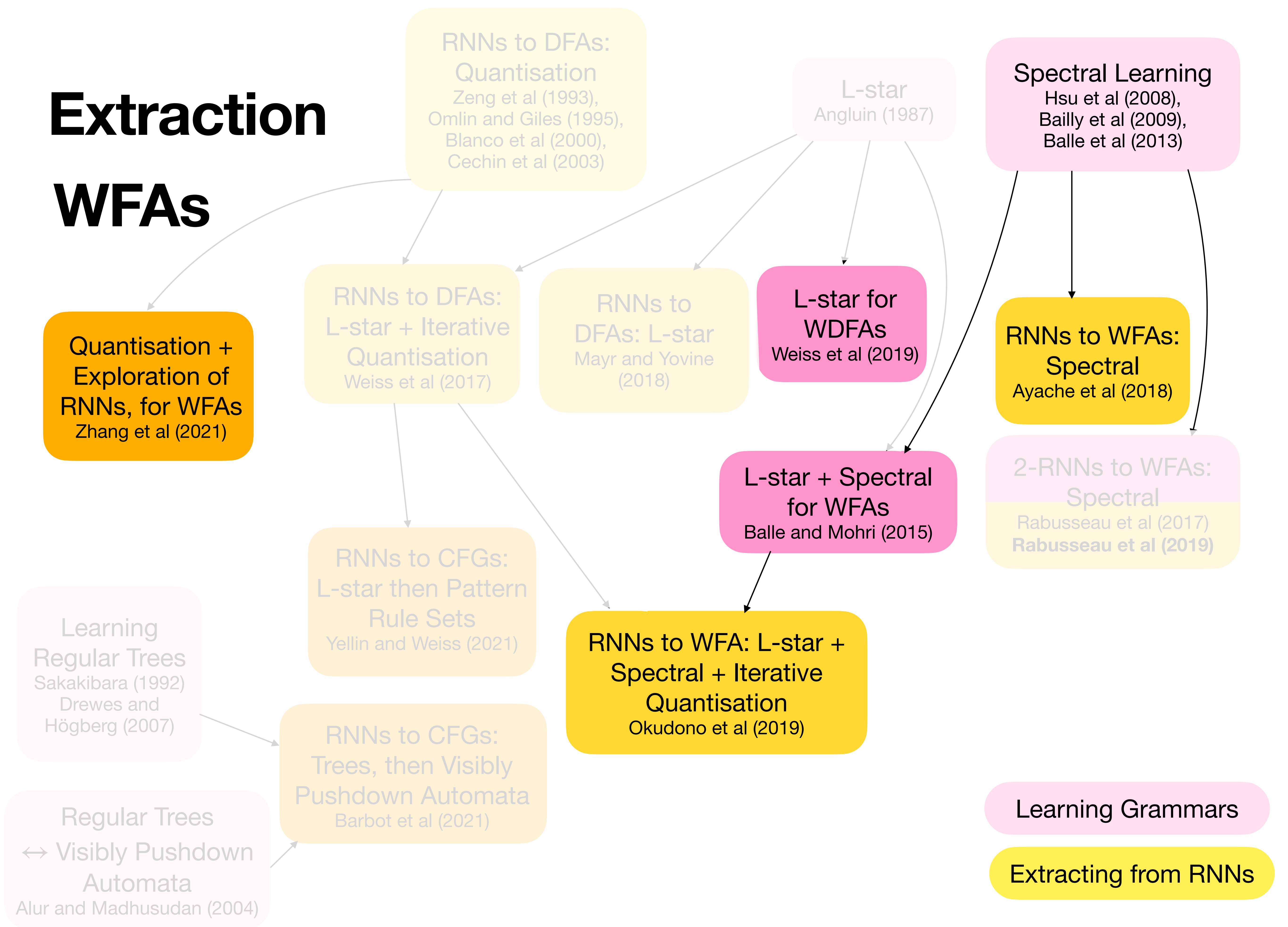


When considering a finite alphabet, second-order simple RNNs are equivalent to weighted finite automata (WFAs)

Connecting Weighted Automata and Recurrent Neural Networks through Spectral Learning

Rabusseau et al, 2019



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- Language-Model RNNs
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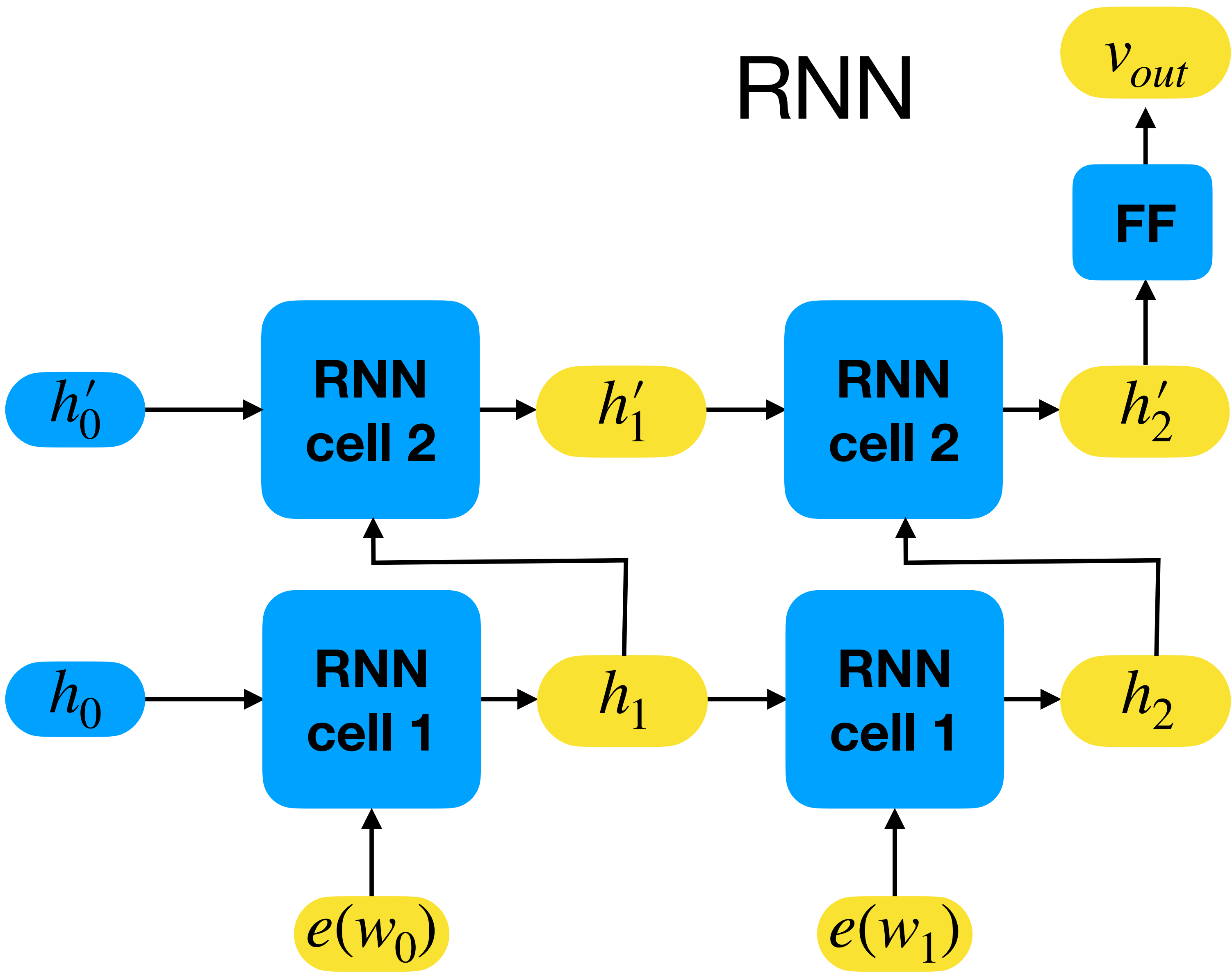

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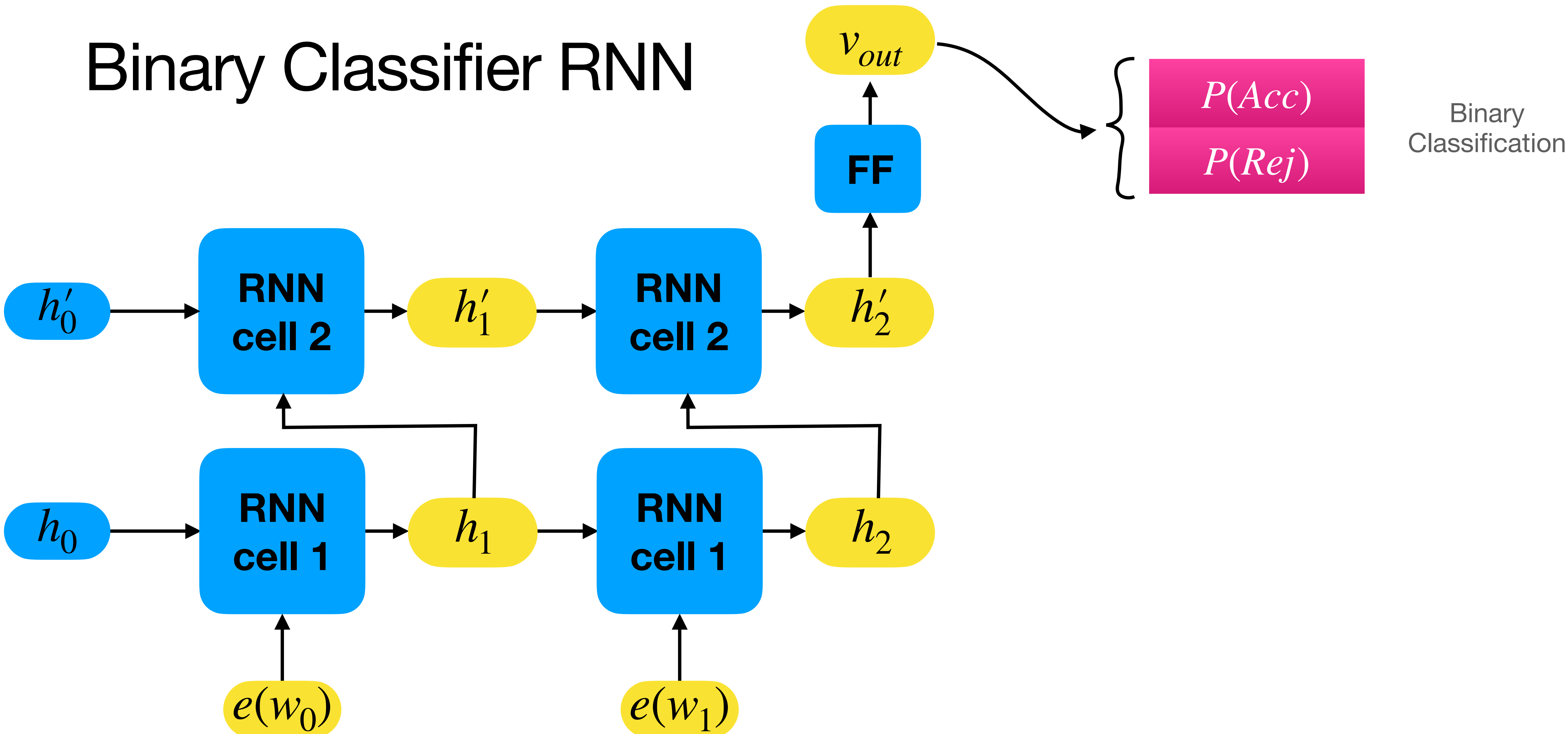

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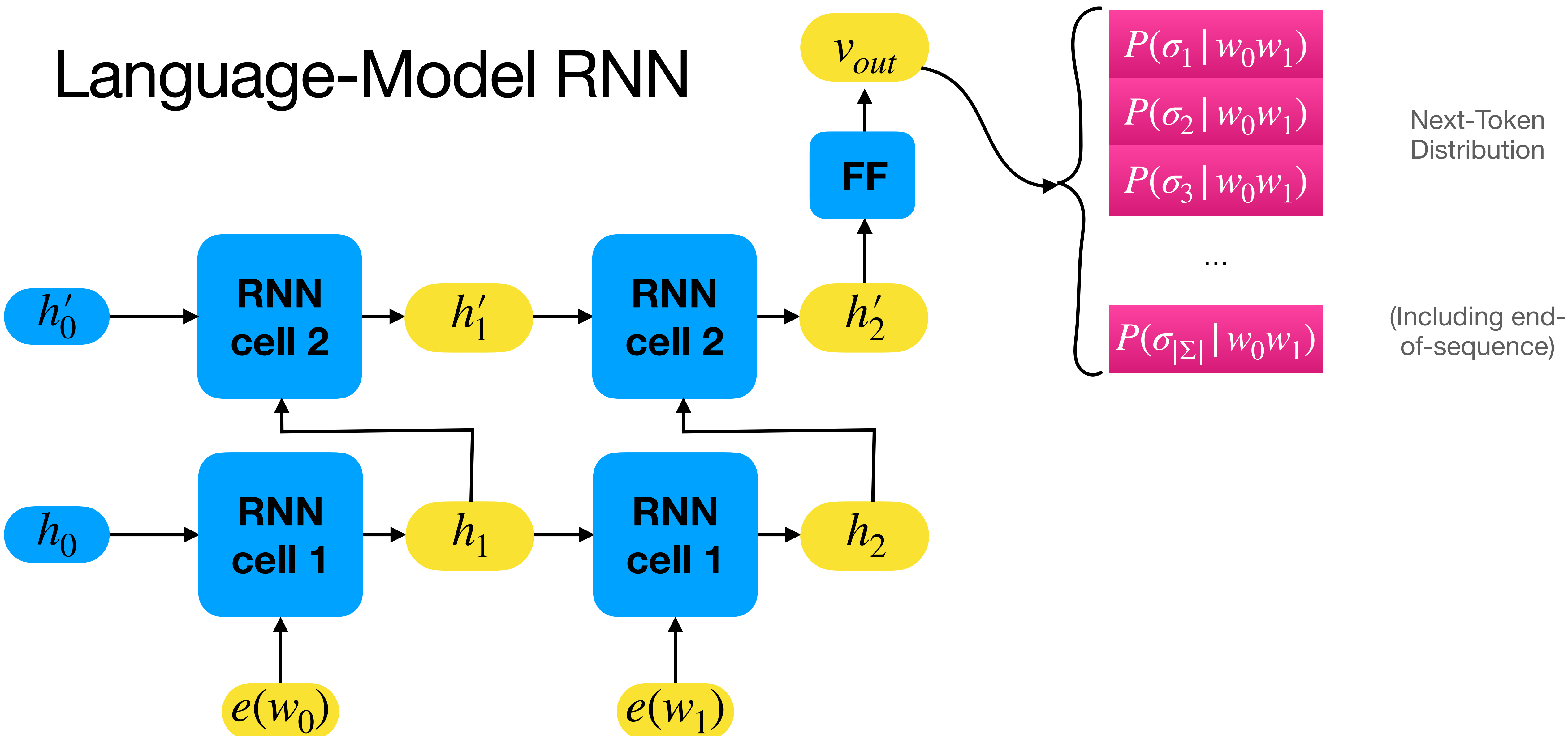

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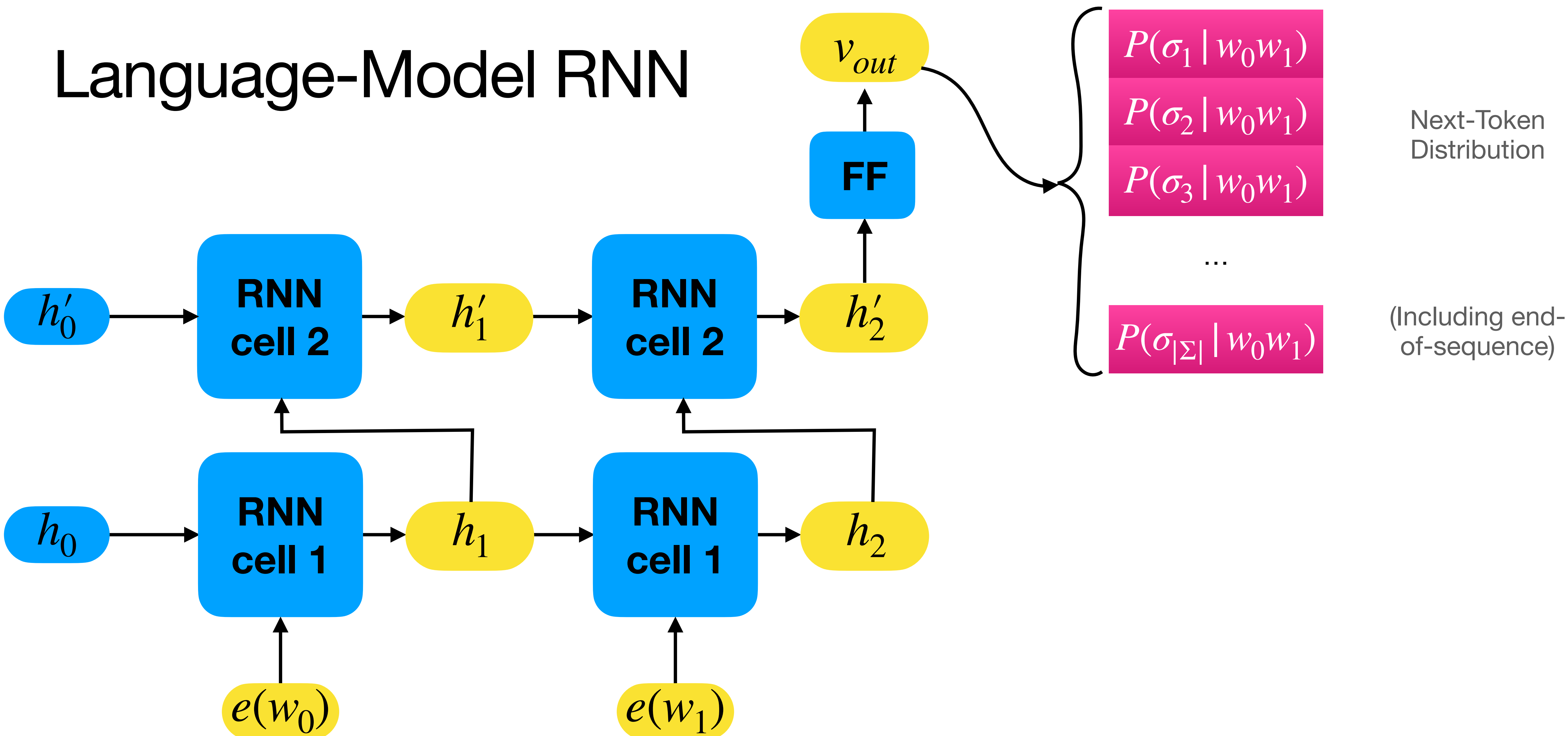

$$\text{RNN}(w_1 w_2) = P(w_1 | \varepsilon) \cdot P(w_2 | w_1) \cdot P(\text{EOS} | w_1 w_2)$$

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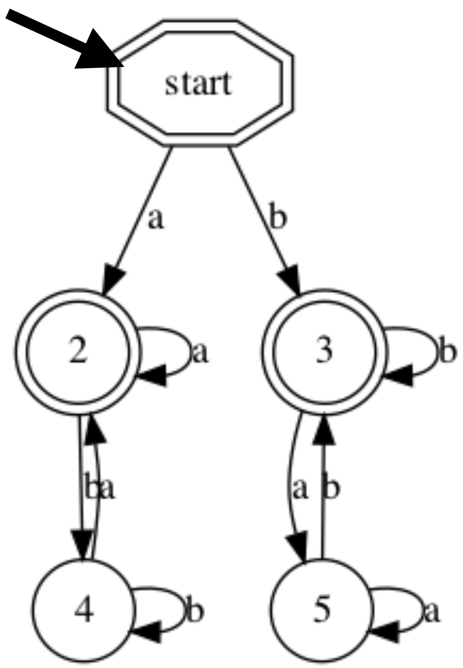

DFA

deterministic

$$A = \langle \Sigma, Q, q_0, F, \delta_Q \rangle$$

$$\delta_Q : Q \times \Sigma \rightarrow Q$$

$$A(w) = \begin{cases} \text{Acc} & \text{if } \hat{\delta}_Q(w) \in F \\ \text{Rej,} & \text{else} \end{cases}$$

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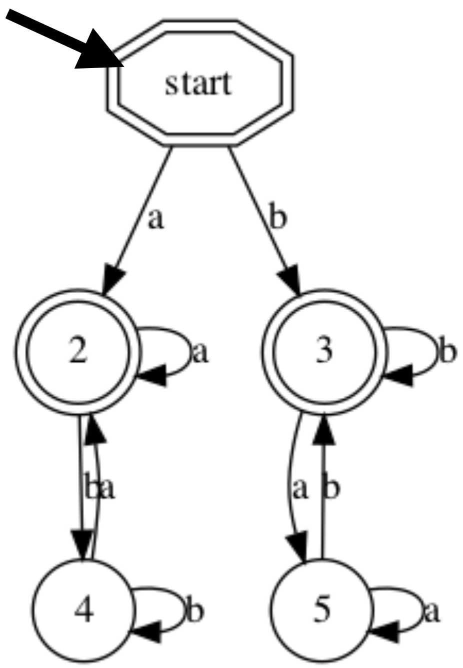

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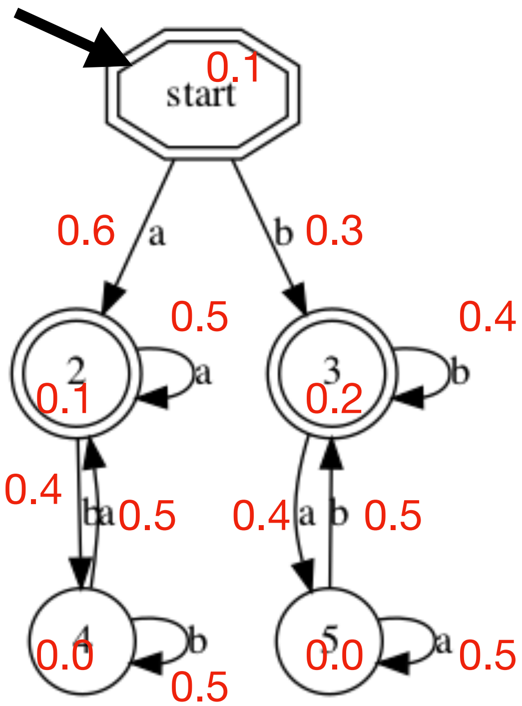


WDFA

weighted deterministic

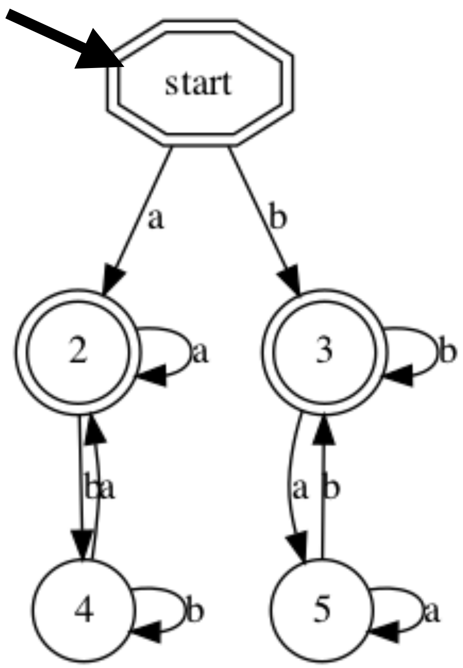
$$A = \langle \Sigma, Q, q_0, \delta_Q, \delta_W, \beta \rangle$$

$$\delta_W \colon Q \times \Sigma \to \mathbb{R}$$

$$\beta \colon Q \to \mathbb{R}$$

$$A(w) = \Big(\prod_{i \in [|w|]} \delta_W(\hat{\delta}_Q(w_{1:i-1}), w_i) \Big) \cdot \beta(\hat{\delta_Q(w)})$$

RNNs: Extracting WFAs: Background!



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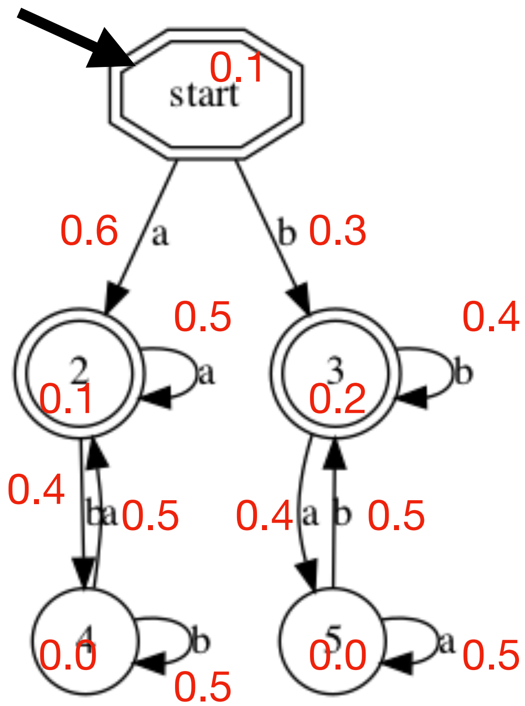

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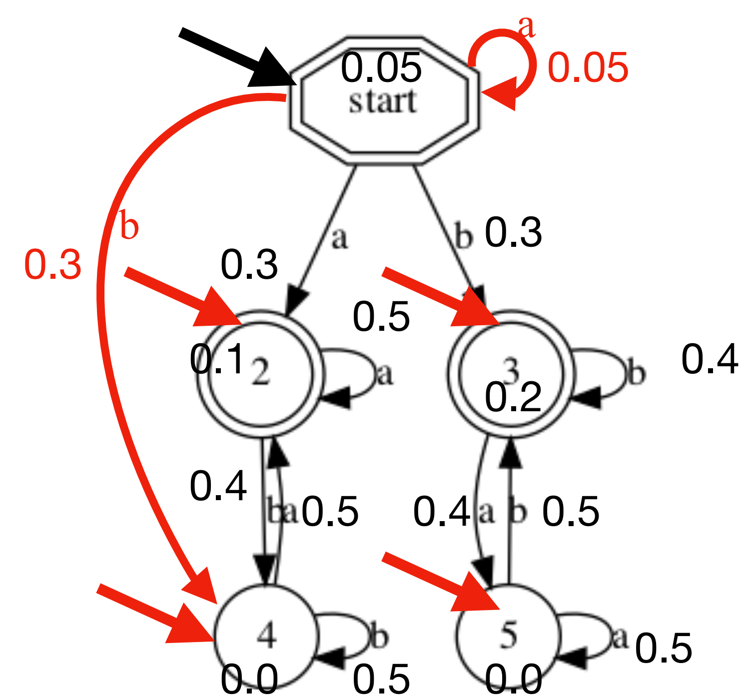


WFA

weighted

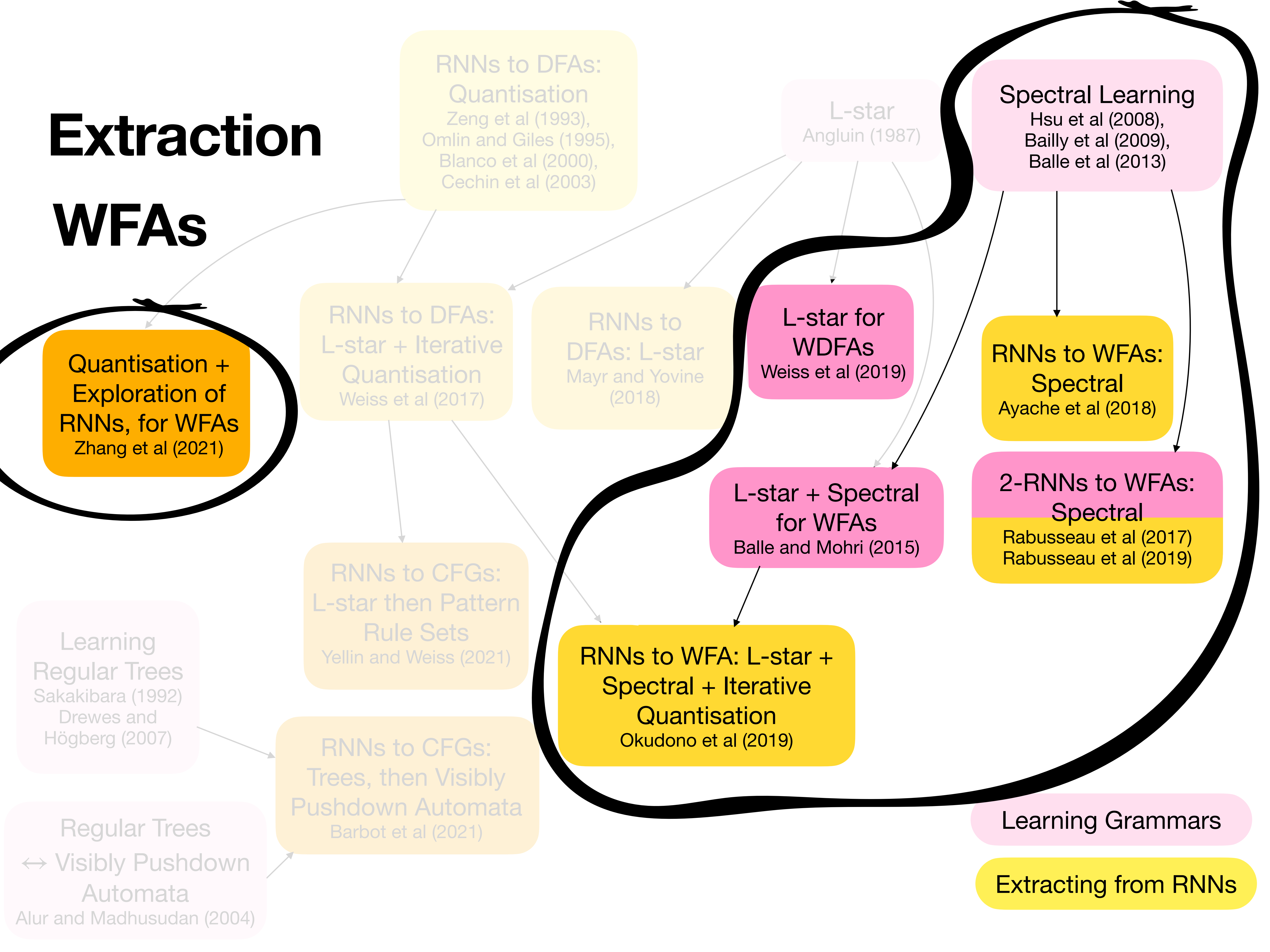
$$A = \langle \Sigma, Q, \alpha, \beta, \{W_\sigma\}_{\sigma \in \Sigma} \rangle$$

$$\alpha \colon Q \to \mathbb{R}$$

$$\beta \colon Q \to \mathbb{R}$$

$$W_\sigma \in \mathbb{R}^{Q \times Q}$$

$$A(w) = \alpha \cdot W_{w_1} \cdot W_{w_2} \cdot \ldots \cdot W_{w_{|w|}} \cdot \beta$$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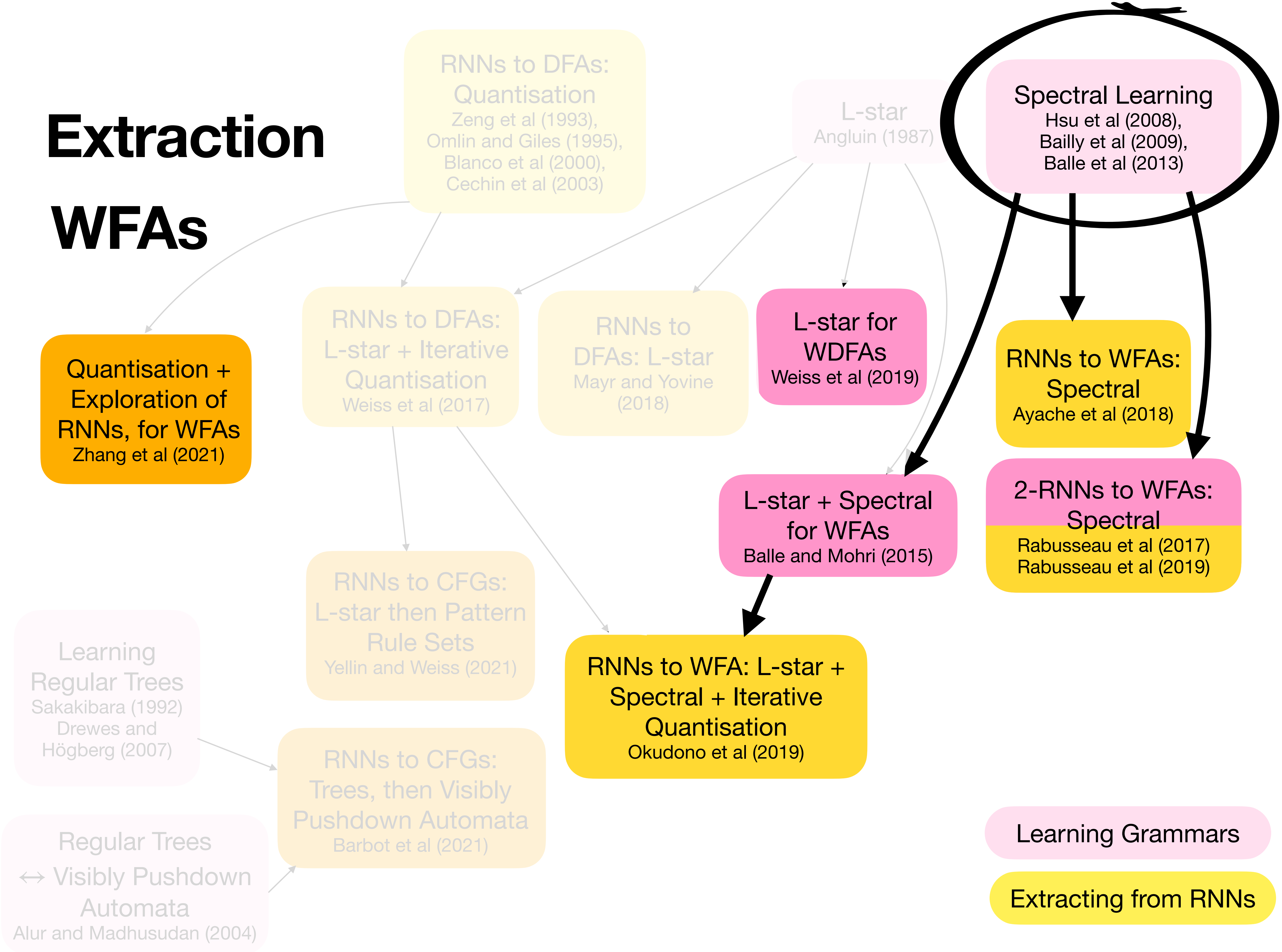

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Spectral Learning of WFAs

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(example on $\Sigma = \{a, b\}$)

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1. Make Hankel Sub-blocks

Hankel sub-block H

P \ S	ε	b	ab	$\cdots$	v
ε	$T(\varepsilon)$	$T(b)$	$T(ab)$		$T(v)$
a	$T(a)$	$T(ab)$	$T(aab)$		$T(a \cdot v)$
ab	$T(ab)$	$T(abb)$	$T(abab)$		$T(ab \cdot v)$
$\cdots$					
u	$T(u)$	$T(u \cdot b)$	$T(u \cdot ab)$		$T(u \cdot v)$

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Hankel sub-block H^b

P \ S	ε	b	ab	$\cdots$	v
ε					
a					
ab					
$\cdots$					
u					$T(u \cdot b \cdot v)$

Hankel sub-block H^a

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a					
ab					
$\cdots$					
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Hankel sub-block H^b

P \ S	ε	b	ab	$\cdots$	v
ε					
a					
ab					
$\cdots$					
u					$T(u \cdot b \cdot v)$

Hankel sub-block H^a

P \ S	ε	b	ab	$\cdots$	v
ε					
a					
ab					
$\cdots$					
u					$T(u \cdot a \cdot v)$

2. $U, d, V = \mathrm{SVD}(H)$

3. (Optional): Trim U, d, V to k largest singular values

4. $\alpha = H_{\varepsilon,:}V \;,\; \beta = (HV)^{\dagger} H_{:,\varepsilon} \;,$
$W_\sigma = (HV)^{\dagger} H^{\sigma} V$

5. $A = \langle \Sigma, [k], \alpha, \beta, \{W_\sigma\}_{\sigma \in \Sigma} \rangle$

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ab	$T(ab)$	$T(abb)$	$T(abab)$		$T(ab\cdot v)$
$\cdots$					
u	$T(u)$	$T(u\cdot b)$	$T(u\cdot ab)$		$T(u\cdot v)$

Hankel sub-block H^b

P \ S	ε	b	ab	$\cdots$	v
ε					
a					
ab					
$\cdots$					
u					$T(u\cdot b\cdot v)$

Hankel sub-block H^a

P \ S	ε	b	ab	$\cdots$	v
ε					
a					
ab					
$\cdots$					
u					$T(u\cdot a\cdot v)$

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Balle et al, 2013

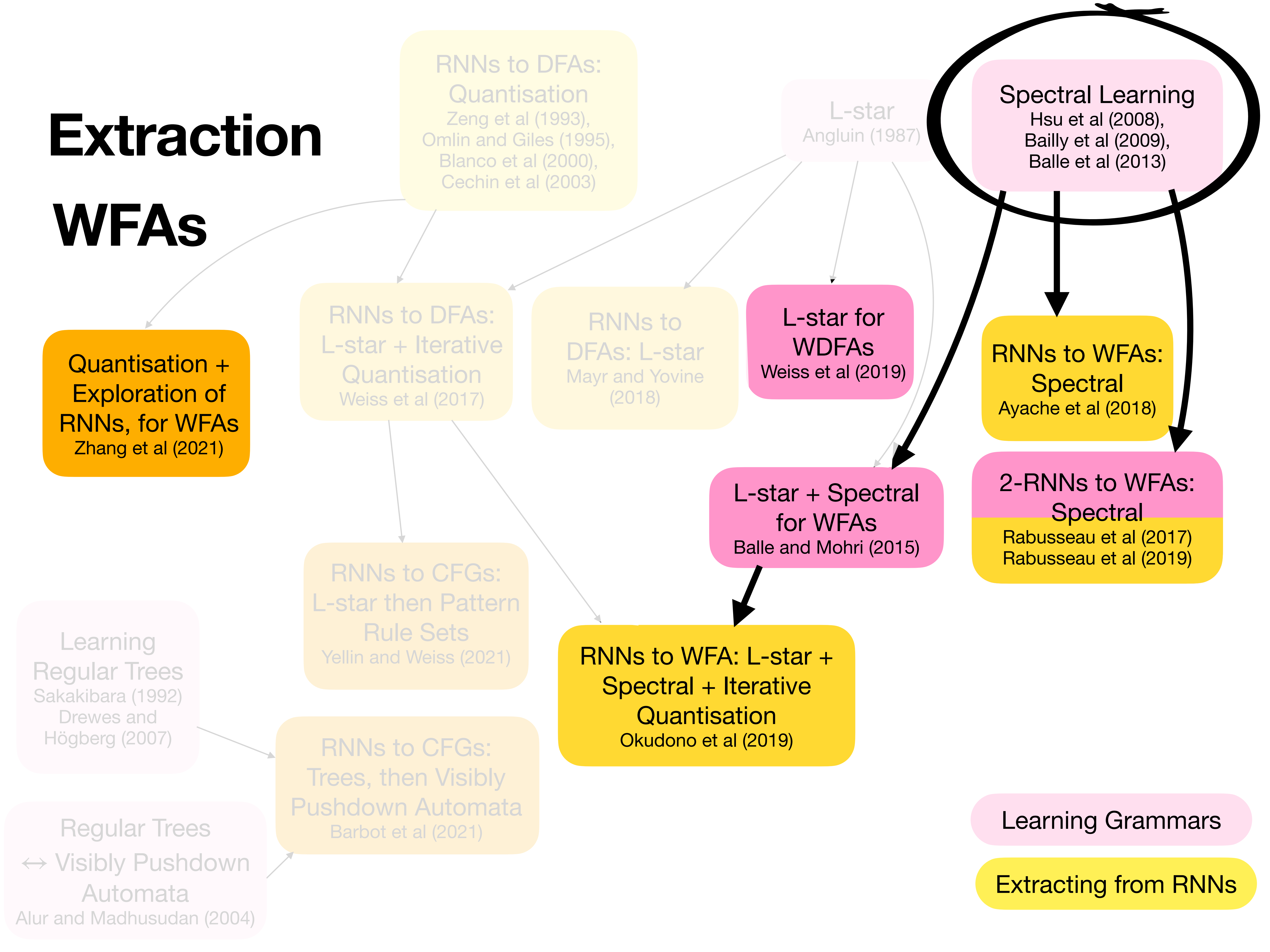
Learning Weighted Automata

Balle and Mohri, 2015

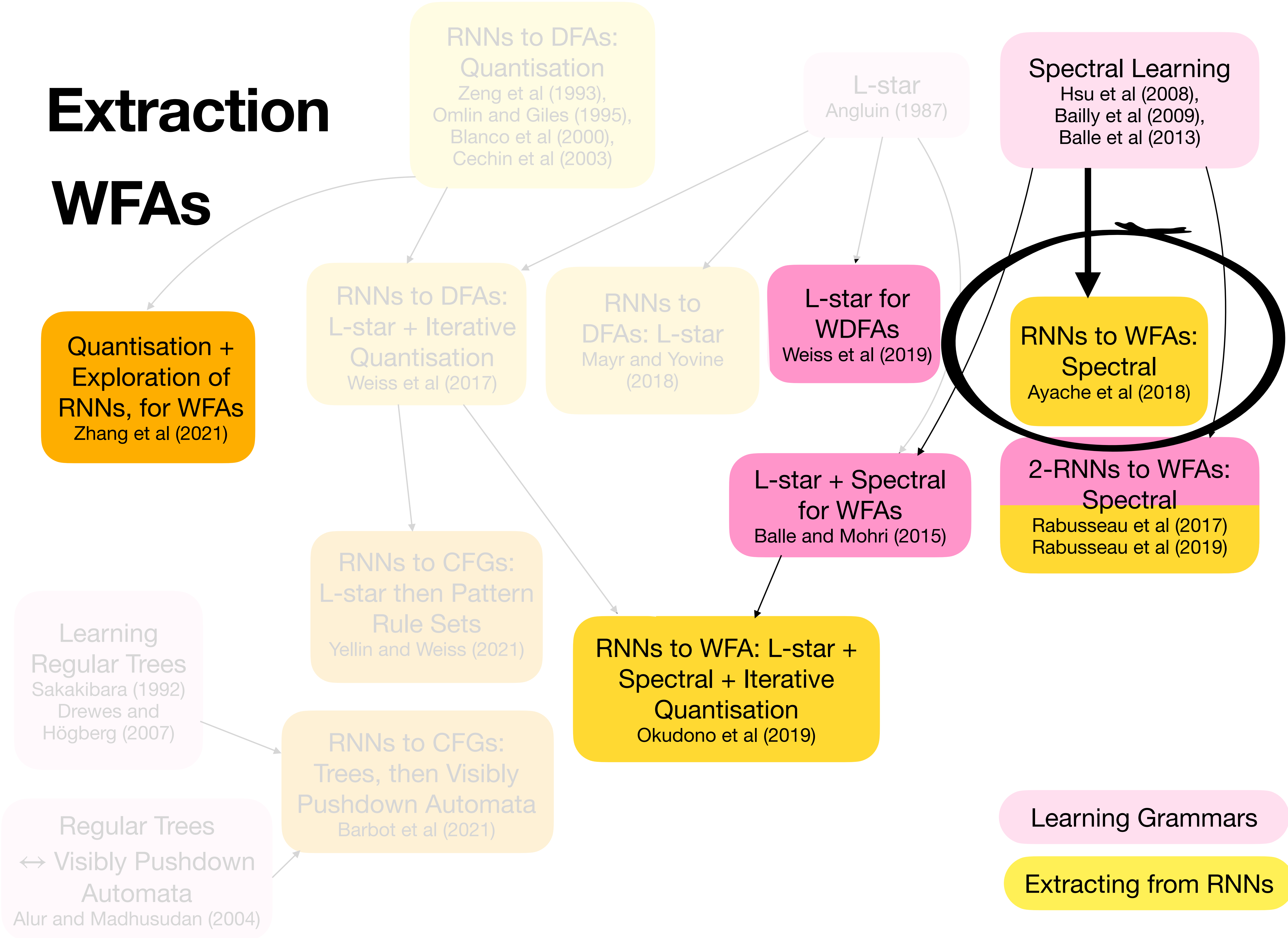
A Maximum Matching Algorithm for Basis Selection in Spectral Learning

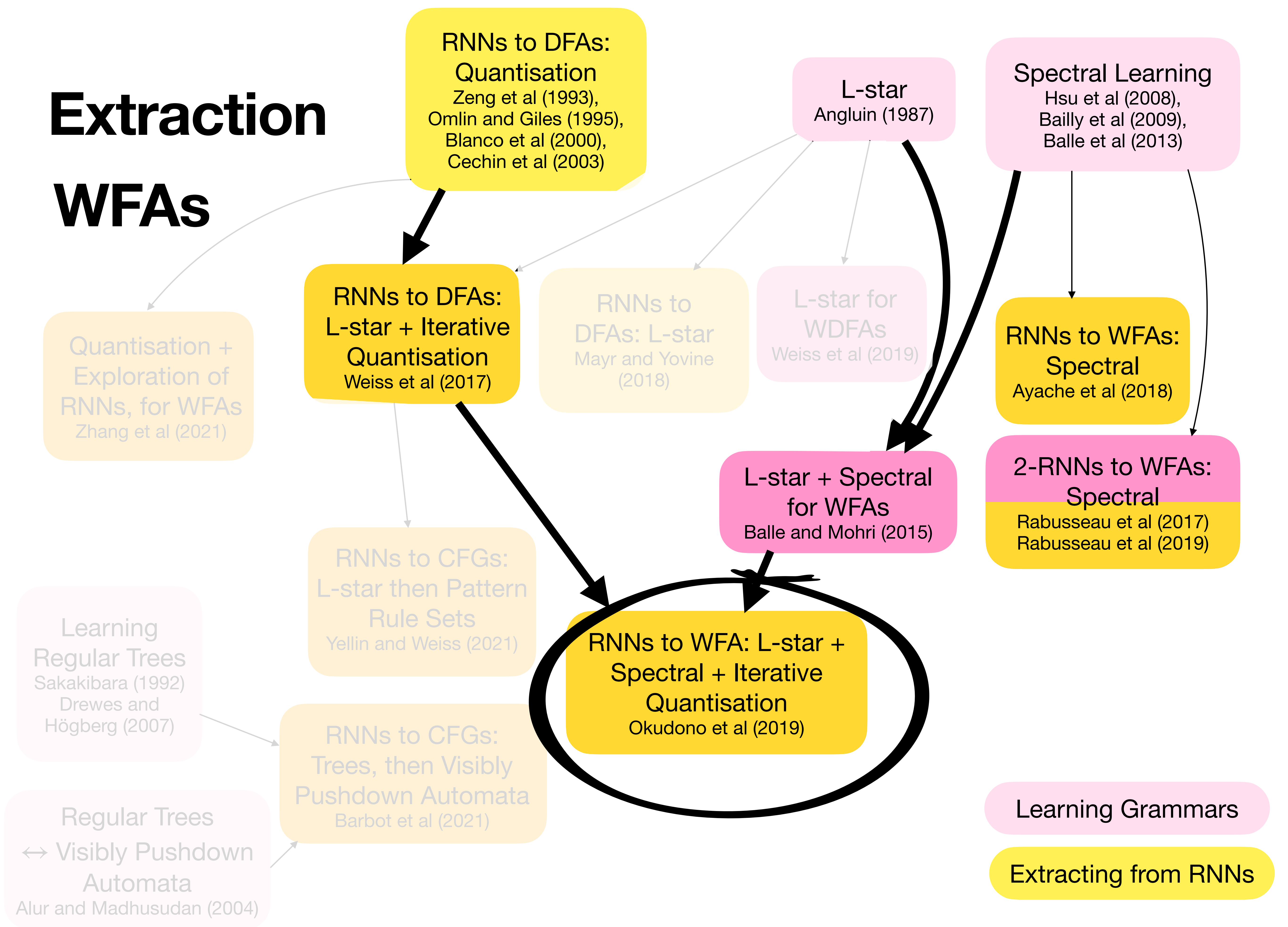
Quattoni et al, 2017

Extraction WFAs



Extraction WFAs





Extraction
WFAs
RNNs to DFAs: Quantisation
Zeng et al (1993), Omlin and Giles (1995), Blanco et al (2000), Cechin et al (2003)
L-star
Angluin (1987)
Spectral Learning
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Quantisation + Exploration of RNNs, for WFAs
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RNNs to DFAs: L-star + Iterative Quantisation
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Yellin and Weiss (2021)
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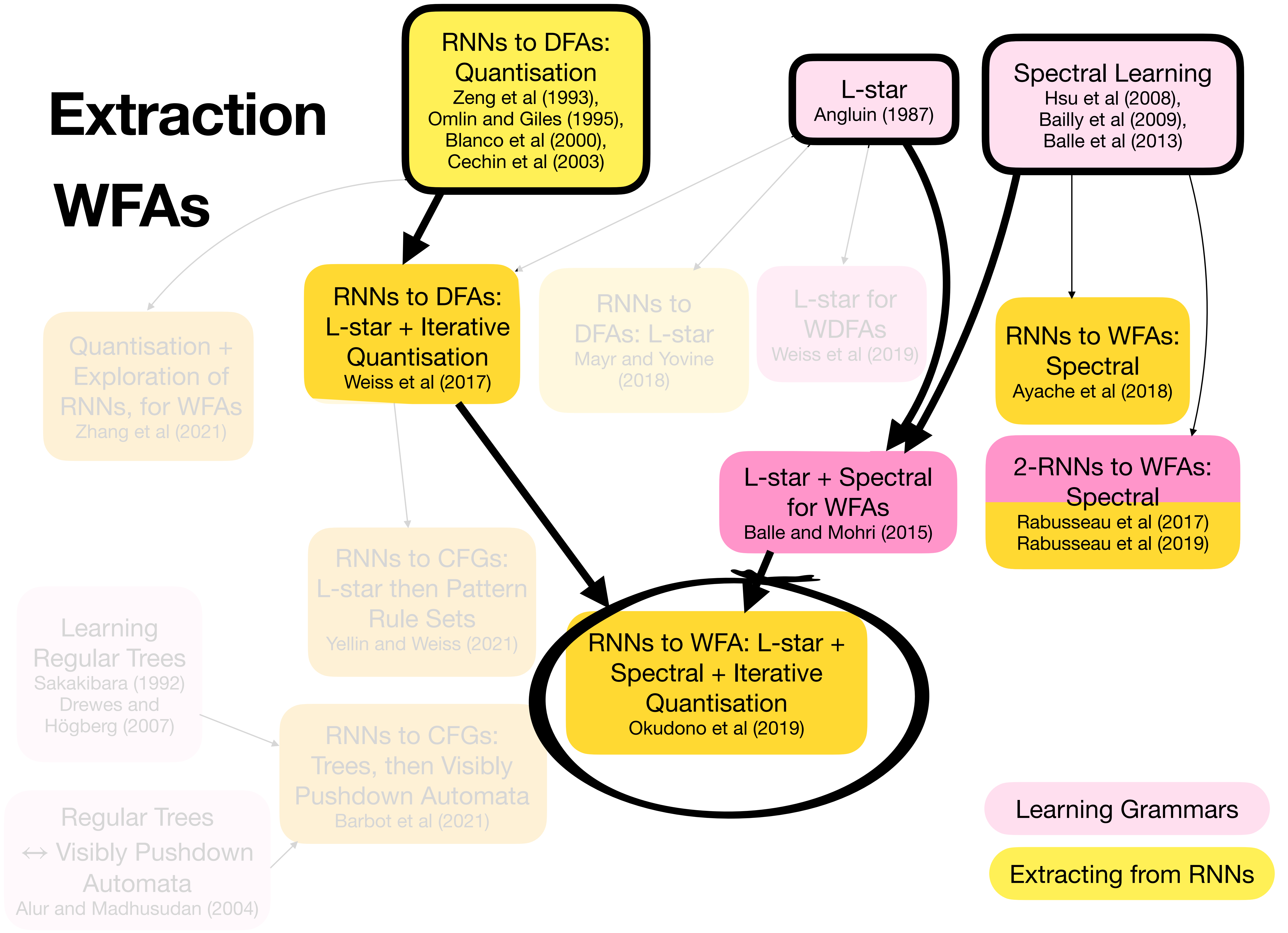
Learning Grammars
Extracting from RNNs



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RNNs: Extracting WFAs: Spectral Methods

Explaining Black Boxes on Sequential Data Using Weighted Automata

Ayache et al, 2018

Black Box Model

Build Hankel basis (P,S) by sampling sequences according to black box's distribution

Try multiple sizes for final WFA (truncations k of SVD decomposition) and choose best result

Spectral Learning

Hsu et al (2008), Bailly et al (2009), Balle et al. (2013)

RNNs: Extracting WFAs: Spectral Methods

Explaining Black Boxes on Sequential Data Using Weighted Automata

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Try multiple sizes for final WFA (truncations k of SVD decomposition) and choose best result

Weighted Automata Extraction from Recurrent Neural Networks via Regression on State Spaces

Okudono et al, 2019

White Box Model (specifically RNN)

Build Hankel basis (P,S) according to queries from and counterexamples to active learning algorithm

Continue until reach equivalence

Spectral Learning

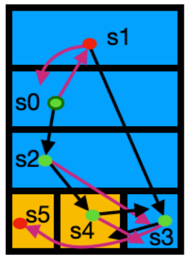
Hsu et al (2008), Bailly et al (2009), Balle et al. (2013)

⊕

Balle and Mohri, 2015

L-star

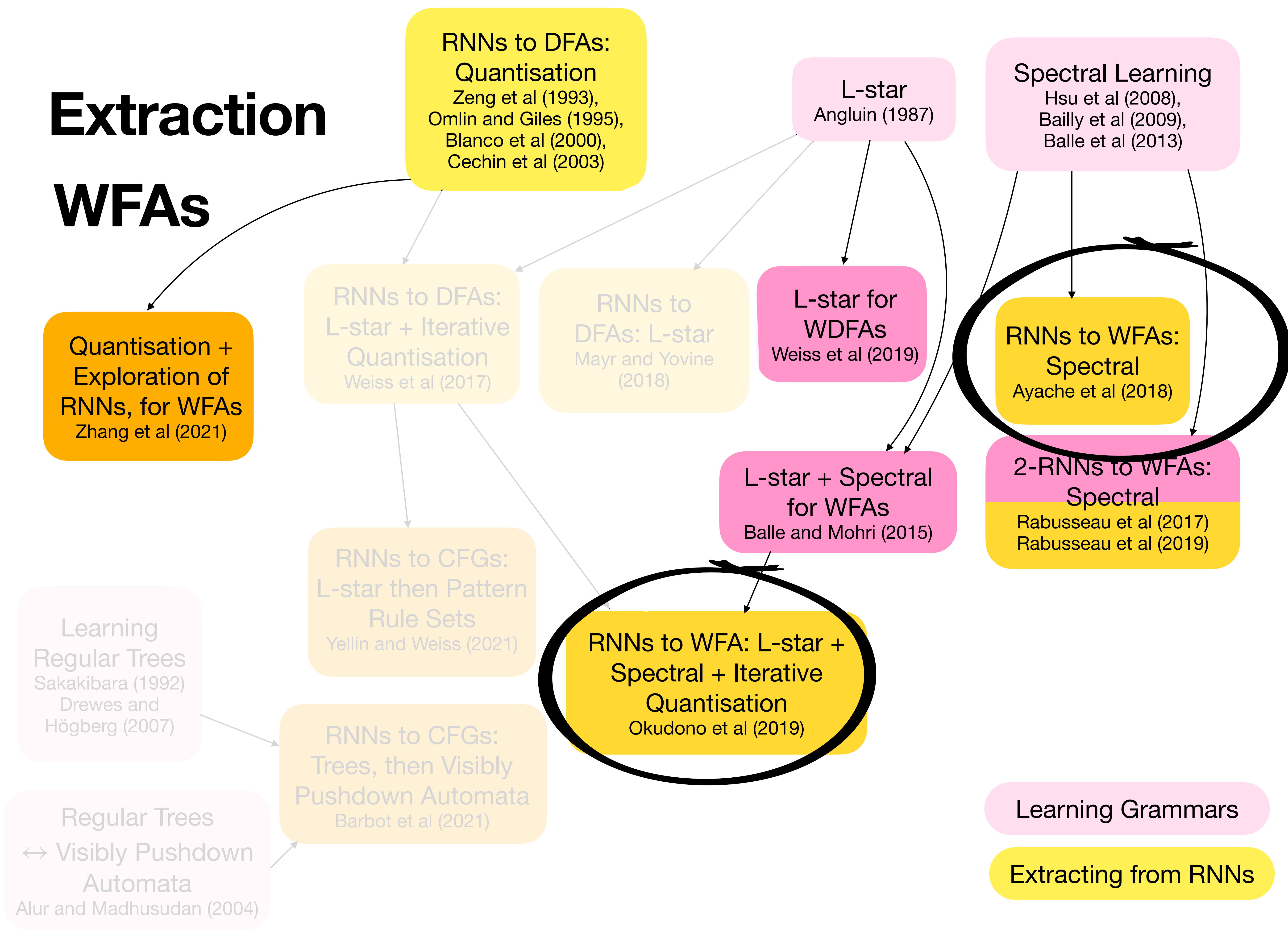
Angluin 1987



Weiss et al, 2017

Quantisation-Exploration

Omlin and Giles, 1996



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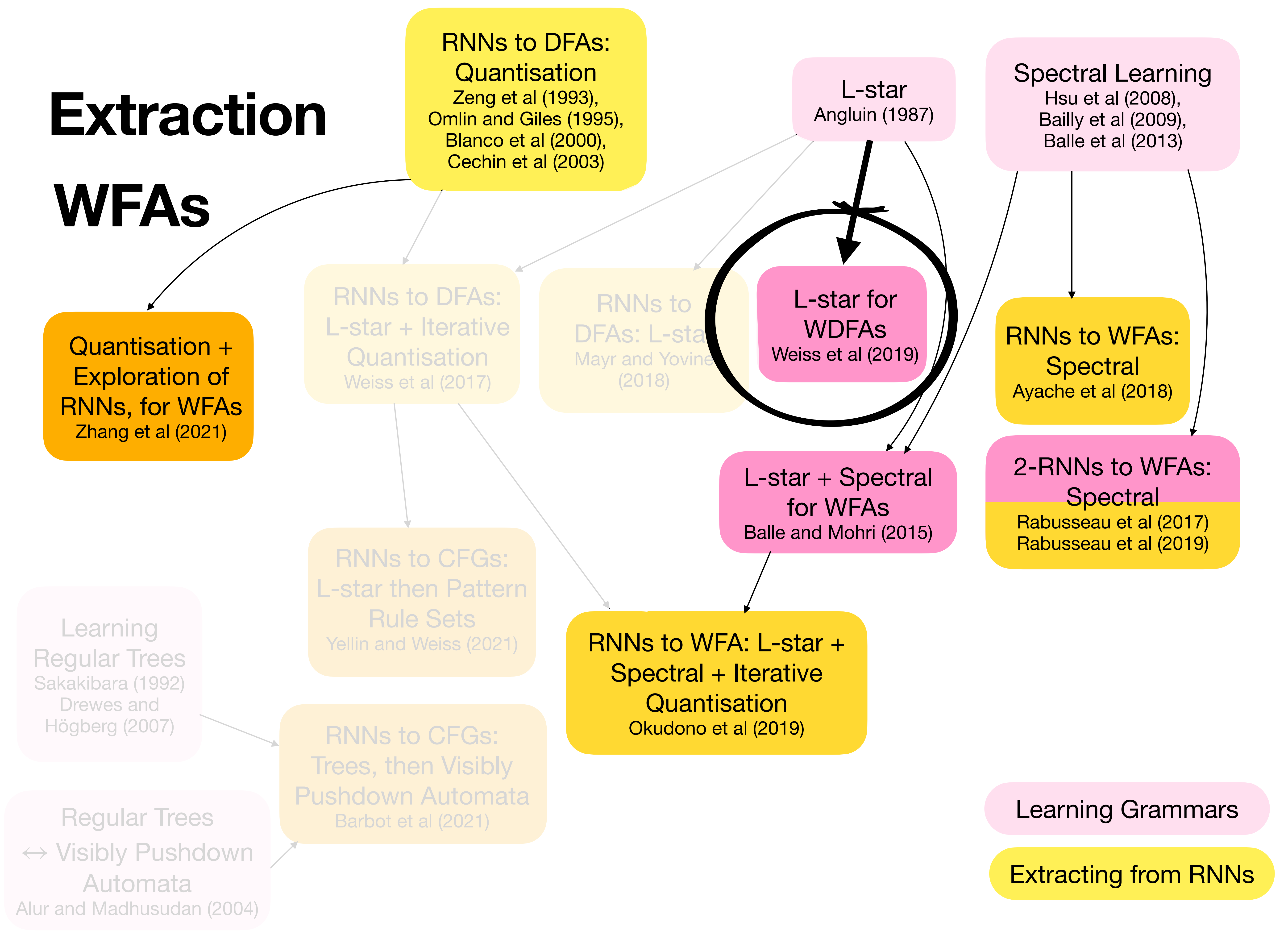

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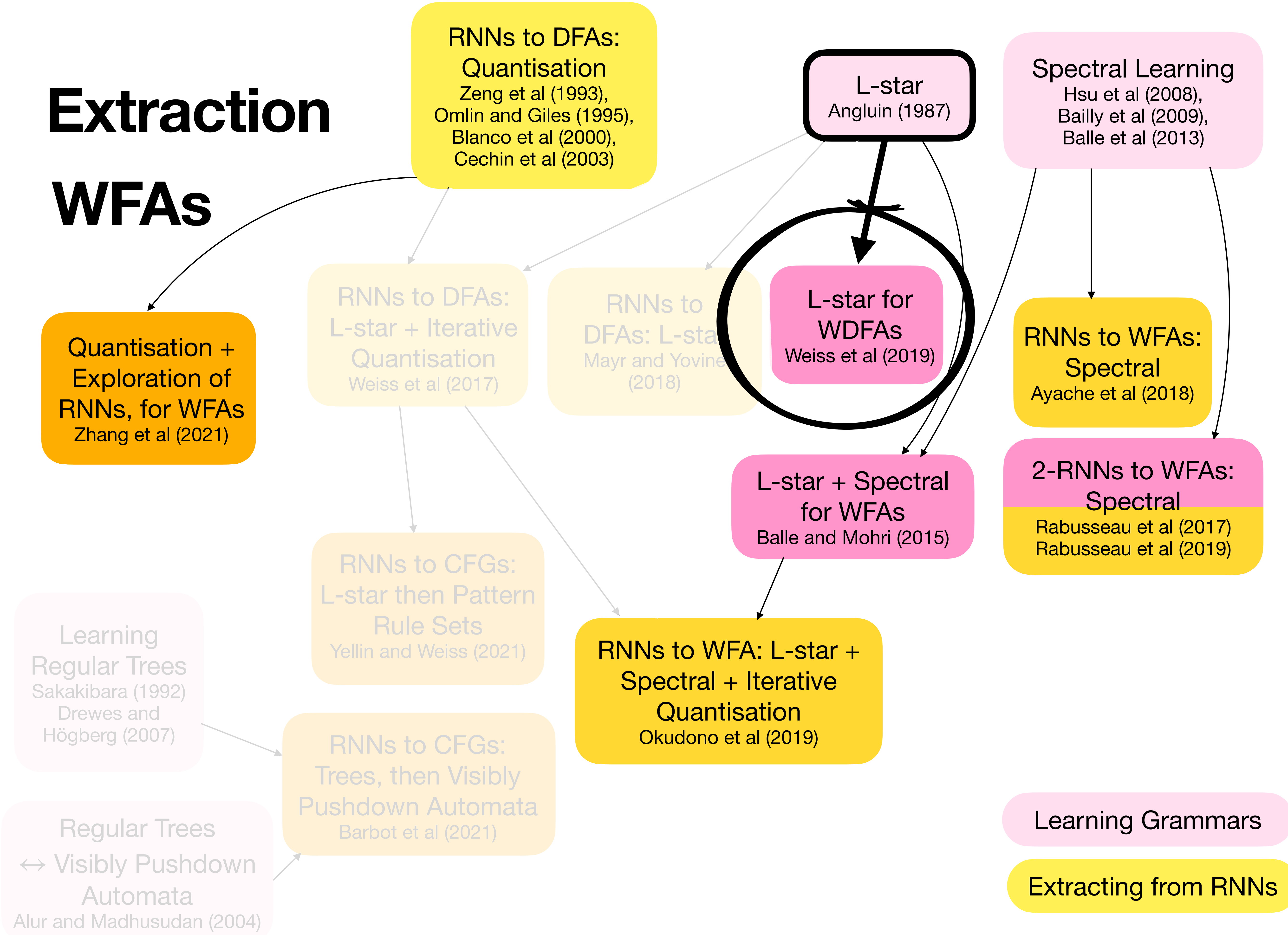
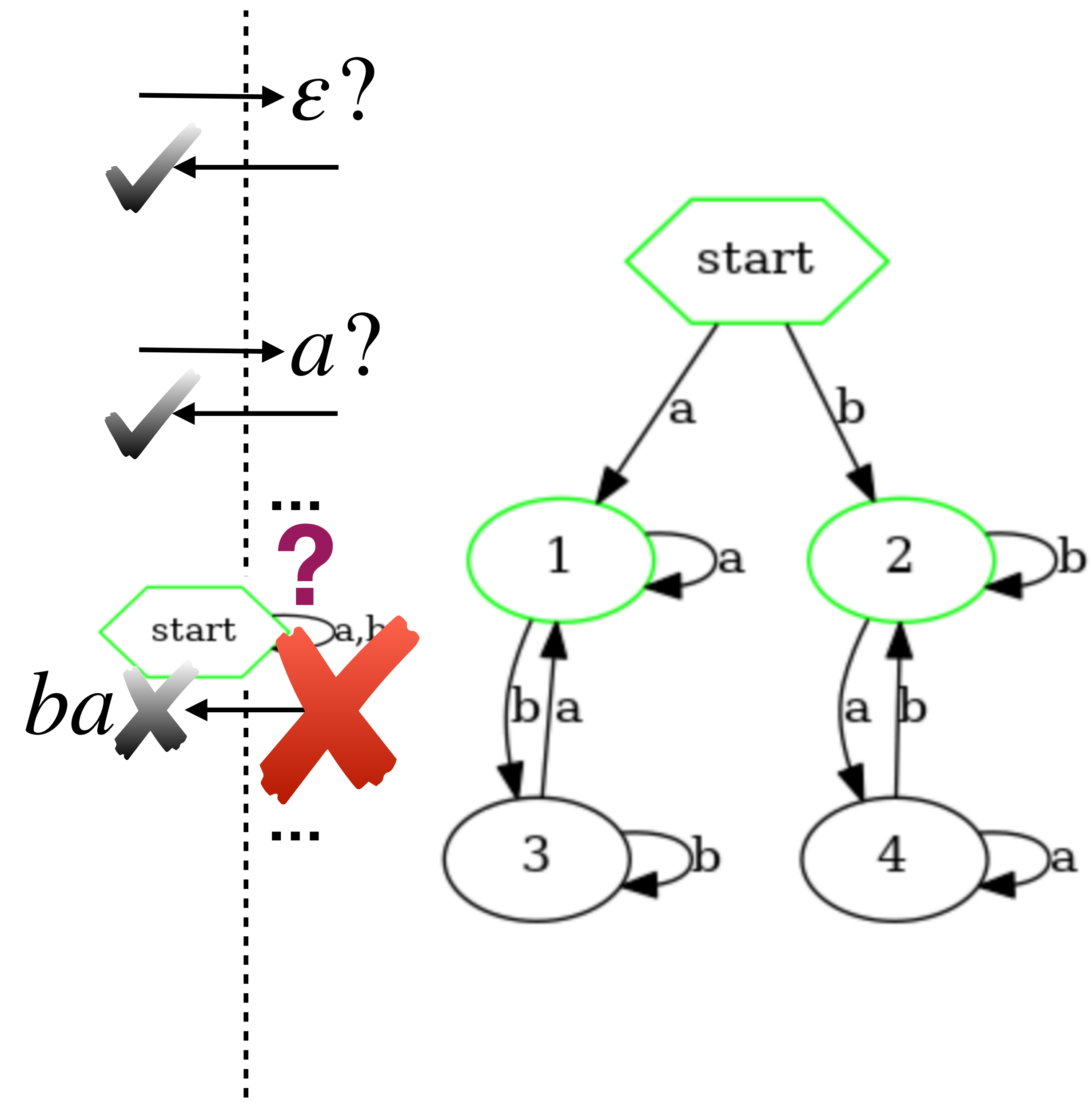
Extraction

WFAs



Background: L*

L*

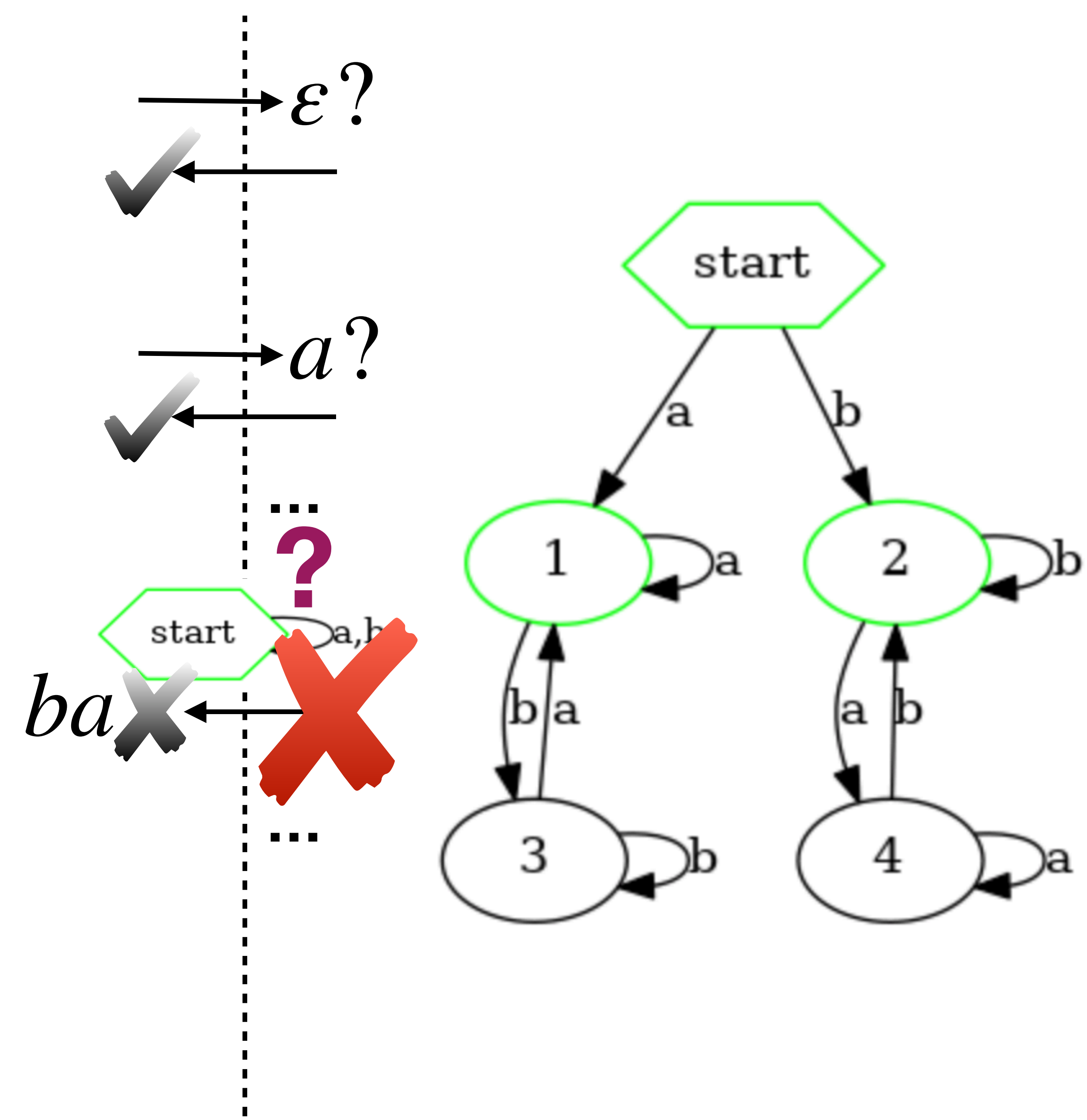


Membership Queries **Equivalence Queries** **Counter-Examples**

Background: L*

The Observation Table

P \ S	ε	a	ba	…
ε	1	1	0	
a	1	1	1	
b	1	0	0	
ba	0	0	0	
bb	1	0	0	
…				

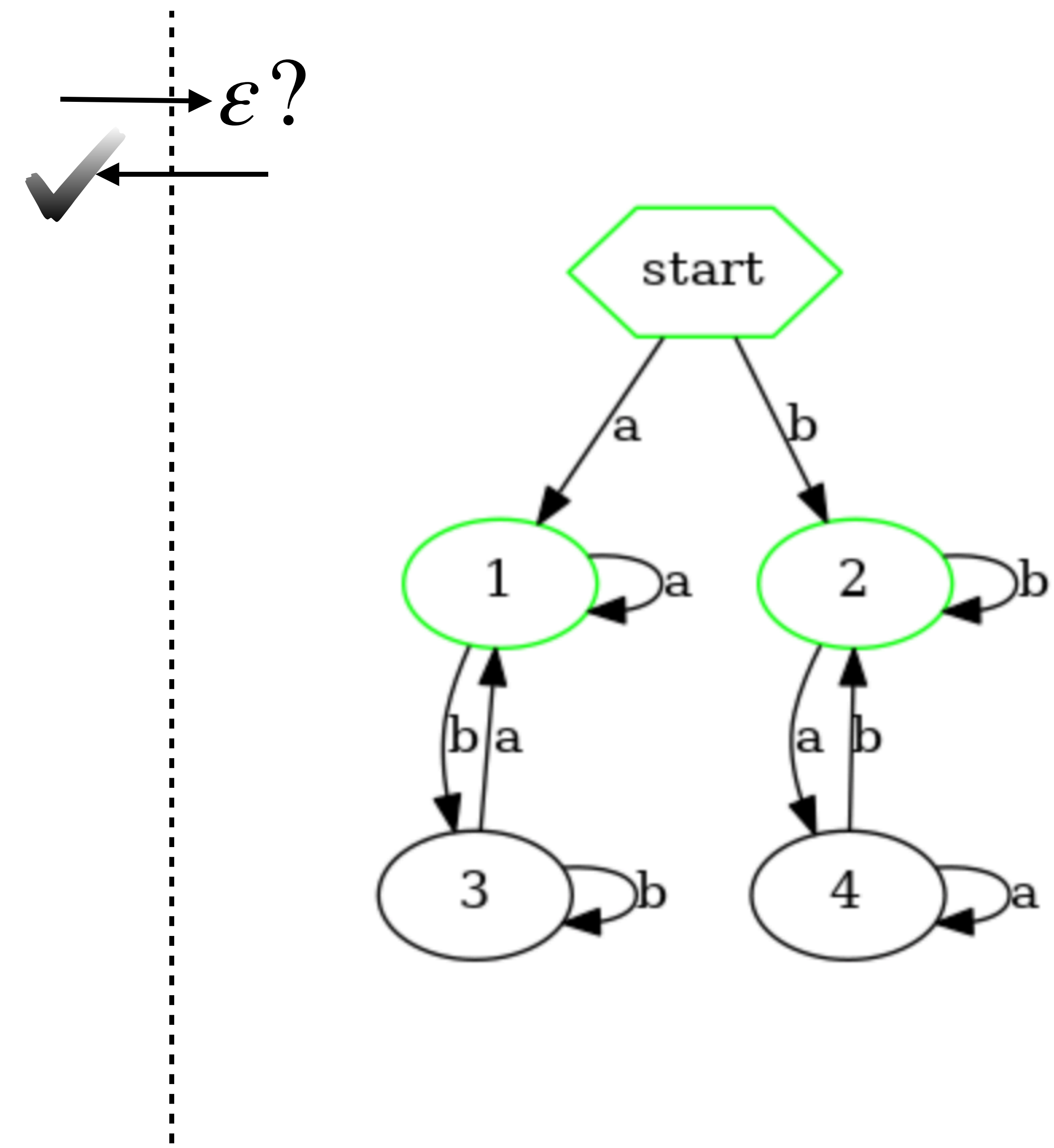


Membership Queries **Equivalence Queries** **Counter-Examples**

Background: L*

The Observation Table

P \ S	ε	a	ba
ε	1	1	0
a	1	1	1
b	1	0	0
ba	0	0	0
bb	1	0	0



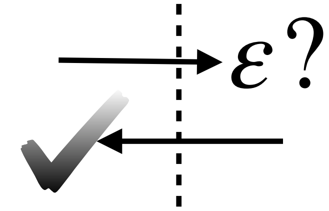
Background: L*

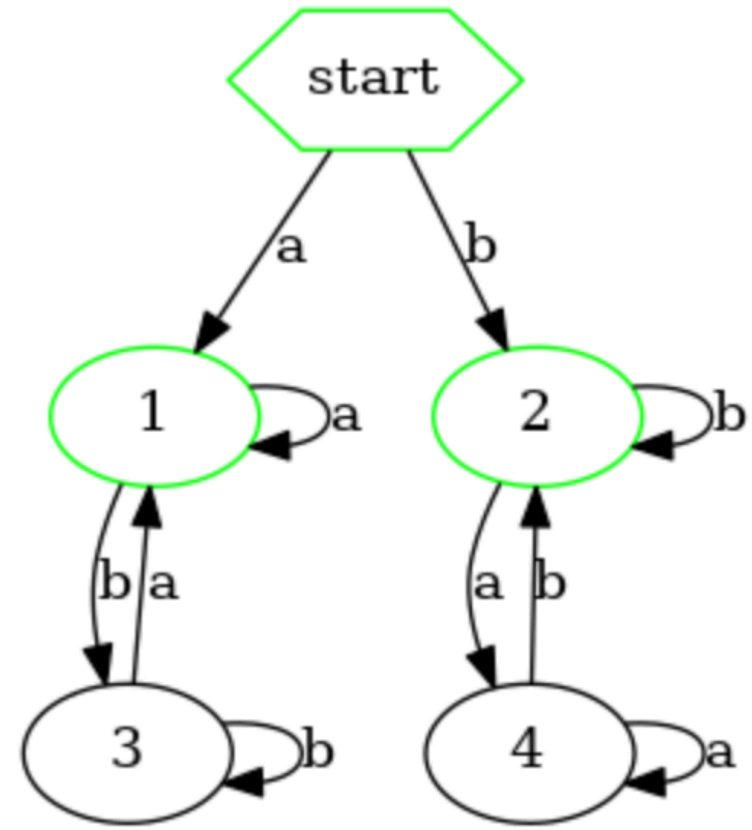
The Observation Table

P \ S	ε	a	ba
ε	1	1	0
a	1	1	1
b	1	0	0
ba	0		
bb	1	0	0

Closedness

Consistency





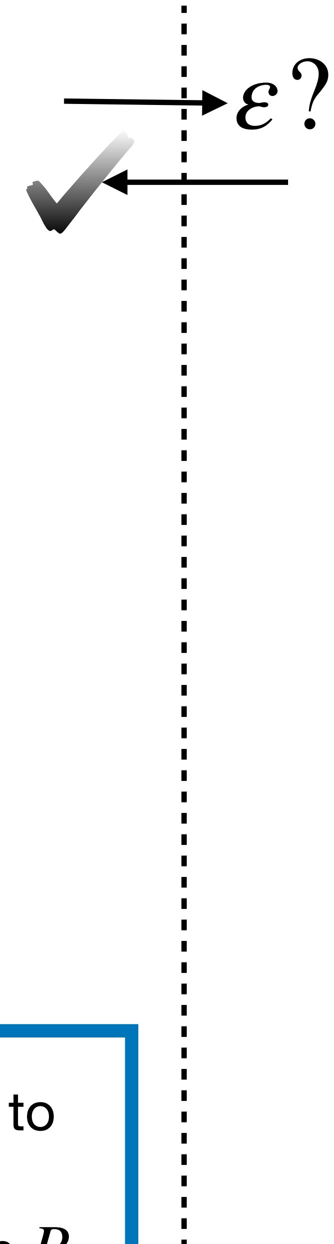
Background: L*

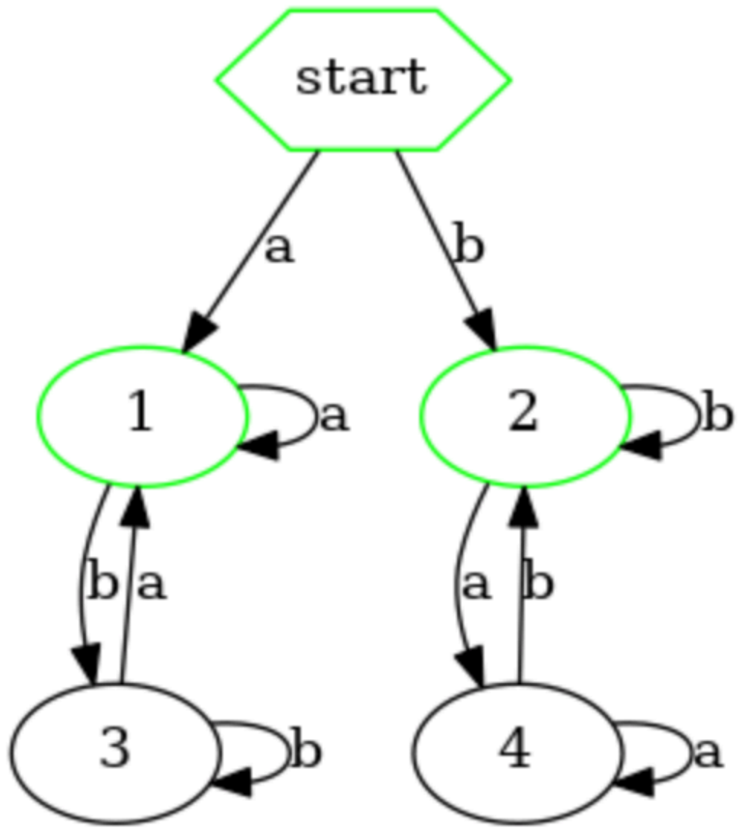
The Observation Table

P \ S	ε	a	ba
ε	1	1	0
a	1	1	1
b	1	0	0
ba	0	[illegible]	[illegible]
bb	1	[illegible]	[illegible]

Closedness

For all $p \in P$ and $\sigma \in \Sigma$, if we were to add $p \cdot \sigma$ to P, its row would be identical to that of some p' already in P





Background: L*

The Observation Table

P \ S	ε	a	ba
ε	1	1	0
a	1	1	1
b	1	0	0
ba	0	0	[illegible]
bb	1	[illegible]	[illegible]

Closedness

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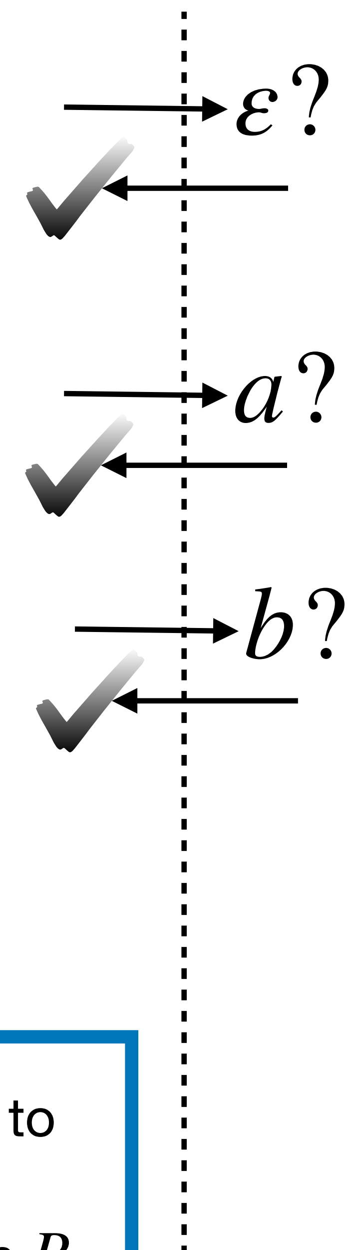
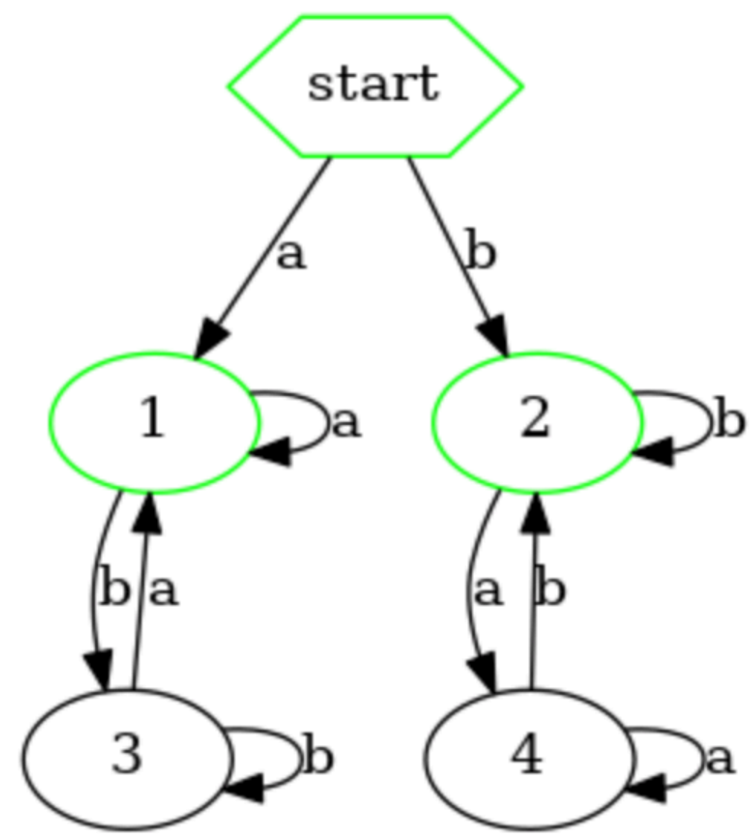




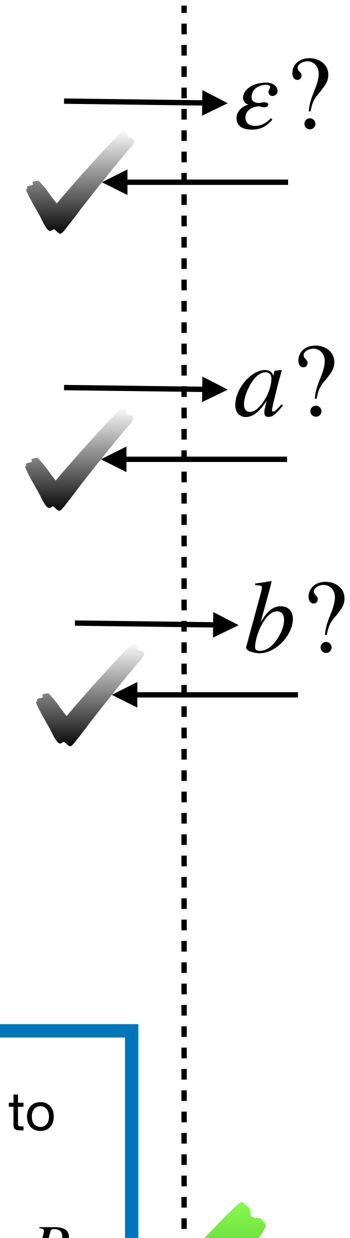
Background: L*

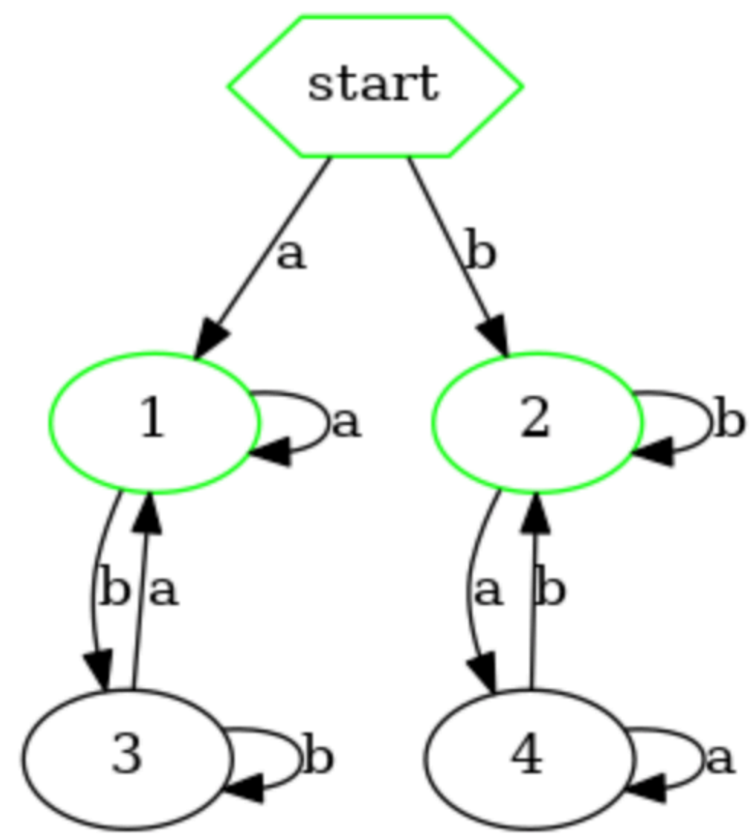
The Observation Table

P \ S	ε	a	ba
ε	1	1	0
a	1	1	1
b	1	0	0
ba	0		
bb	1		

Closedness

For all $p \in P$ and $\sigma \in \Sigma$, if we were to add $p \cdot \sigma$ to P, its row would be identical to that of some p' already in P

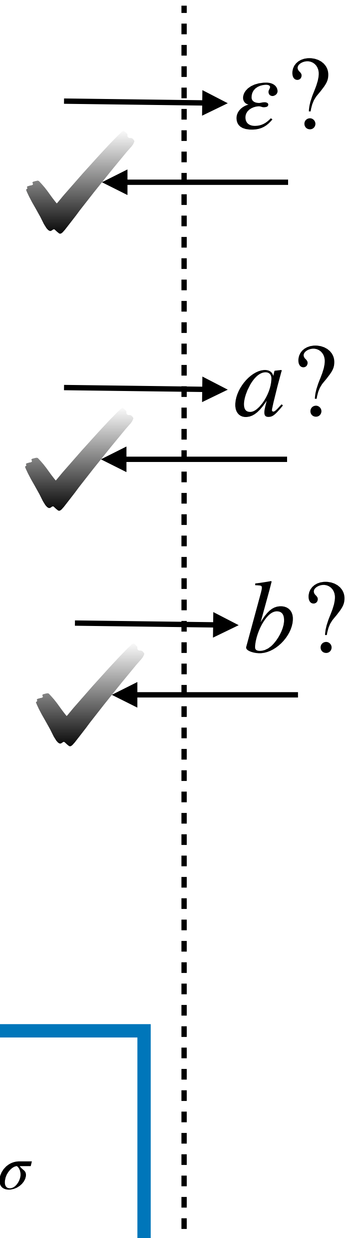


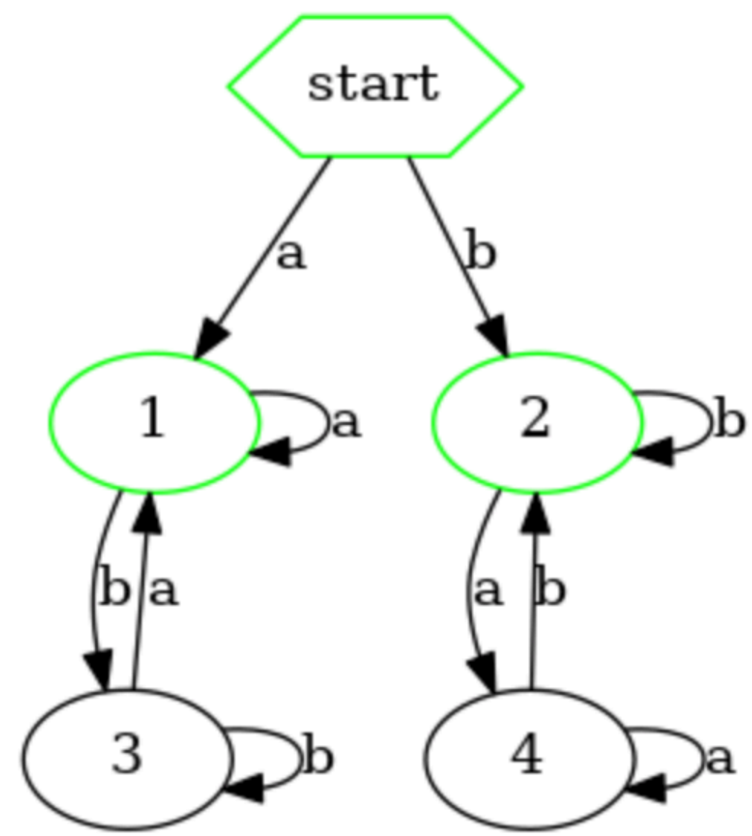


Background: L*

The Observation Table

P \ S	ε	a	ba
ε	1	1	0
a	1	1	1
b	1	0	0
ba			
bb			





Consistency

For all $p_1, p_2 \in P$ with identical rows, and all $\sigma \in \Sigma$, if we were to add $p_1 \cdot \sigma$ and $p_2 \cdot \sigma$ to P, their rows would be identical to each other

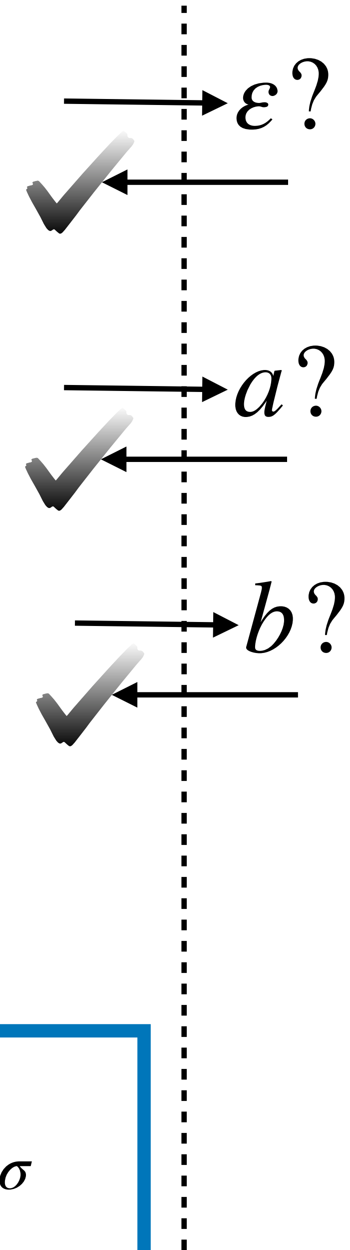
Background: L*

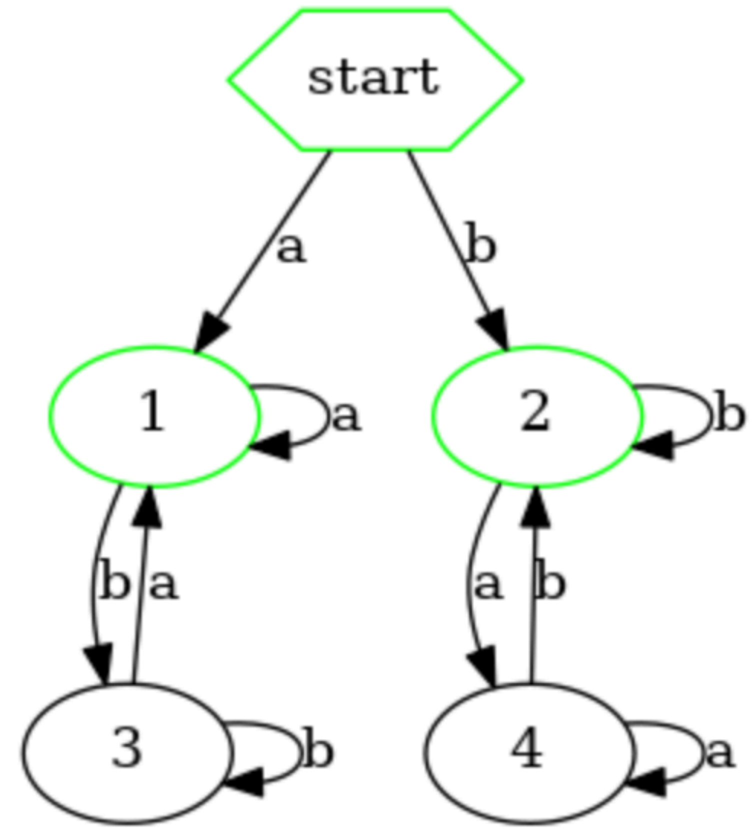
The Observation Table

P \ S	ε	a	ba
ε	1	1	0
a	1	1	1
b	1	0	0
ba	[illegible]	[illegible]	[illegible]
bb	[illegible]	[illegible]	[illegible]

Consistency

For all $p_1, p_2 \in P$ with identical rows, and all $\sigma \in \Sigma$, if we were to add $p_1 \cdot \sigma$ and $p_2 \cdot \sigma$ to P, their rows would be identical to each other



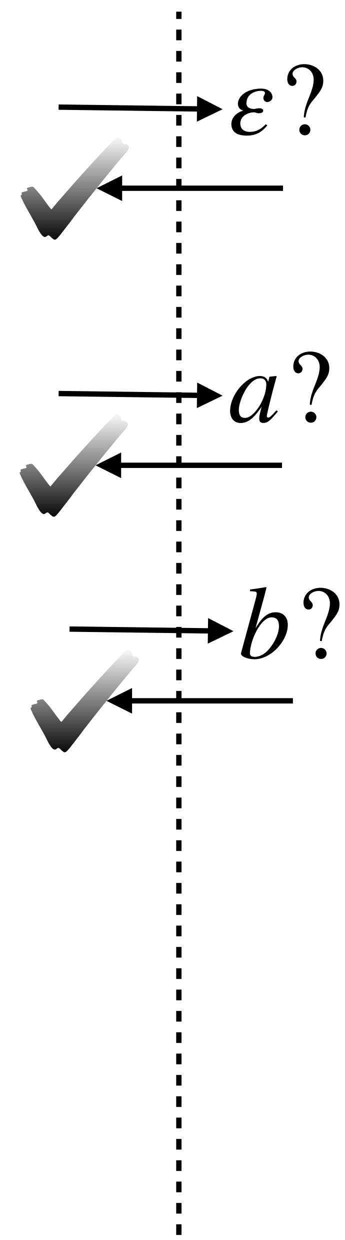


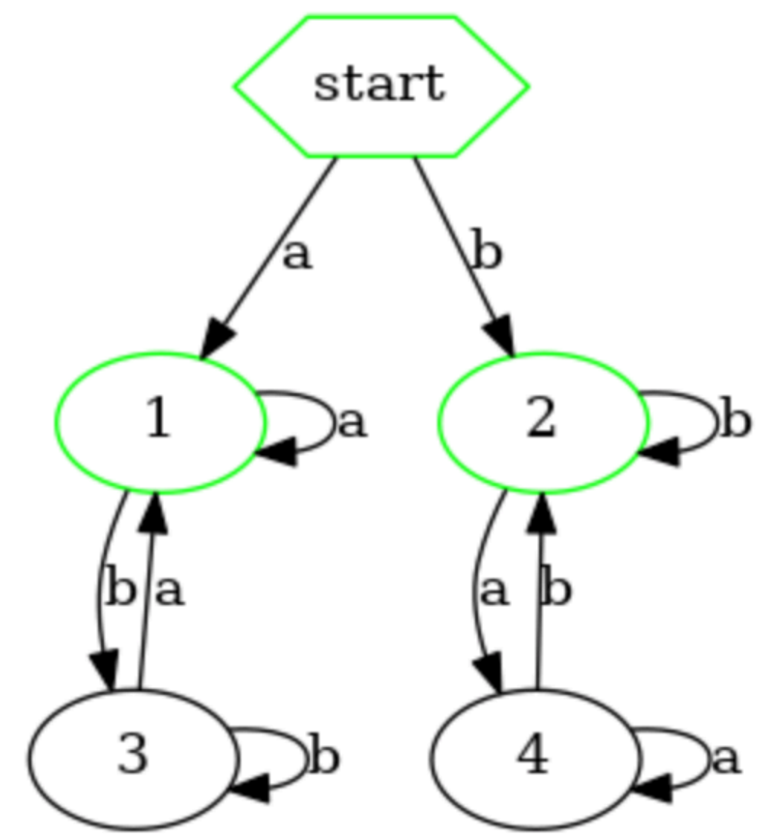
Background: L*

The Observation Table

P \ S	ε	a	ba
ε	1	1	0
a	1	1	1
b	1	0	0
ba	0	0	0
bb	1	0	0

Equivalence Query



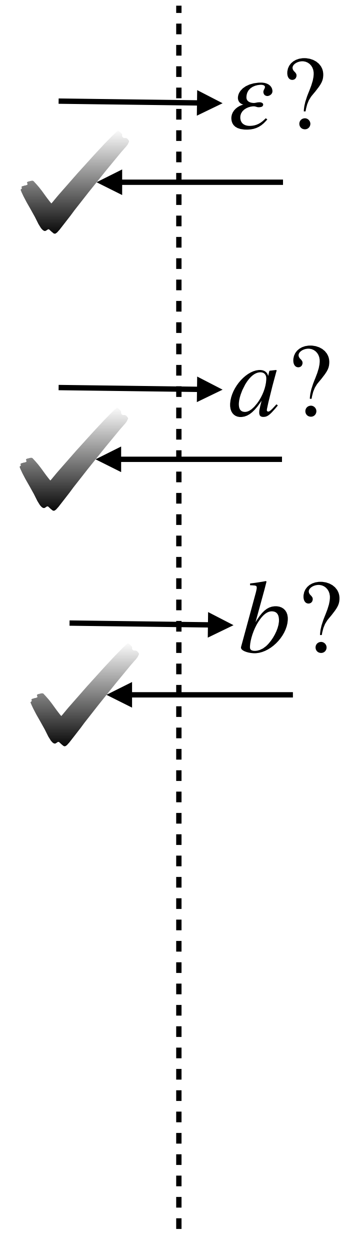


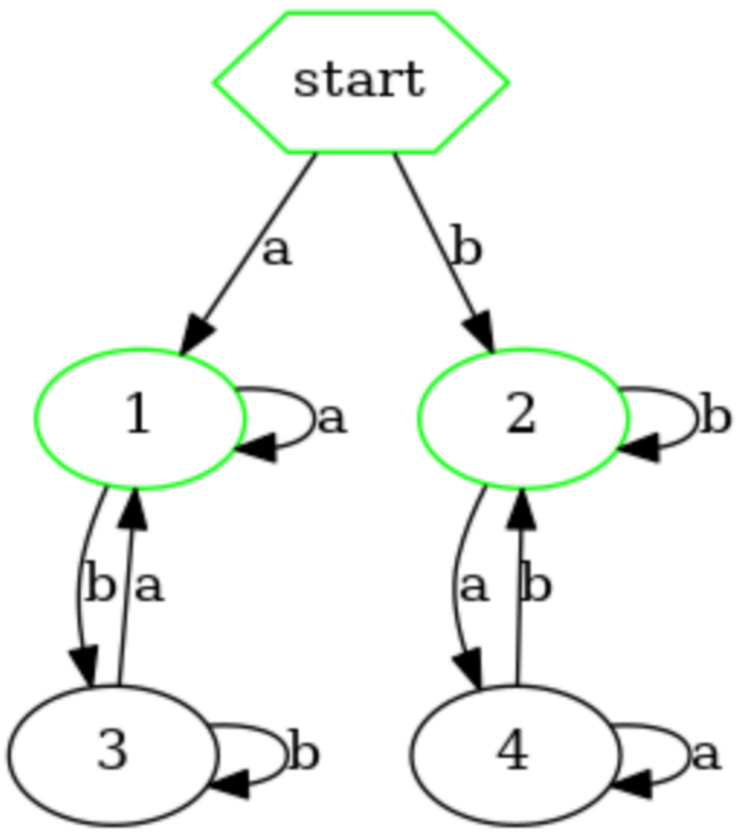
Background: L*

The Observation Table

P \ S	ε	a	ba
ε	1	1	0
a	1	1	1
b	1	0	0
ba	0		
bb	1	[illegible]	[illegible]

Equivalence Query



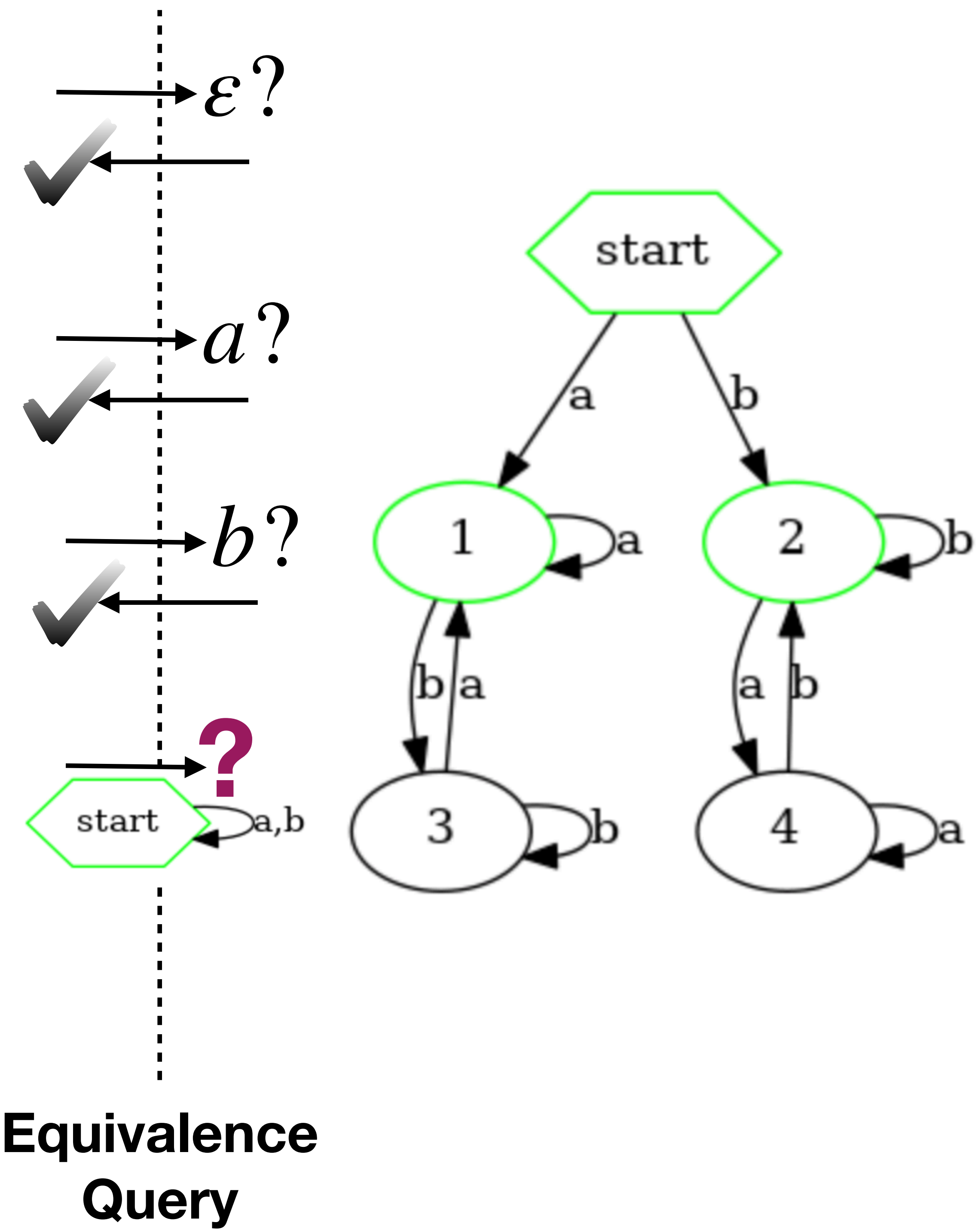


Each group of identical rows describes a single state

Background: L*

The Observation Table

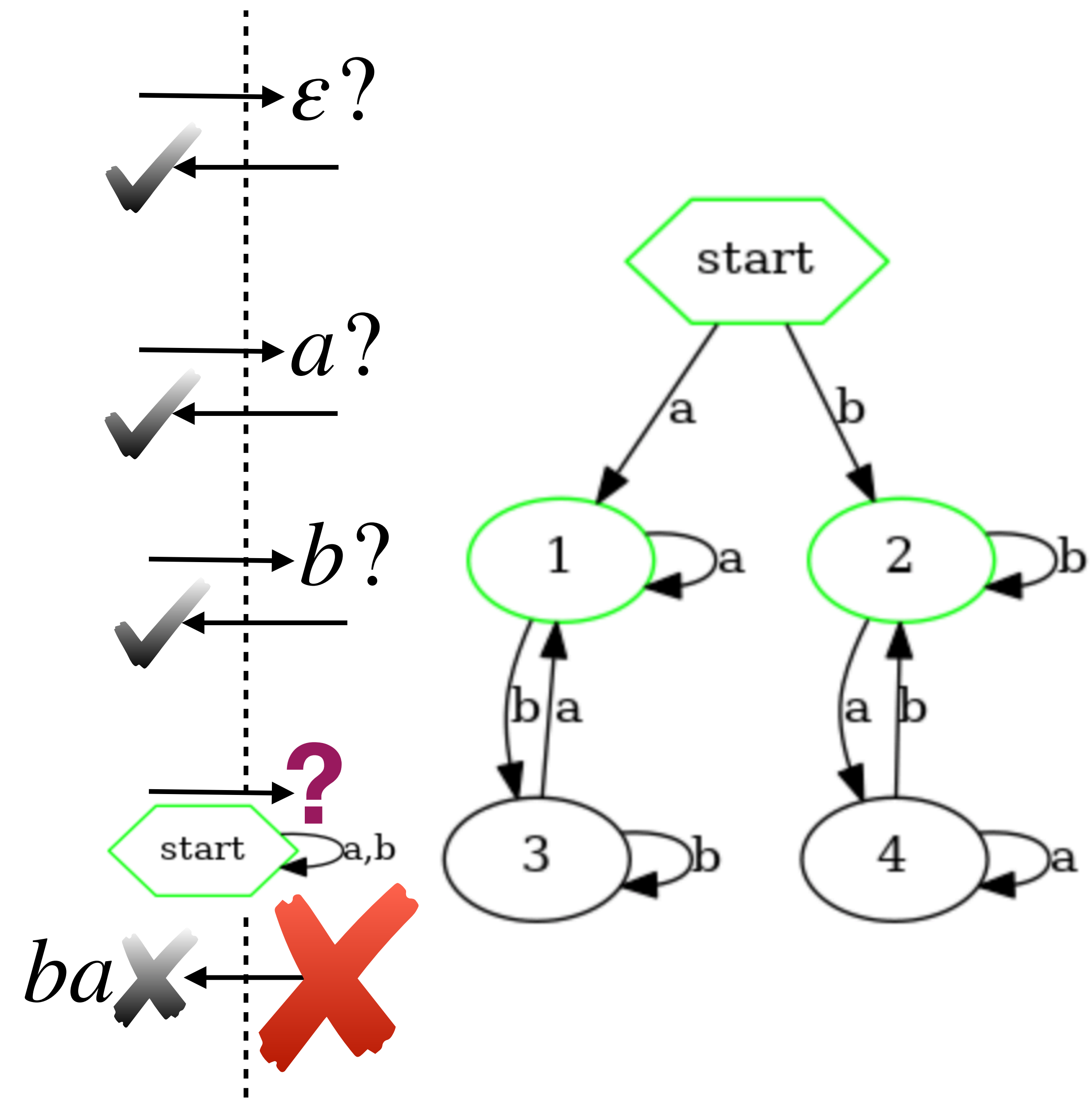
P \ S	ε	a	ba
ε	1	1	0
a	1	1	1
b	1	0	0
ba	0	0	0
bb	1	0	0



Background: L*

The Observation Table

P \ S	ε	a	ba
ε	1	1	0
a	1	1	1
b	1	0	0
ba	0	0	0
bb	1	0	0

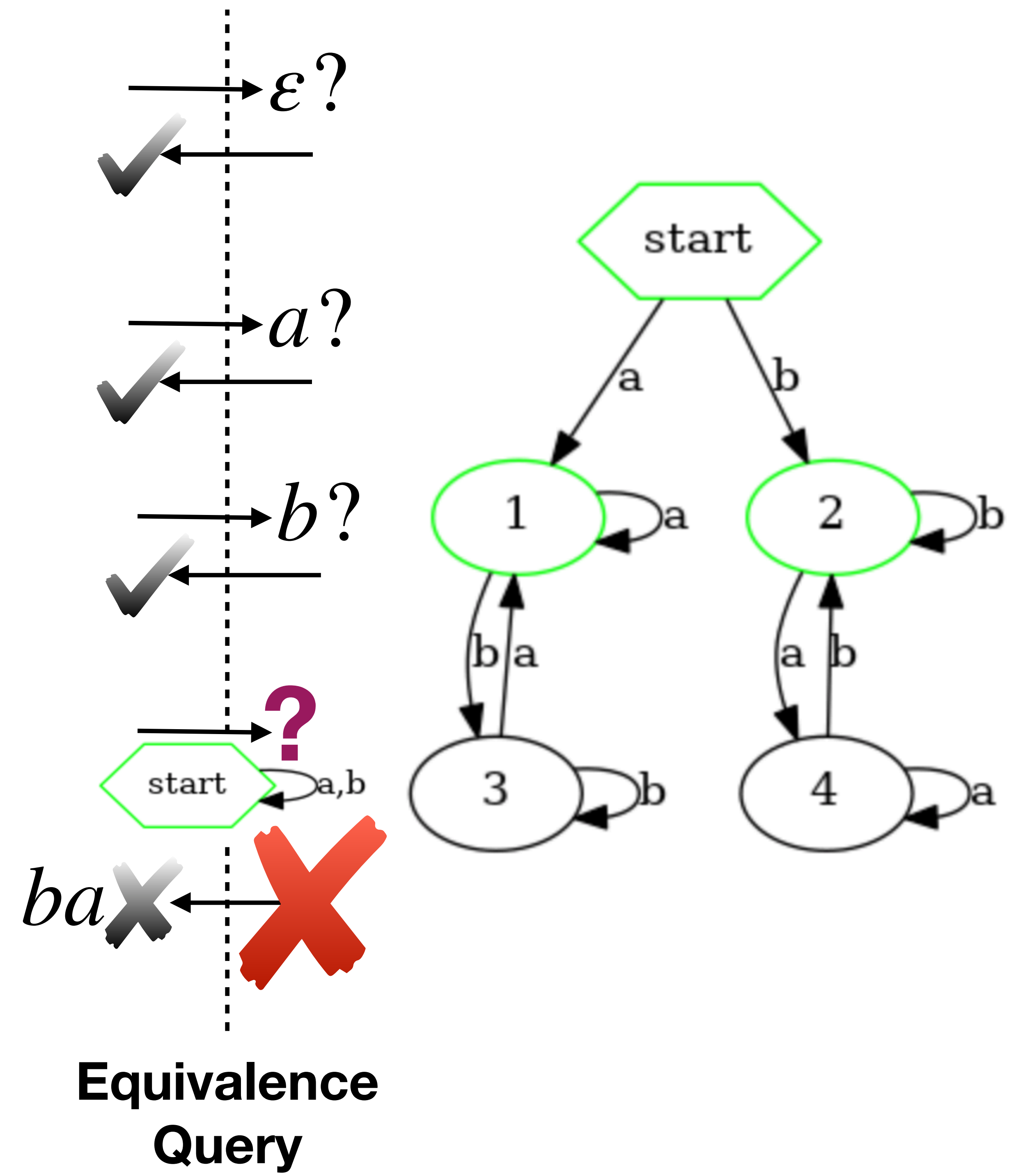


Equivalence Query

Background: L*

The Observation Table

P \ S	ε	a	ba
ε	1	1	0
a	1	1	1
b	1	0	0
ba	0	0	0
bb	1	0	0

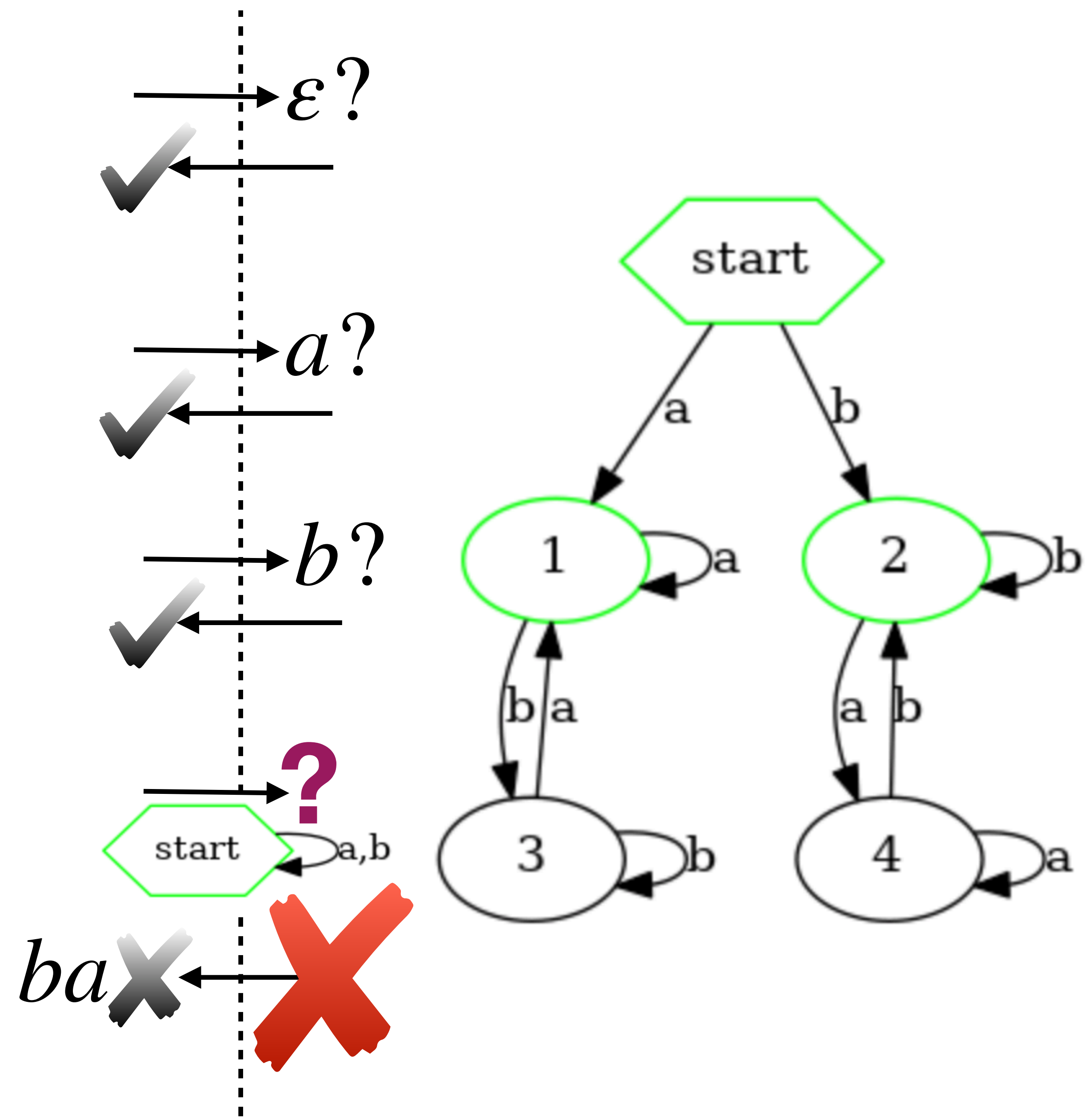


(this is simplified: it also adds to S)

Background: L*

The Observation Table

P \ S	ε	a	ba
ε	1	1	0
a	1	1	1
b	1	0	0
ba	0	0	0
bb	1	0	0



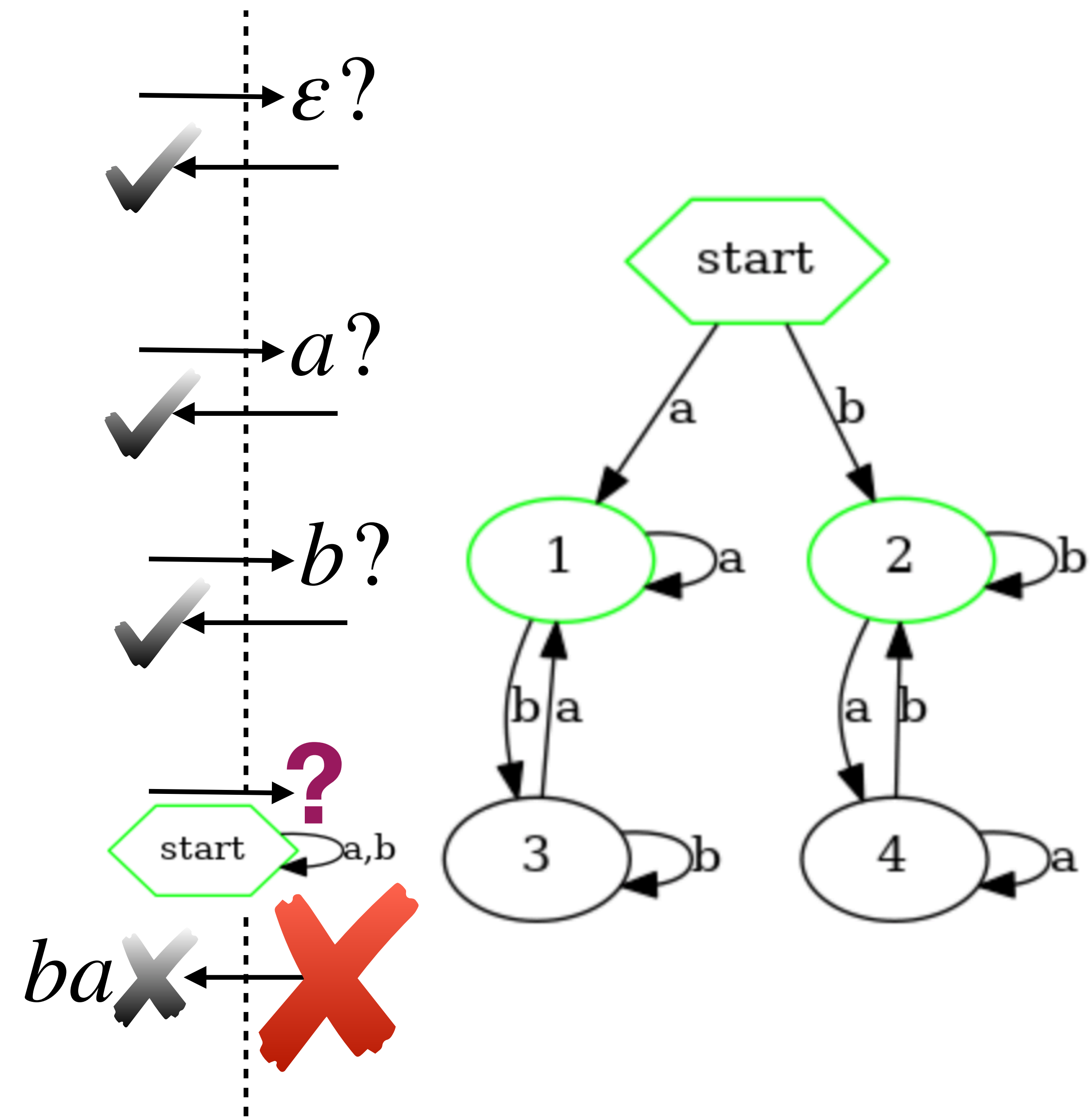
Equivalence Query

Background: L*

The Observation Table

P \ S	ε	a	ba
ε	1	1	0
a	1	1	1
b	1	0	0
ba	0	0	0
bb	1	0	0

Closedness



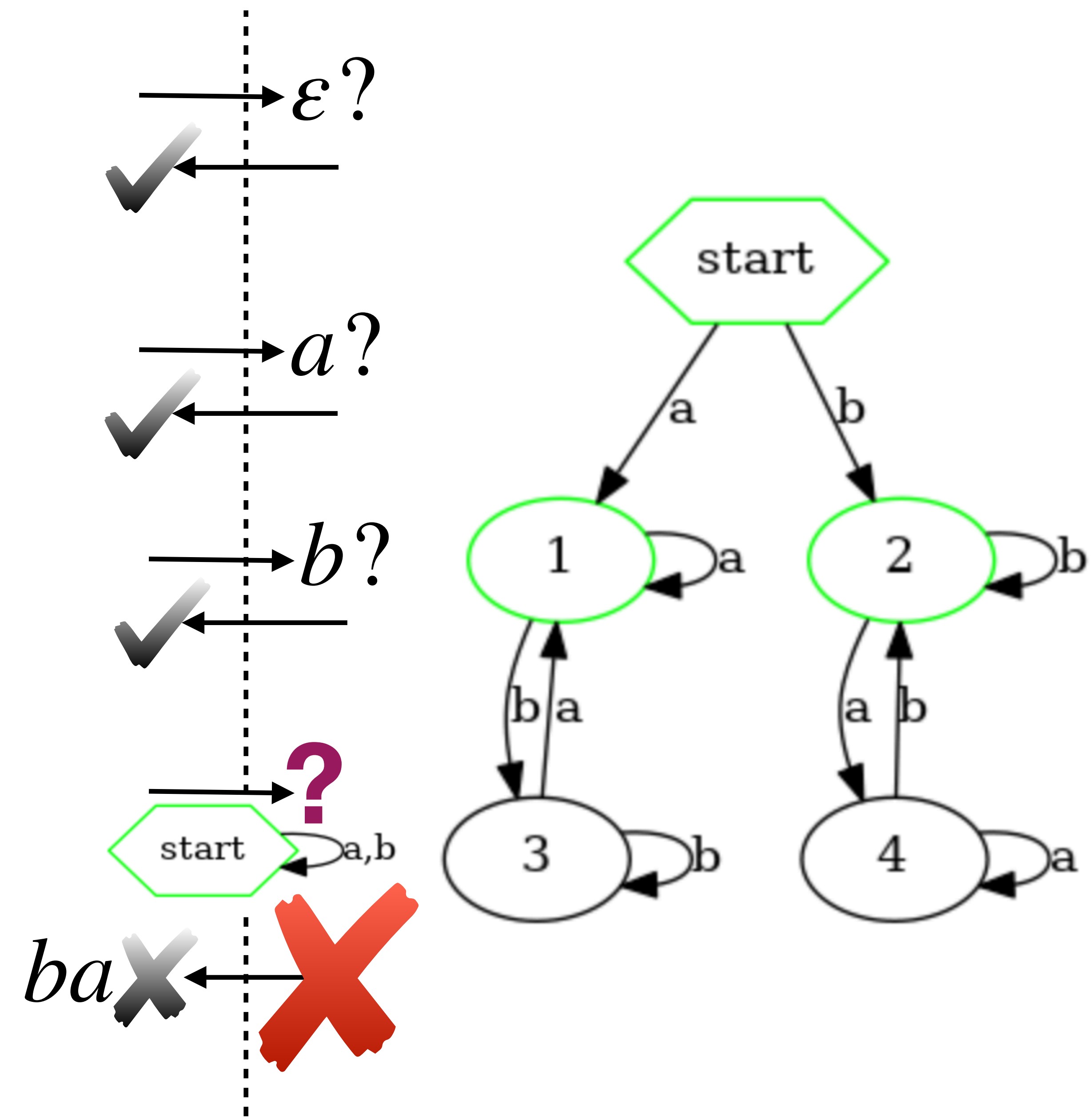
Equivalence Query

Background: L*

The Observation Table

P \ S	ε	a	ba
ε	1	1	0
a	1	1	1
b	1	0	0
ba	0	0	0
bb	1	0	0

Consistency?

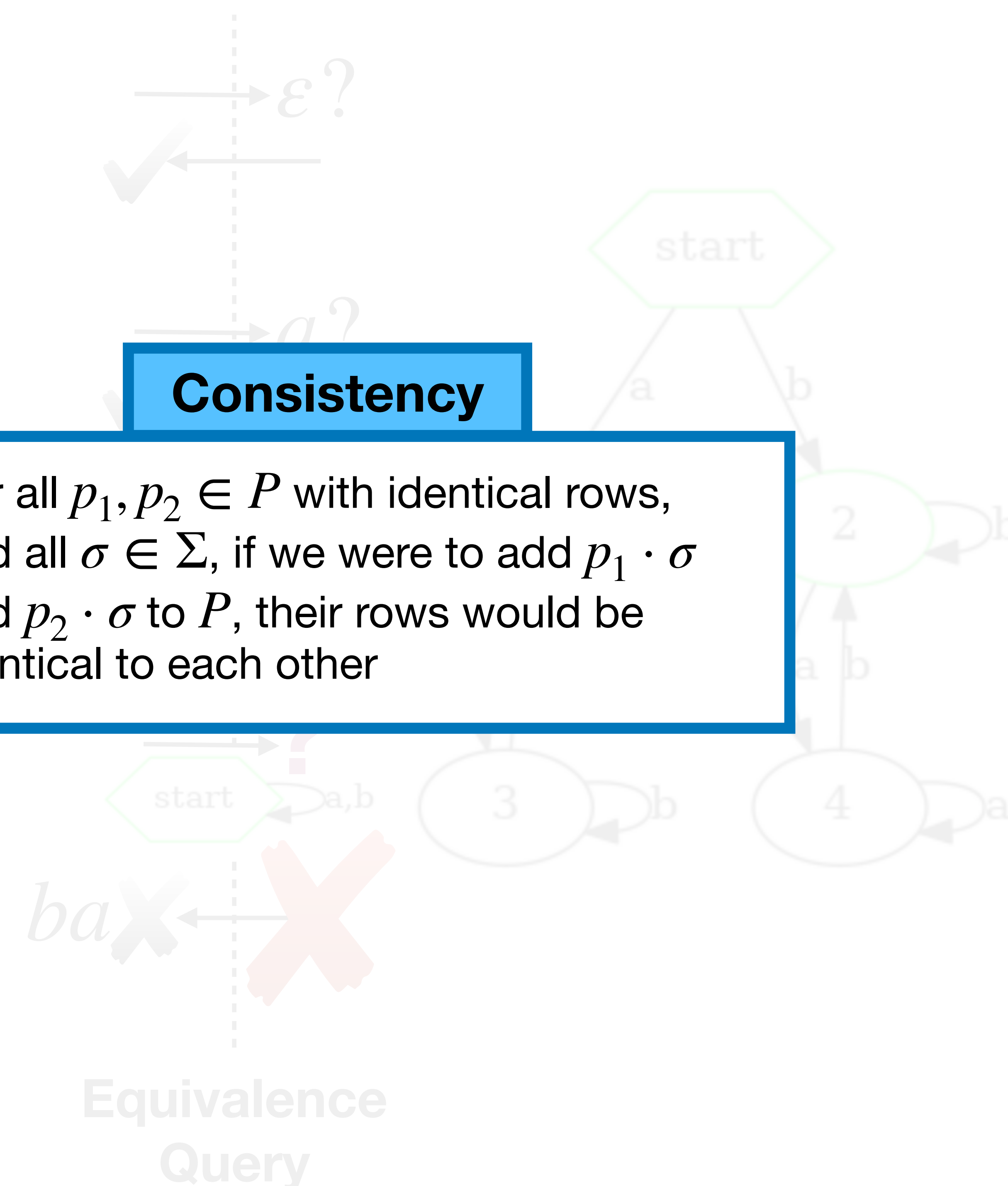


Equivalence Query

Background: L*

The Observation Table

P \ S	ε	a	ba
ε	1	1	0
a	1	1	1
b	1	0	0
ba	0	0	0
bb	1	0	0



Consistency

For all $p_1, p_2 \in P$ with identical rows, and all $\sigma \in \Sigma$, if we were to add $p_1 \cdot \sigma$ and $p_2 \cdot \sigma$ to P, their rows would be identical to each other

Background: L*

The Observation Table

P \ S	ε	a	ba
ε	1	1	0
a	1	1	1
b	1	0	0
ba	0	0	0
bb	1	0	0

Agree

Consistency

For all $p_1, p_2 \in P$ with identical rows, and all $\sigma \in \Sigma$, if we were to add $p_1 \cdot \sigma$ and $p_2 \cdot \sigma$ to P, their rows would be identical to each other

Background: L*

The Observation Table

P \ S	ε
ε	**1**
a	**1**
b	**1**
ba	**0**

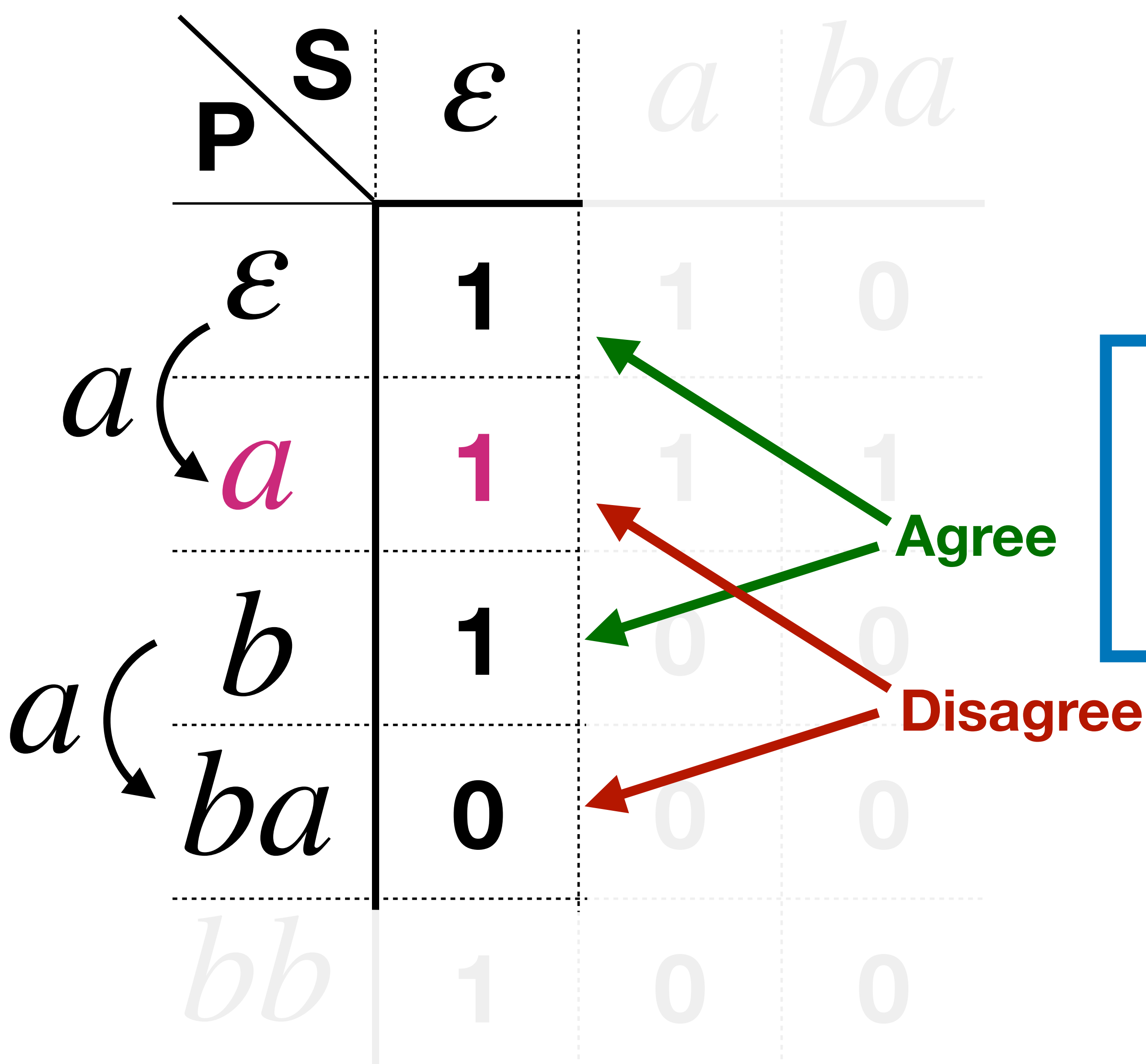
Agree

Consistency

For all $p_1, p_2 \in P$ with identical rows, and all $\sigma \in \Sigma$, if we were to add $p_1 \cdot \sigma$ and $p_2 \cdot \sigma$ to P, their rows would be identical to each other

Background: L*

The Observation Table



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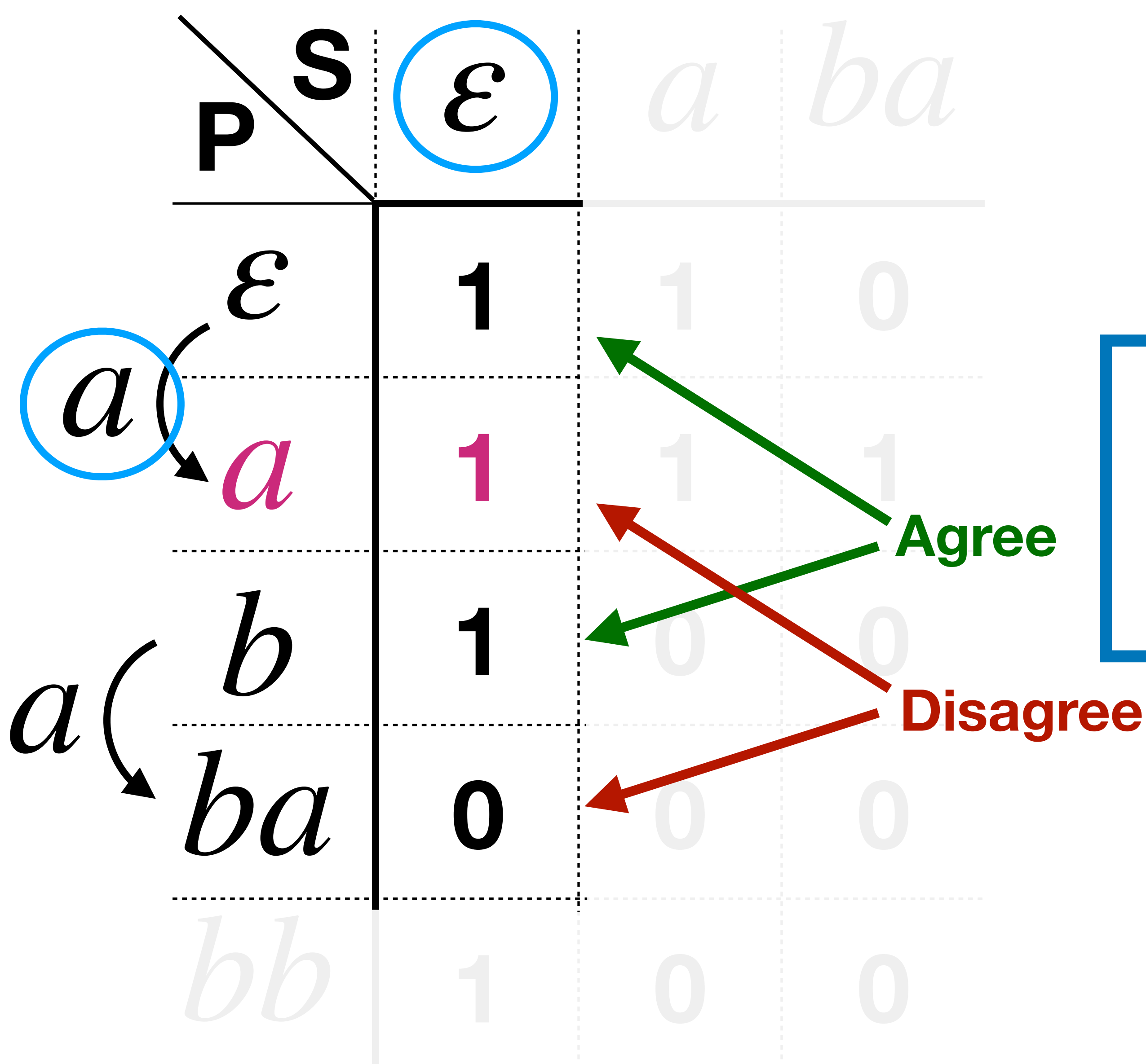
Background: L*

The Observation Table



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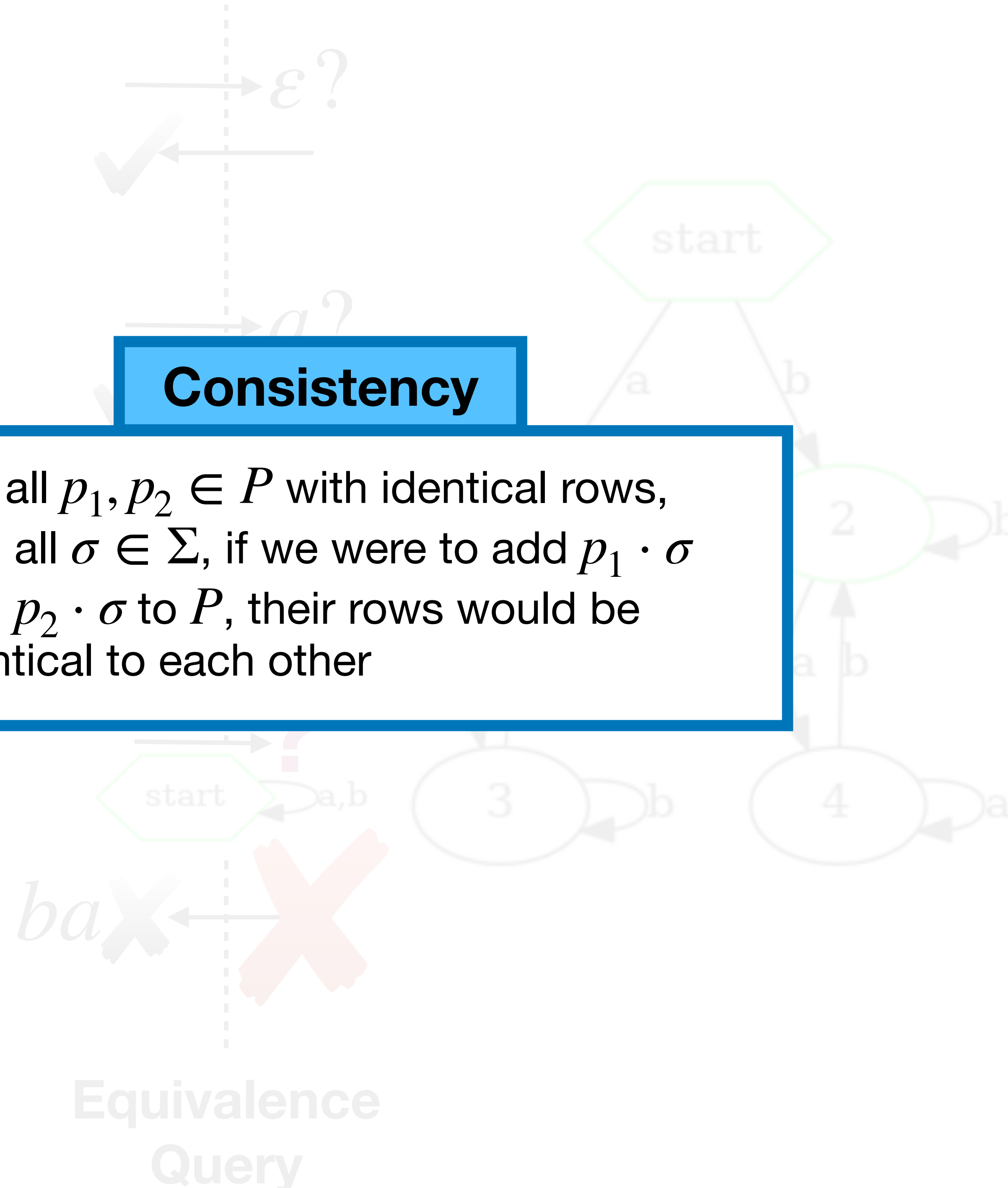
Background: L*

The Observation Table

P \ S	ε	a	ba
ε	1	1	0
a	1	1	1
b	1	0	0
ba	0	0	0
bb	1	0	0

Consistency

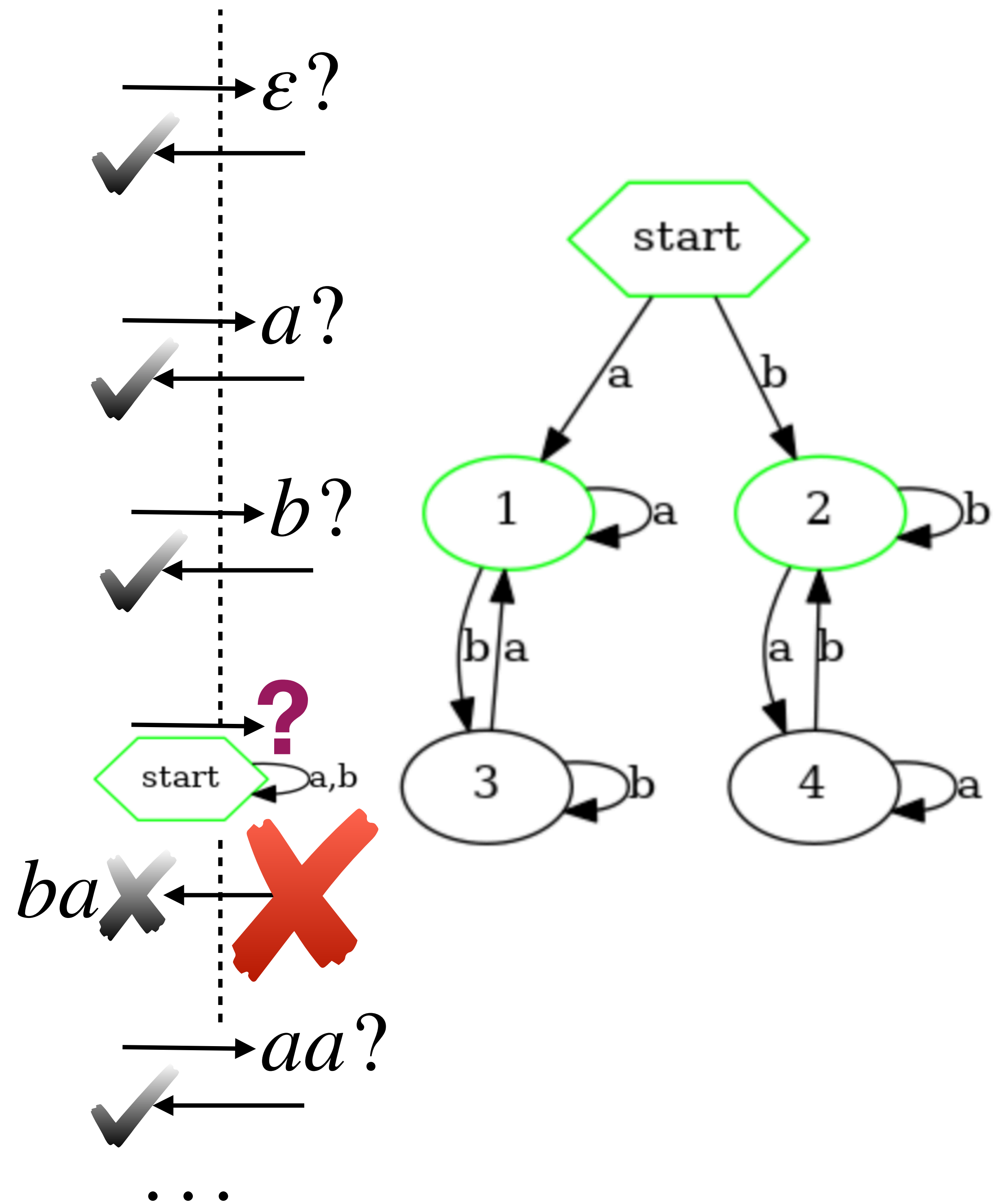
For all $p_1, p_2 \in P$ with identical rows, and all $\sigma \in \Sigma$, if we were to add $p_1 \cdot \sigma$ and $p_2 \cdot \sigma$ to P, their rows would be identical to each other

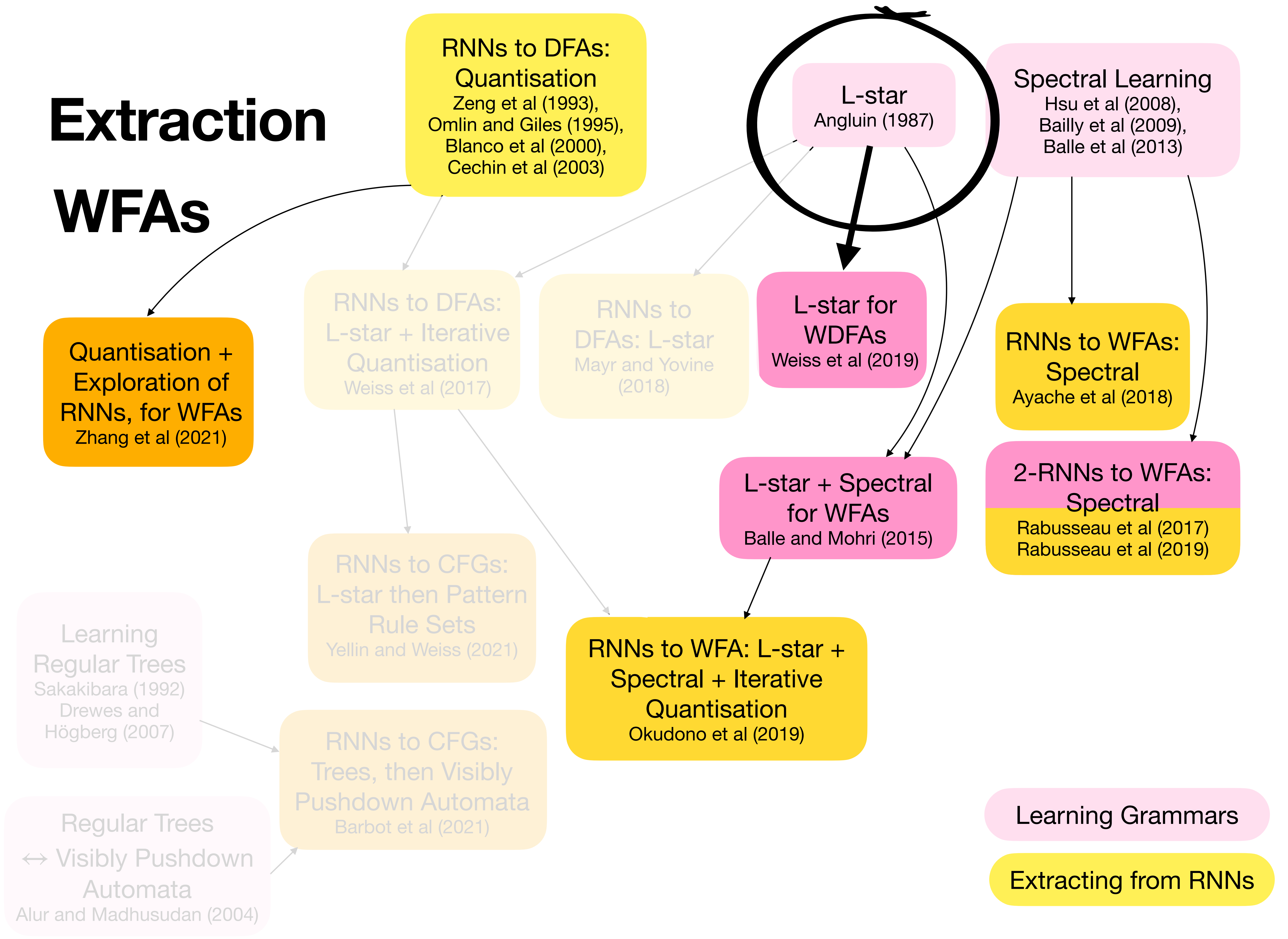


Background: L*

The Observation Table

P \ S	ε	a	ba
ε	1	1	0
a	1	1	1
b	1	0	0
ba	0	0	0
bb	1	0	0





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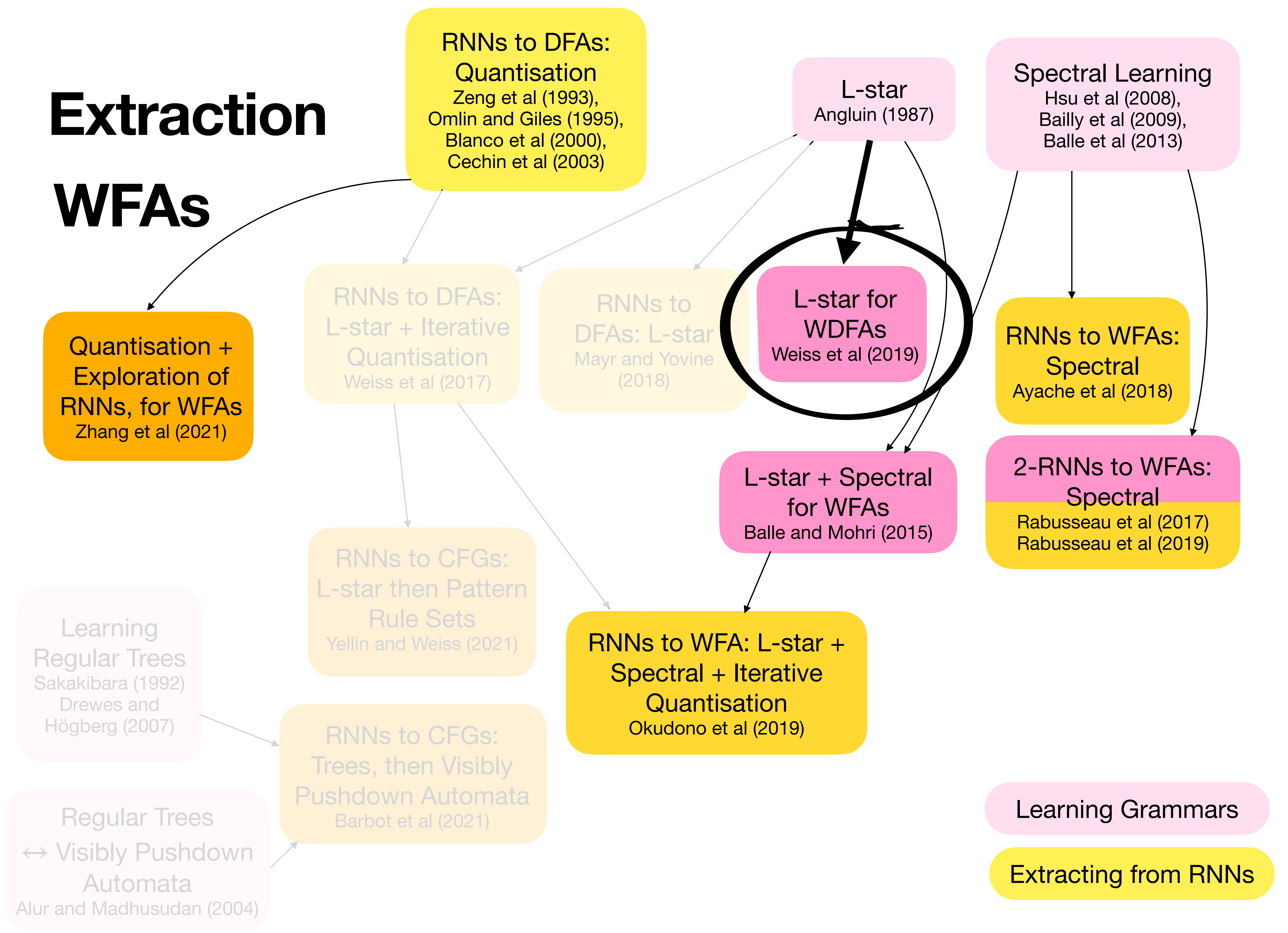

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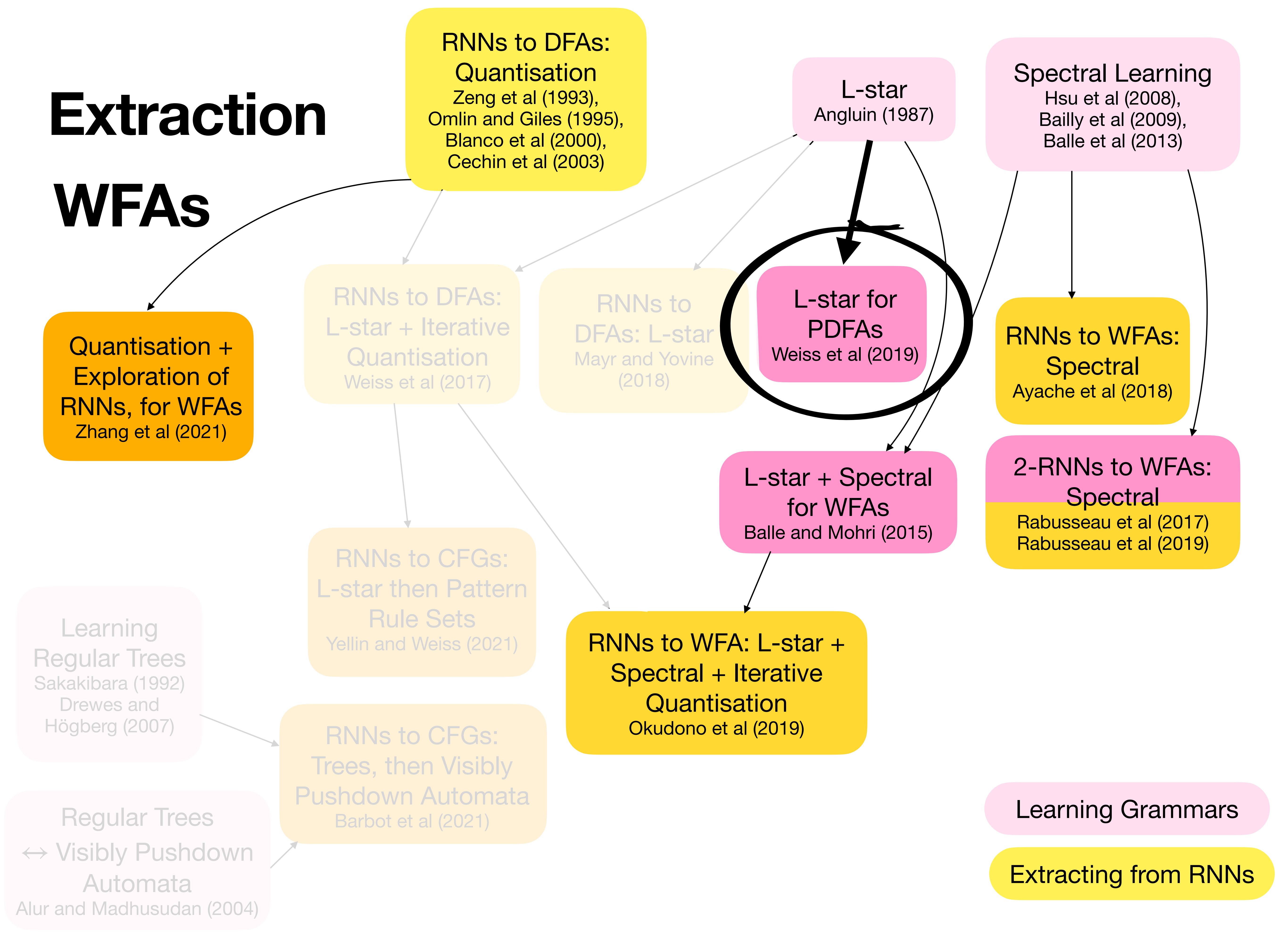
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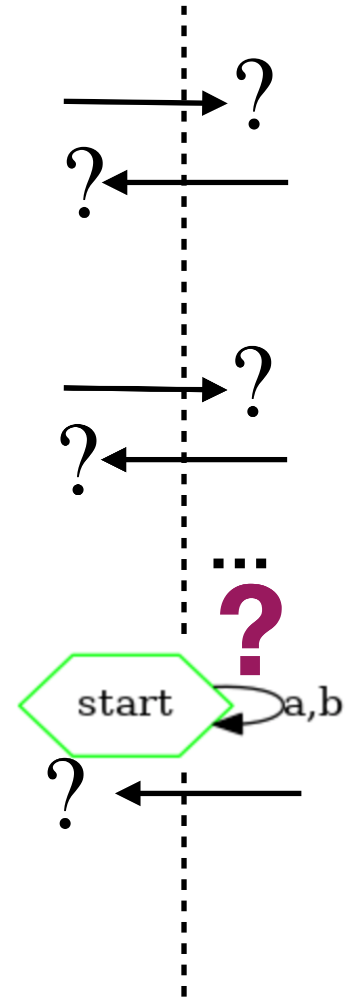
Adapting L*

The Observation Table

P \ S	ε	a	ba
ε	?	?	?
a	?	?	?
b	?	?	?
ba	?	?	?
bb	?	?	?



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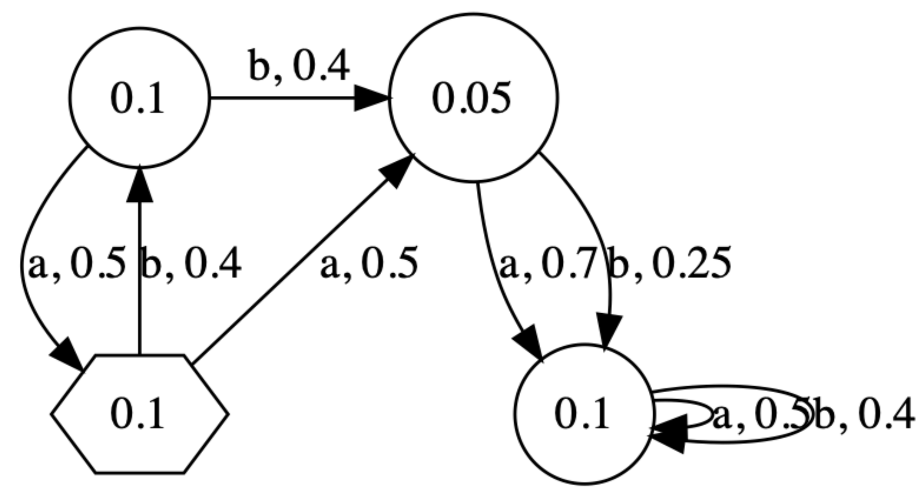


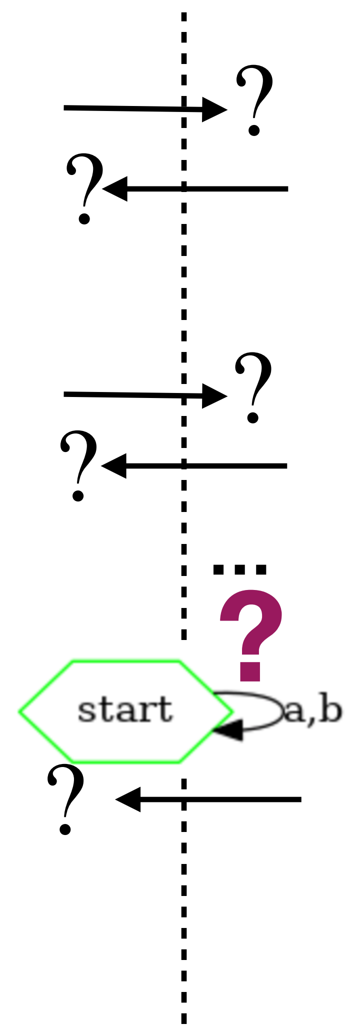
there may be some noise...

What shall we put in the table?

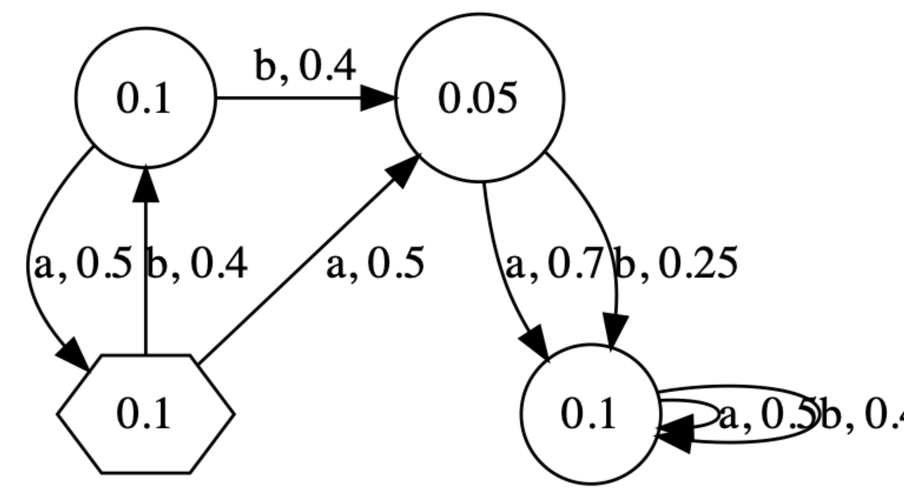
Adapting L*

The Observation Table

P \ S	ε	a	ba
ε	?	?	?
a	?	?	?
b	?	?	?
ba	?	?	?
bb	?	?	?



RNN, trained on



there may be some noise…

What shall we put in the table?

Direct approach: Full sequence weight

Flaw: Will quickly degrade

Intuition: Conditional probabilities

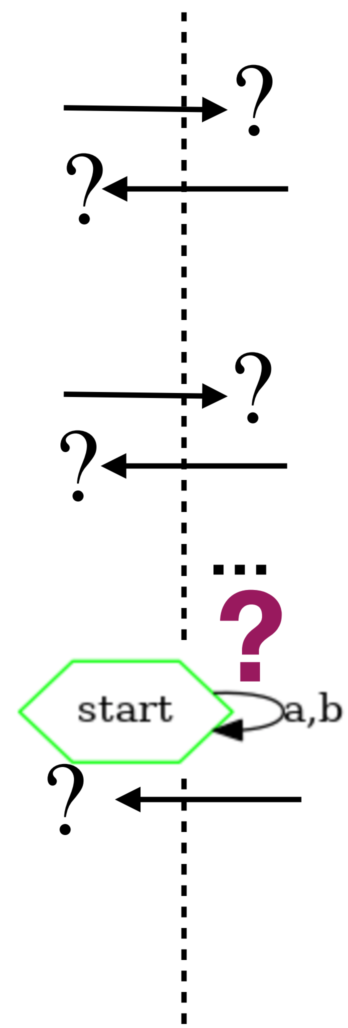
Flaw: Also degrade as S grows

Fix: Last token probabilities

Adapting L*

The Observation Table

P \ S	ε	a	ba
ε	?	?	?
a	?	?	?
b	?	?	?
ba	?	?	?
bb	?	?	?



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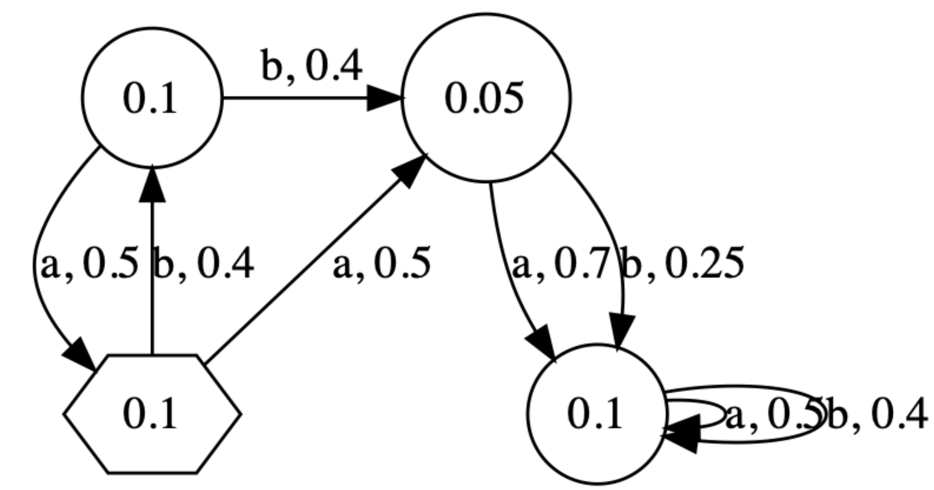


there may be some noise…

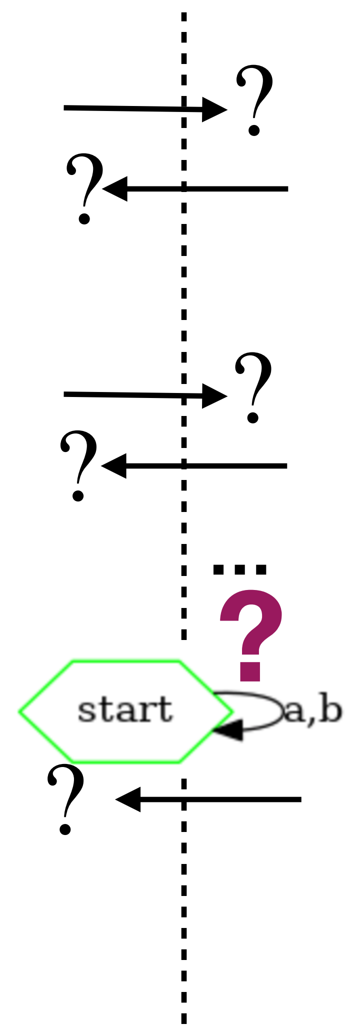
What shall we put in the table?

Final Choice: Last Token Probabilities

Adapting L*

The Observation Table

P \ S	ε	a	ba
ε	?	0.5	0.4
a	?	0.7	0.5
b	?	0.5	0.7
ba	?	0.5	0.5
bb	?	0.7	0.5



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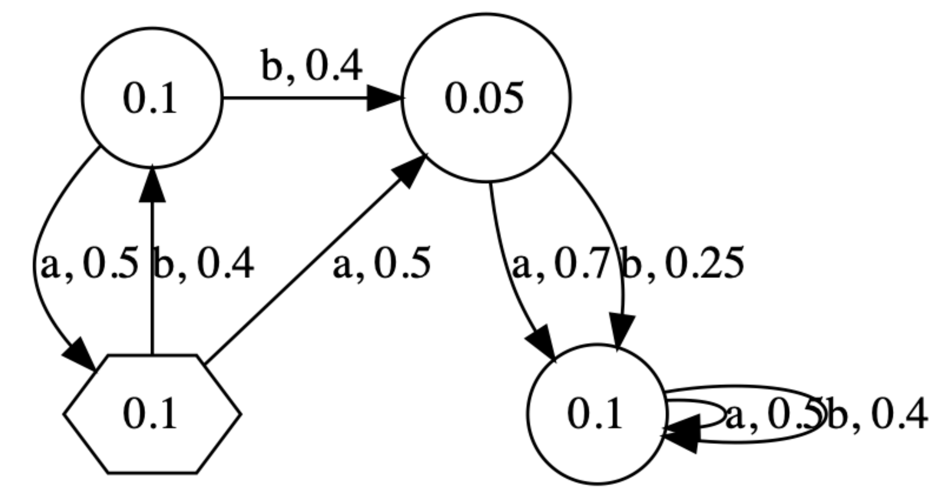


there may be some noise…

What shall we put in the table?

Final Choice: Last Token Probabilities

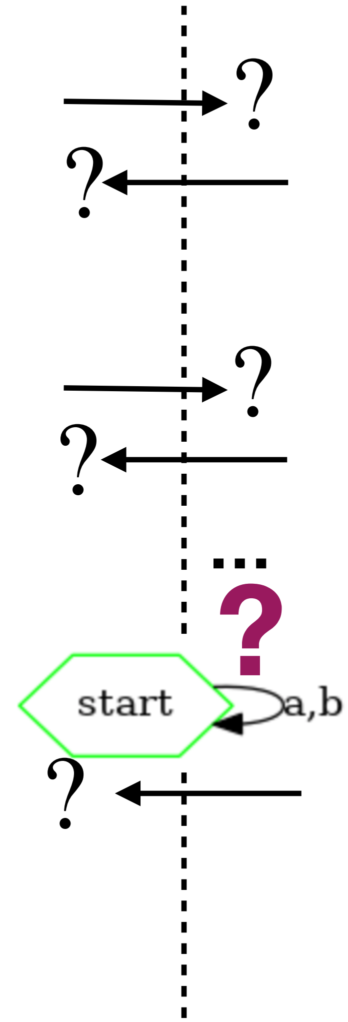
Realisation:

empty suffix doesn't mean anything anymore…

Adapting L*

The Observation Table

P \ S	$	a	ba
ε	0.1	0.5	0.4
a	0.05	0.7	0.5
b	0.1	0.5	0.7
ba	0.1	0.5	0.5
bb	0.05	0.7	0.5



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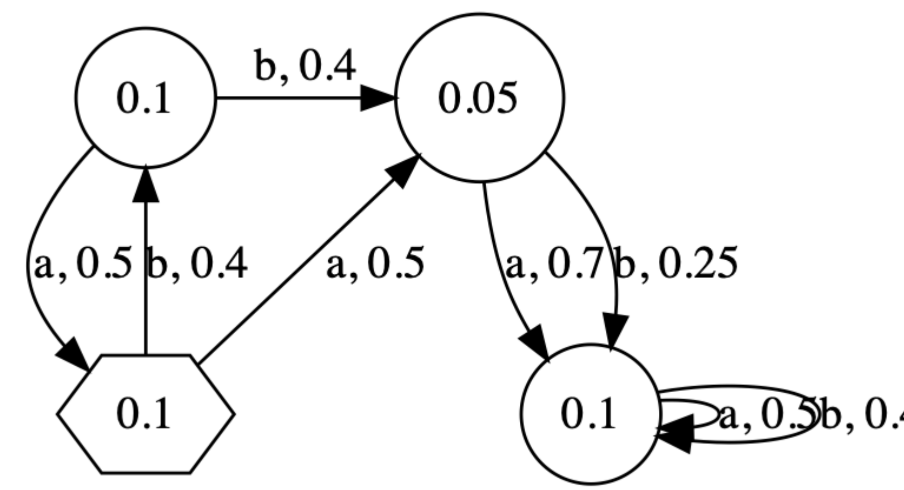

there may be some noise…

What shall we put in the table?

Final Choice: Last Token Probabilities

Realisation:

empty suffix doesn’t mean anything anymore…
but end-of-sequence does

Adapting L*

The Observation Table

P \ S	$	a	ba
ε	0.1	0.5	0.4
a	0.05	0.7	0.5
b	0.1	0.5	0.7
ba	0.1	0.5	0.5
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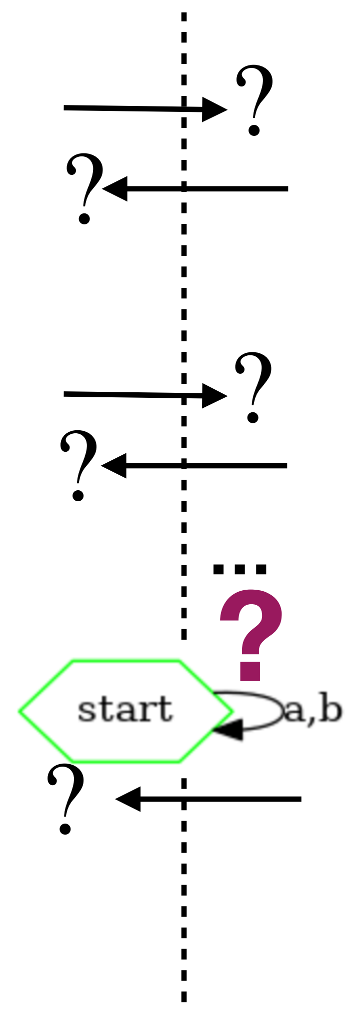
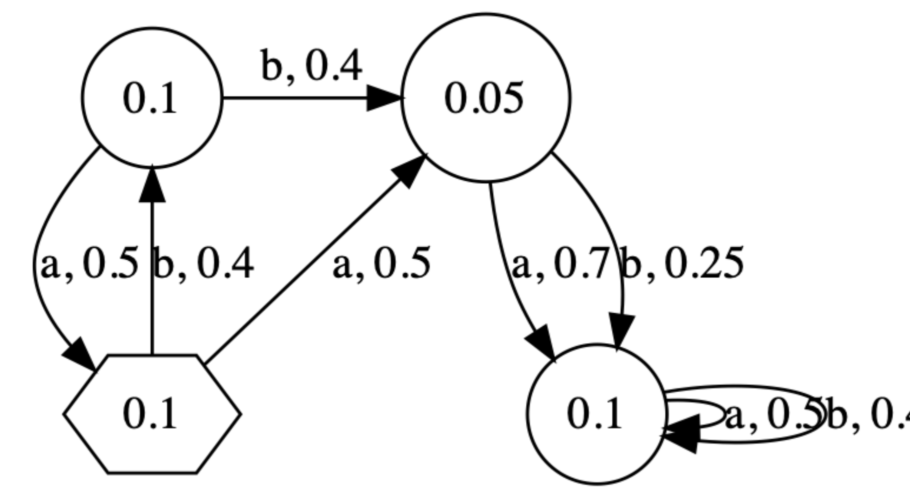


RNN, trained on



there may be some noise...

What shall we put in the table?

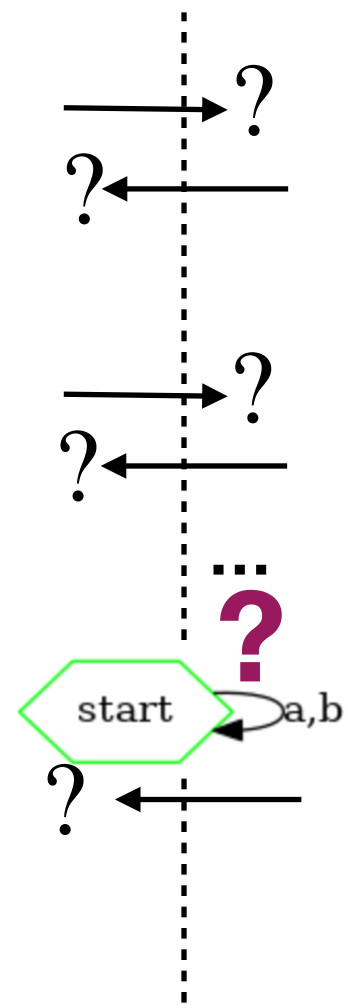
Final Choice: Last Token Probabilities

Okay, we have our adaptation. Let's go!?

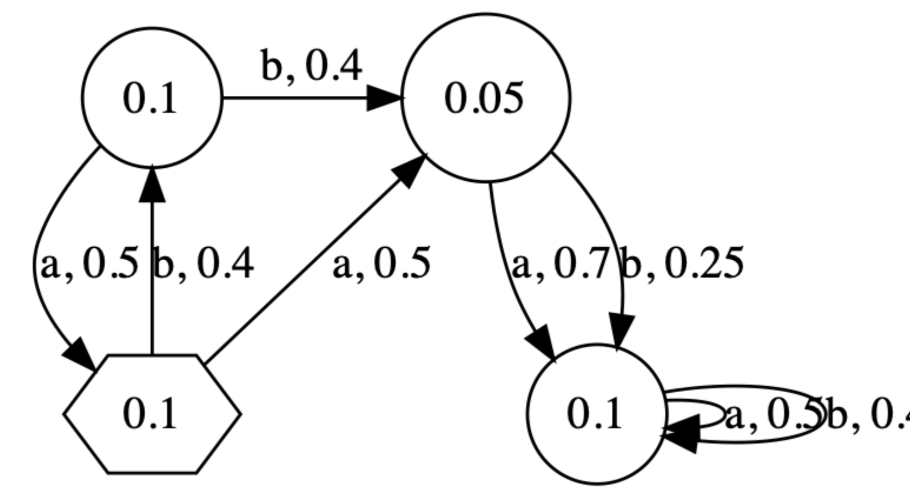
Adapting L*

The Observation Table

P \ S	$	a	ba
ε	0.1	0.5	0.4
a	0.05	0.7	0.5
b	0.1	0.5	0.7
ba	0.1	0.5	0.5
bb	0.05	0.7	0.5



RNN, trained on



there may be some noise…

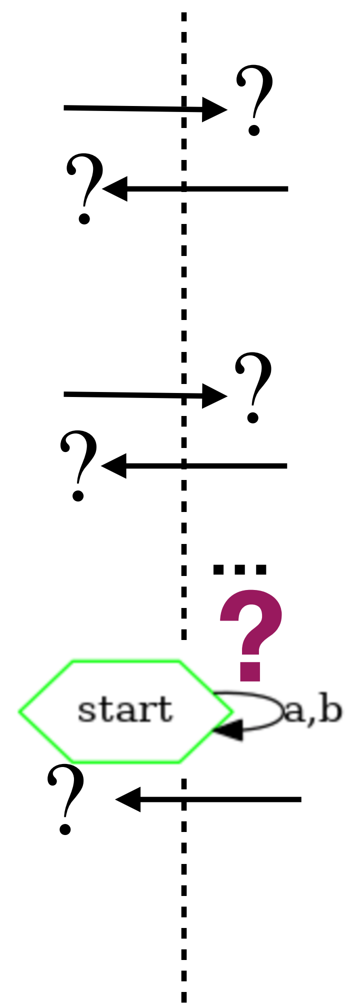
What shall we put in the table?

Final Choice: Last Token Probabilities

Adapting L*

The Observation Table

P \ S	$	a	ba
ε	0.1	0.5	0.4
a	0.05	0.7	0.5
b	0.1	0.5	0.7
ba	0.1	0.5	0.5
bb	0.05	0.7	0.5



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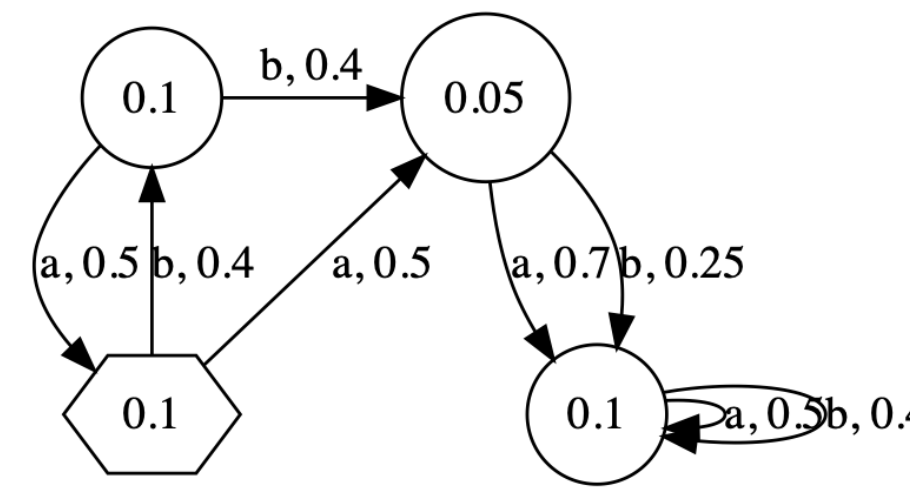

there may be some noise…

What shall we put in the table?

Final Choice: Last Token Probabilities
Nice Realisation: Can use additive tolerance

Adapting L*

The Observation Table

P \ S	$	a	ba
ε	0.1	0.5	0.4
a	0.05	0.7	0.5
b	0.1	0.5	0.7
ba	0.1	0.5	0.5
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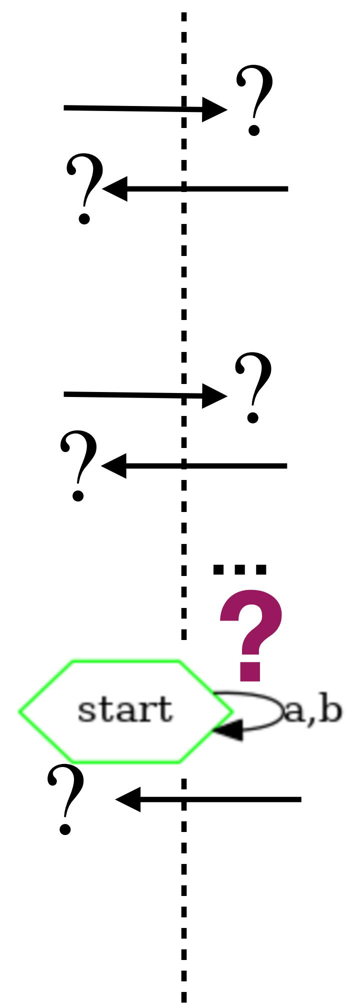

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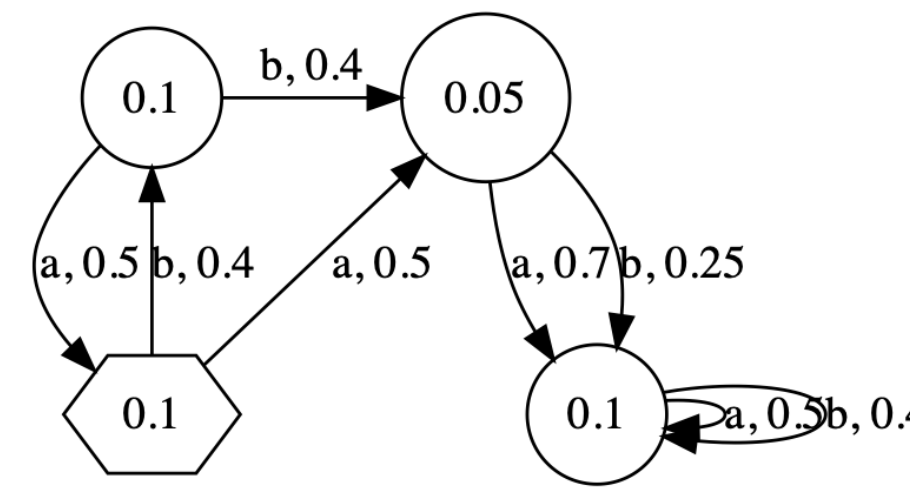


there may be some noise…

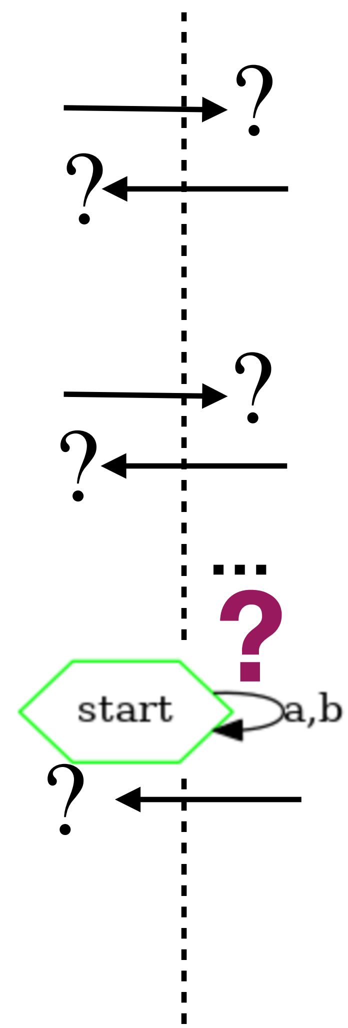
What shall we put in the table?

Final Choice: Last Token Probabilities
Nice Realisation: Can use additive tolerance
Challenge: Non-transitivity of tolerance

Adapting L*

The Observation Table

P \ S	$	a	ba
ε	0.1	0.5	0.4
a	0.05	0.7	0.5
b	0.1	0.5	0.7
ba	0.1	0.5	0.5
bb	0.05	0.7	0.5



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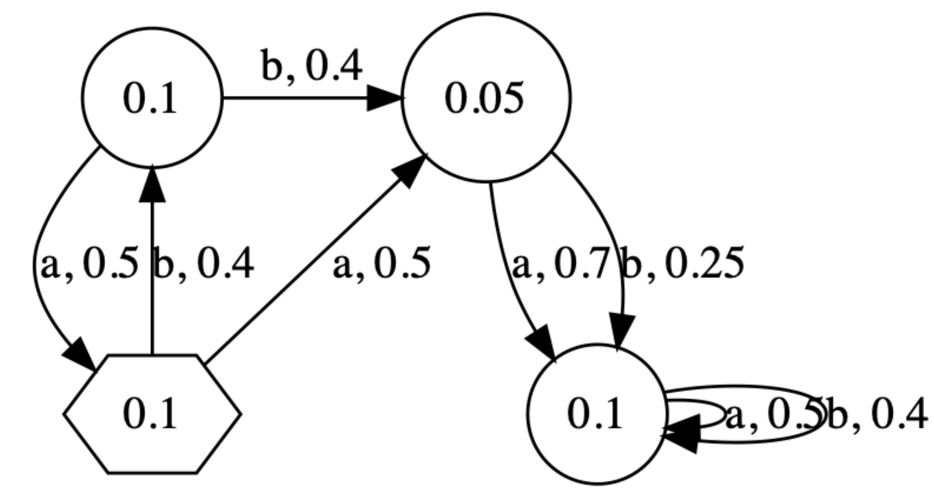


there may be some noise…

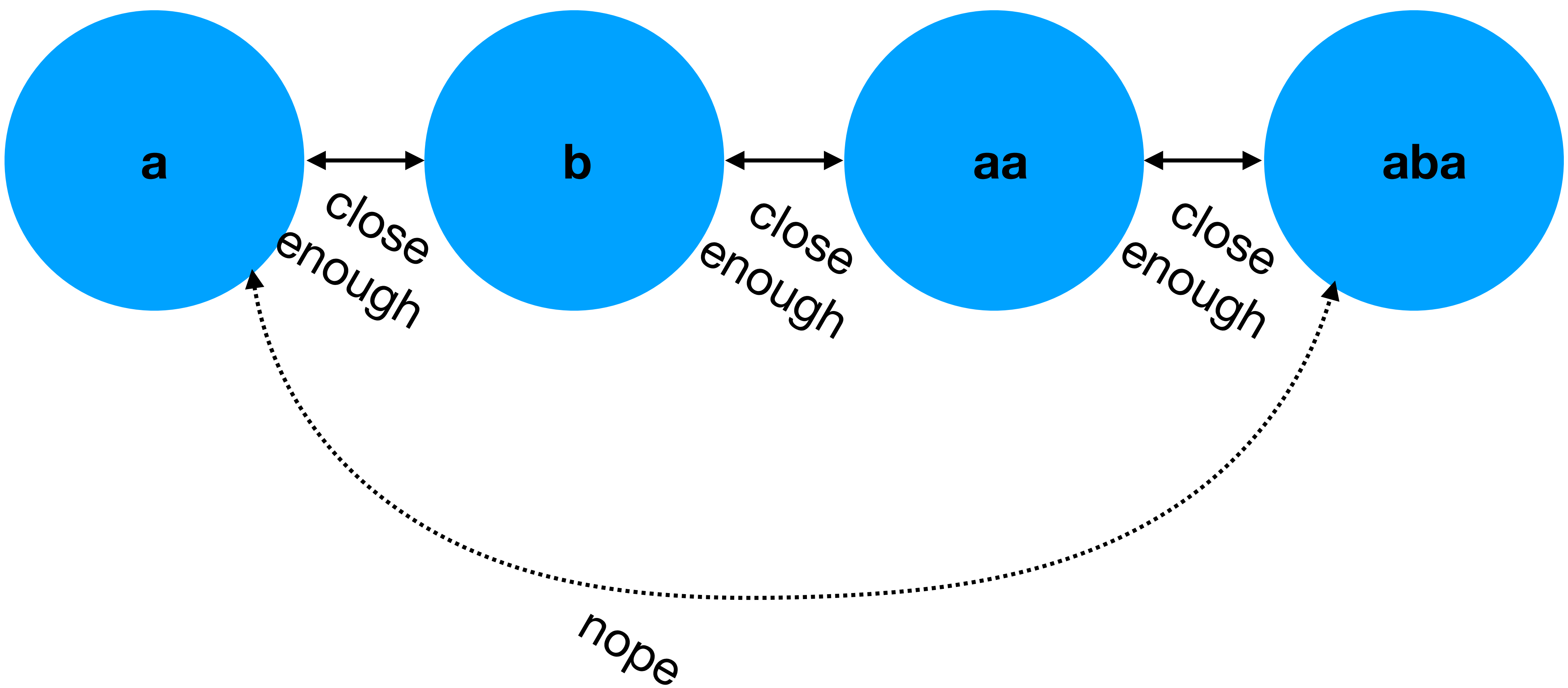
What shall we put in the table?

Final Choice: Last Token Probabilities
Nice Realisation: Can use additive tolerance
Challenge: Non-transitivity of tolerance

Adapting L*

Dealing with the Additive Tolerance

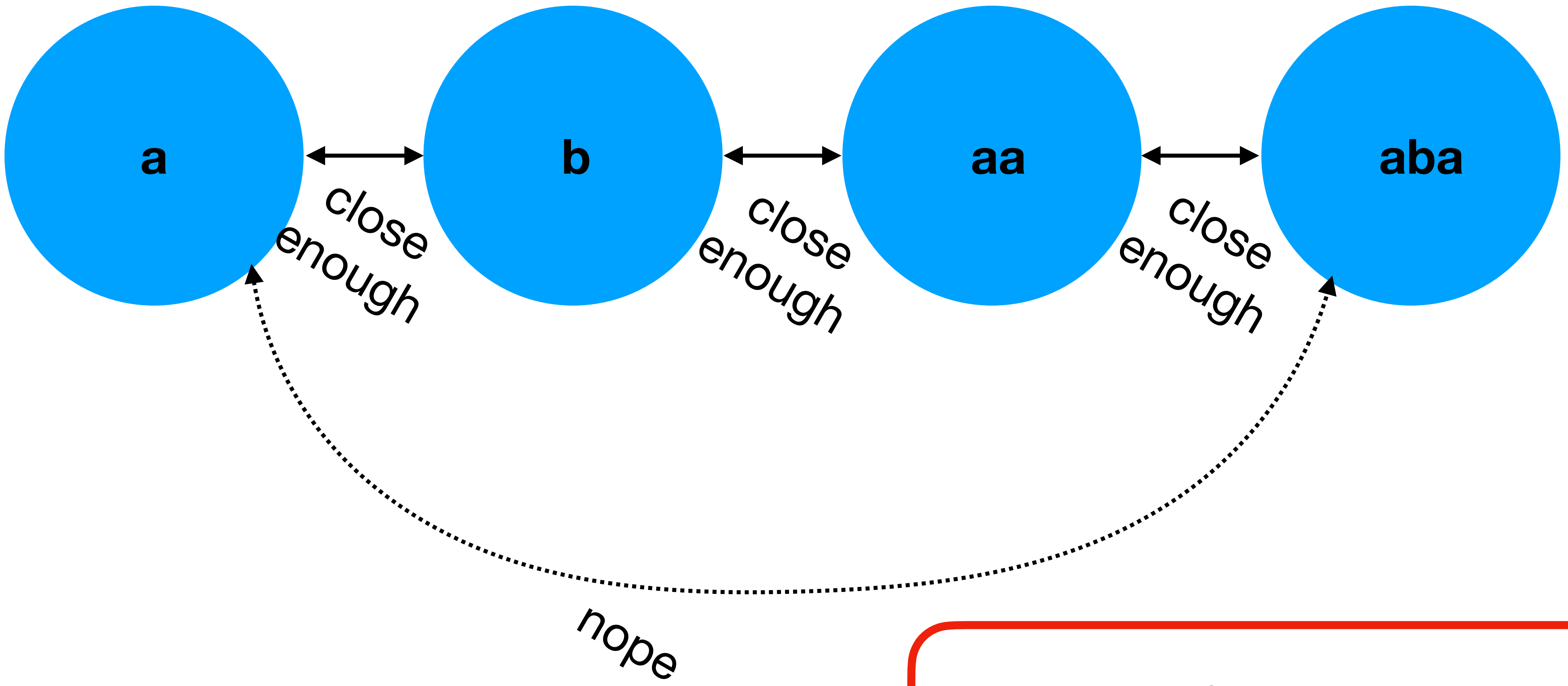
In particular: dealing with 'chains' of similar prefixes



Adapting L*

Dealing with the Additive Tolerance

In particular: dealing with ‘chains’ of similar prefixes



How can we fix the “**closedness**” and “**consistency**” definitions, to avoid mistaken groupings?

Adapting L*

Dealing with the Additive Tolerance

In particular: dealing with ‘chains’ of similar prefixes

Immediate realisation: Attempting to fix definitions for table is painful

Adapting L*

Dealing with the Additive Tolerance

In particular: dealing with ‘chains’ of similar prefixes

Immediate realisation: Attempting to fix definitions for table is painful

Solution:

Fill table optimistically, and fix problems post-hoc

Adapting L*

Optimistic Table and Post-Hoc Fixes

Adapting L*

Optimistic Table and Post-Hoc Fixes

1. **Check closedness as normal**,
   just with the additive tolerance

2. **Check consistency as normal**,
   just with the additive tolerance

3. **Make hypothesis with caution!**

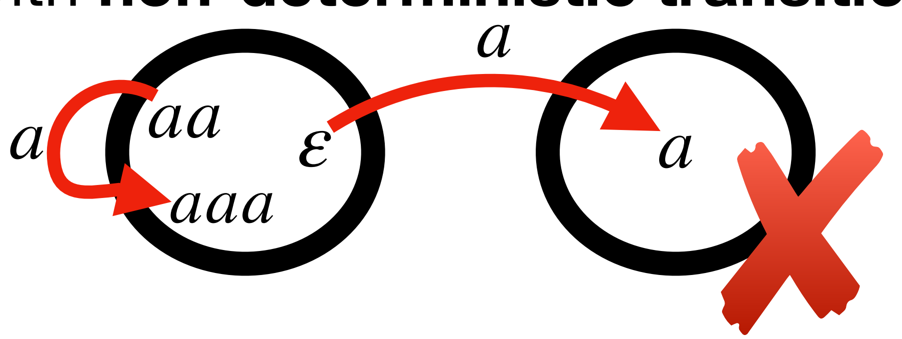
Adapting L*

Optimistic Table and Post-Hoc Fixes

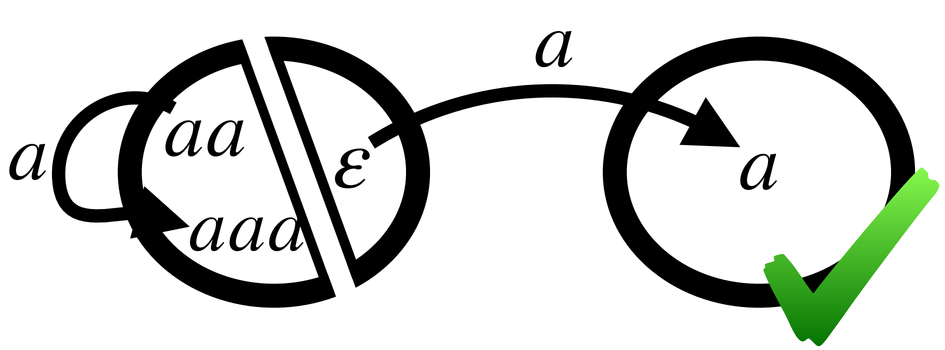
3. Make hypothesis with caution!

Potential Problems:

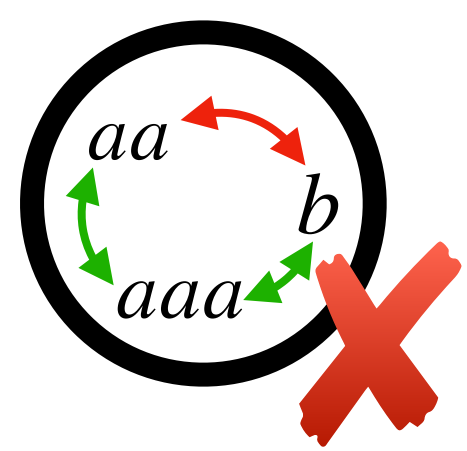
1. Clustering of prefixes causes states with **non-deterministic transitions**



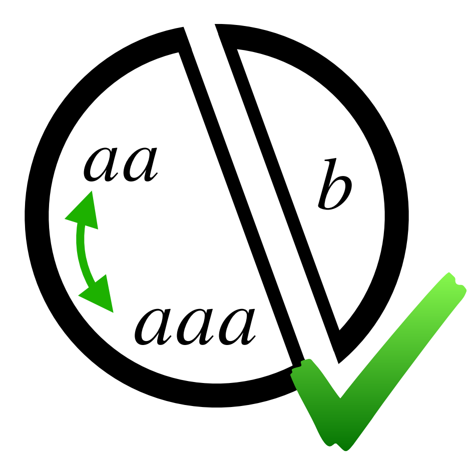
post hoc fix: refine



2. Clustering of prefixes creates states with prefixes **beyond threshold** of each other



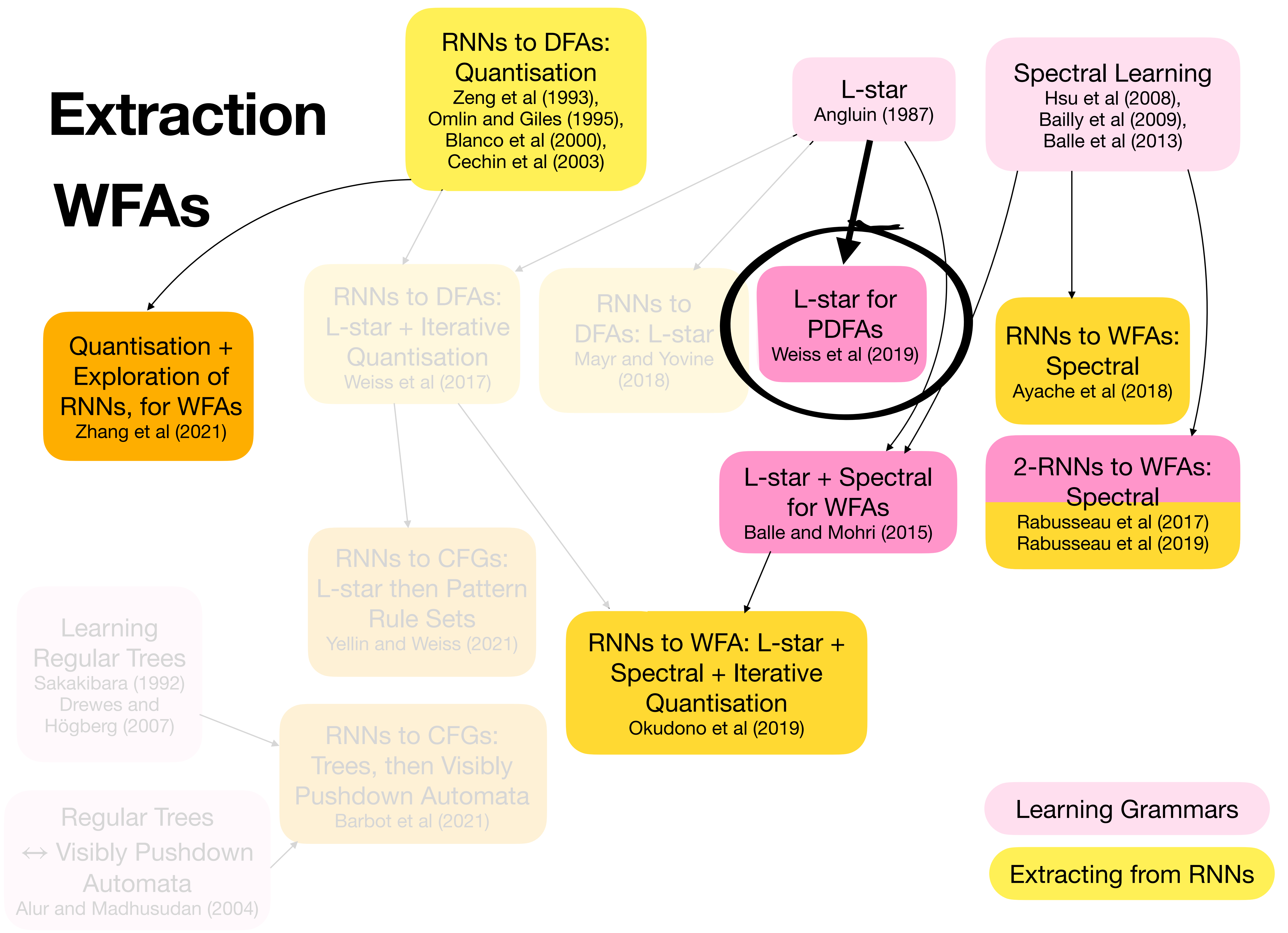
post hoc fix: refine



Anytime Stopping

This algorithm is unlikely to complete on real-world tasks. Thus, we allow anytime stopping:

- Prioritise high-weight prefixes
- Avoid very low-weight separating suffixes
- On stop, map remaining prefixes to best match
  - This is actually quite slow, and might not be very beneficial *(needs to be tested!)*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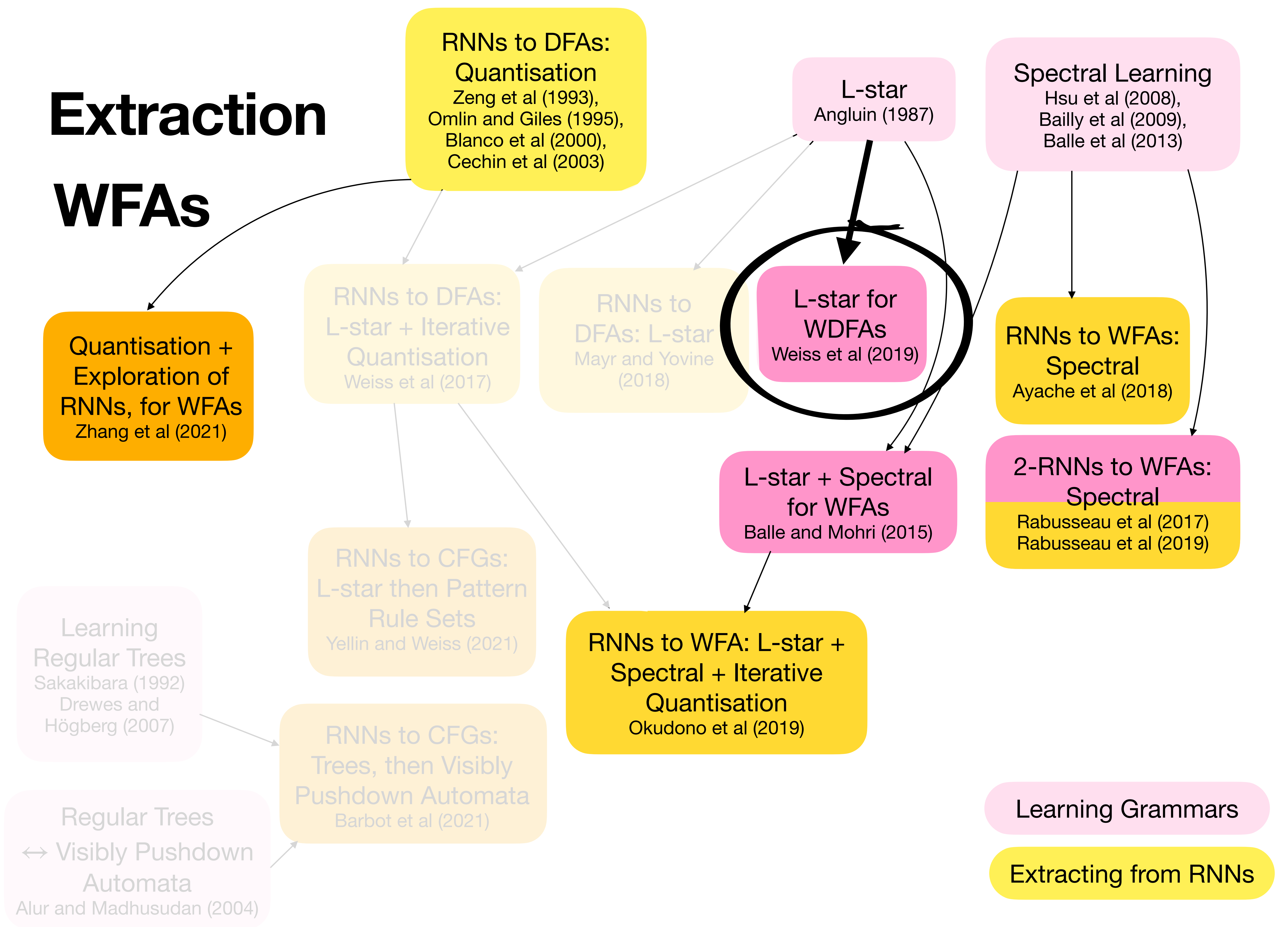
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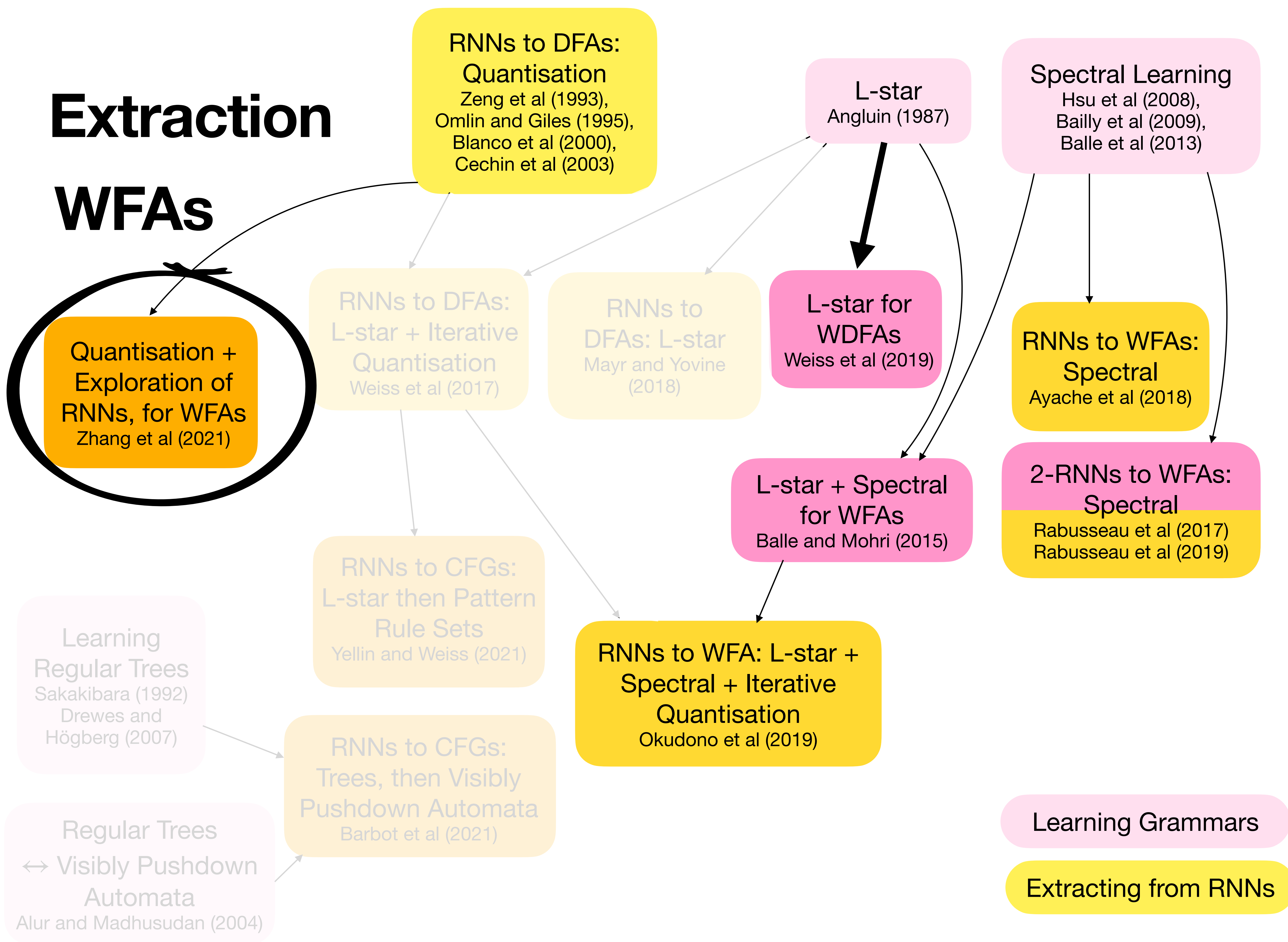
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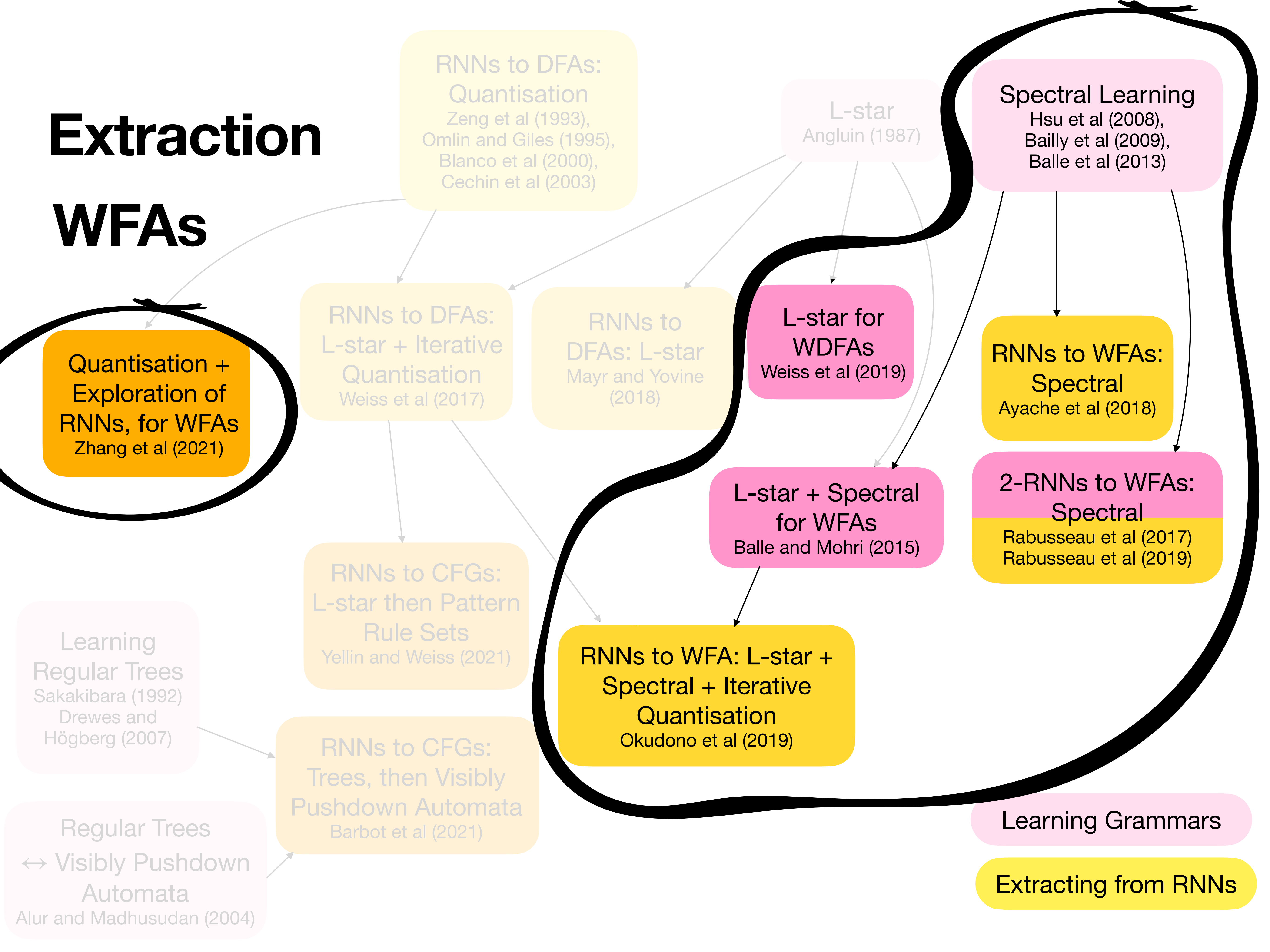
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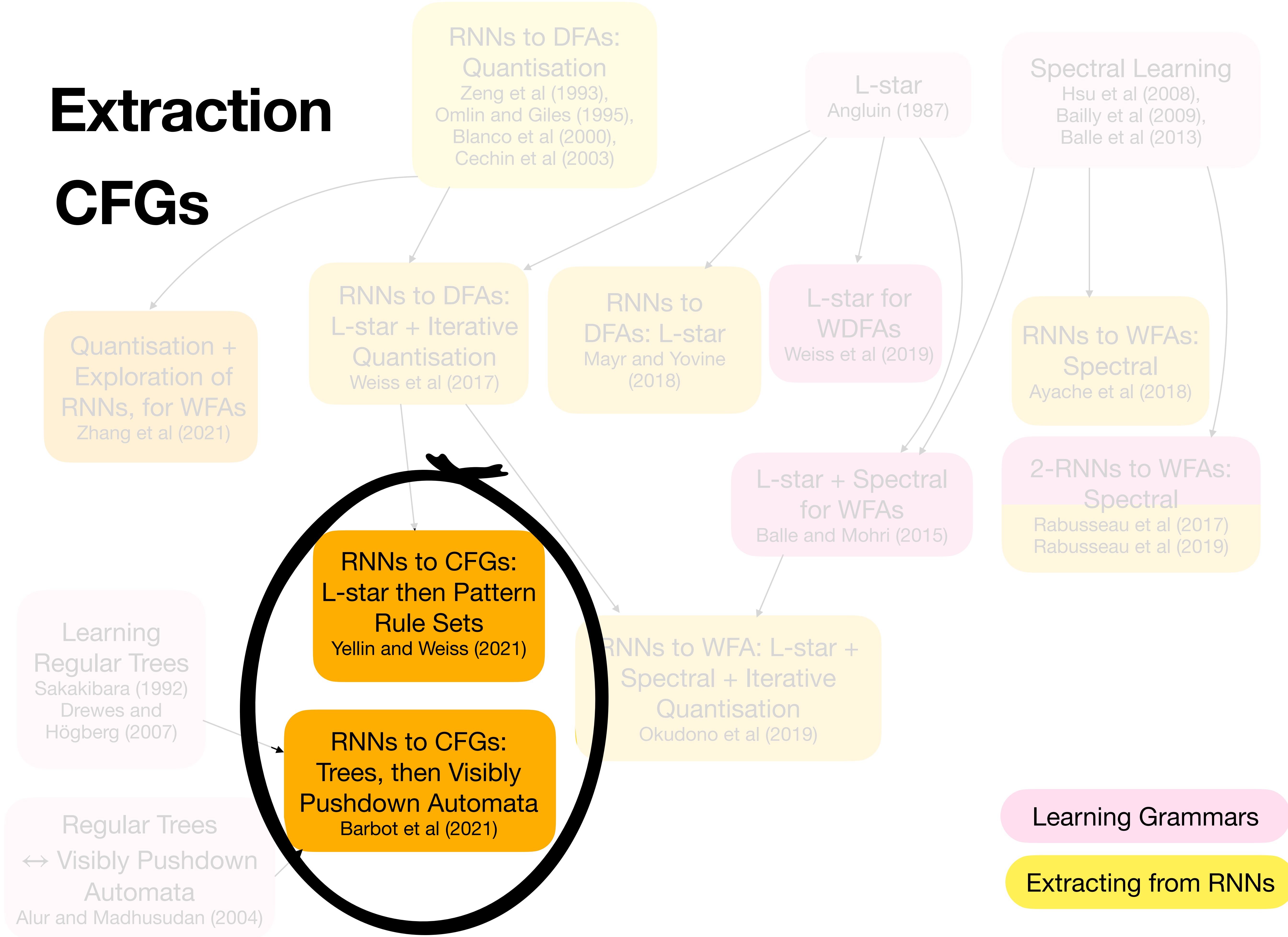
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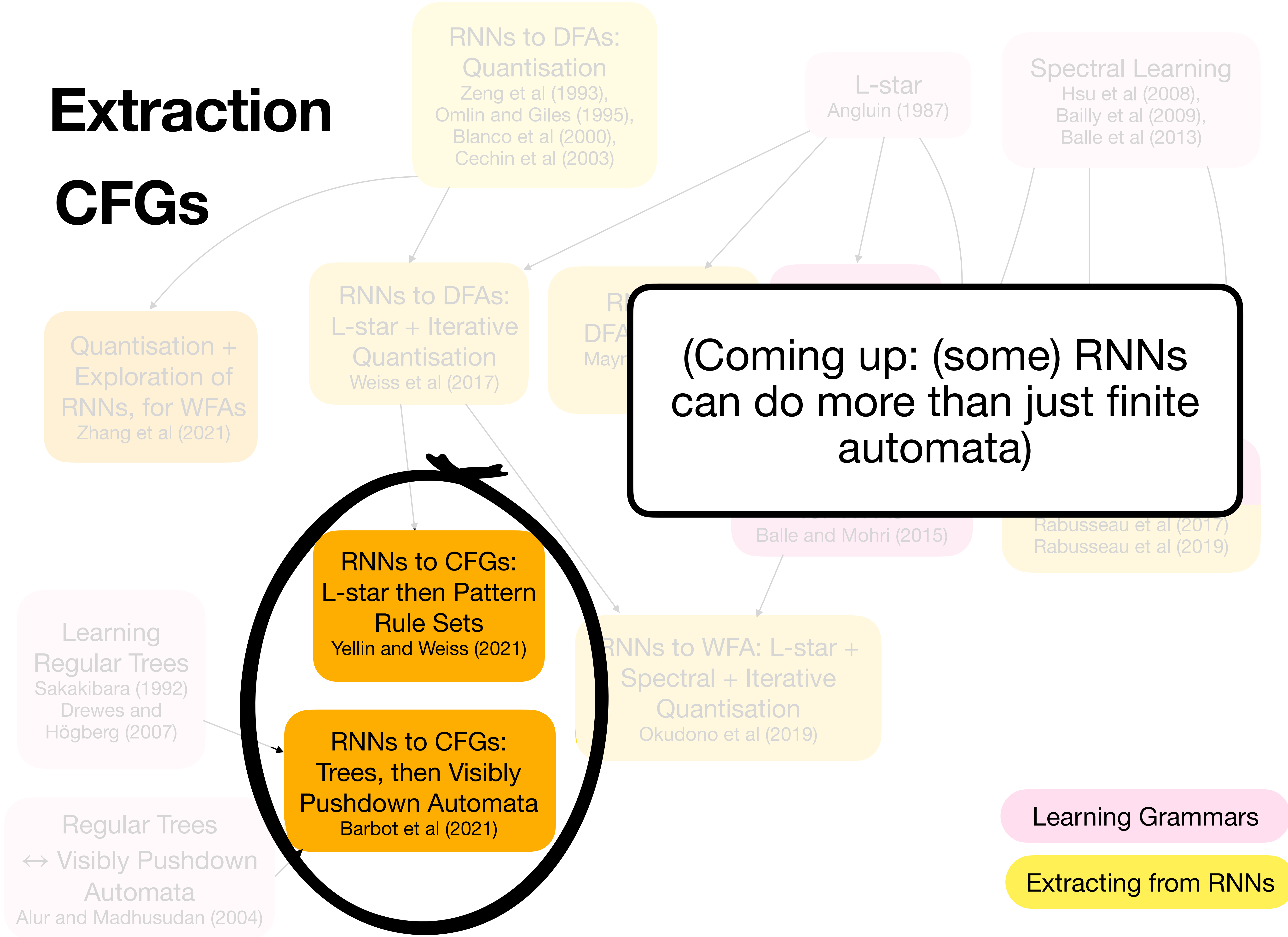

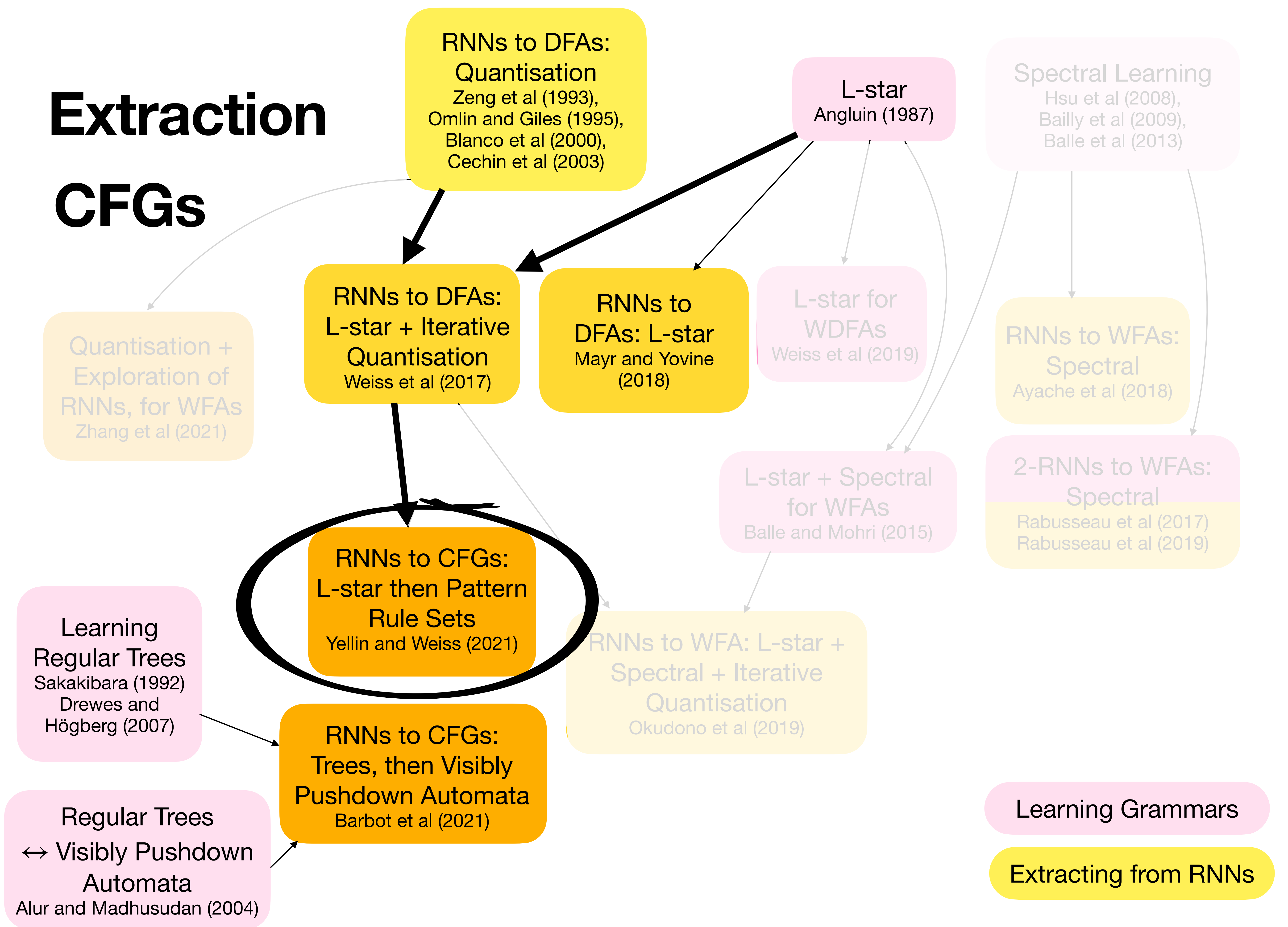

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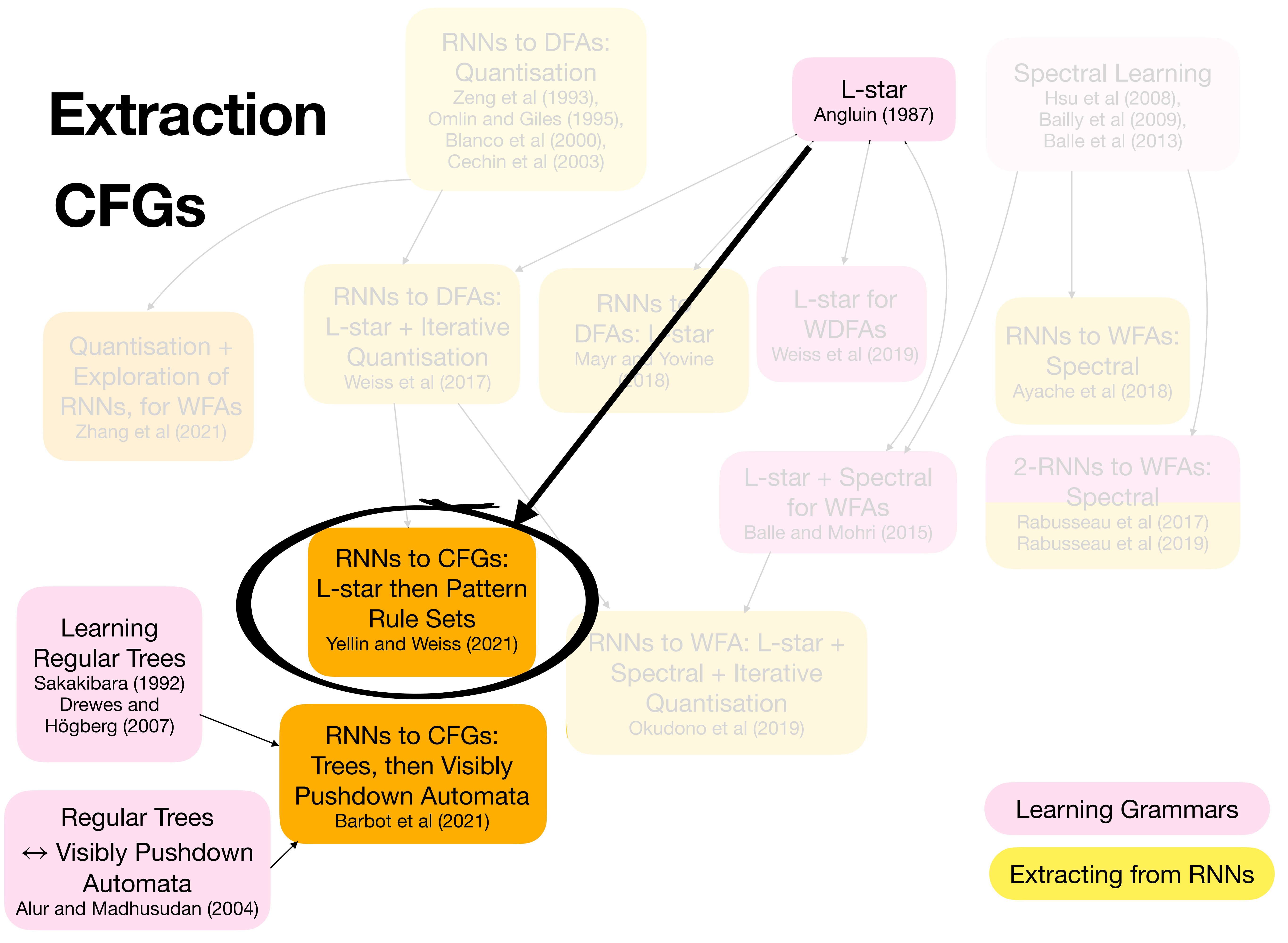
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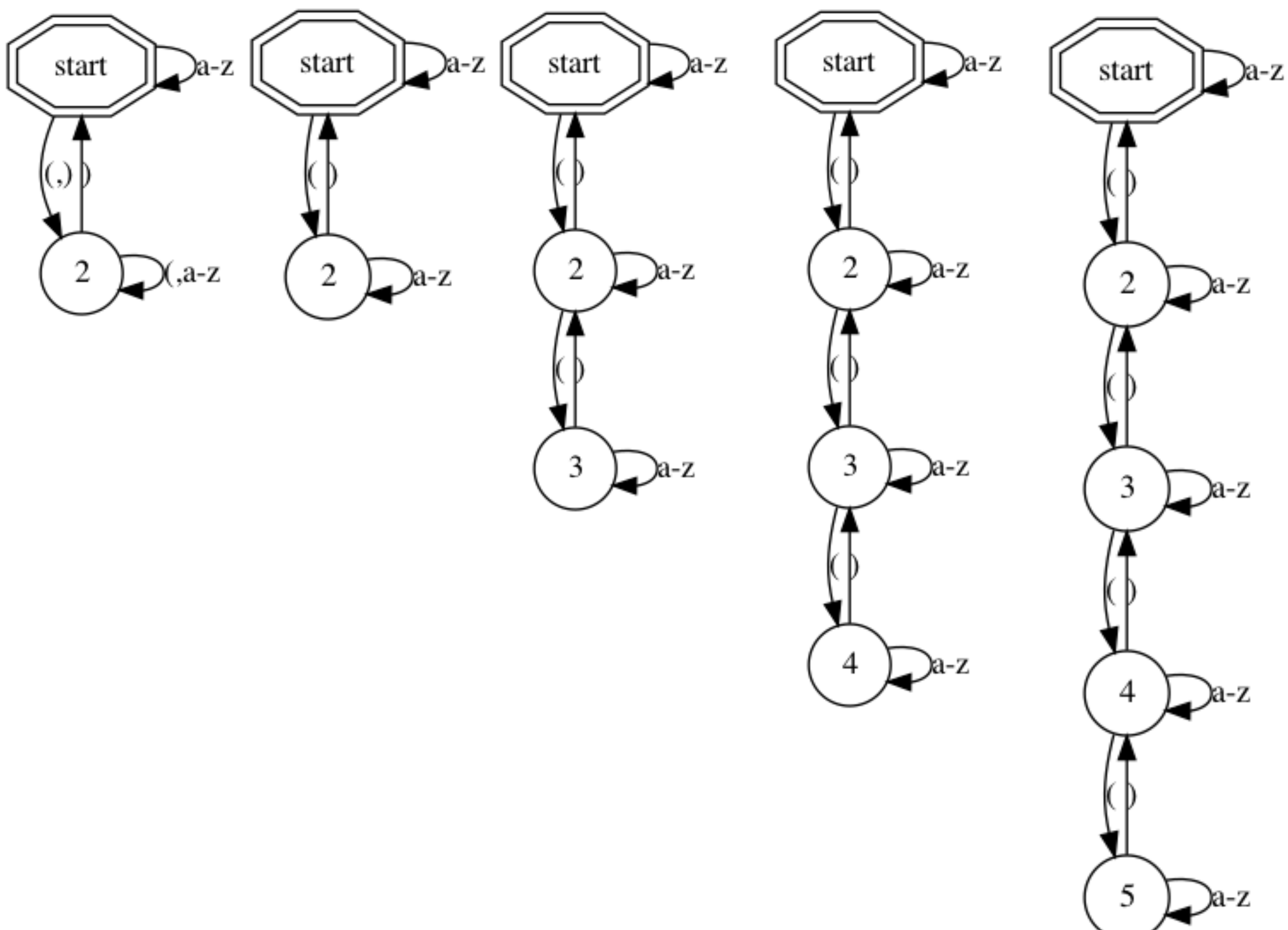
RNNs: Extraction: CFGs: **Pattern Rule Sets**

Yellin and Weiss (2021)

Observation: L-star learning a CFG seems to have structured increases (example on balanced parentheses)



etc…

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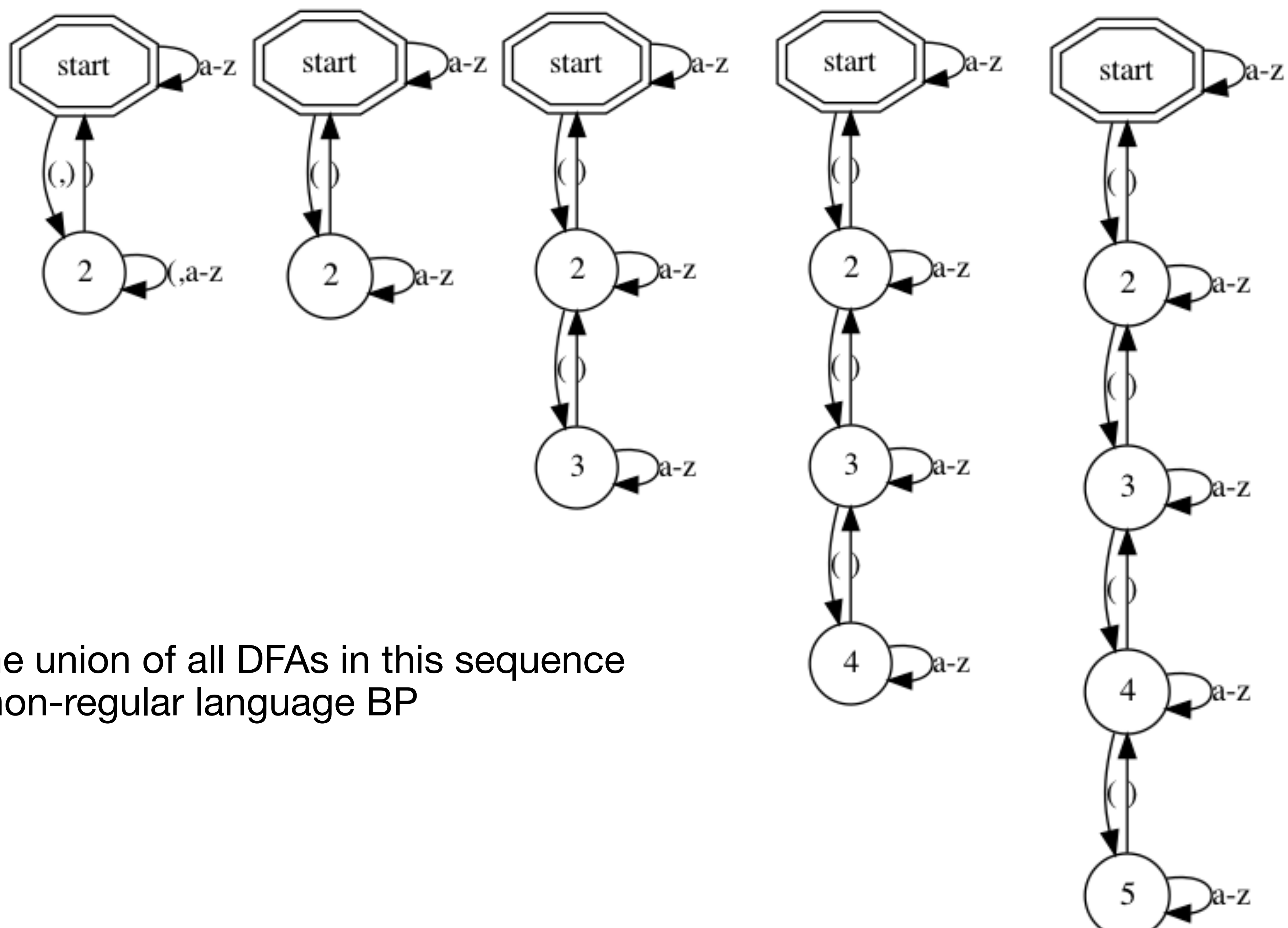

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1. In the limit, the union of all DFAs in this sequence accepts the non-regular language BP

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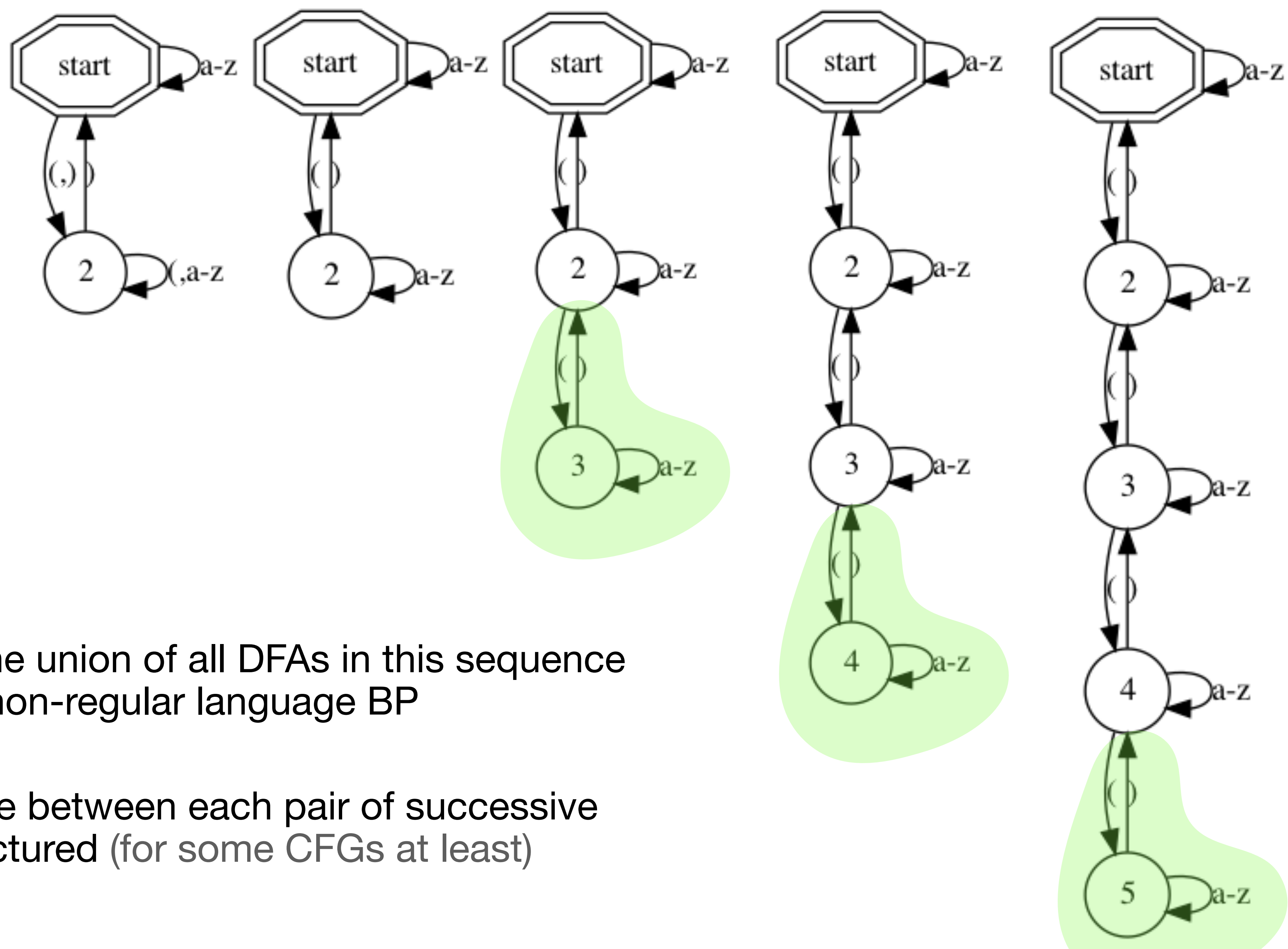

etc…

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RNNs: Extraction: CFGs: **Pattern Rule Sets**

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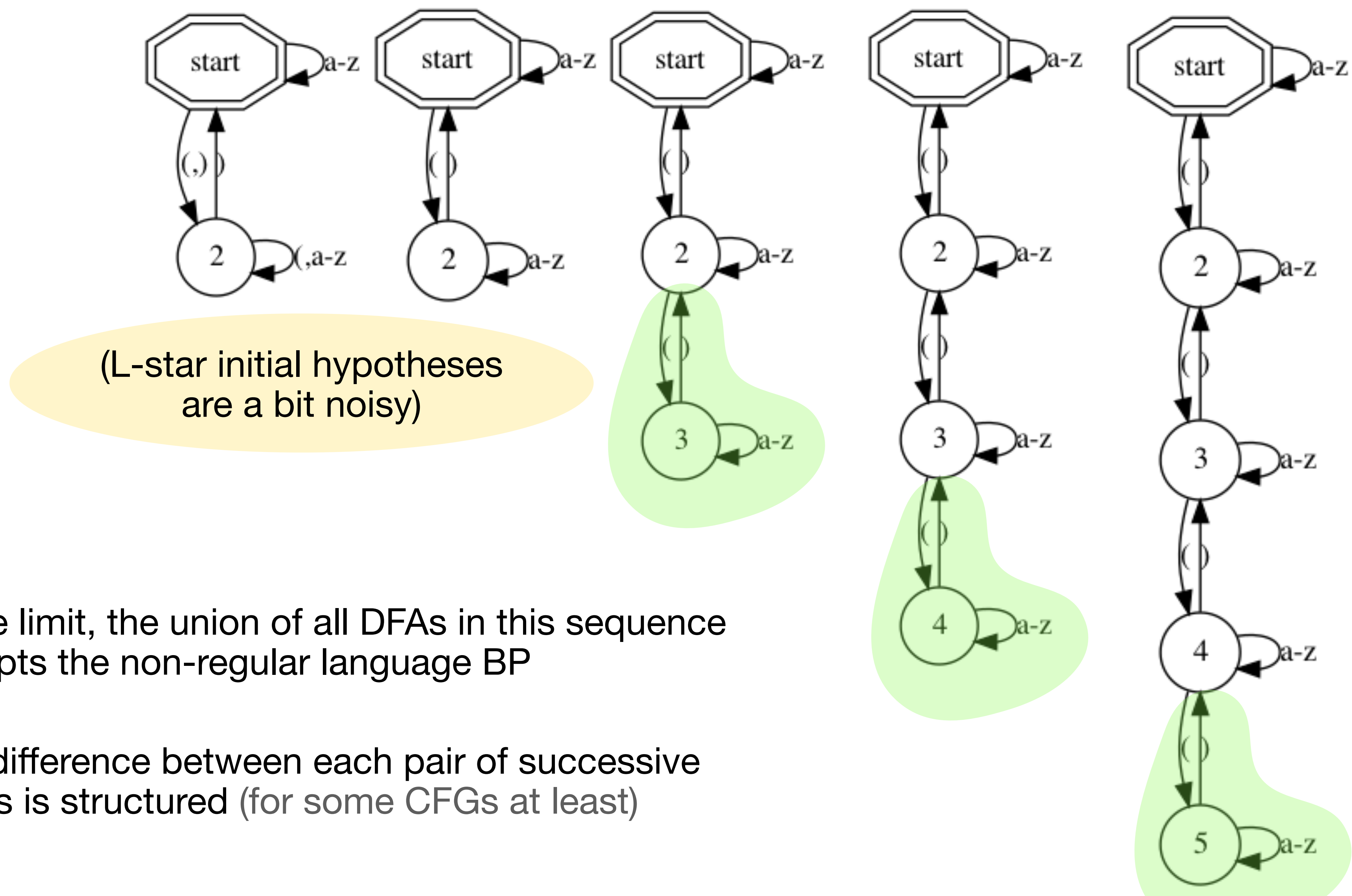

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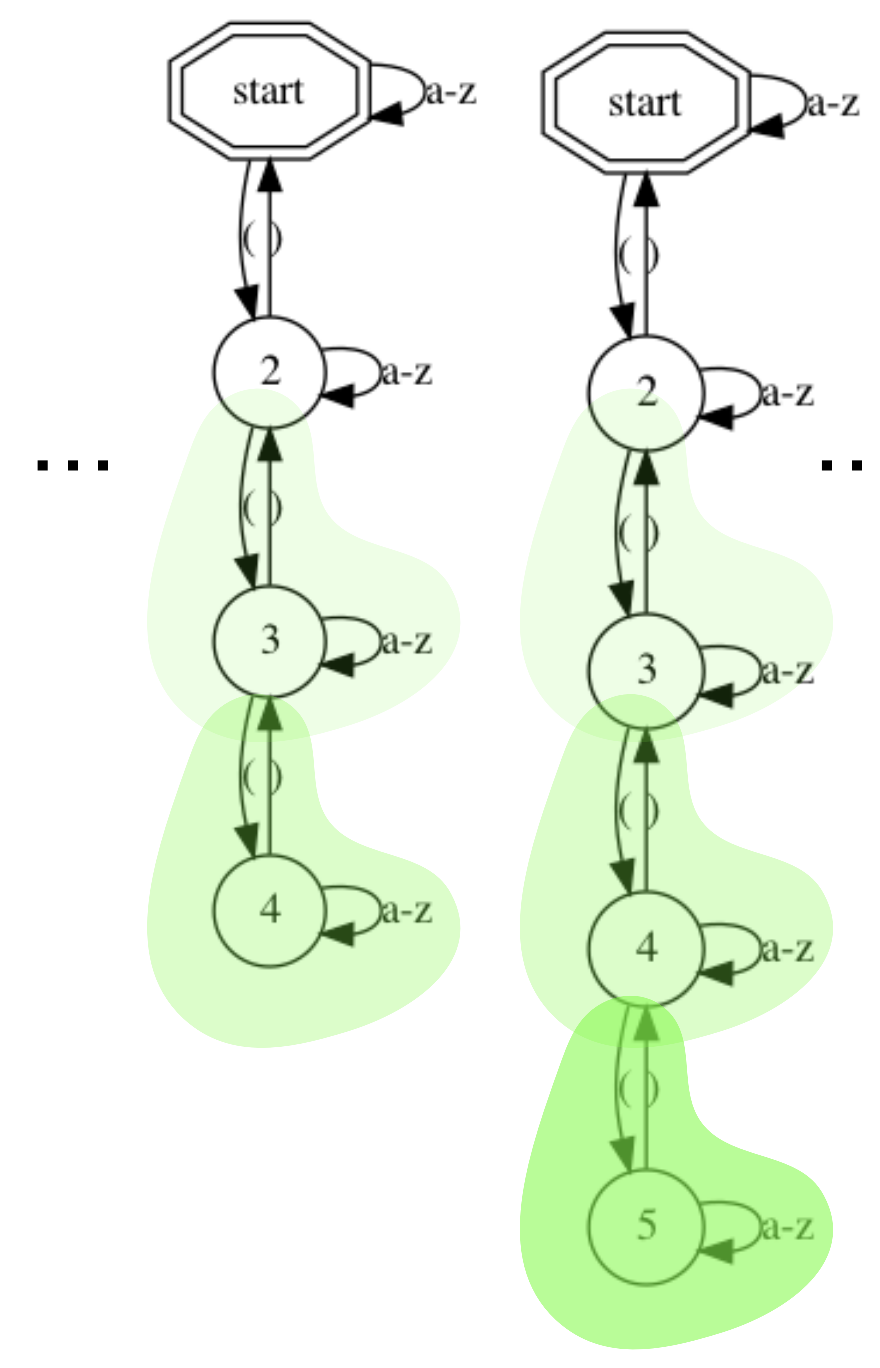
Yellin and Weiss (2021)

Patterns

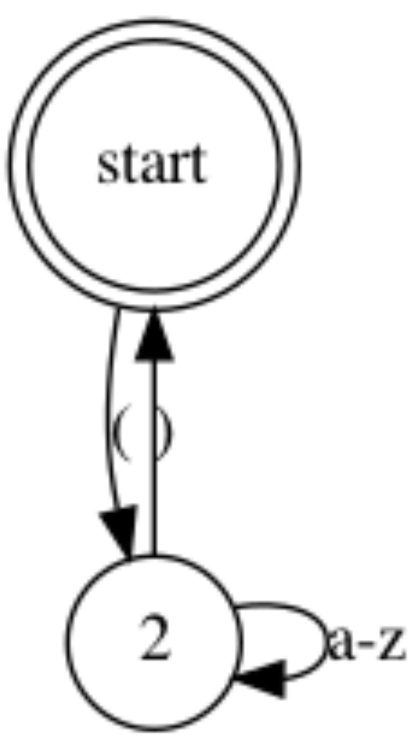


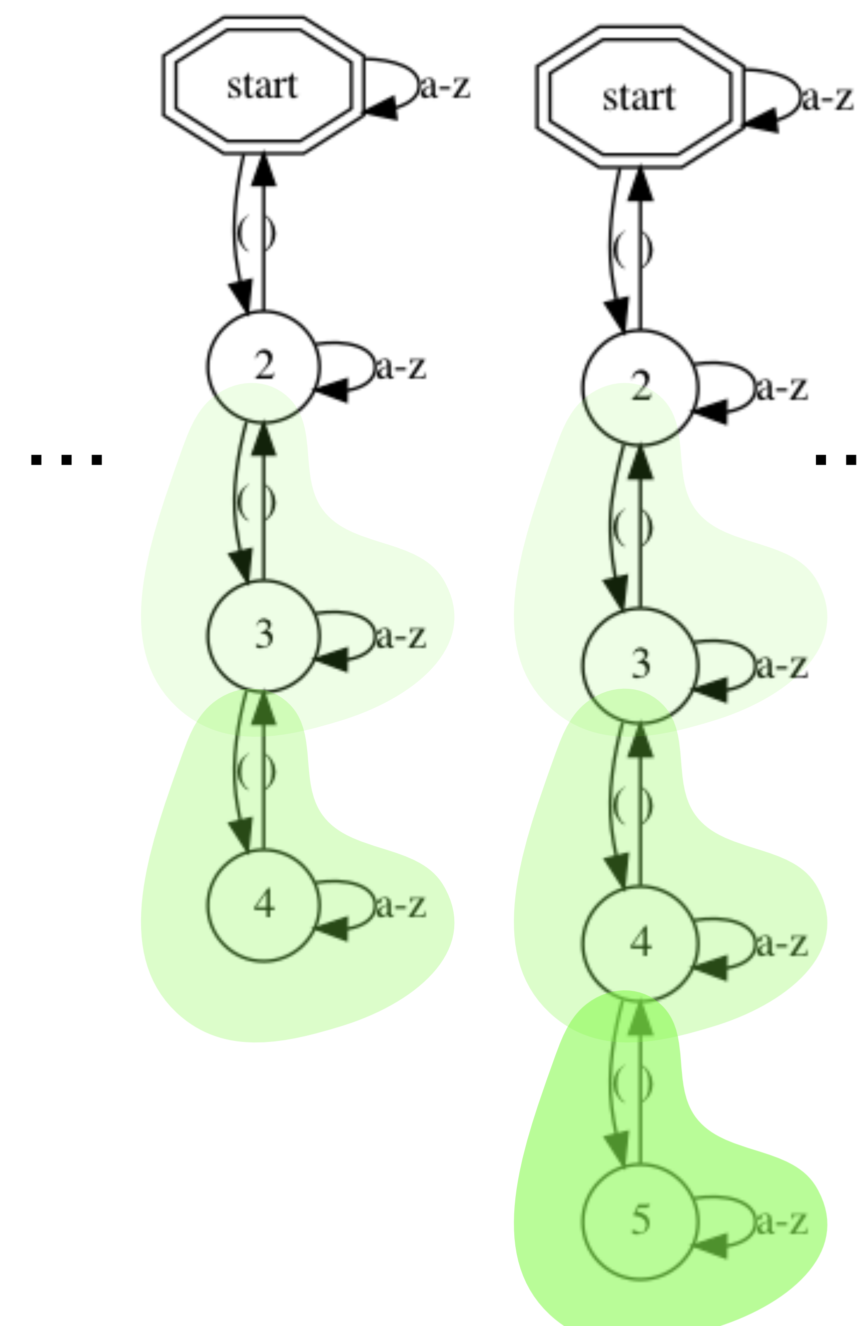
RNNs: Extraction: CFGs: **Pattern Rule Sets**

Yellin and Weiss (2021)

Patterns

- Structure





RNNs: Extraction: CFGs: **Pattern Rule Sets**

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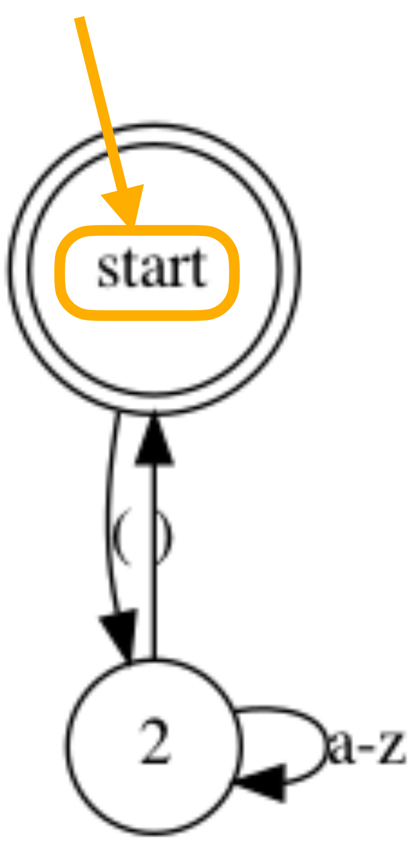
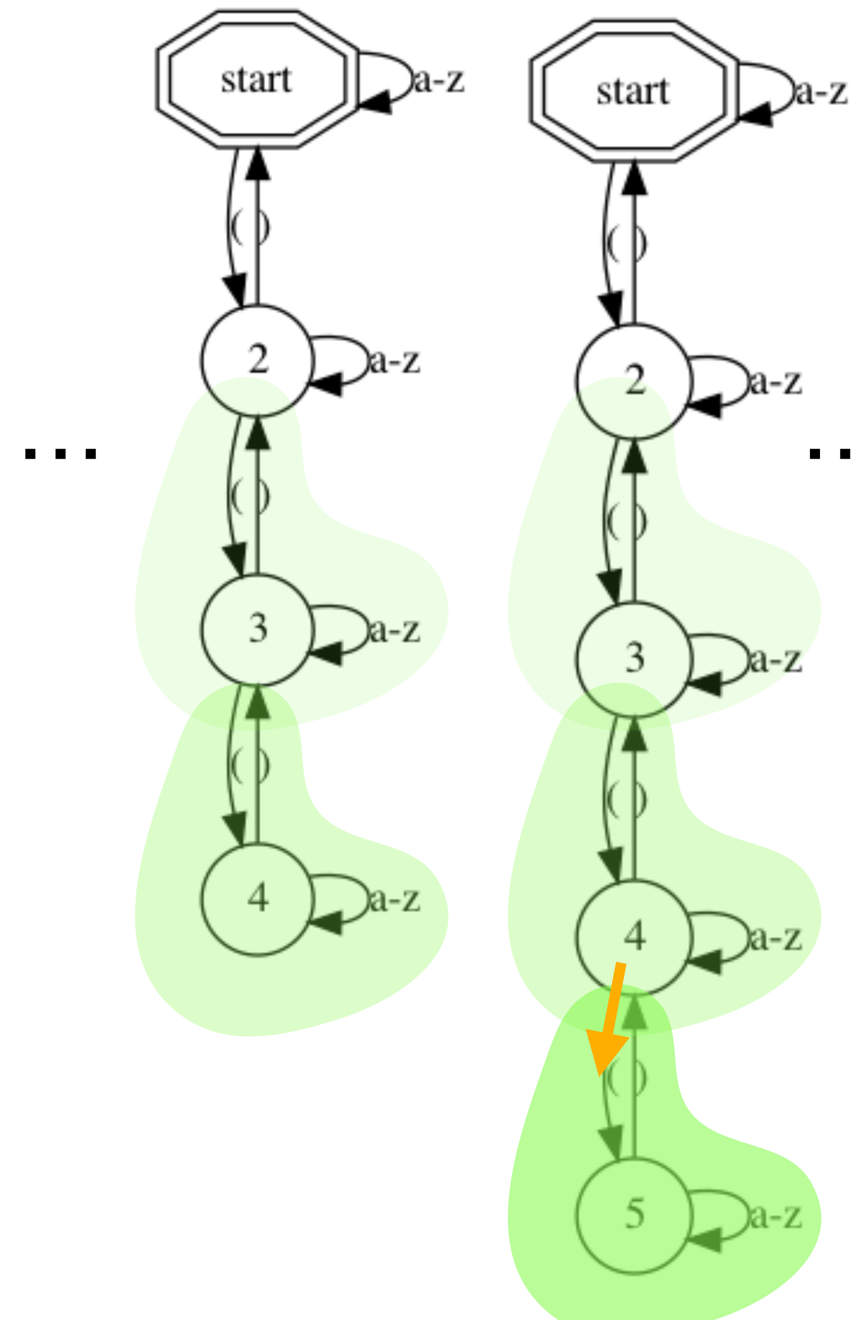
Patterns

- Structure
  - Entry





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Patterns

- Structure
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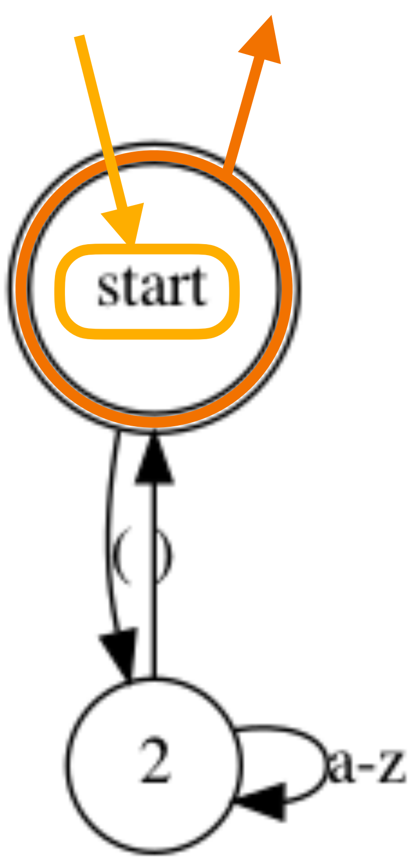
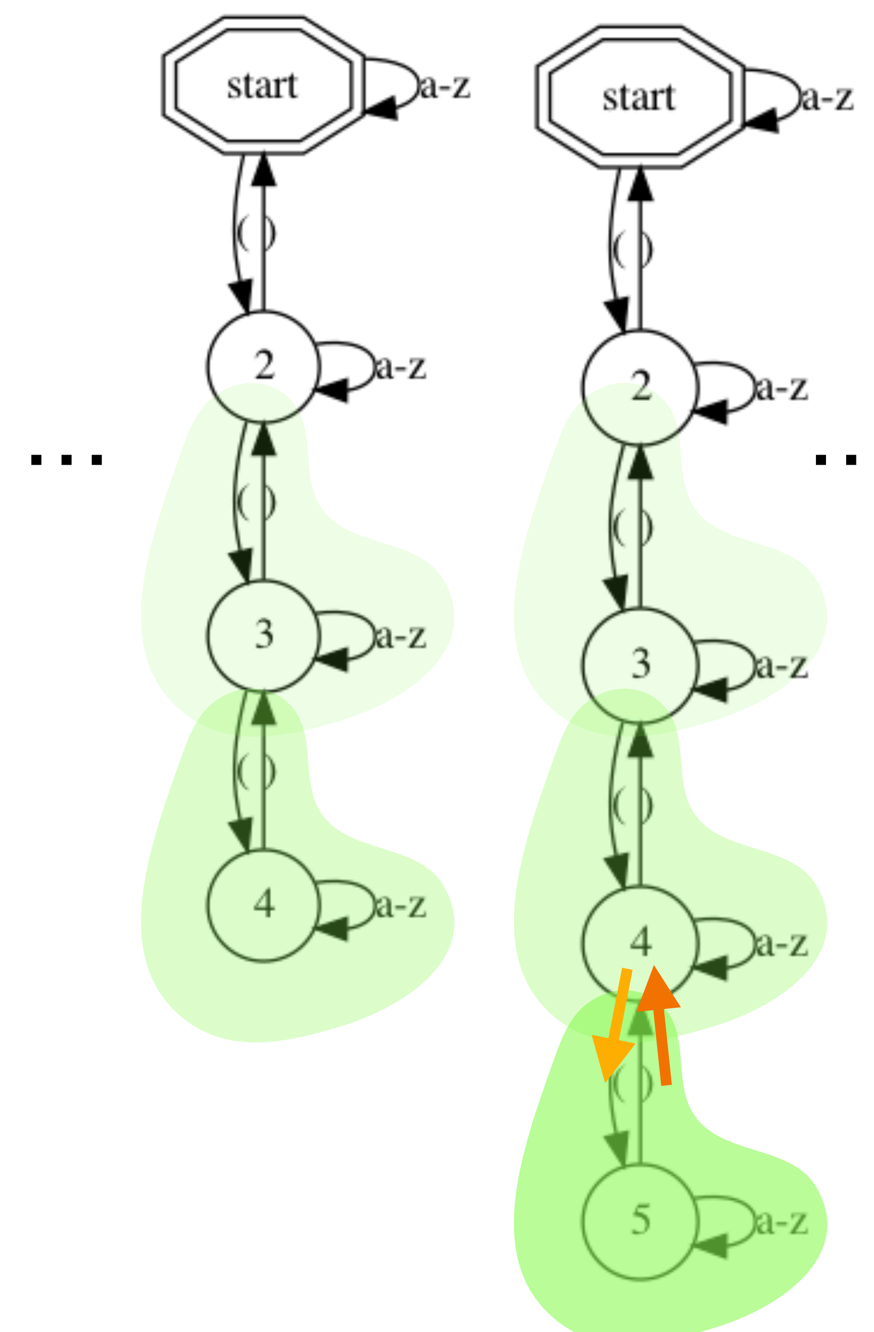
  - Exit





RNNs: Extraction: CFGs: **Pattern Rule Sets**

Yellin and Weiss (2021)

Patterns

- Structure
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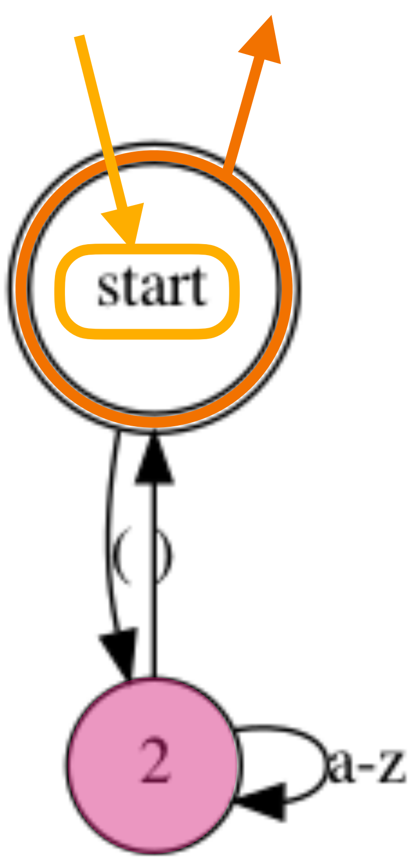
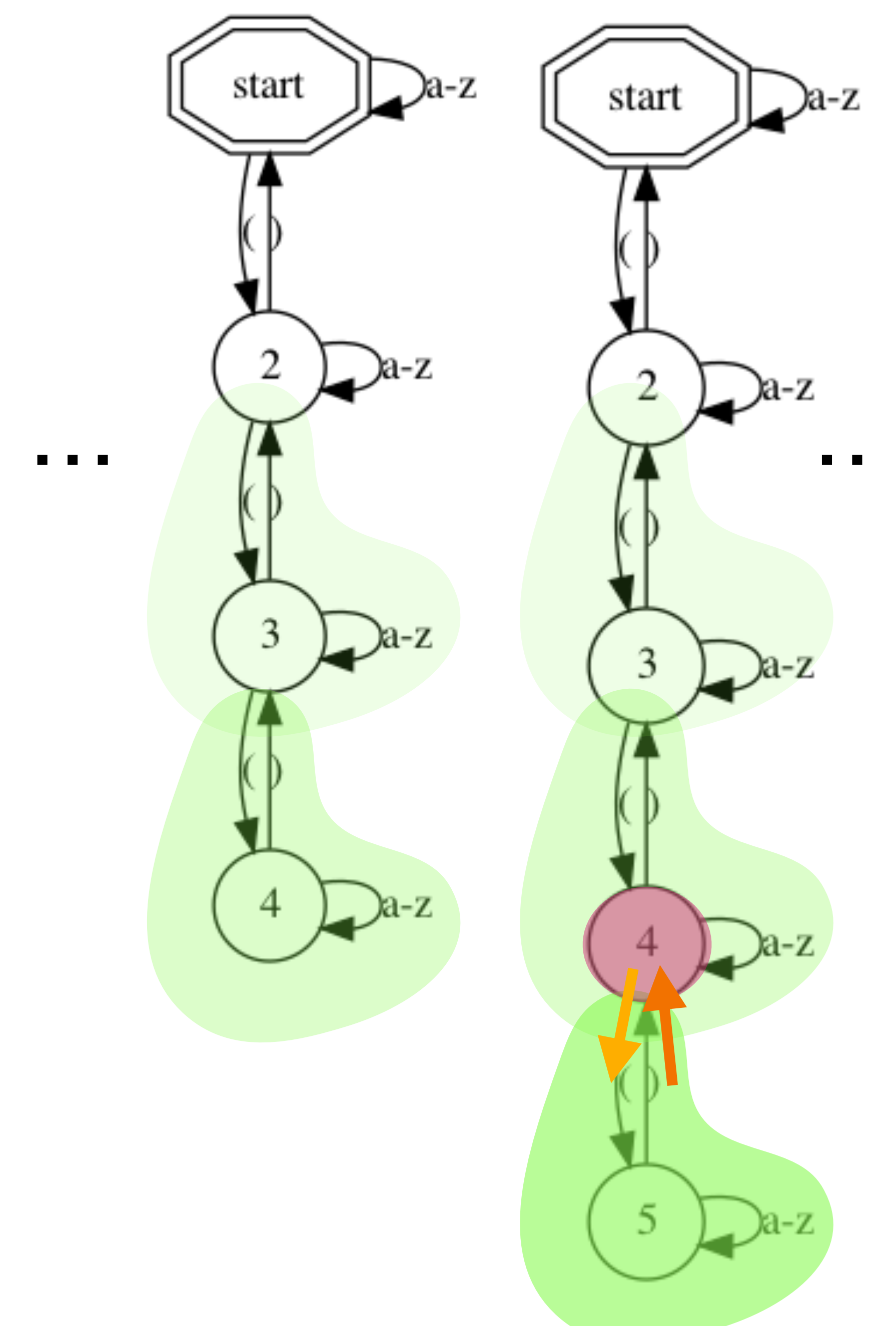
  - Exit
- Connection Point(s)



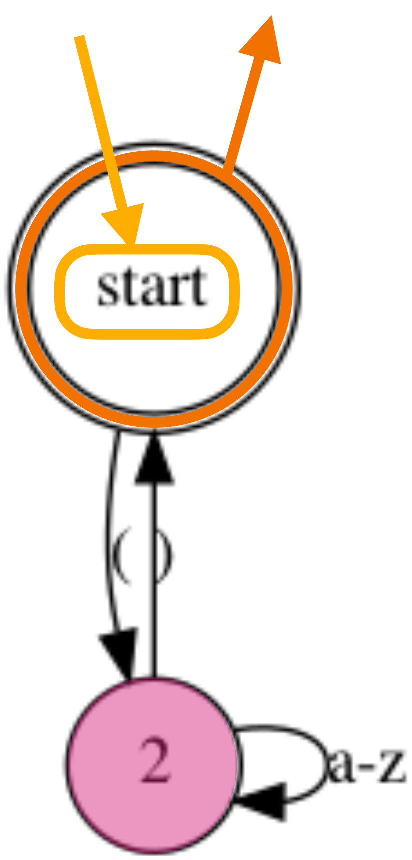


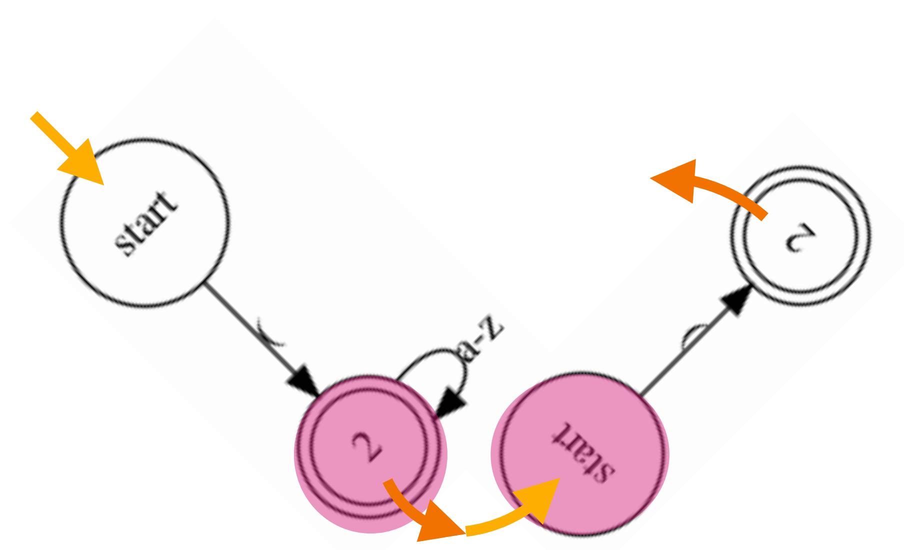
RNNs: Extraction: CFGs: **Pattern Rule Sets**

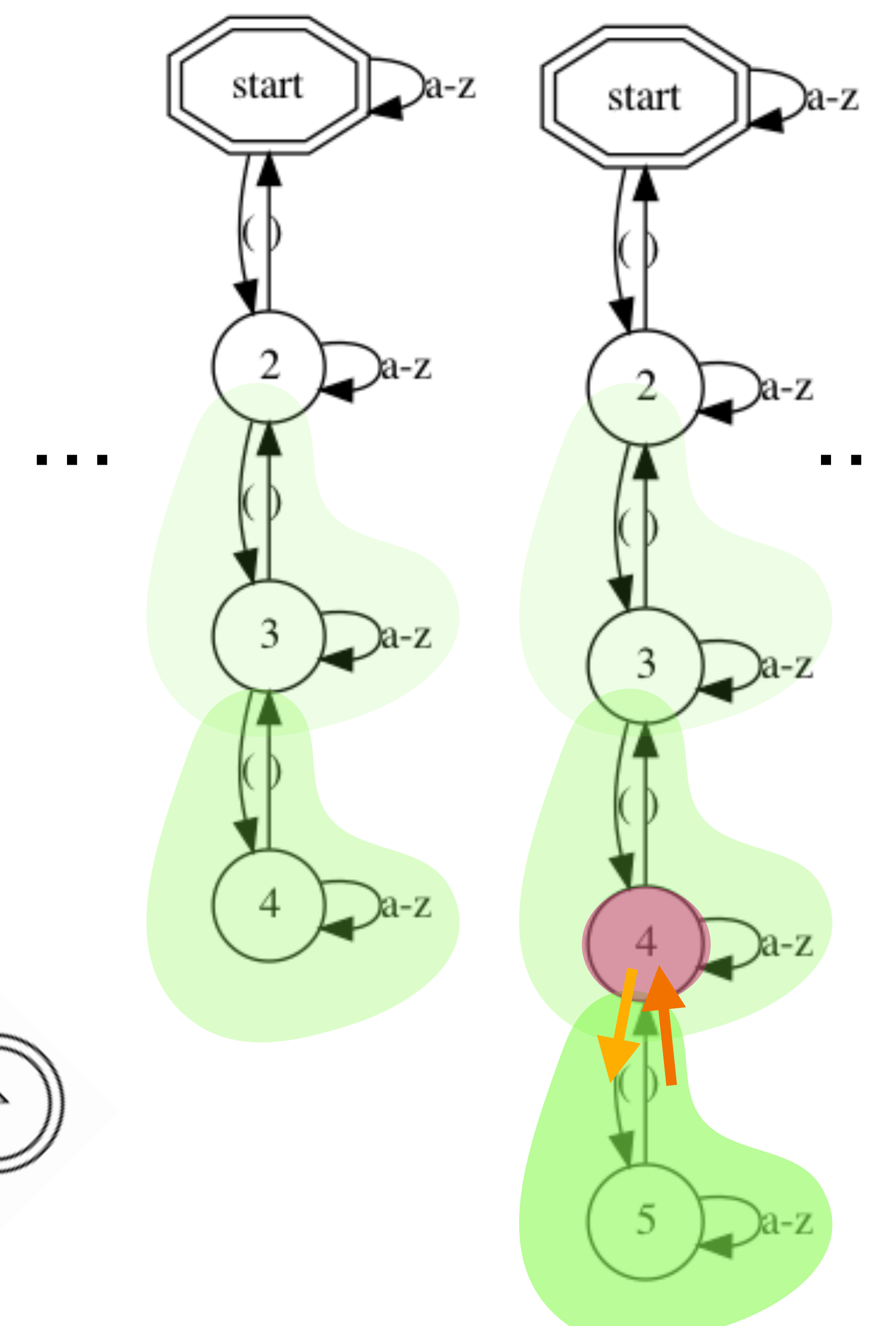
Yellin and Weiss (2021)

Patterns

- Structure
  - Entry
  - Exit
- Connection Point(s)
- Composable
  - Connection points are on compositions





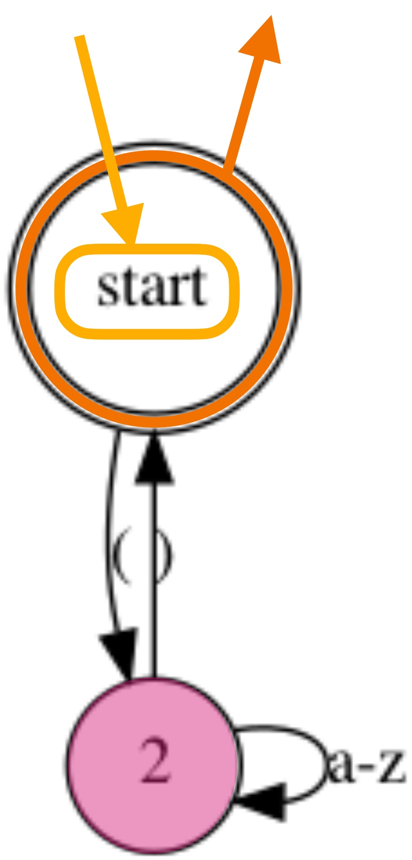


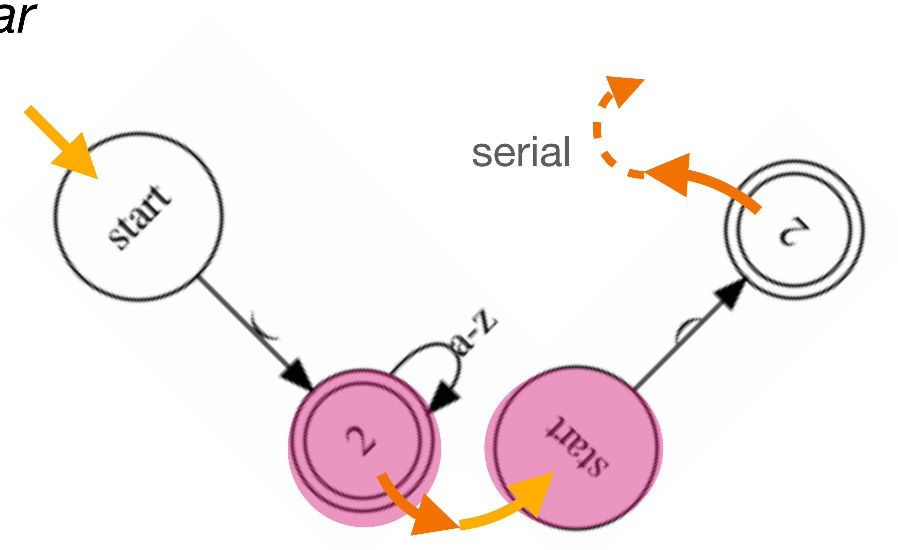
RNNs: Extraction: CFGs: **Pattern Rule Sets**

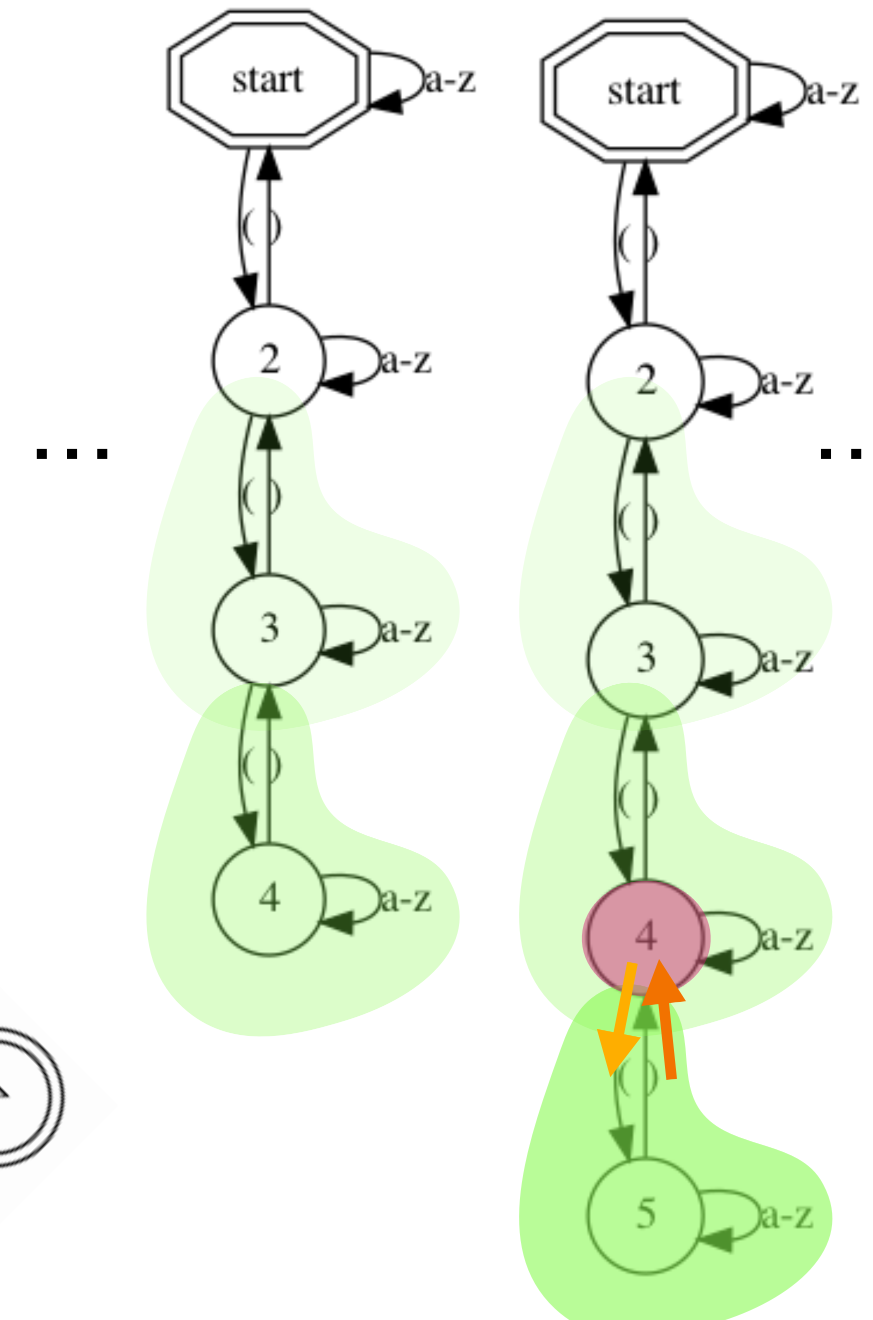
Yellin and Weiss (2021)

Patterns

- Structure
  - Entry
  - Exit
- Connection Point(s)
- Composable
  - Connection points are on compositions
  - Composition can be *serial* or *circular*







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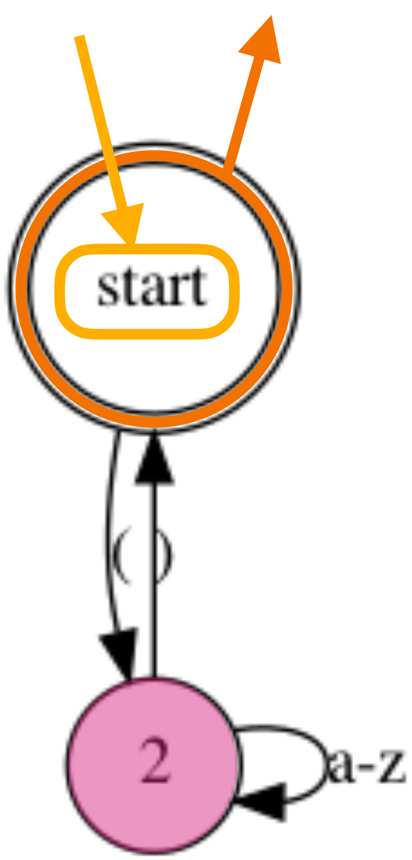

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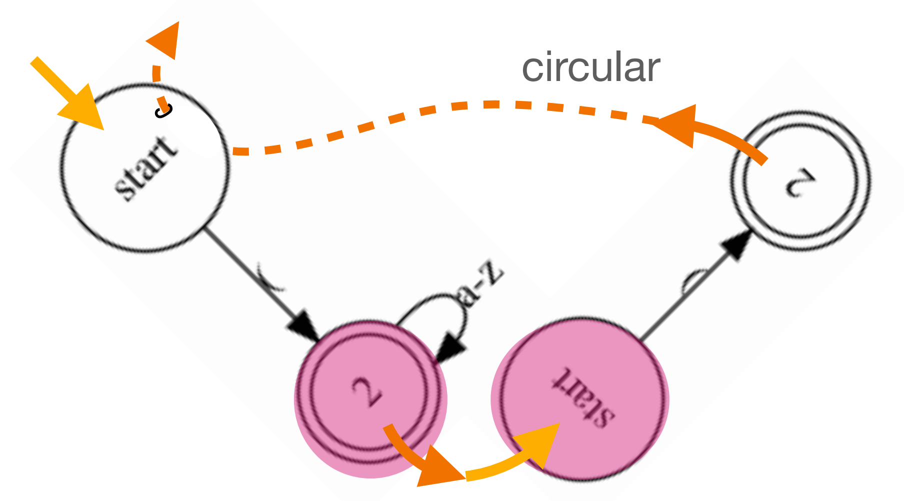

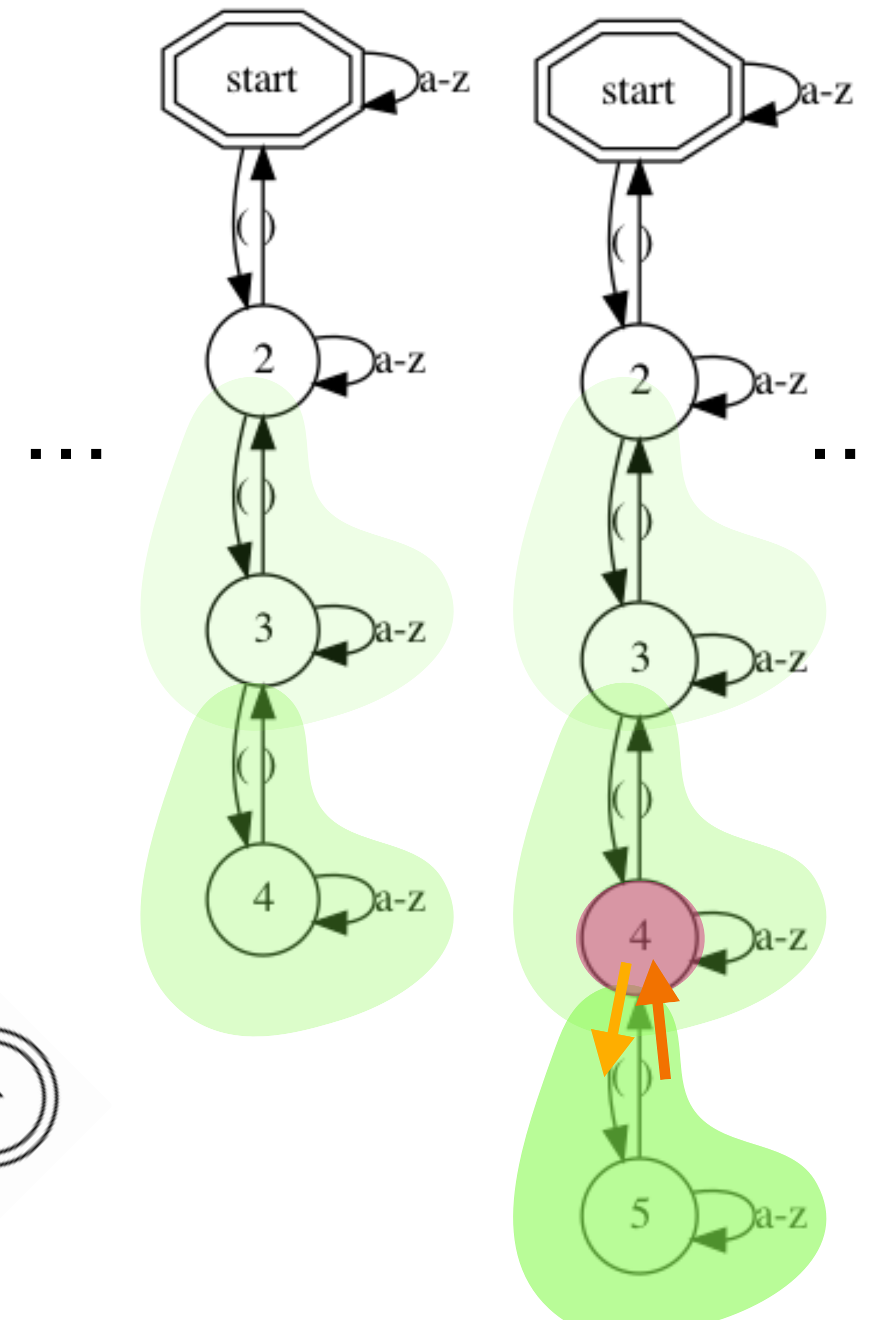

RNNs: Extraction: CFGs: **Pattern Rule Sets**

Yellin and Weiss (2021)

Rules

Rules describe how specific patterns initiate and expand the DFAs. There are three types:

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(When we get to extraction:
this might not be the same
first DFA that L-star suggests)

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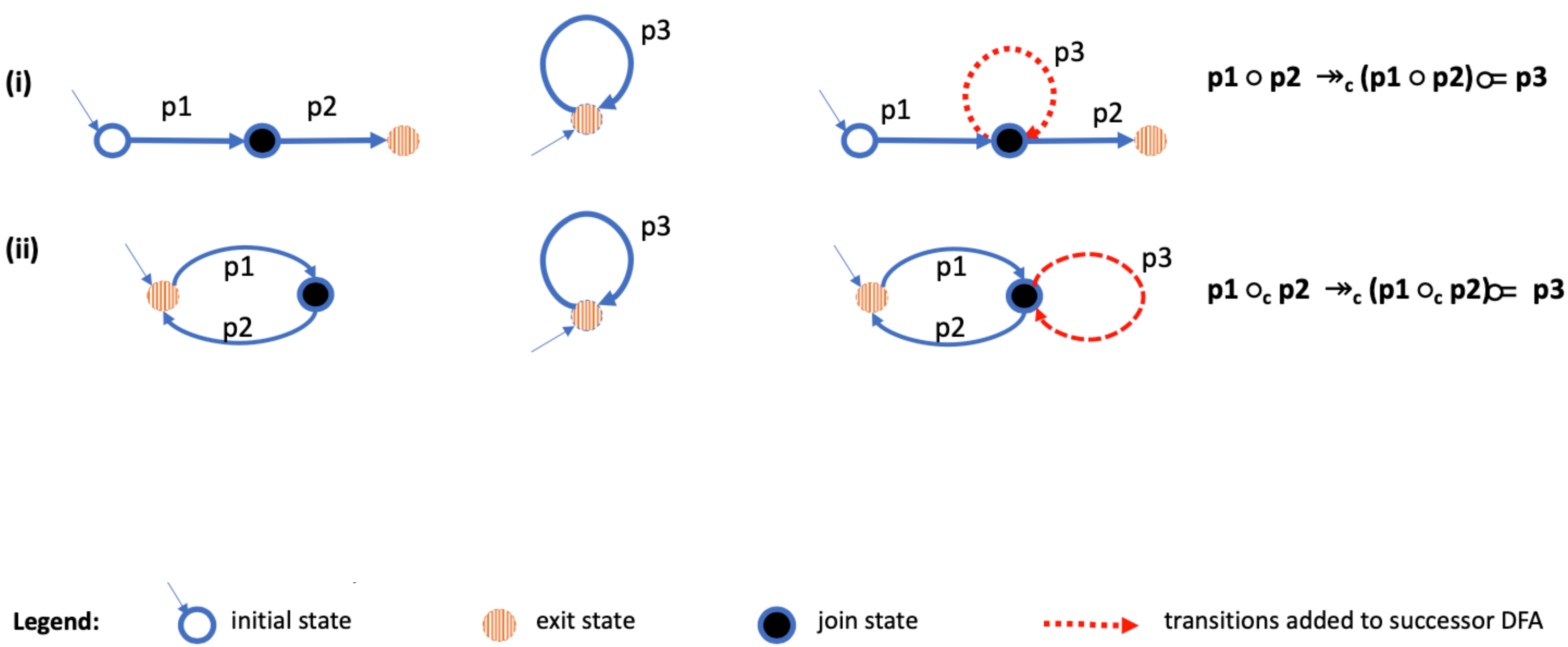

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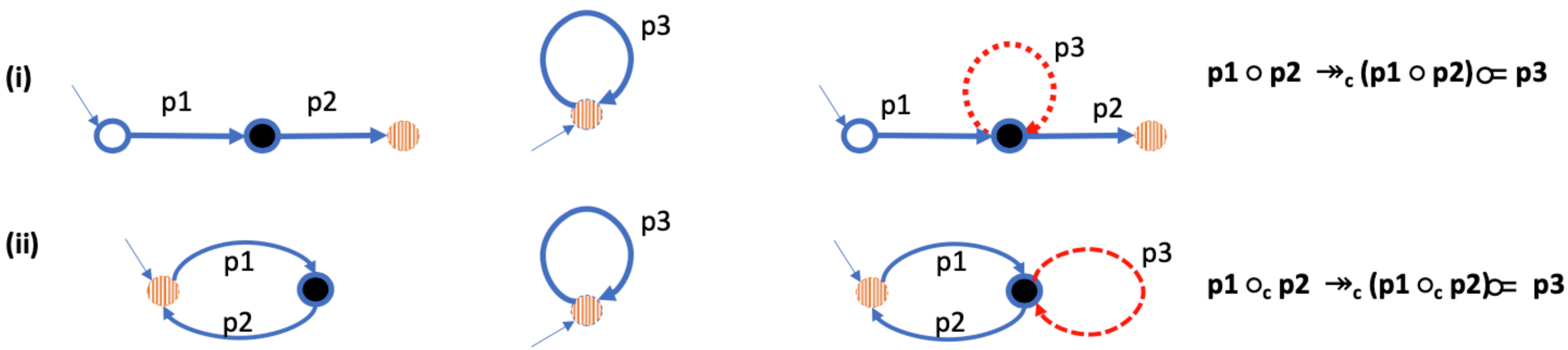

What happens when adding another (different) circular pattern to the same state?

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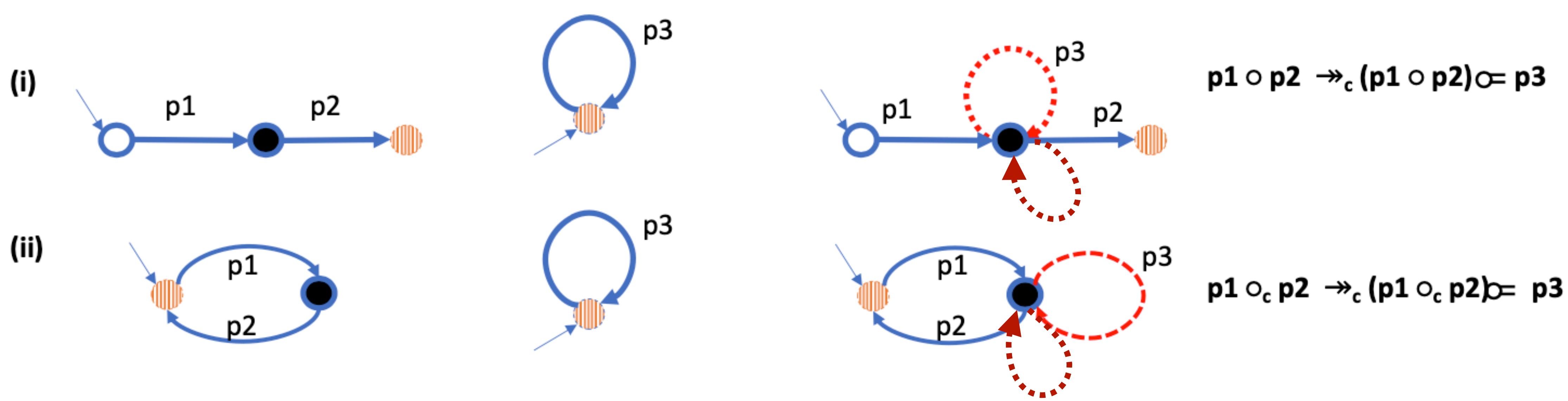

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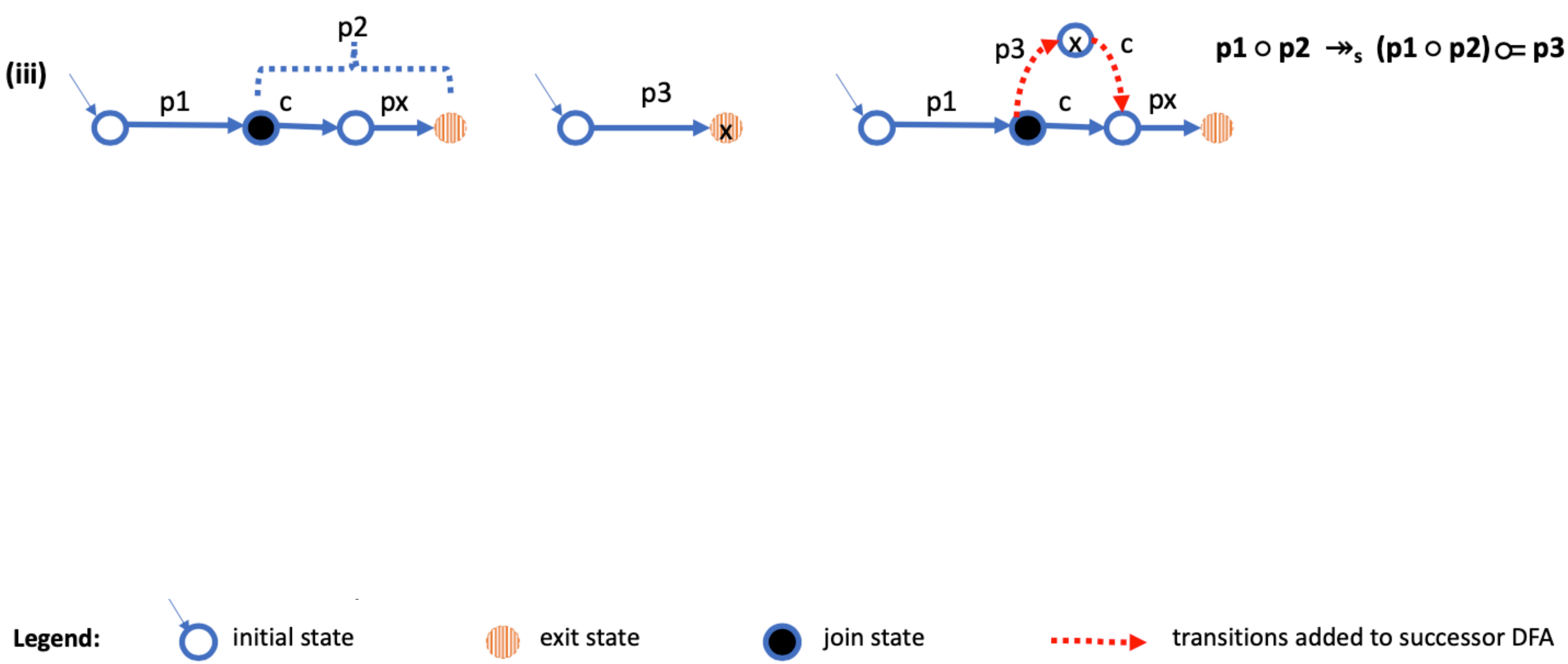

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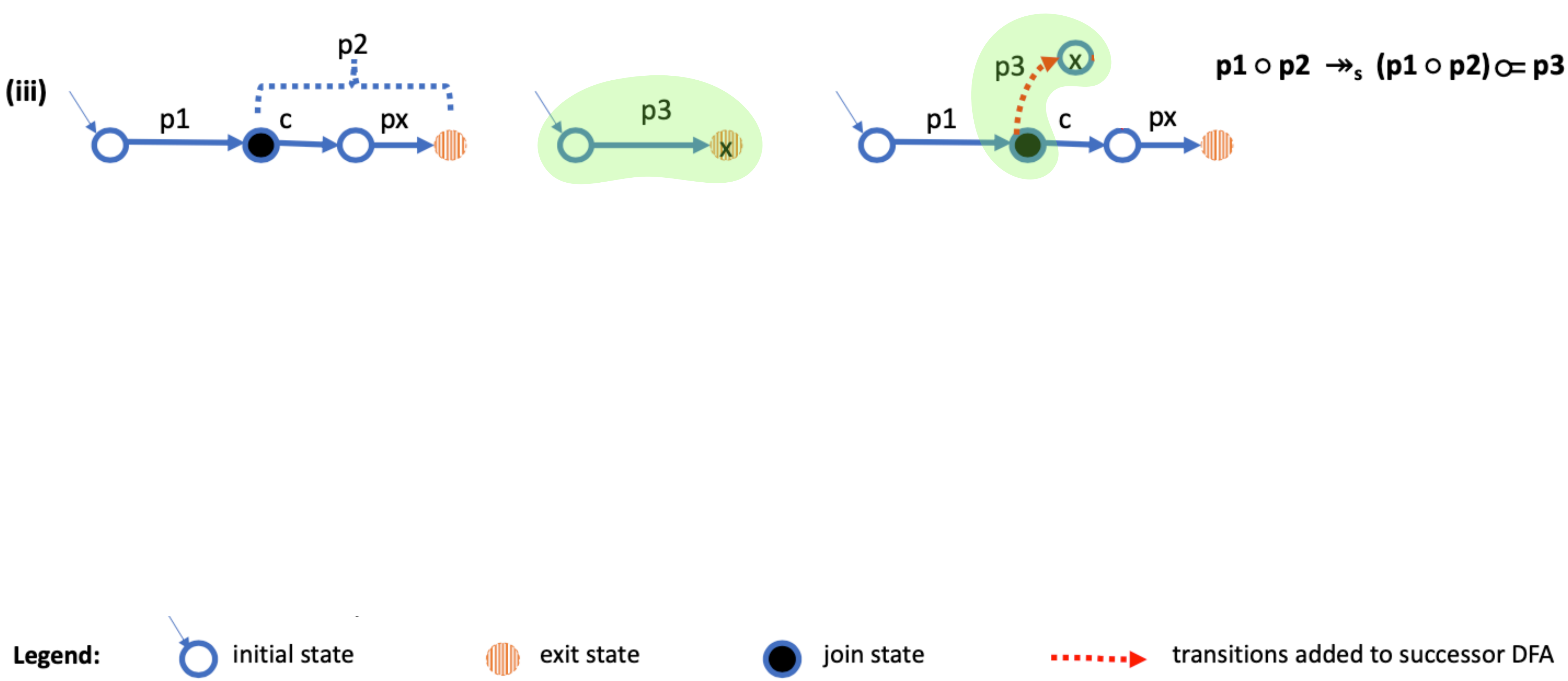

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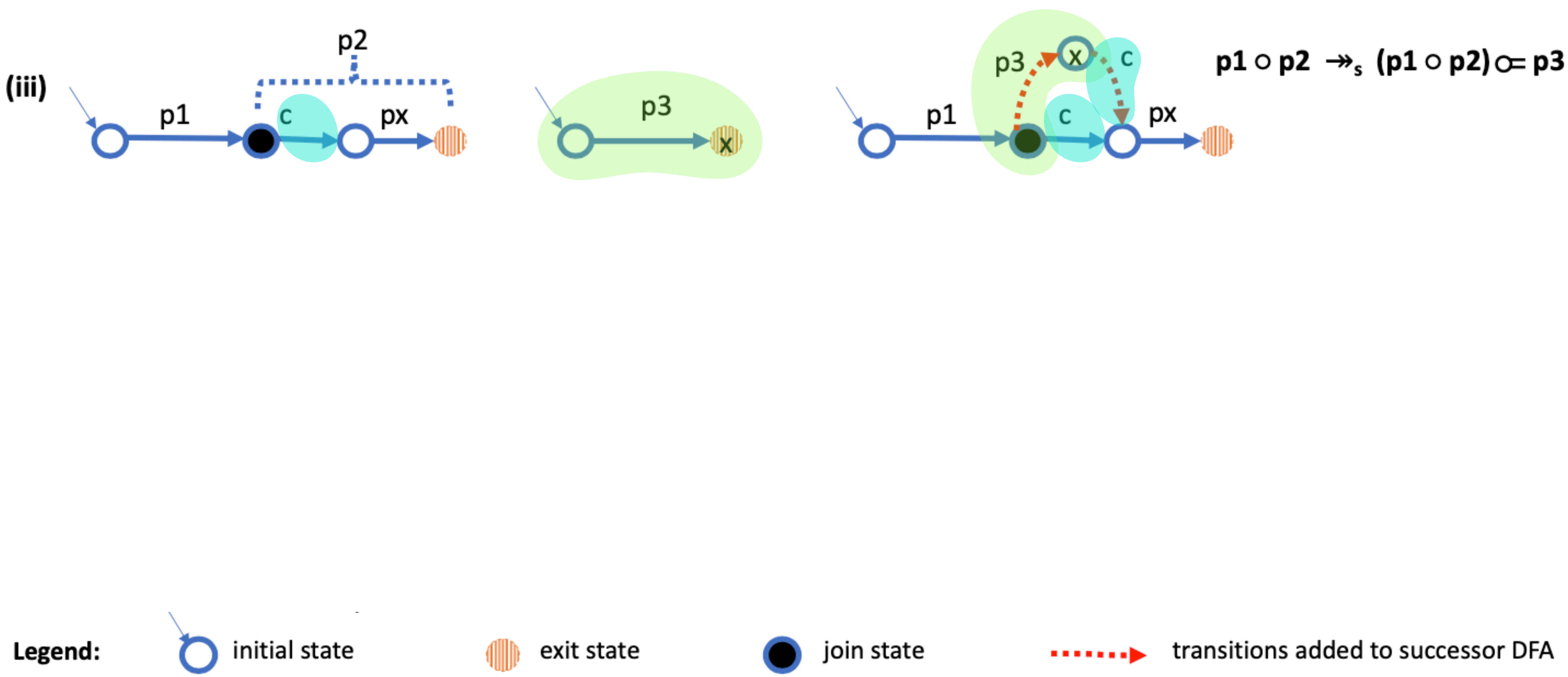

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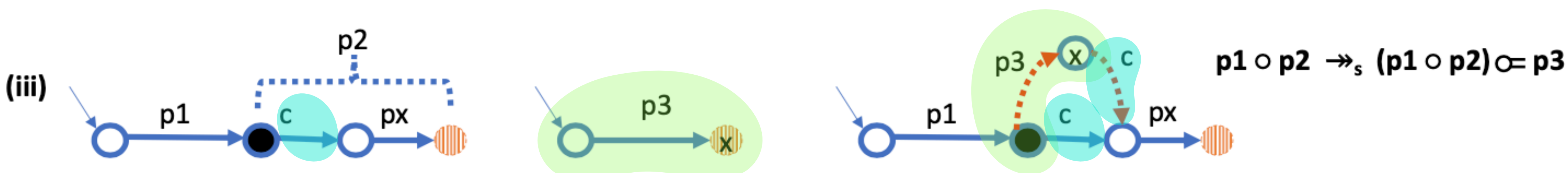

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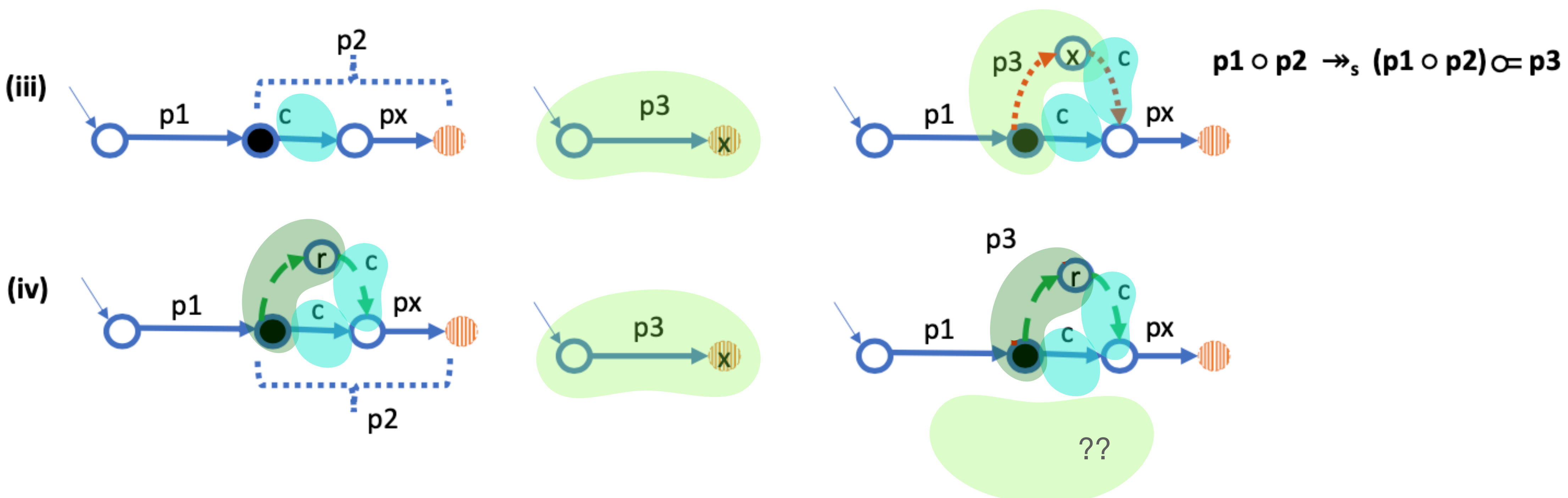

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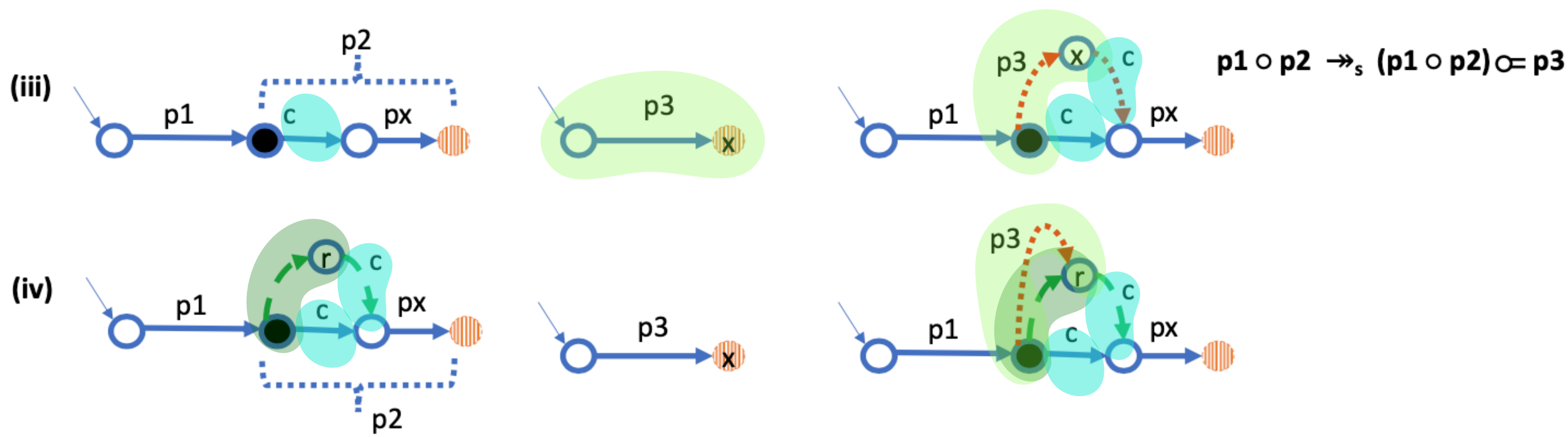

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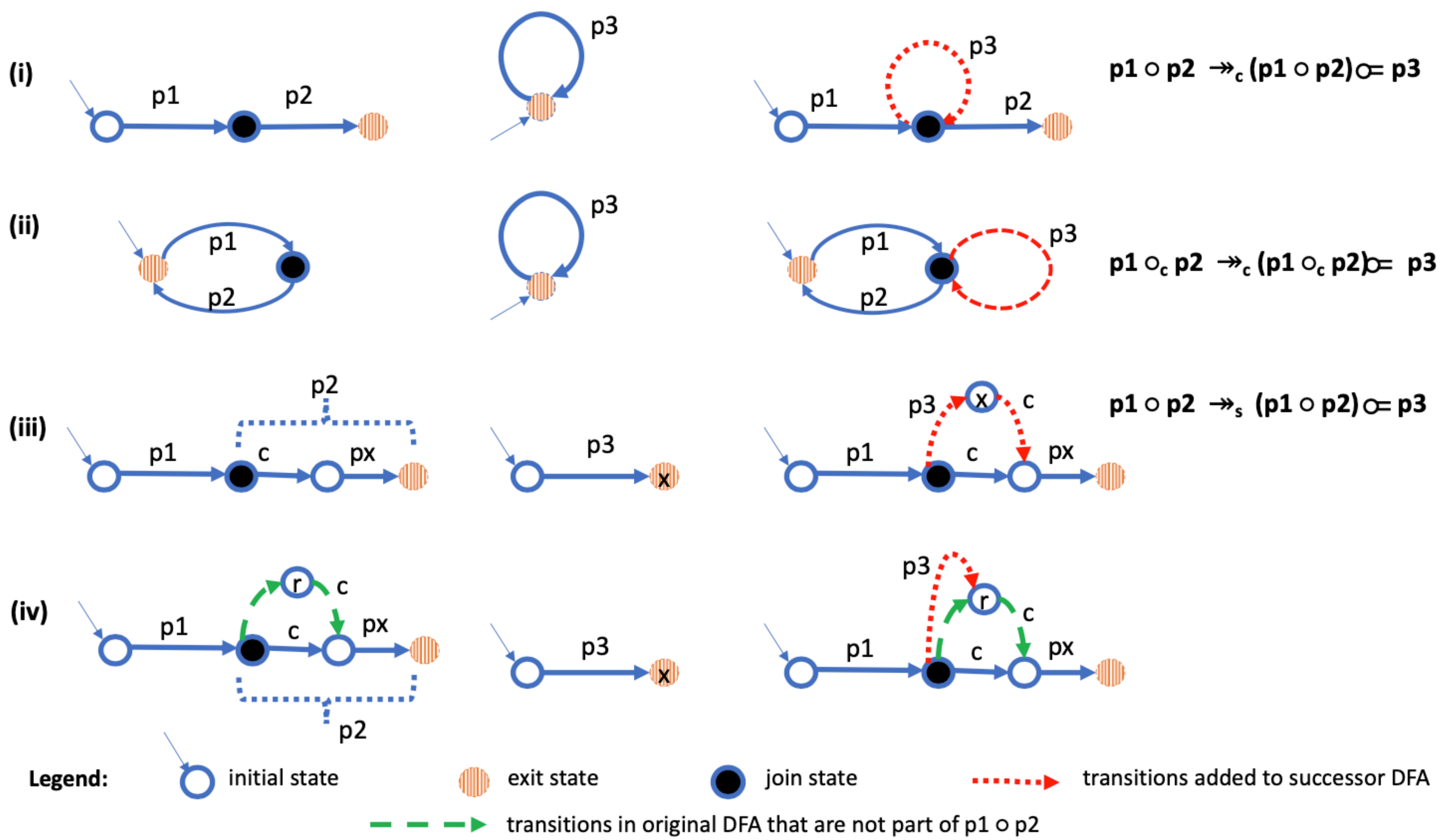
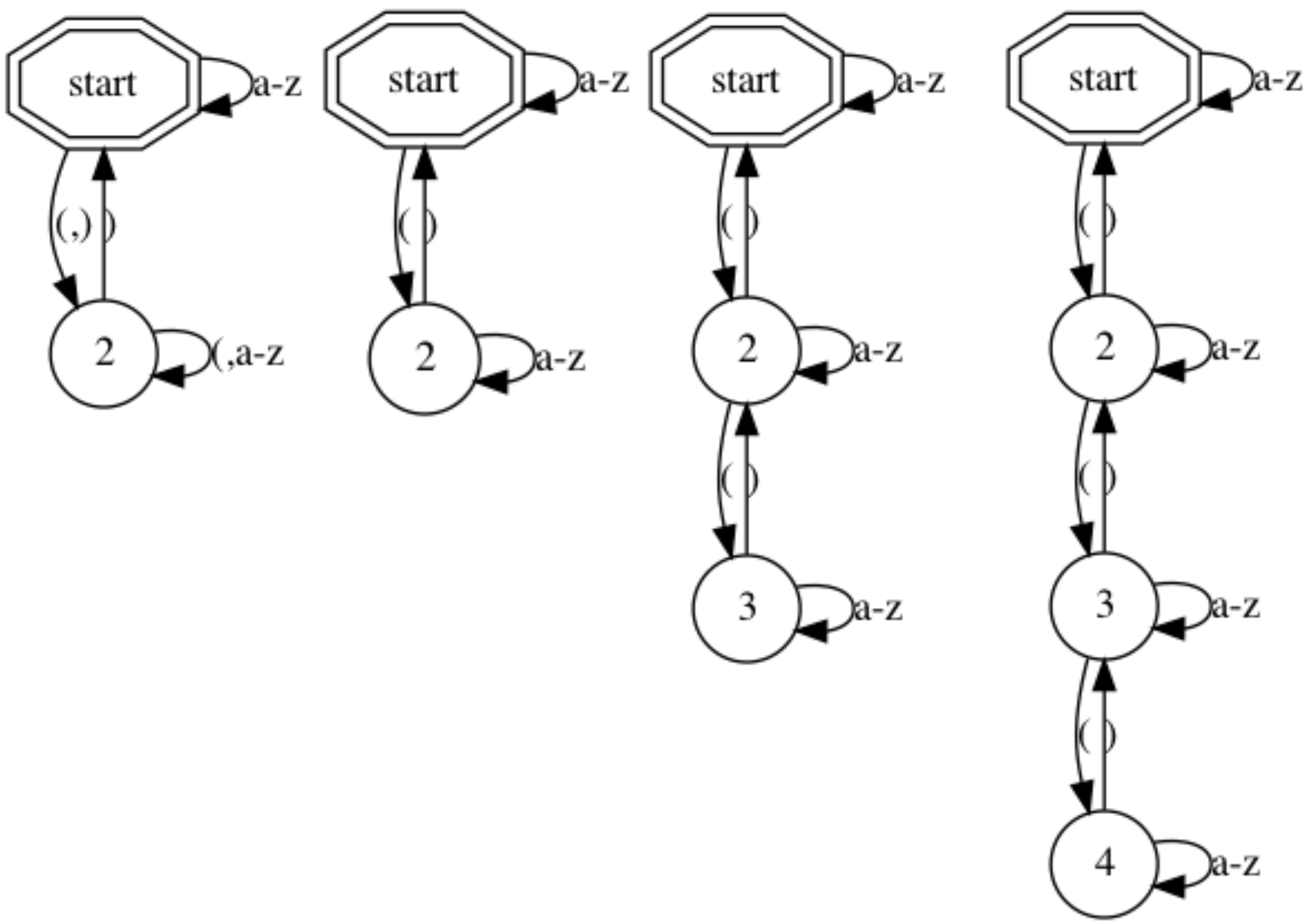


RNNs: Extraction: CFGs: **Pattern Rule Sets**

Yellin and Weiss (2021)

Recovering a Pattern Rule Set



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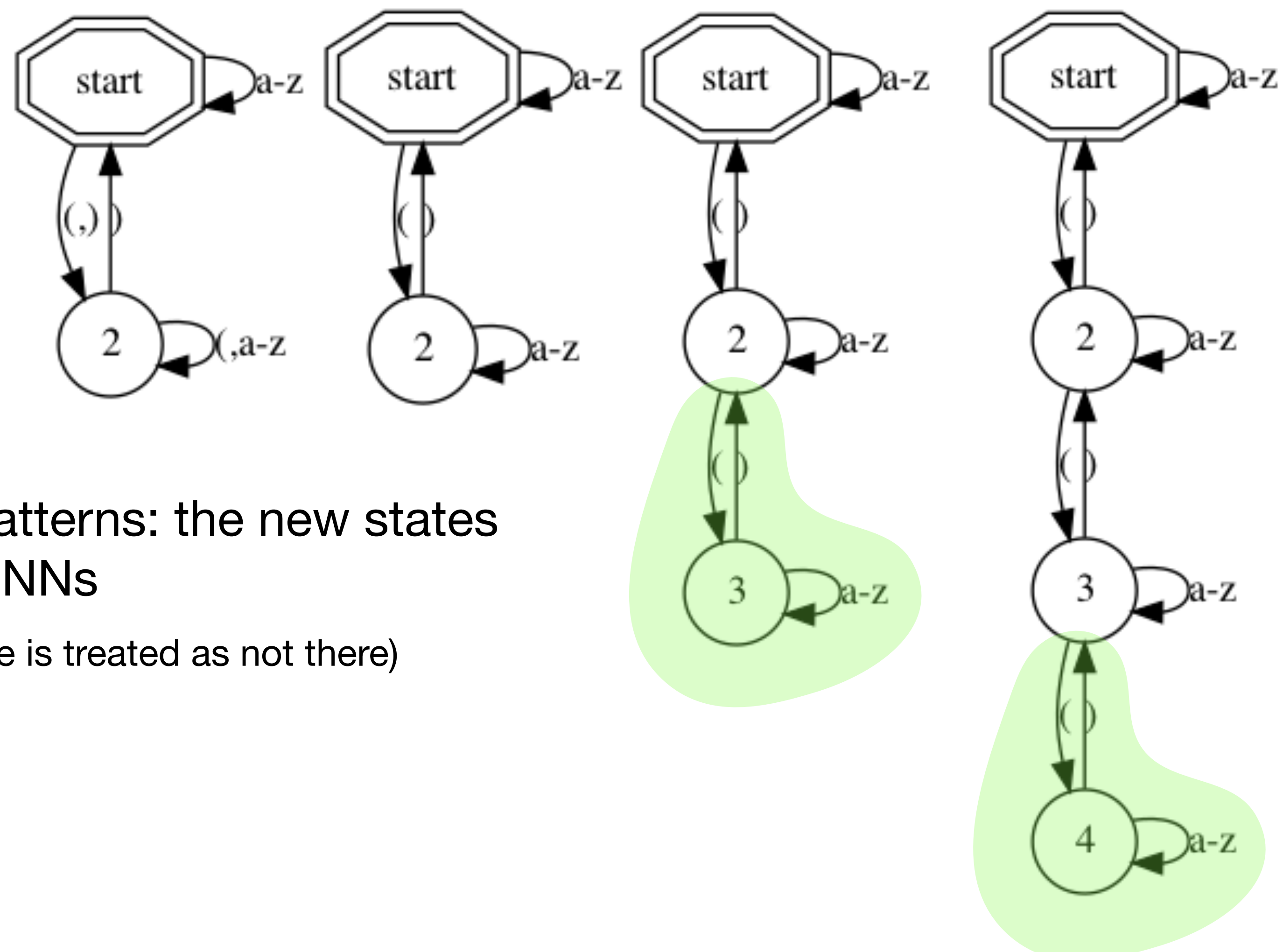

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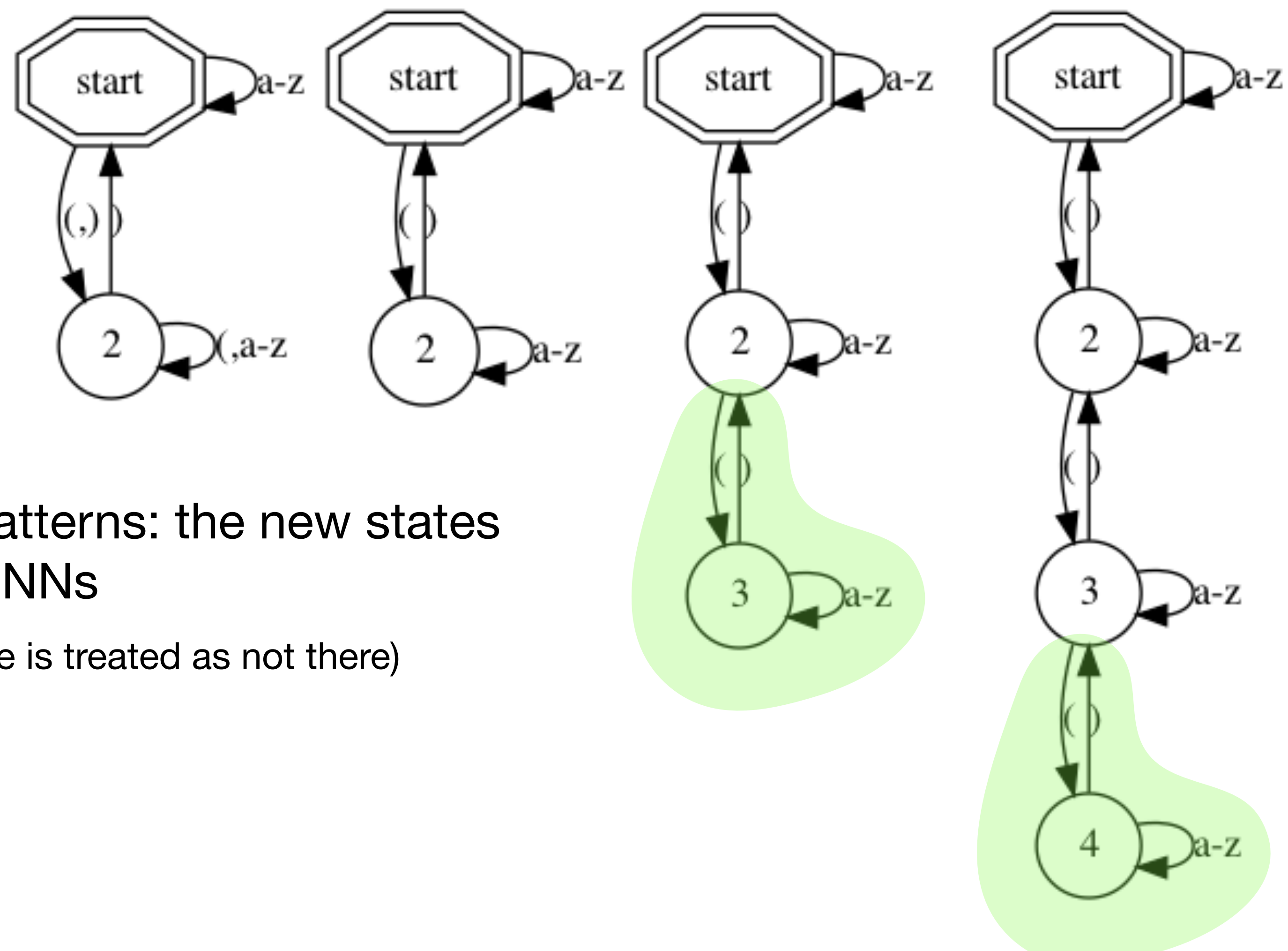

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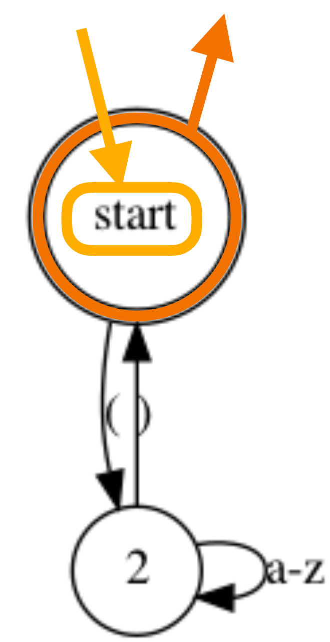
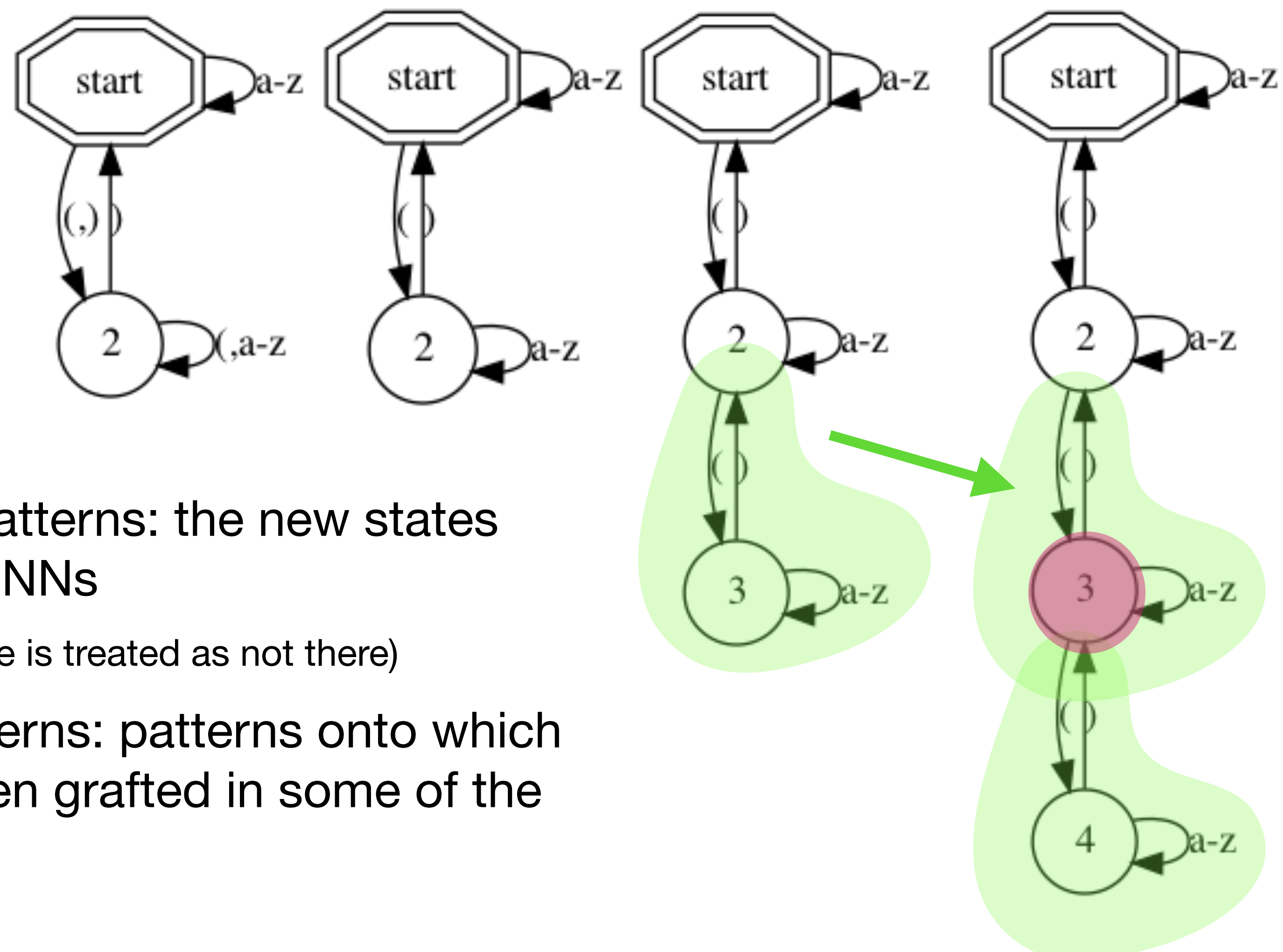


RNNs: Extraction: CFGs: **Pattern Rule Sets**

Yellin and Weiss (2021)

Recovering a Pattern Rule Set



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    1. (Note that reject state is treated as not there)
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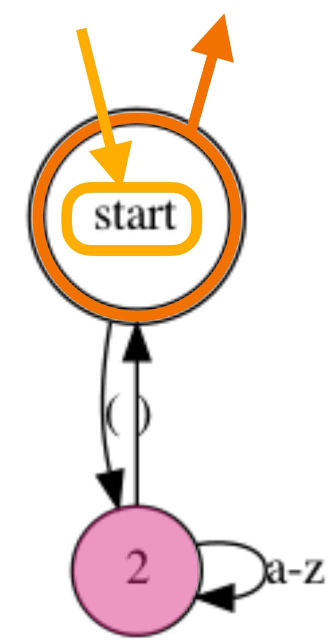

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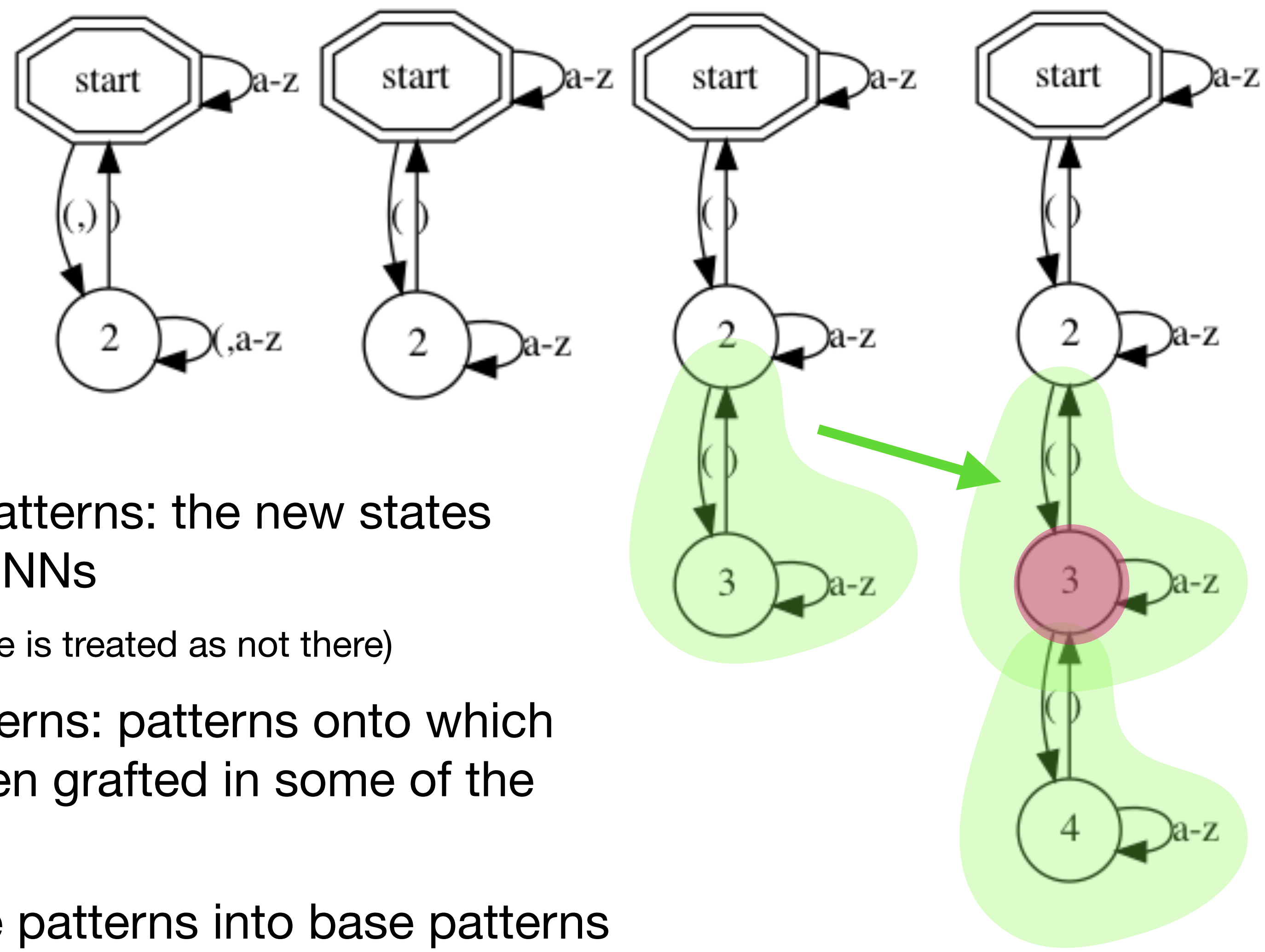

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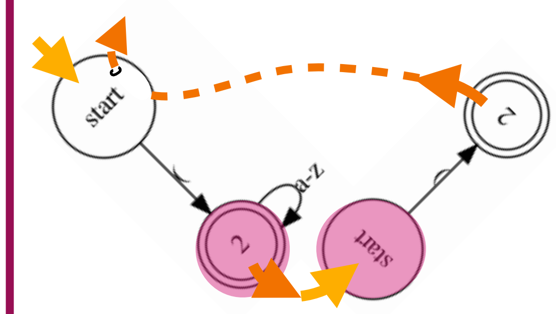

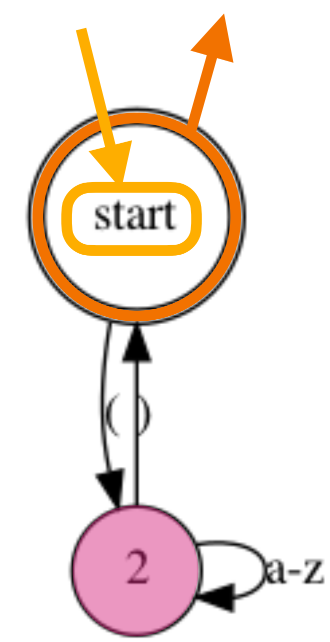

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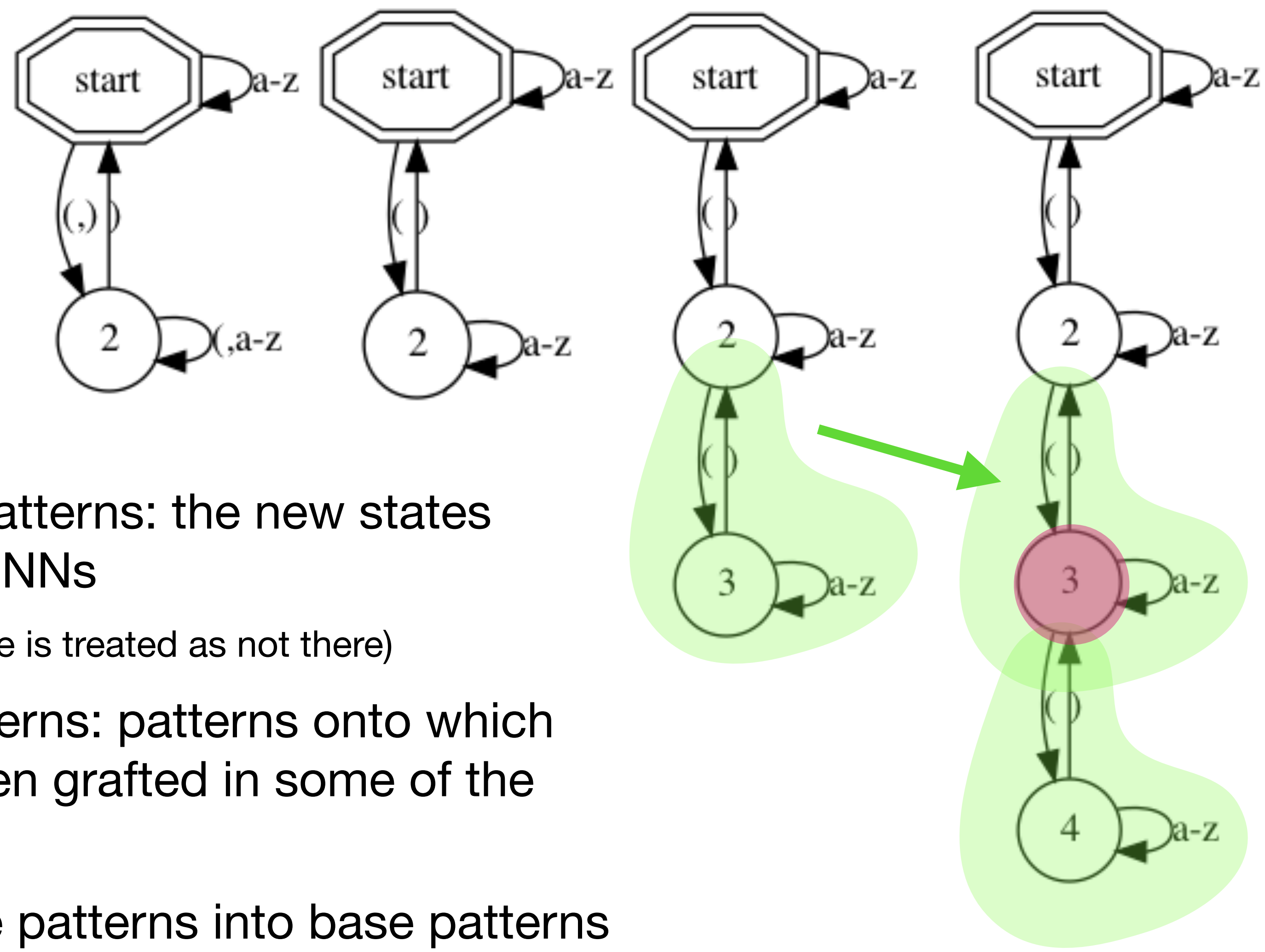

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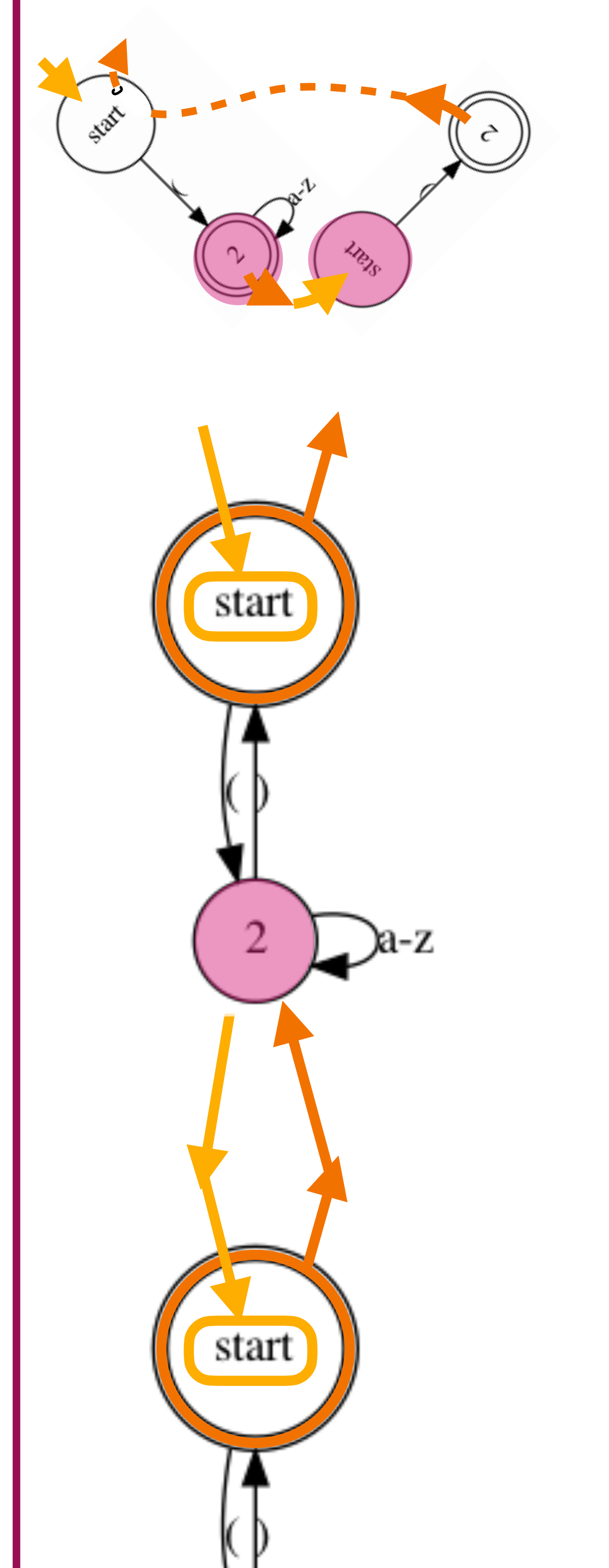

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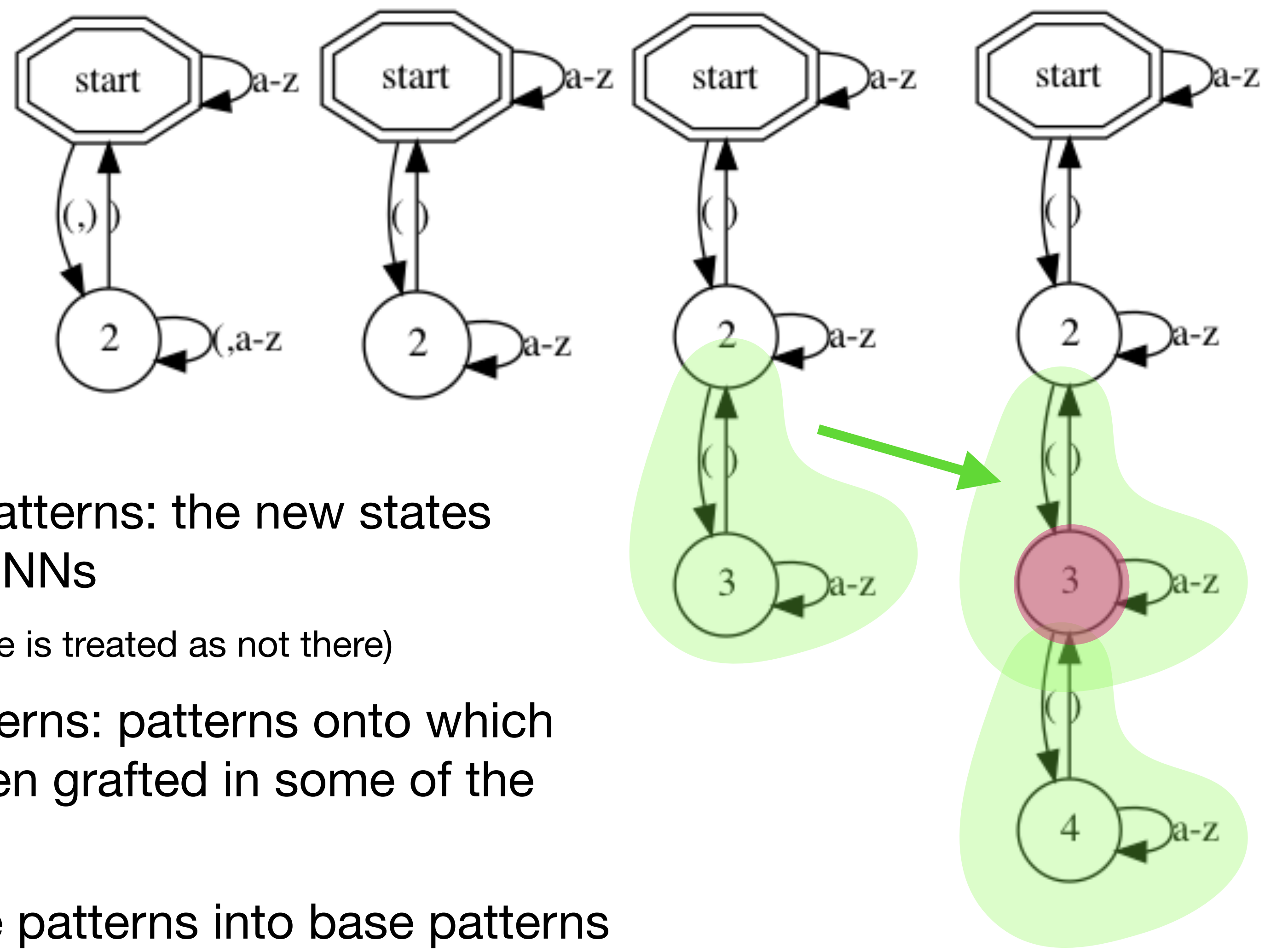

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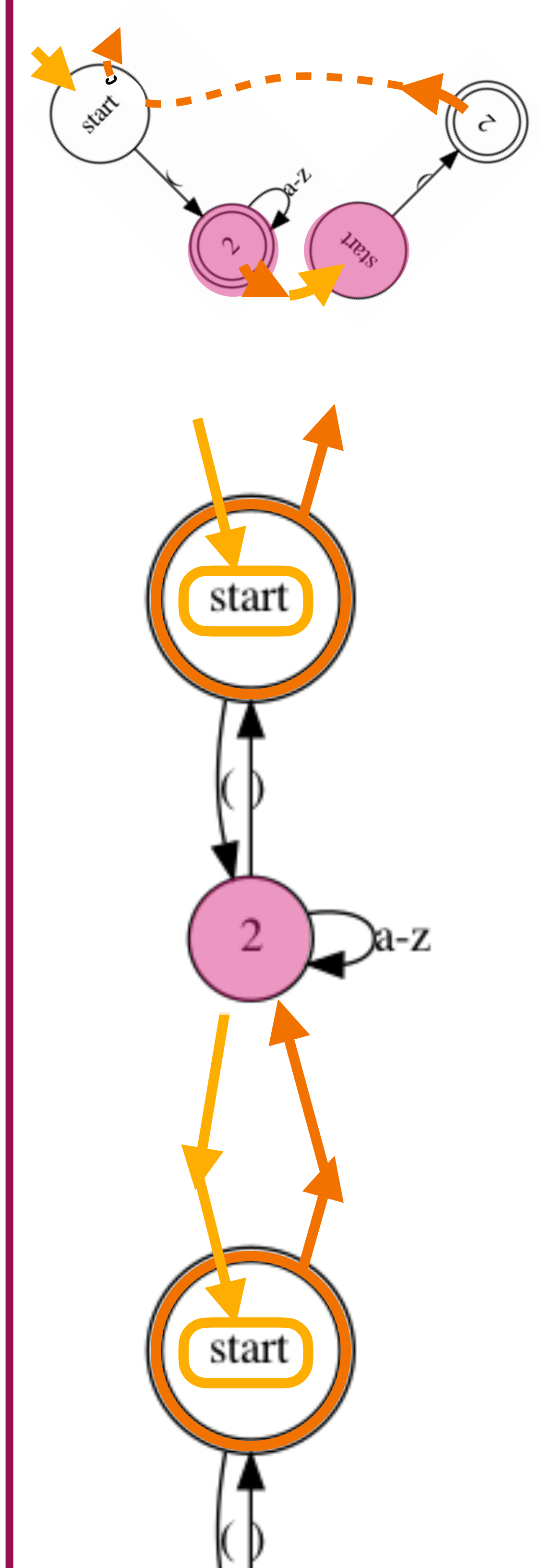
3. To handle noise: have threshold, and only keep patterns and rules that have frequency above that threshold



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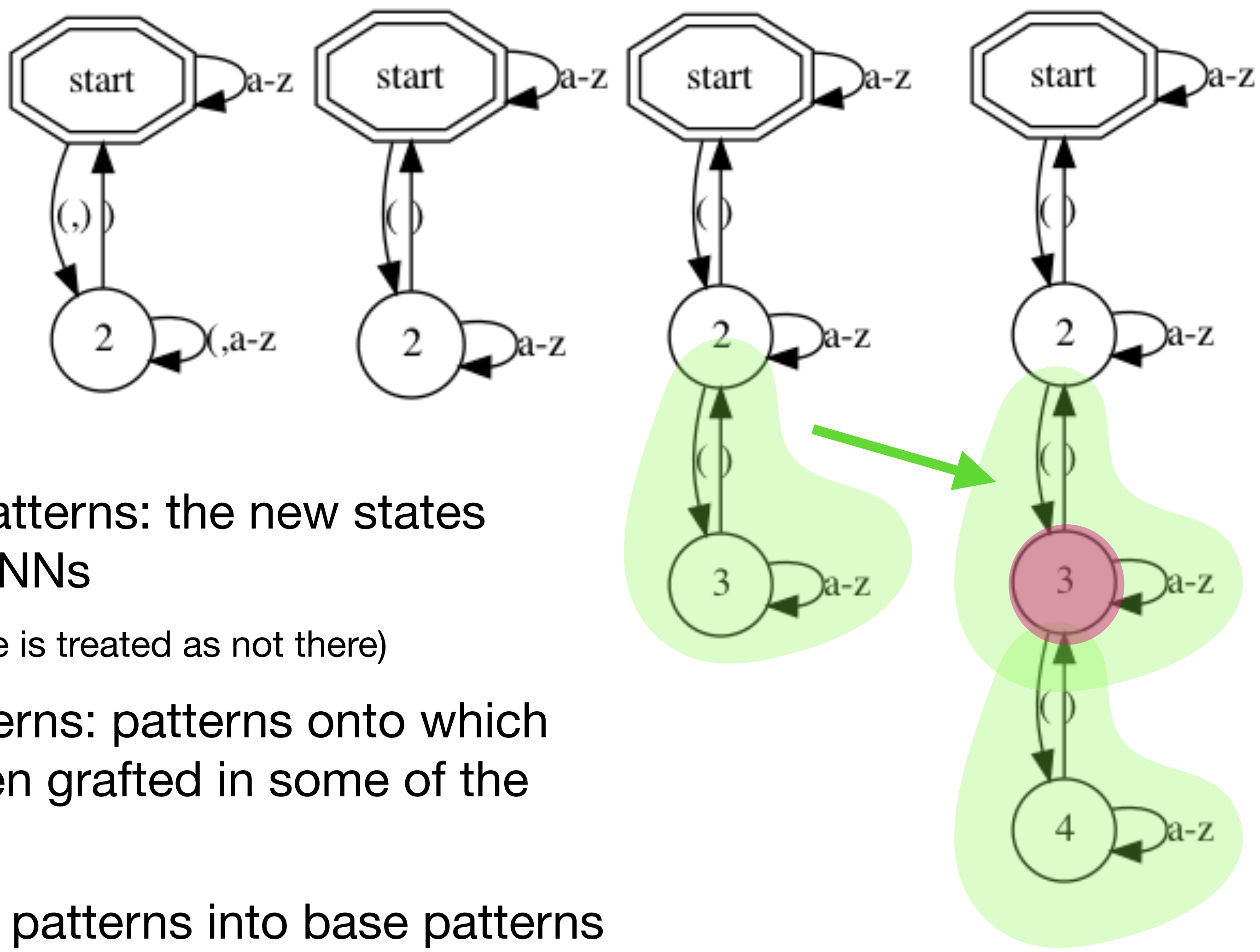

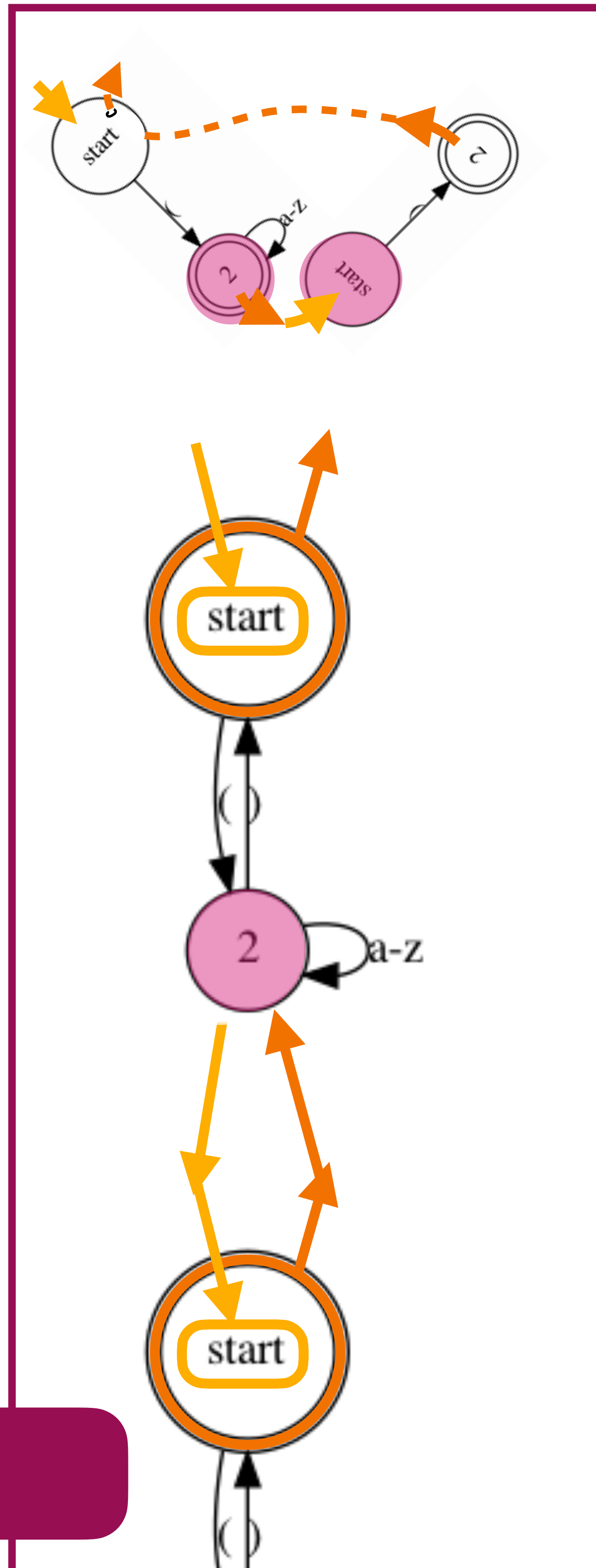

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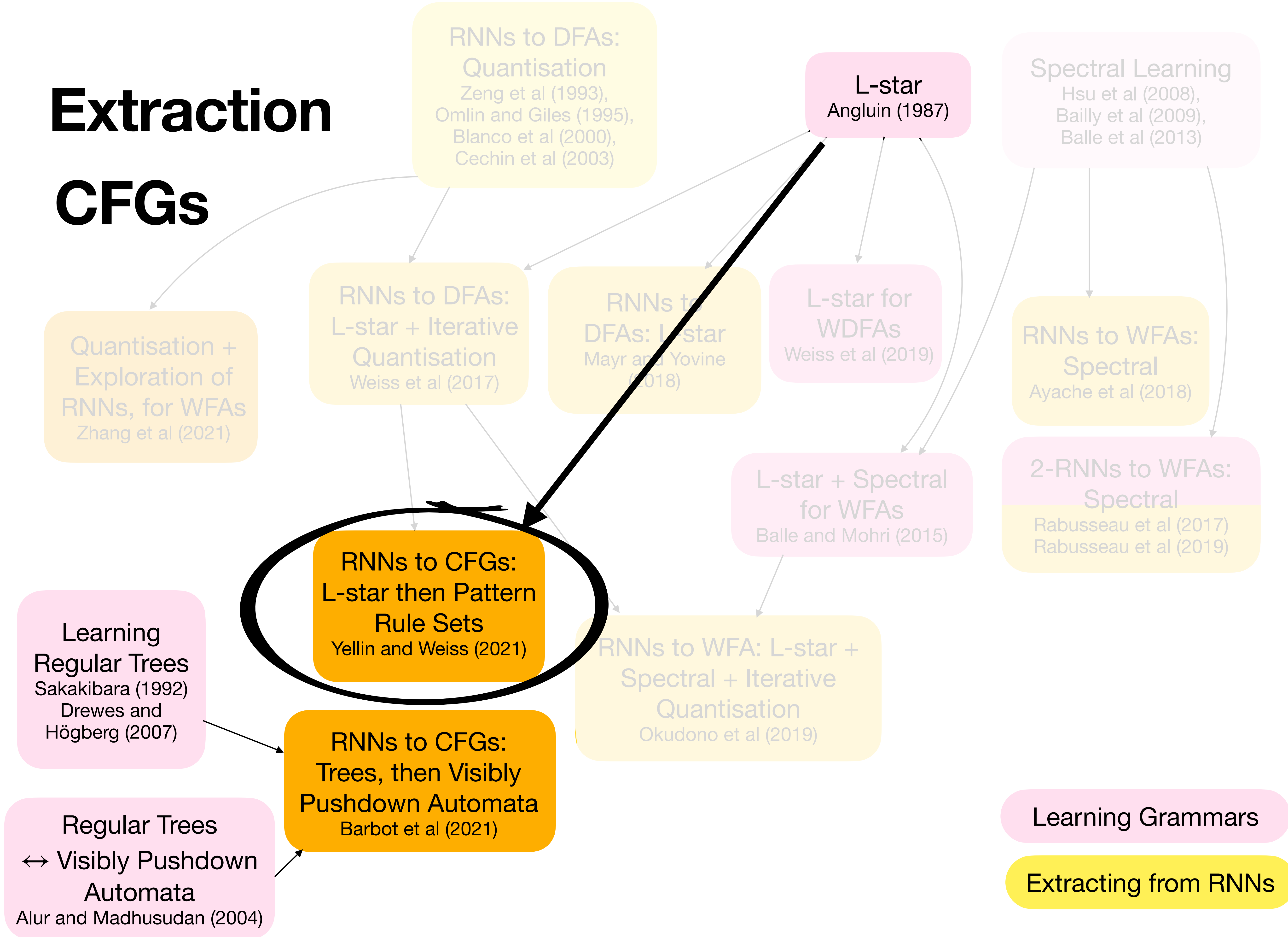
4. Convert PRS to CFG!



Extraction
CFGs
RNNs to DFAs: Quantisation
Zeng et al (1993), Omlin and Giles (1995), Blanco et al (2000), Cechin et al (2003)
L-star
Angluin (1987)
Spectral Learning
Hsu et al (2008), Bailly et al (2009), Balle et al (2013)
Quantisation + Exploration of RNNs, for WFAs
Zhang et al (2021)
RNNs to DFAs: L-star + Iterative Quantisation
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2-RNNs to WFAs: Spectral
Rabusseau et al (2017)
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RNNs to CFGs: L-star then Pattern Rule Sets
Yellin and Weiss (2021)
Learning Regular Trees
Sakakibara (1992)
Drewes and Högberg (2007)
RNNs to WFA: L-star + Spectral + Iterative Quantisation
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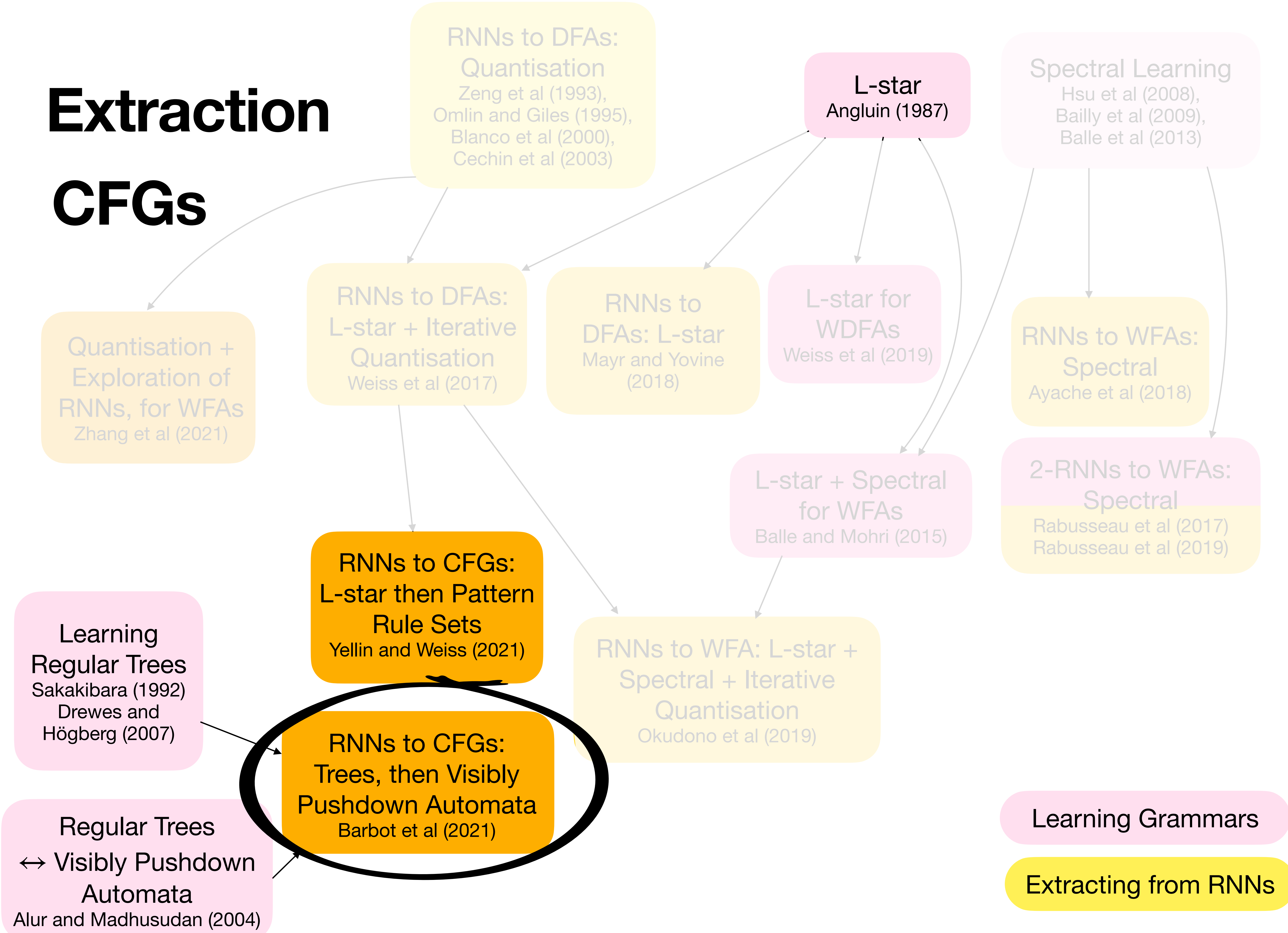
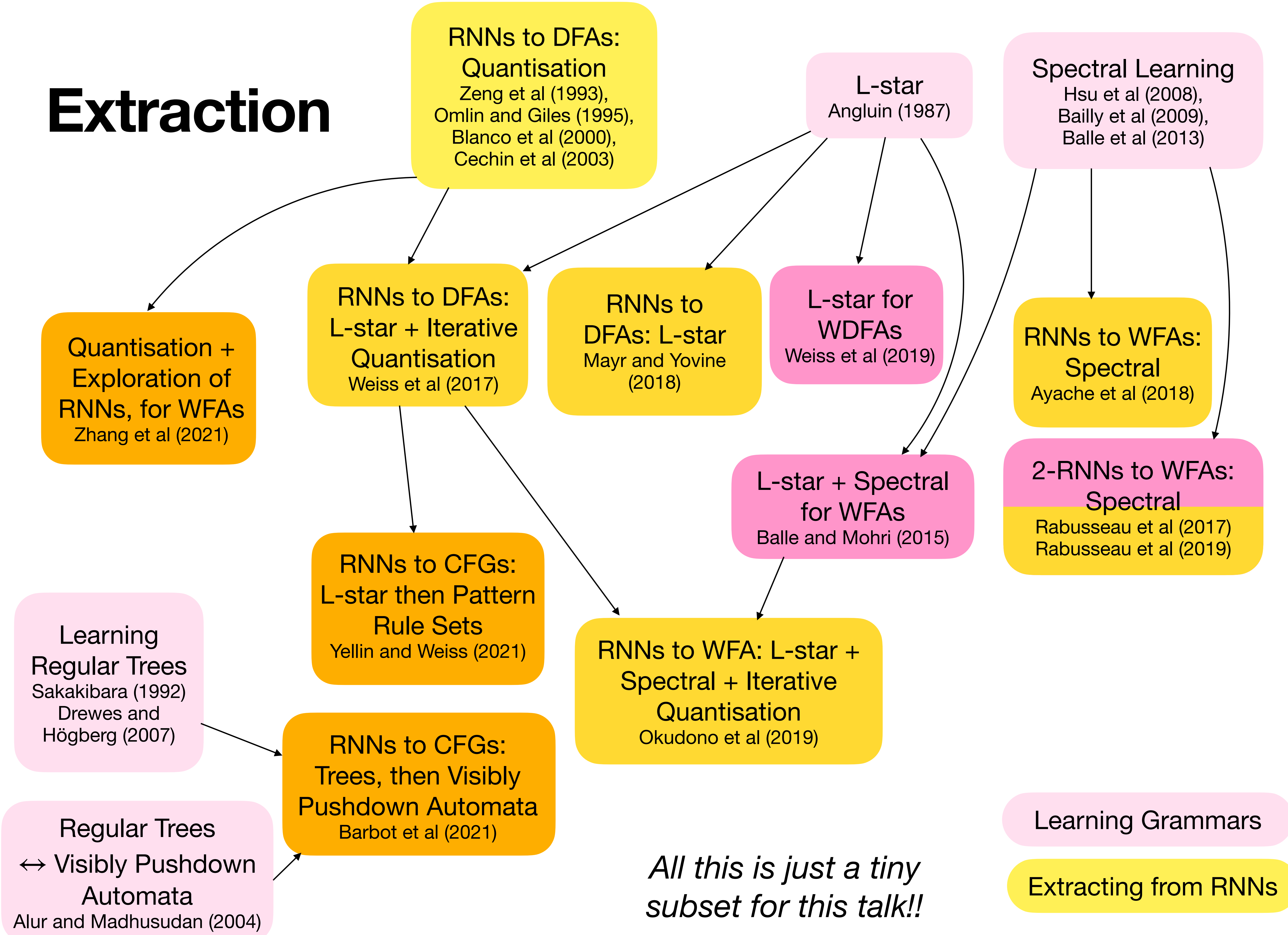
RNNs to CFGs: Trees, then Visibly Pushdown Automata
Barbot et al (2021)
Regular Trees ↔ Visibly Pushdown Automata
Alur and Madhusudan (2004)
Learning Grammars
Extracting from RNNs

Extraction

CFGs



Extraction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All this is just a tiny subset for this talk!!
Learning Grammars
Extracting from RNNs

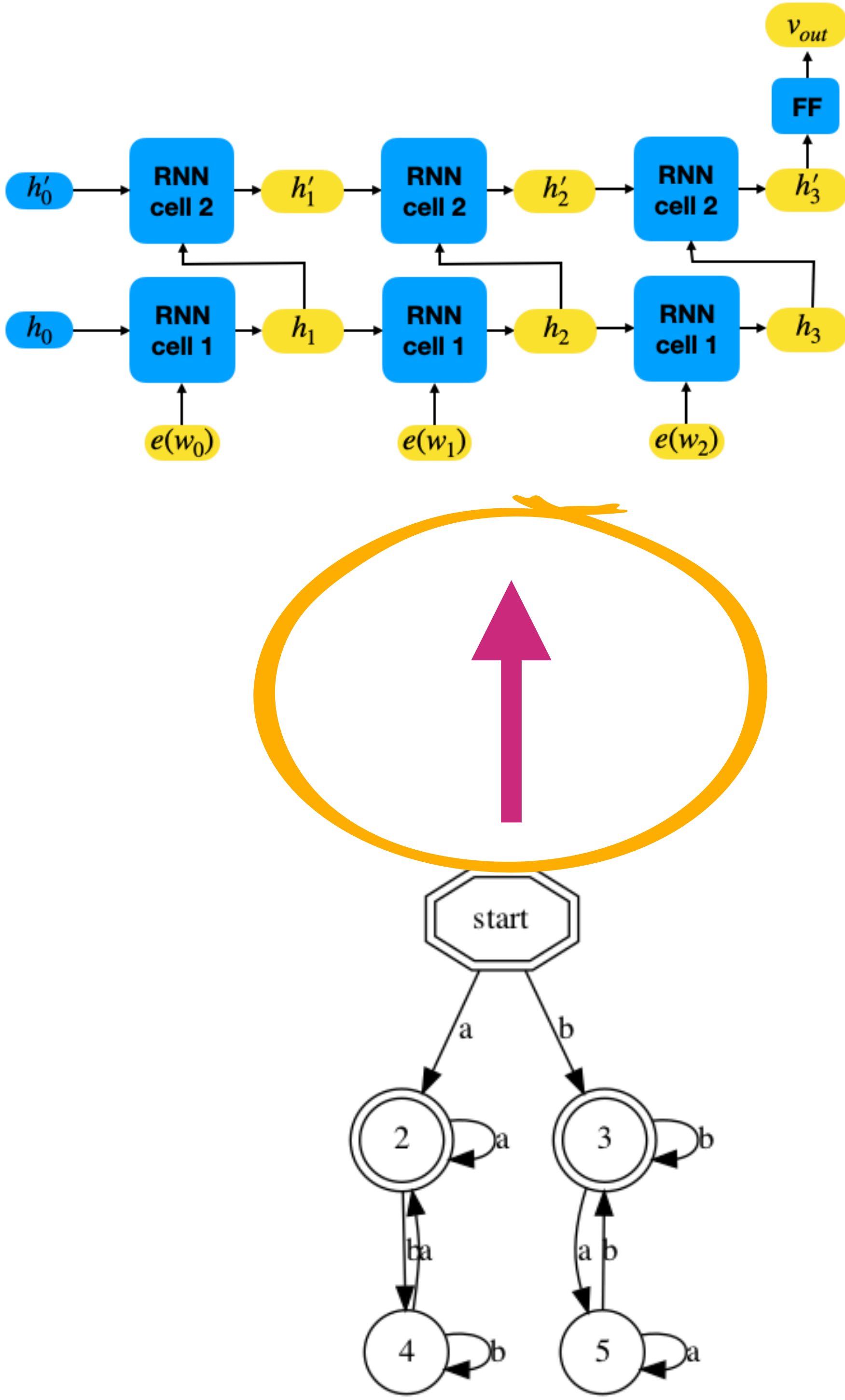
Overview

Recurrent Neural Networks (RNNs)

- Introduction
- RNN-Automata relation
- Extraction
  - DFAs
  - WFAs
  - More
- Analysis

Transformers

- Introduction
- A formal abstraction



RNNs: Expressive Power

Simple RNNs
Elman 1990 (/1988)

LSTMs
Hochreiter and Schmidhuber 1997

GRUs
Cho et al 2014, Chung et al 2014

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RNNs are like DFAs
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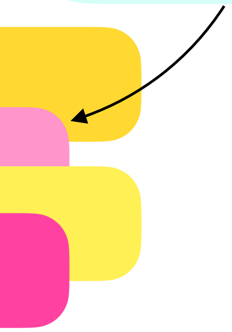

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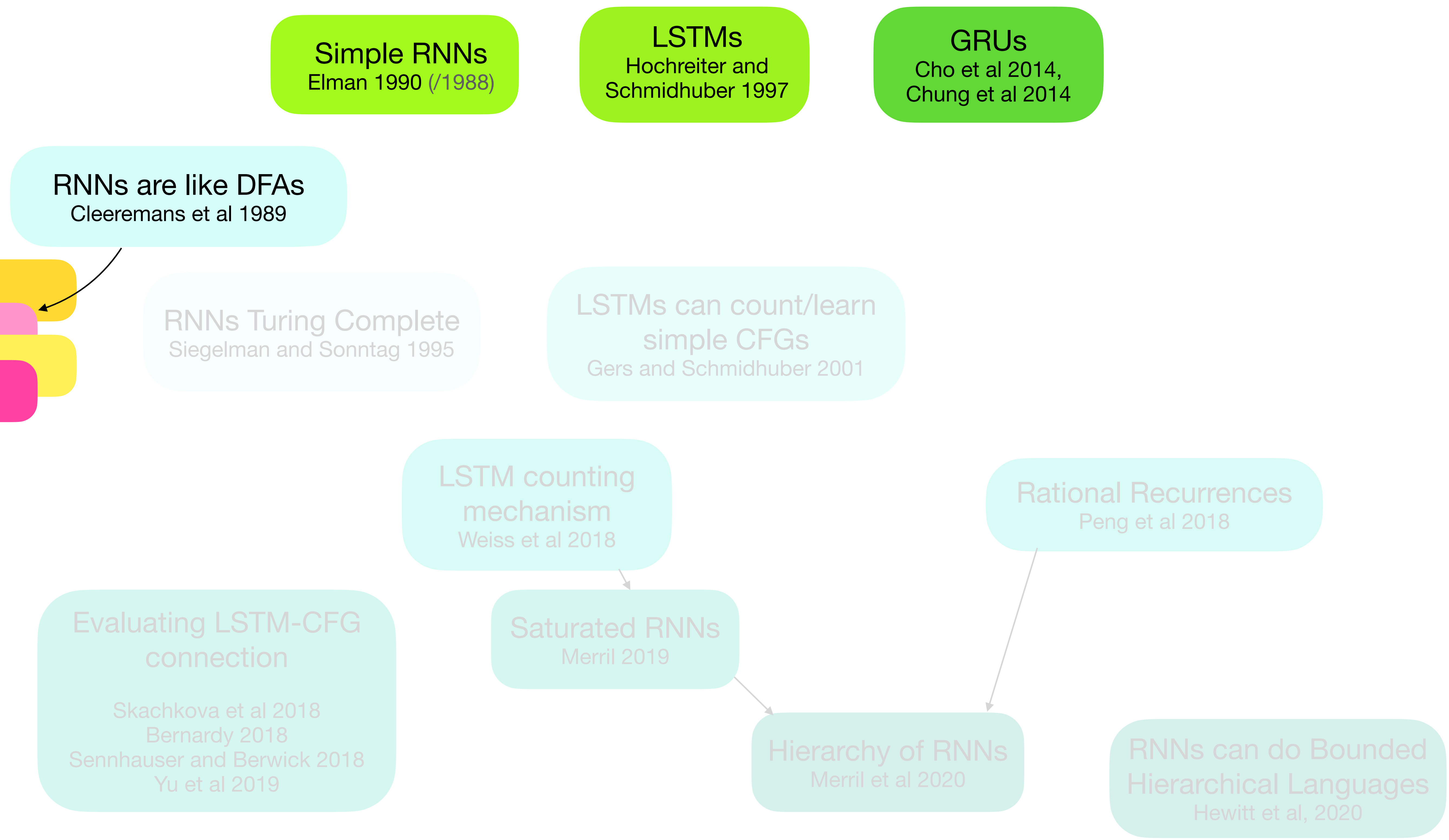

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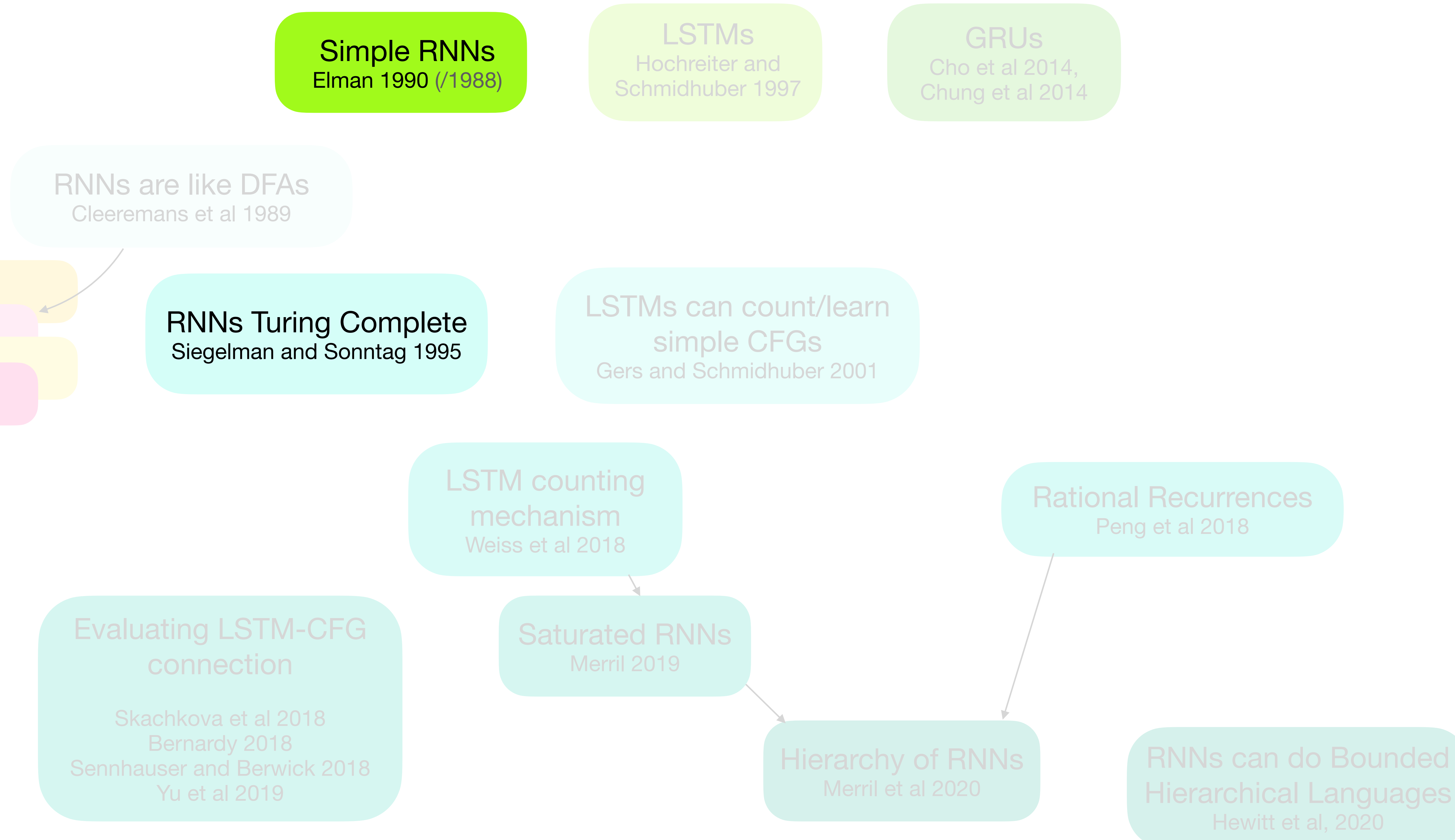


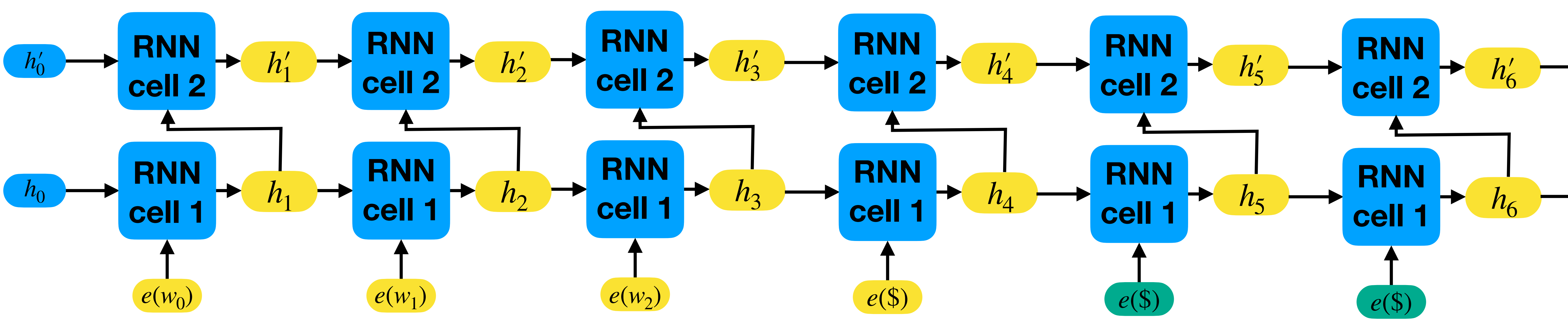
RNNs: Expressive Power: Theory

RNNs are Turing Complete:

Given infinite precision, RNNs can emulate pushing and popping to/from stacks in their hidden state. Thus, given also infinite time, they can simulate any Turing Machine

On the computational power of Neural Nets

Siegelmann and Sonntag (1995)



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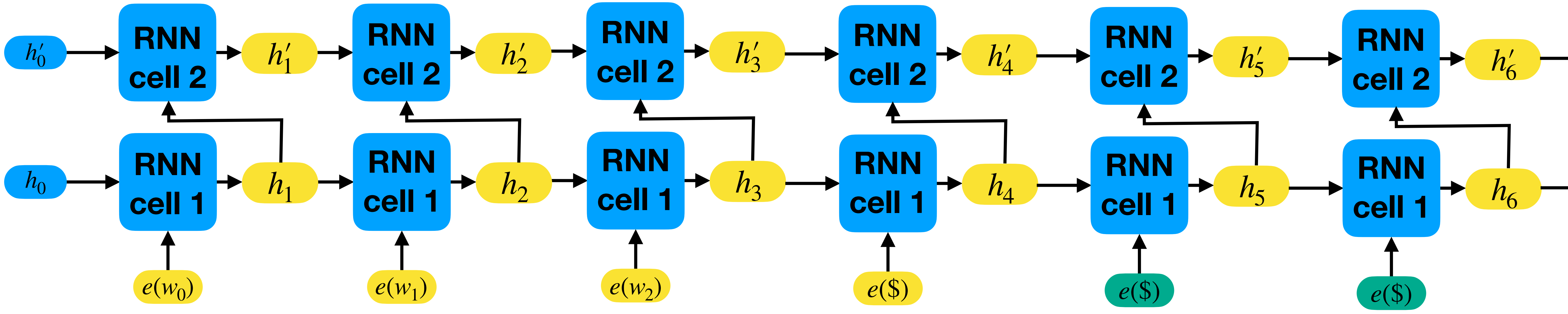

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LSTM counting mechanism
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Rational Recurrences
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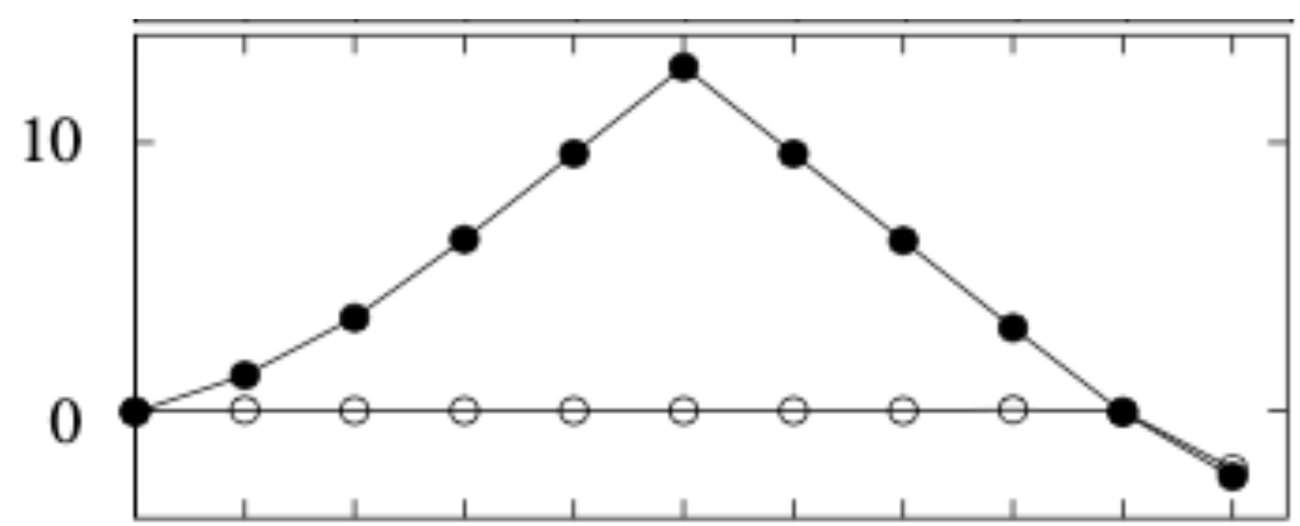
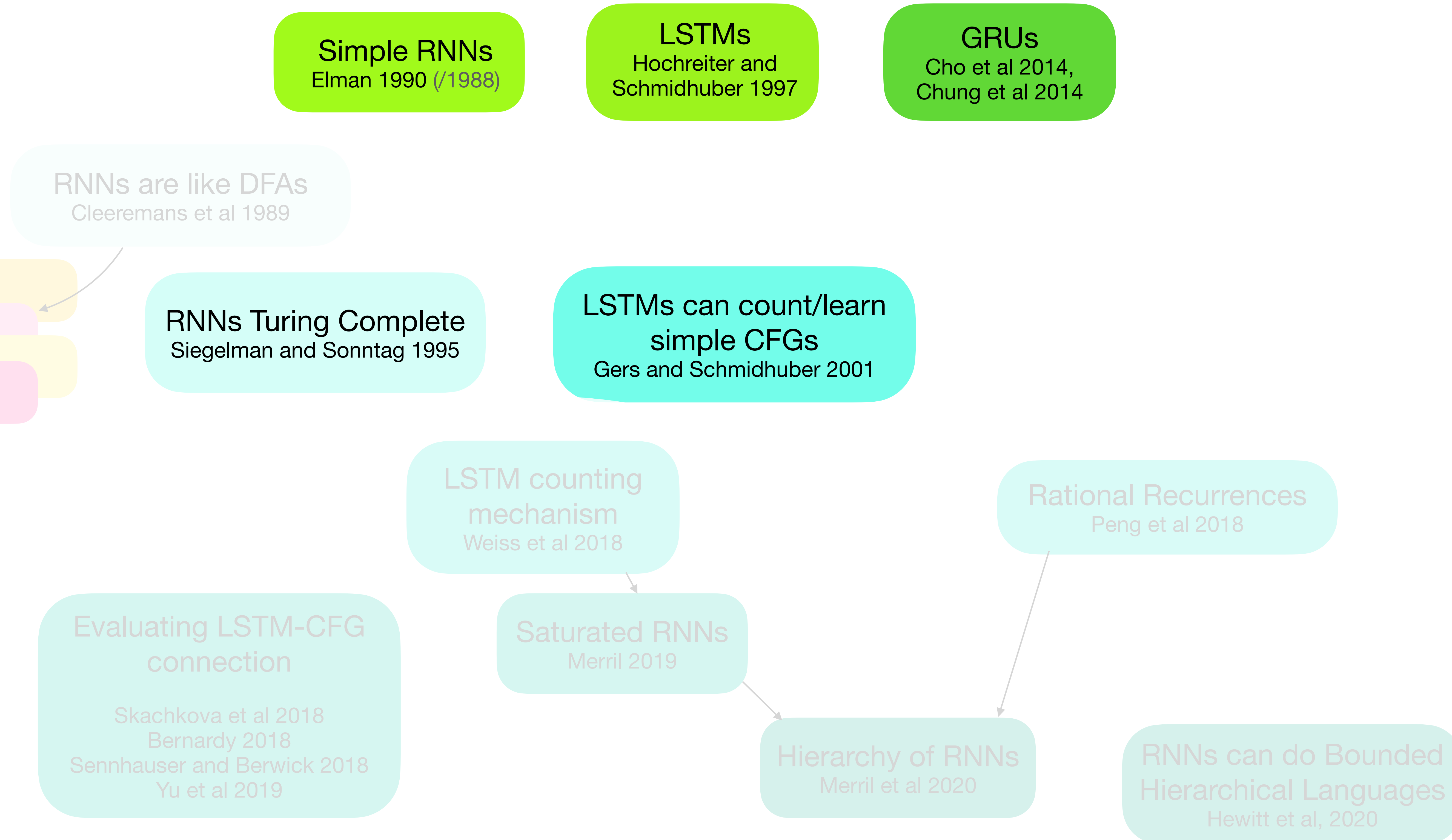
RNNs: Expressive Power: Practice

LSTMs can count



LSTM recurrent networks learn simple context-free and context-sensitive languages
Gers and Schmidhuber, 2001

RNNs: Expressive Power



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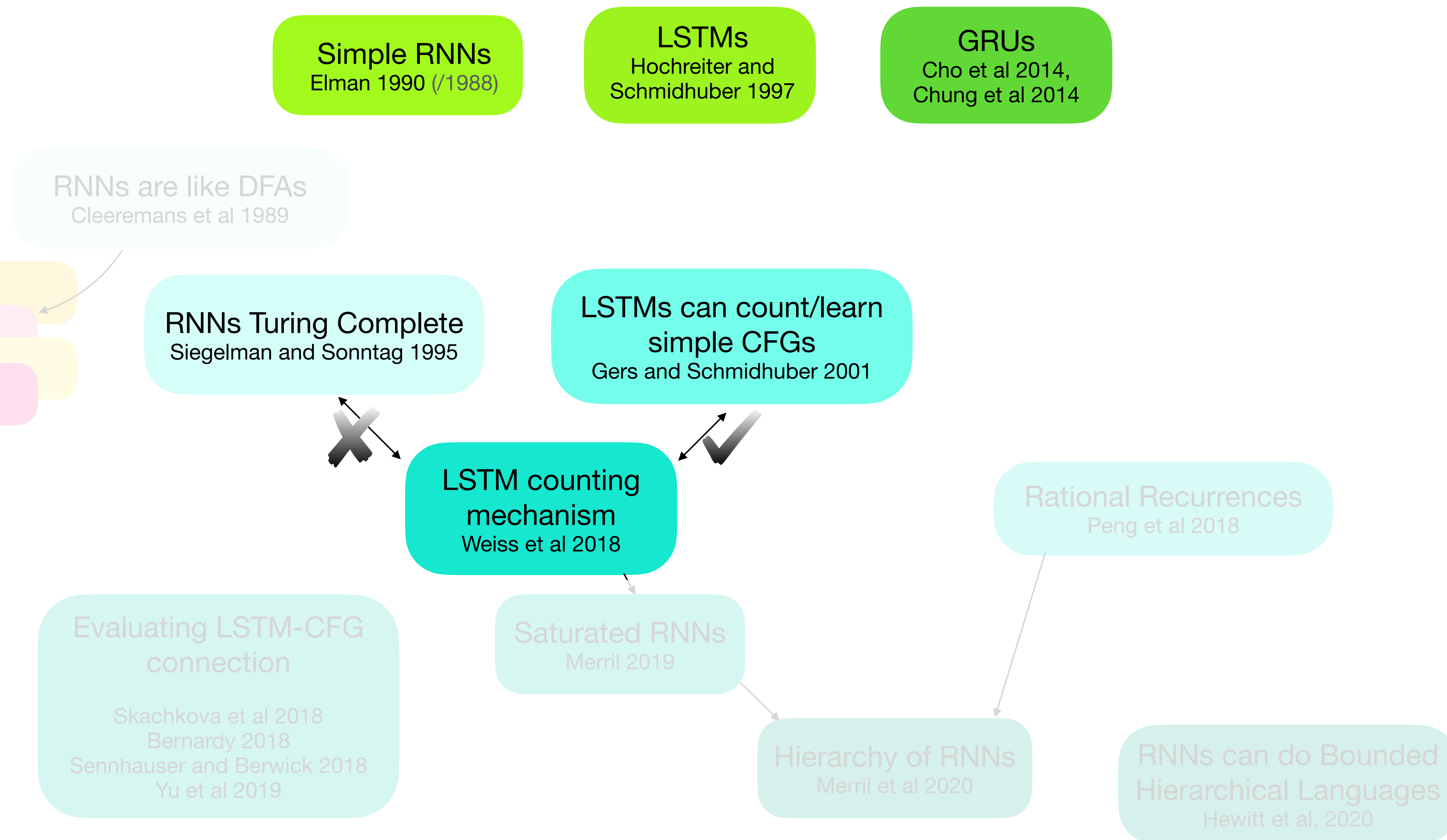
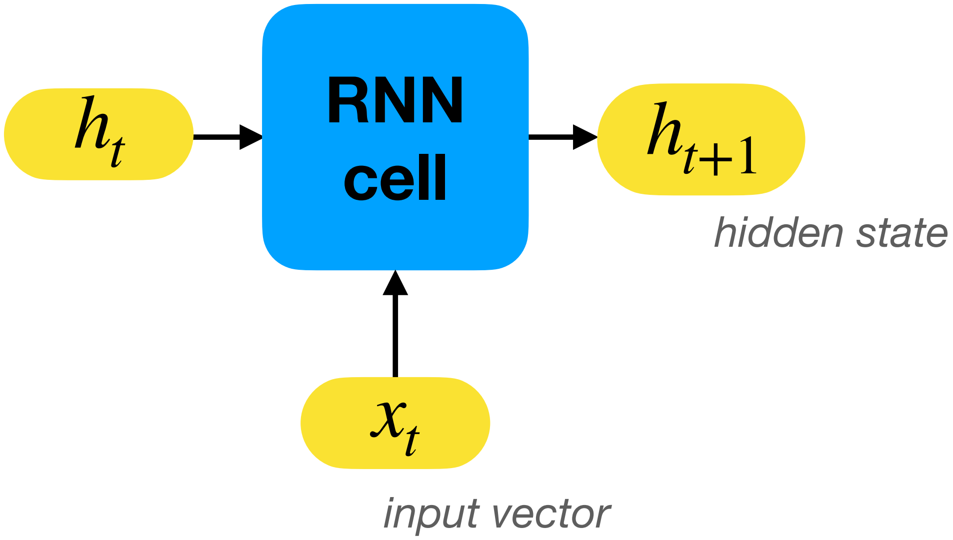


LSTMs: Counting Mechanism

Simple RNN $h_{t+1} = \tanh(W^h h_t + W^x x_t + b)$ Elman (1990)



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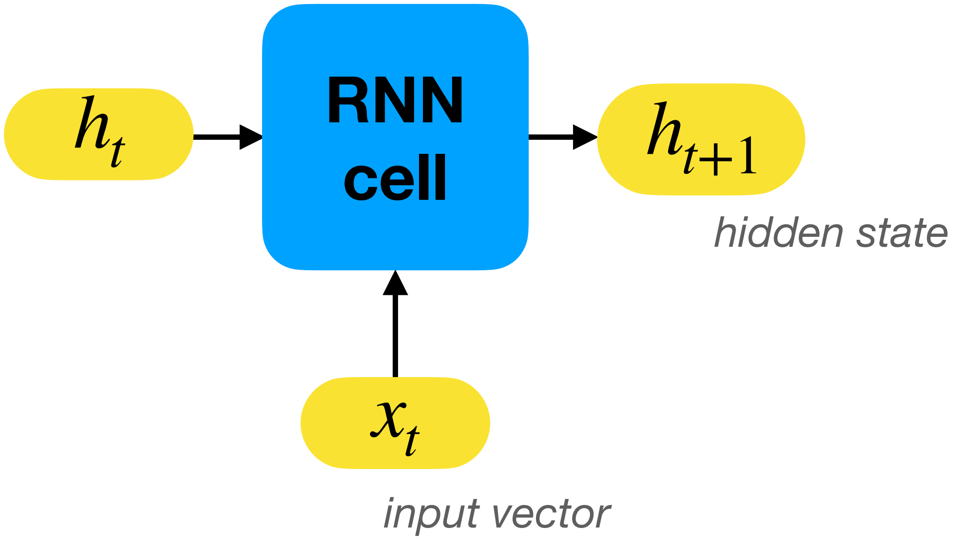

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GRU

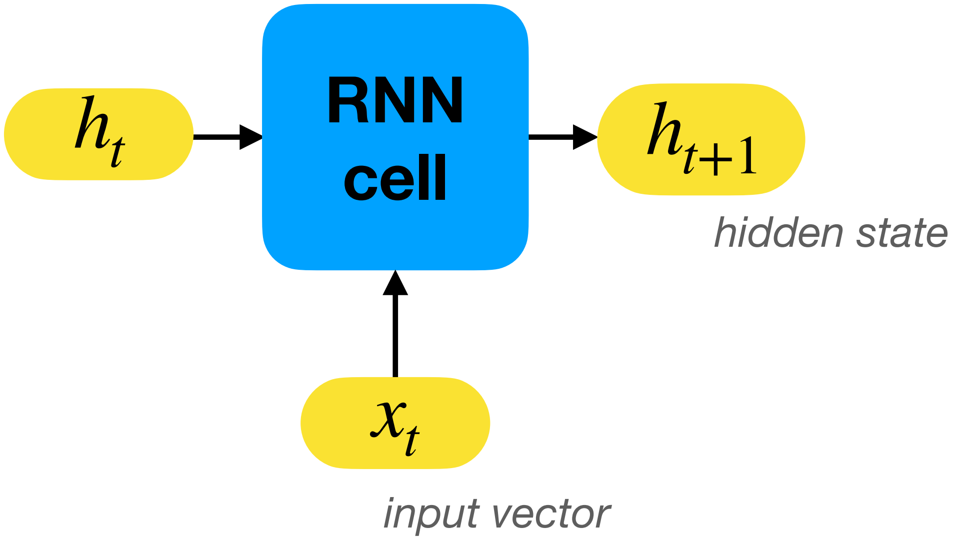
$$z_t = \sigma(W^z x_t + U^z h_{t-1} + b^z)$$
$$r_t = \sigma(W^r x_t + U^r h_{t-1} + b^r)$$
$$\tilde{h}_t = \tanh(W^h x_t + U^h (r_t \circ h_{t-1}) + b^h)$$
$$h_t = z_t \circ h_{t-1} + (1 - z_t) \circ \tilde{h}_t$$

Cho et al (2014), Chung et al (2014)

LSTM

$$f_t = \sigma(W^f x_t + U^f h_{t-1} + b^f)$$
$$i_t = \sigma(W^i x_t + U^i h_{t-1} + b^i)$$
$$o_t = \sigma(W^o x_t + U^o h_{t-1} + b^o)$$
$$\tilde{c}_t = \tanh(W^c x_t + U^c h_{t-1} + b^c)$$
$$c_t = f_t \circ c_{t-1} + i_t \circ \tilde{c}_t$$
$$h_t = o_t \circ g(c_t)$$

Hochreiter and Schmidhuber (1997)



LSTMs: Counting Mechanism

LSTMs can count (and GRUs cannot)

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LSTM

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$$i_t = \sigma(W^i x_t + U^i h_{t-1} + b^i)$$

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gates

candidate vectors

update functions

LSTMs: Counting Mechanism

LSTMs can count (and GRUs cannot)

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$$z_t \in (0,1)$$
$$r_t \in (0,1)$$
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GRU	LSTM
$z_t \in (0,1)$	$f_t \in (0,1)$
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LSTMs: Counting Mechanism

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GRU	**LSTM**
$z_t \in (0,1)$	$f_t \in (0,1)$
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Interpolation

LSTMs: Counting Mechanism

LSTMs can count (and GRUs cannot)

GRU

$z_t \in (0,1)$

$r_t \in$

Bounded!

$\tilde{h}_t \in (-1,1)$

$h_t = z_t \circ h_{t-1} + (1 - z) \circ \tilde{h}_t$

Interpolation

LSTM

$f_t \in (0,1)$

$i_t \in (0,1)$

$o_t \in (0,1)$

$\tilde{c}_t \in (-1,1)$

$c_t = f_t \circ c_{t-1} + i_t \circ \tilde{c}_t$

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Interpolation

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Interpolation

LSTM

$f_t \in (0,1)$

$i_t \in (0,1)$

$o_t \in (0,1)$

$\tilde{c}_t \in (-1,1)$

$c_t = f_t \circ c_{t-1} + i_t \circ \tilde{c}_t$

$h_t = o_t \circ g(c_t)$

Addition

LSTMs: Counting Mechanism

LSTMs can count (and GRUs cannot)

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$z_t \in (0,1)$

$r_t \in$

Bounded!

$\tilde{h}_t \in (-1,1)$

$h_t = z_t \circ h_{t-1} + (1 - z) \circ \tilde{h}_t$

Interpolation

LSTM

$f_t \approx 1$

$i_t \approx 1$

$o_t \in (0,1)$

$\tilde{c}_t \in (-1,1)$

$c_t \approx c_{t-1} + \tilde{c}_t$

$h_t = o_t \circ g(c_t)$

Addition

$c_t = f_t \circ c_{t-1} + i_t \circ \tilde{c}_t$

LSTMs: Counting Mechanism

LSTMs can count (and GRUs cannot)

GRU

$z_t \in (0,1)$

$r_t \in$

Bounded!

$\tilde{h}_t \in (-1,1)$

$h_t = z_t \circ h_{t-1} + (1-z) \circ \tilde{h}_t$

Interpolation

LSTM

$f_t \approx 1$

$i_t \approx 1$

$o_t \in (0,1)$

$\tilde{c}_t \approx 1$

$c_t \approx c_{t-1} + 1$

$h_t = o_t \circ g(c_t)$

Increase by 1

$c_t = f_t \circ c_{t-1} + i_t \circ \tilde{c}_t$

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LSTMs can count (and GRUs cannot)

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$z_t \in (0,1)$

$r_t \in$

Bounded!

$\tilde{h}_t \in (-1,1)$

$h_t = z_t \circ h_{t-1} + (1-z) \circ \tilde{h}_t$

Interpolation

LSTM

$f_t \approx 1$

$i_t \approx 1$

$o_t \in (0,1)$

$\tilde{c}_t \approx -1$

$c_t \approx c_{t-1} - 1$

$h_t = o_t \circ g(c_t)$

Decrease by 1

$c_t = f_t \circ c_{t-1} + i_t \circ \tilde{c}_t$

LSTMs: Counting Mechanism

LSTMs can count (and GRUs cannot)

GRU

$z_t \in (0,1)$

$r_t \in$

Bounded!

$\tilde{h}_t \in (-1,1)$

$h_t = z_t \circ h_{t-1} + (1-z) \circ \tilde{h}_t$

Interpolation

LSTM

$f_t \approx 1$

$i_t \approx 0$

$o_t \in (0,1)$

$\tilde{c}_t \in (-1,1)$

$c_t \approx c_{t-1}$

$h_t = o_t \circ g(c_t)$

Do Nothing

$c_t = f_t \circ c_{t-1} + i_t \circ \tilde{c}_t$

LSTMs: Counting Mechanism

LSTMs can count (and GRUs cannot)

GRU

$z_t \in (0,1)$

$r_t \in$ ...

Bounded!

$\tilde{h}_t \in (-1,1)$

$h_t = z_t \circ h_{t-1} + (1-z) \circ \tilde{h}_t$

Interpolation

LSTM

$f_t \approx 0$

$i_t \approx 0$

$o_t \in (0,1)$

$\tilde{c}_t \in (-1,1)$

$c_t \approx 0$

$h_t = o_t \circ g(c_t)$

Reset

$c_t = f_t \circ c_{t-1} + i_t \circ \tilde{c}_t$

LSTMs: Counting Mechanism

LSTMs can count (and GRUs cannot)

GRU

$z_t \in (0,1)$

$r_t \in$

Bounded!

$\tilde{h}_t \in (-1,1)$

$h_t = z_t \circ h_{t-1} + (1 - z) \circ \tilde{h}_t$

Interpolation

LSTM

$f_t \approx 0$

$i_t \approx 0$

Can Count!

$o_t \in$

$\tilde{c}_t \in (-1,1)$

$c_t \approx 0$

$h_t = o_t \circ g(c_t)$

Reset

$c_t = f_t \circ c_{t-1} + i_t \circ \tilde{c}_t$

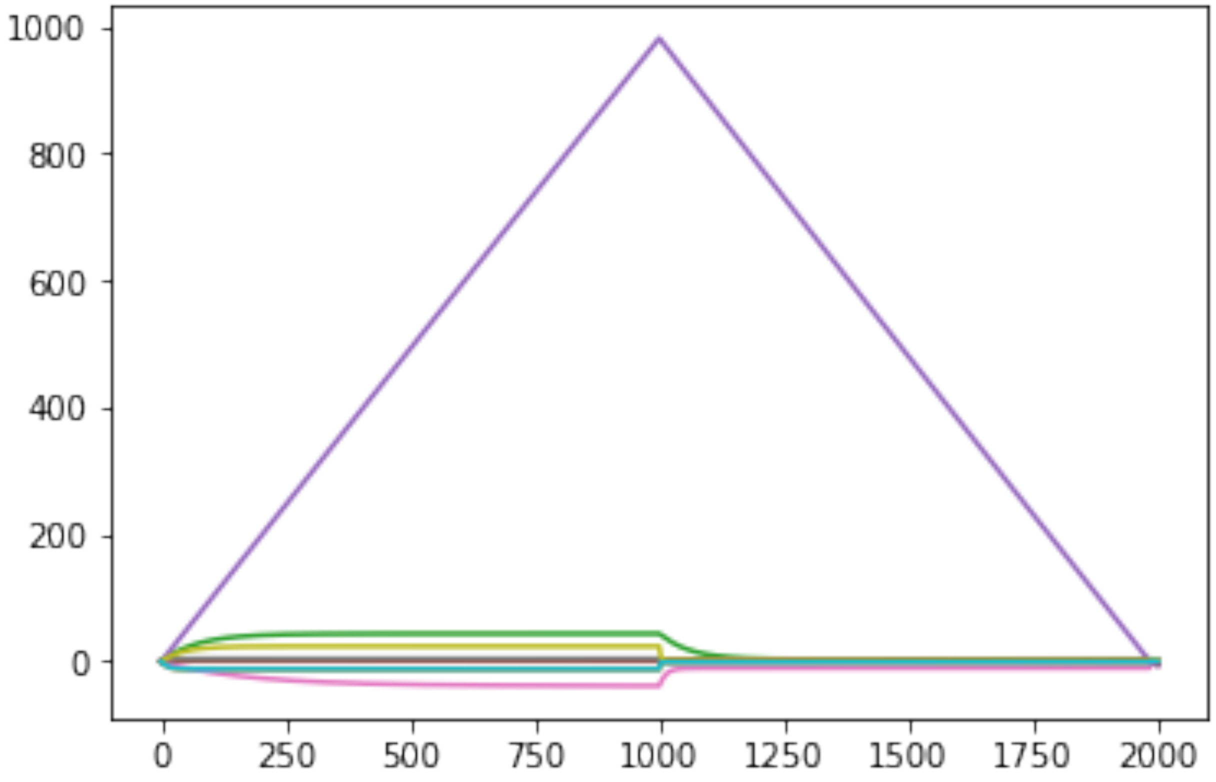
LSTMs: Counting Mechanism

LSTMs can count (and GRUs cannot)

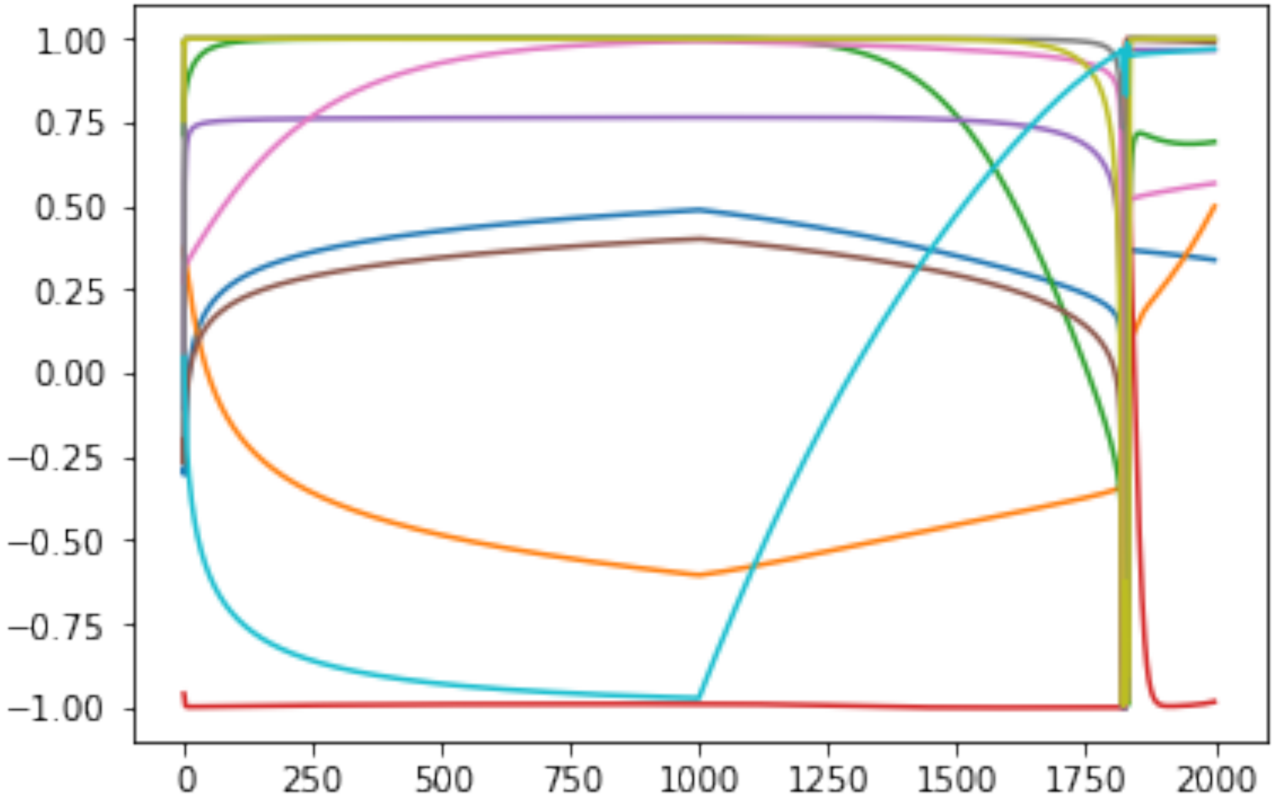
Trained $a^n b^n$**,** (on positive examples up to length 100)

Activations on $a^{1000} b^{1000}$ **:**

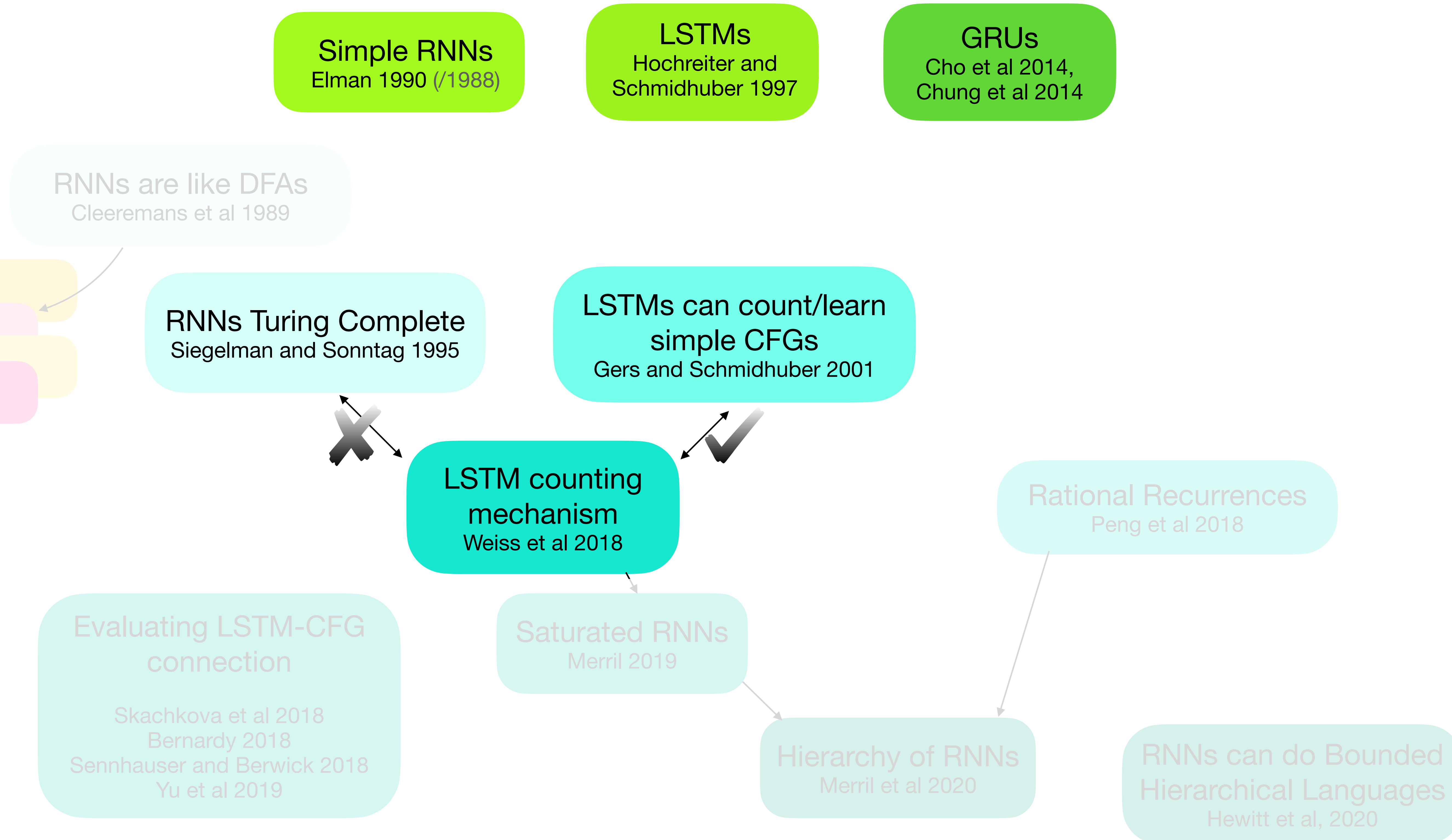
LSTM



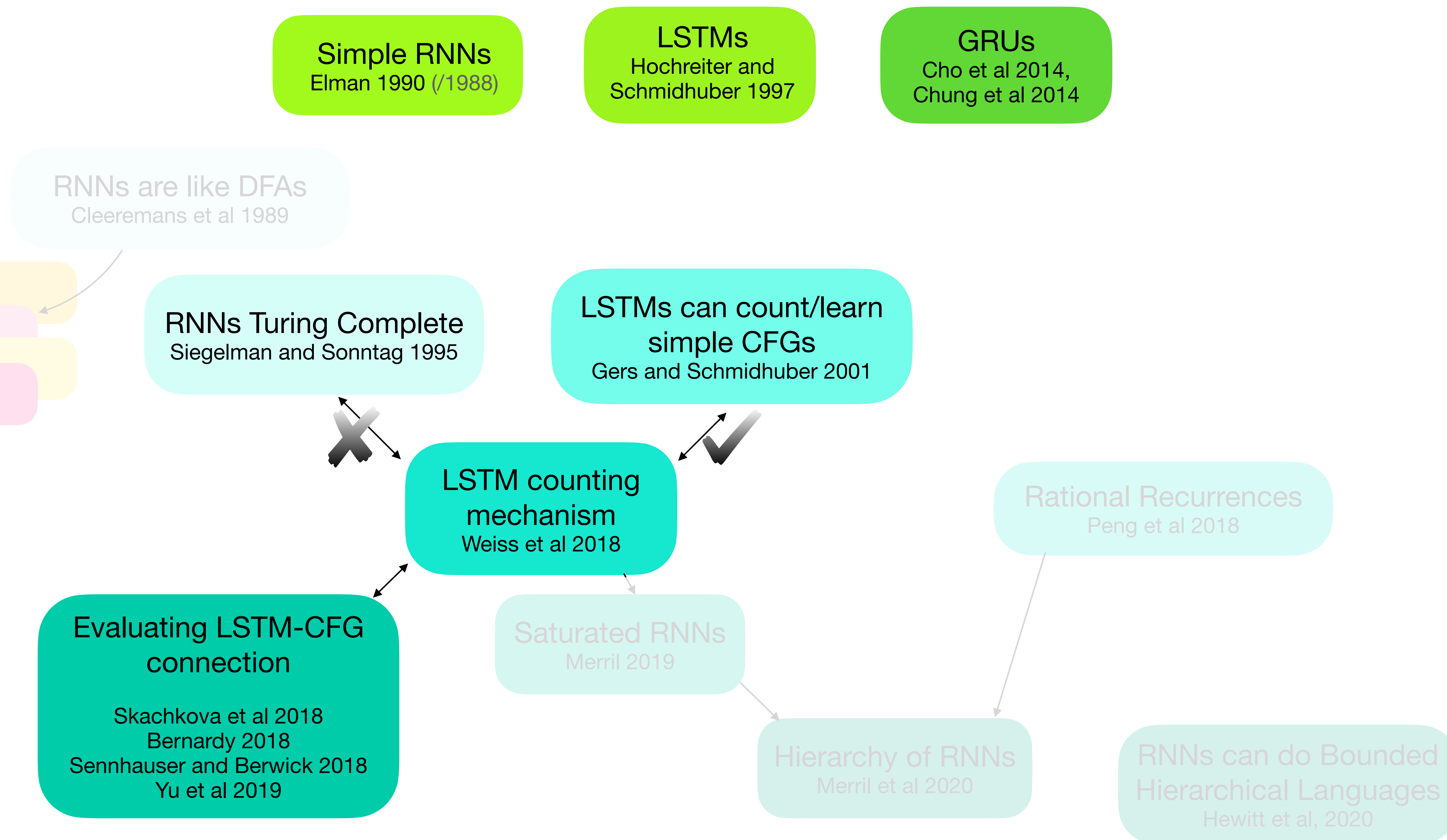
GRU



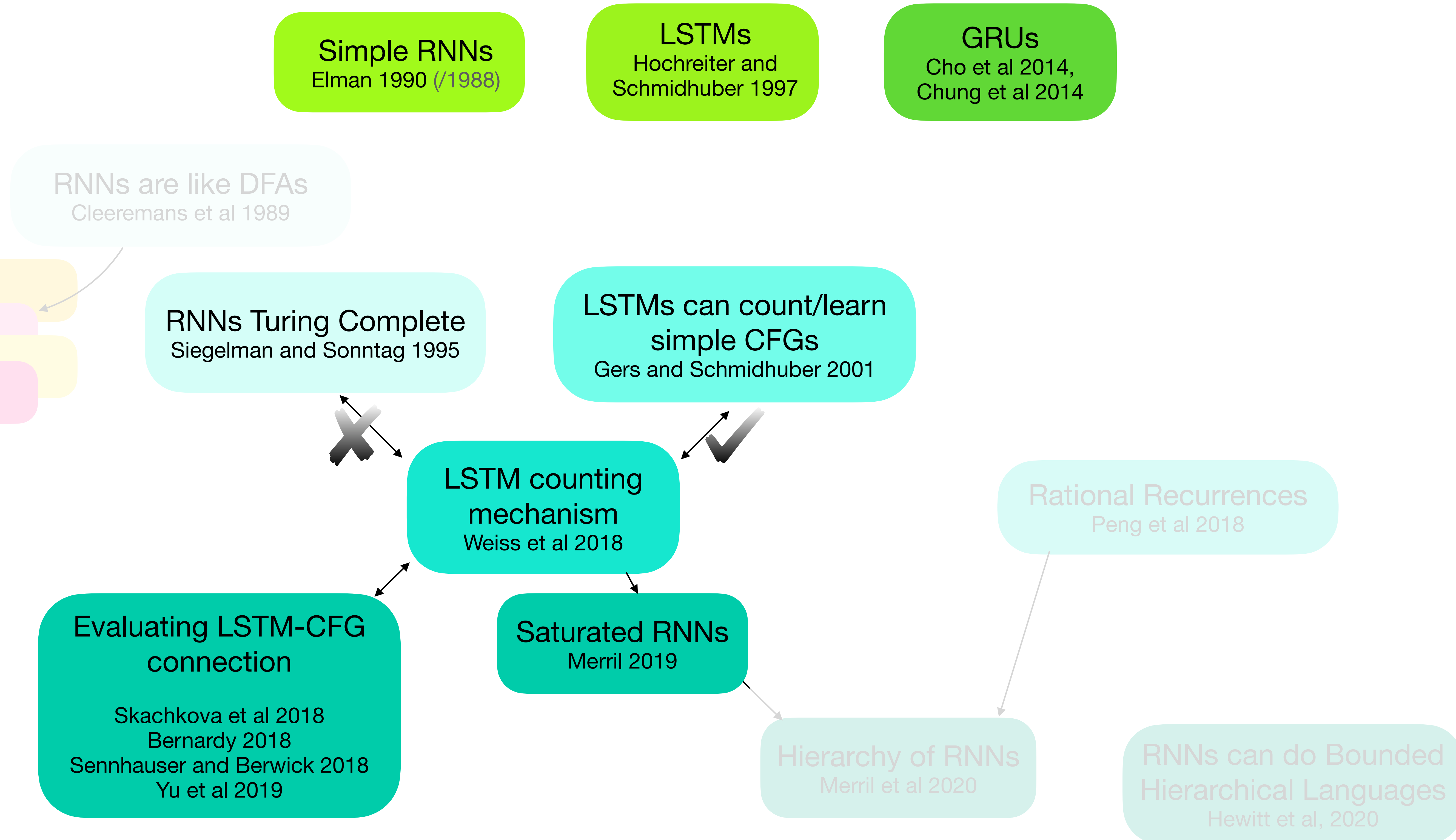
RNNs: Expressive Power



RNNs: Expressive Power



RNNs: Expressive Power



Saturated RNNs

$$f_t = \sigma(W^f x_t + U^f h_{t-1} + b^f)$$
$$i_t = \sigma(W^i x_t + U^i h_{t-1} + b^i)$$
$$o_t = \sigma(W^o x_t + U^o h_{t-1} + b^o)$$

$$f_t \in (0,1)$$
$$i_t \in (0,1)$$
$$o_t \in (0,1)$$

Saturated RNNs

$$f_t = \sigma(W^f x_t + U^f h_{t-1} + b^f)$$
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$$f_t \in (0,1)$$
$$i_t \in (0,1)$$
$$o_t \in (0,1)$$

$$\sigma : \mathbb{R} \to (0,1)$$
$$\tanh : \mathbb{R} \to (-1,1)$$

Saturated RNNs

$$f_t = \sigma(W^f x_t + U^f h_{t-1} + b^f)$$
$$i_t = \sigma(W^i x_t + U^i h_{t-1} + b^i)$$
$$o_t = \sigma(W^o x_t + U^o h_{t-1} + b^o)$$

$$f_t \approx 1$$
$$i_t \approx 0$$
$$o_t \in (0,1)$$

$$\sigma : \mathbb{R} \to (0,1)$$
$$\tanh : \mathbb{R} \to (-1,1)$$

Saturated RNNs

$$f_t = \sigma(W^f x_t + U^f h_{t-1} + b^f)$$
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?

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Saturated RNNs

Sequential Neural Networks as Automata - Merrill (2019)

$$f_t = \sigma(W^f x_t + U^f h_{t-1} + b^f)$$
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Saturated RNNs

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?

$$\sigma : \mathbb{R} \rightarrow (0,1)$$
$$\tanh : \mathbb{R} \rightarrow (-1,1)$$

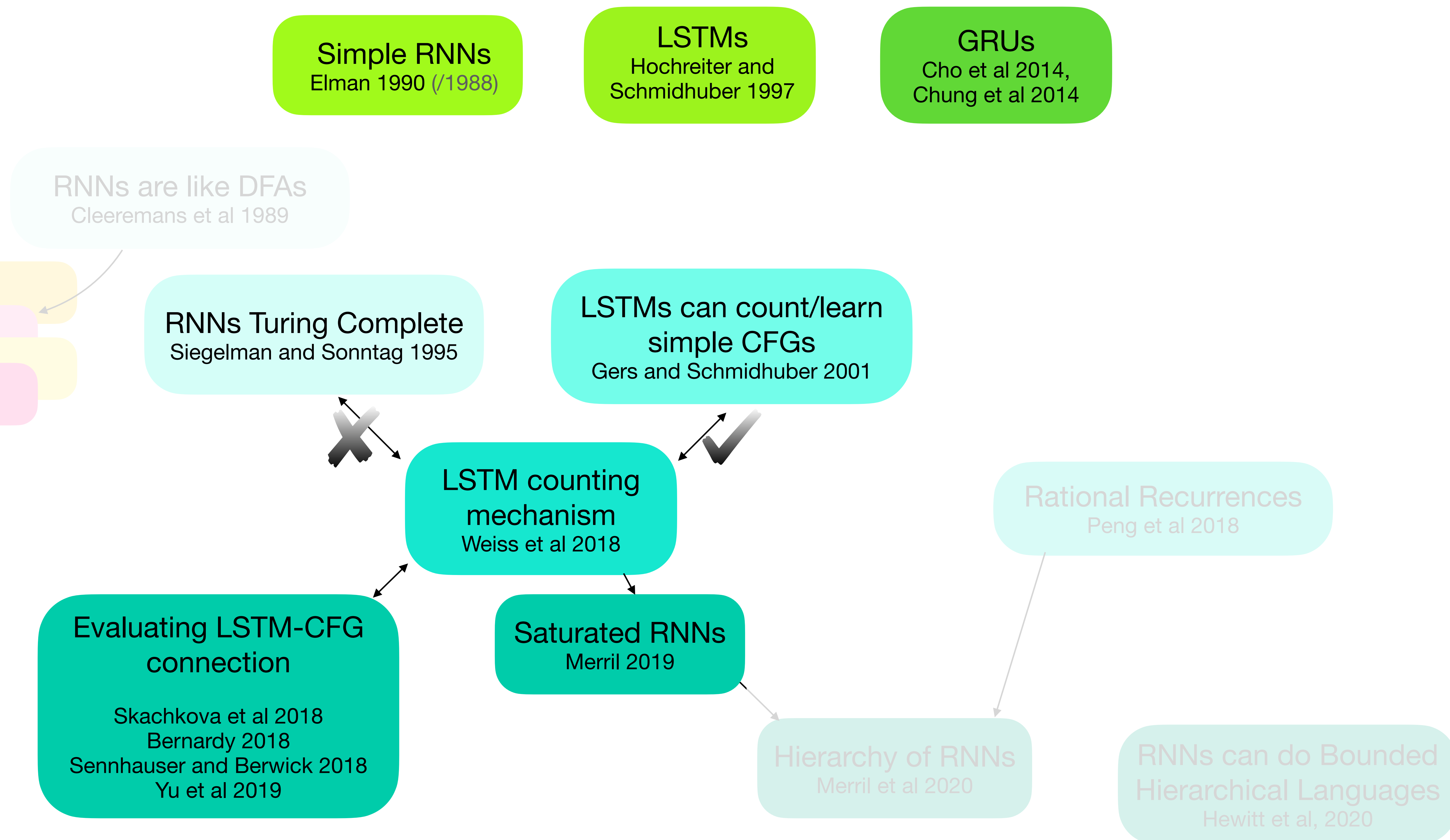
$$\theta$$

RNN is a parameterised function, $R(w : \theta)$

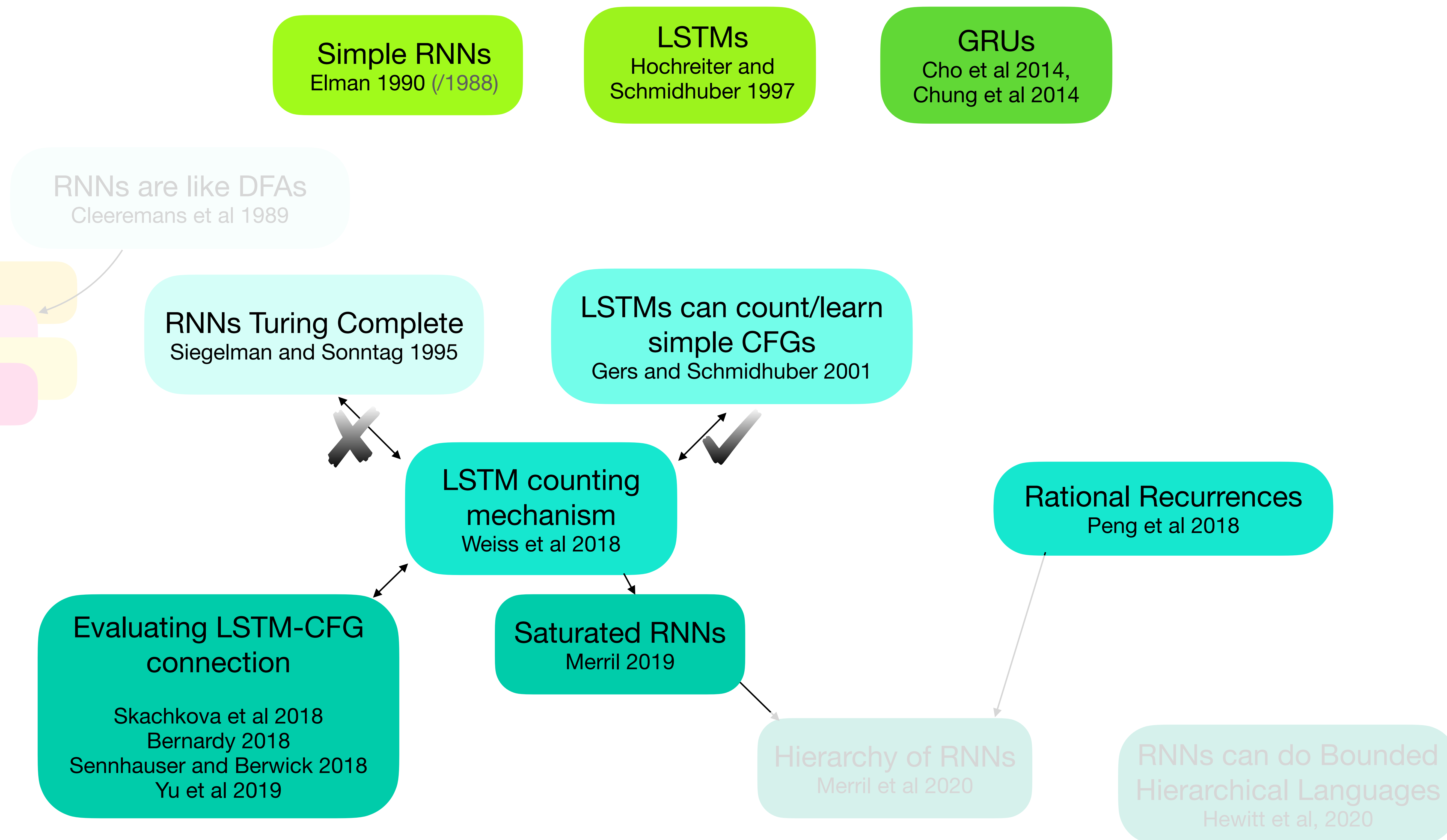
As θ “increases”, inputs to activations increase, saturating them

Saturated RNN: $sat\text{-}R(w : \theta) = \lim_{N \rightarrow \infty} R(w : N\theta)$

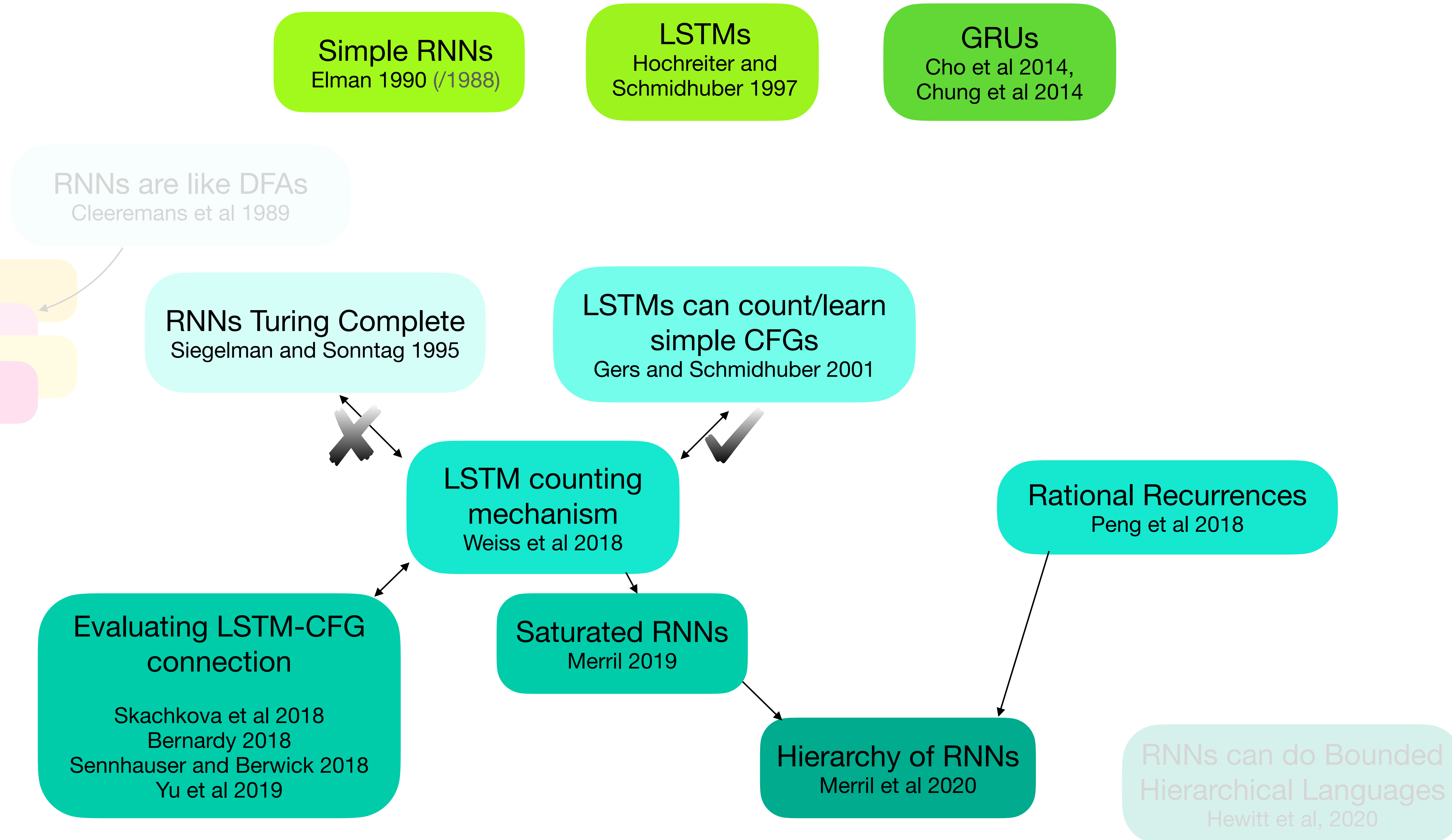
RNNs: Expressive Power



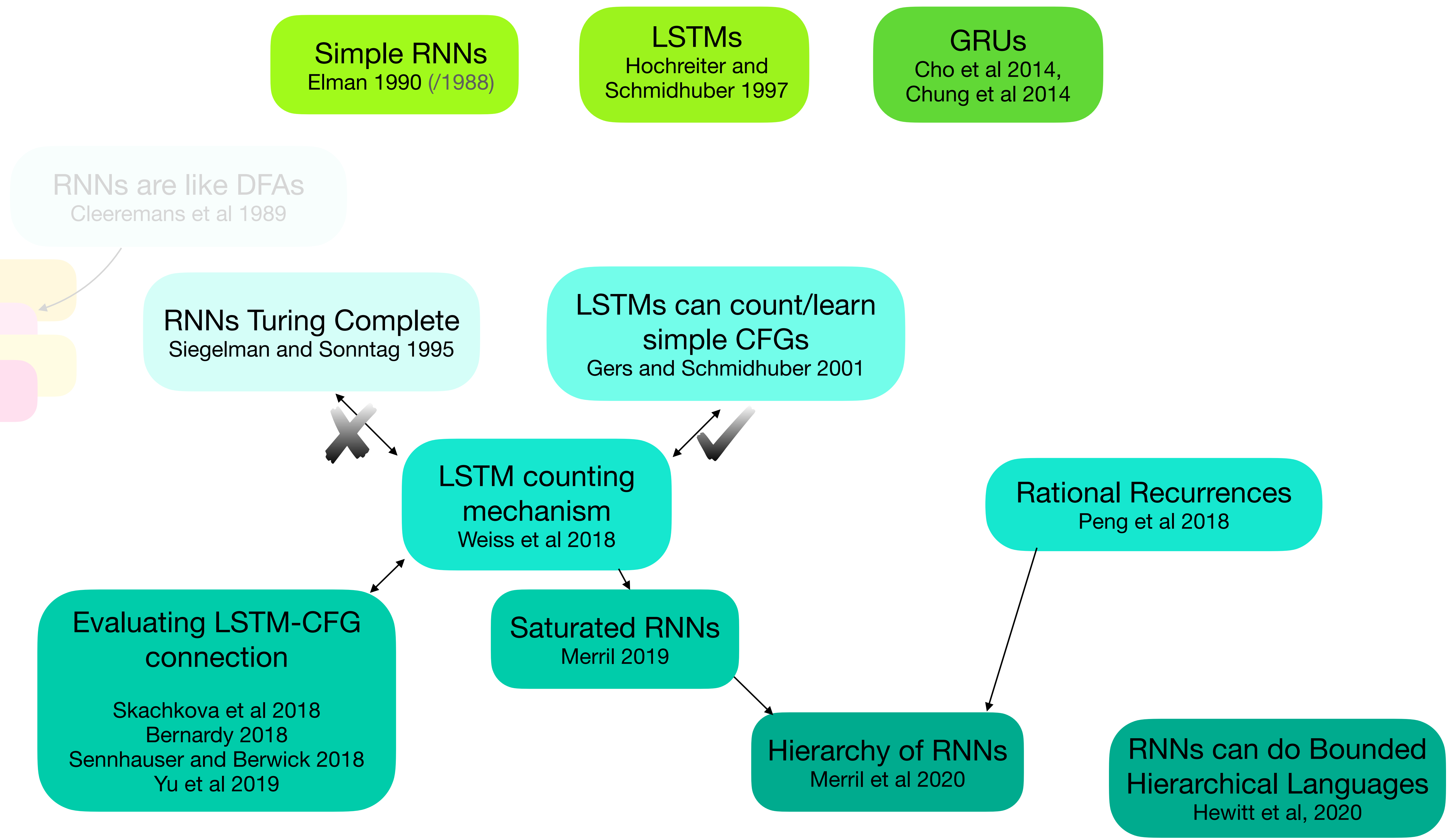
RNNs: Expressive Power



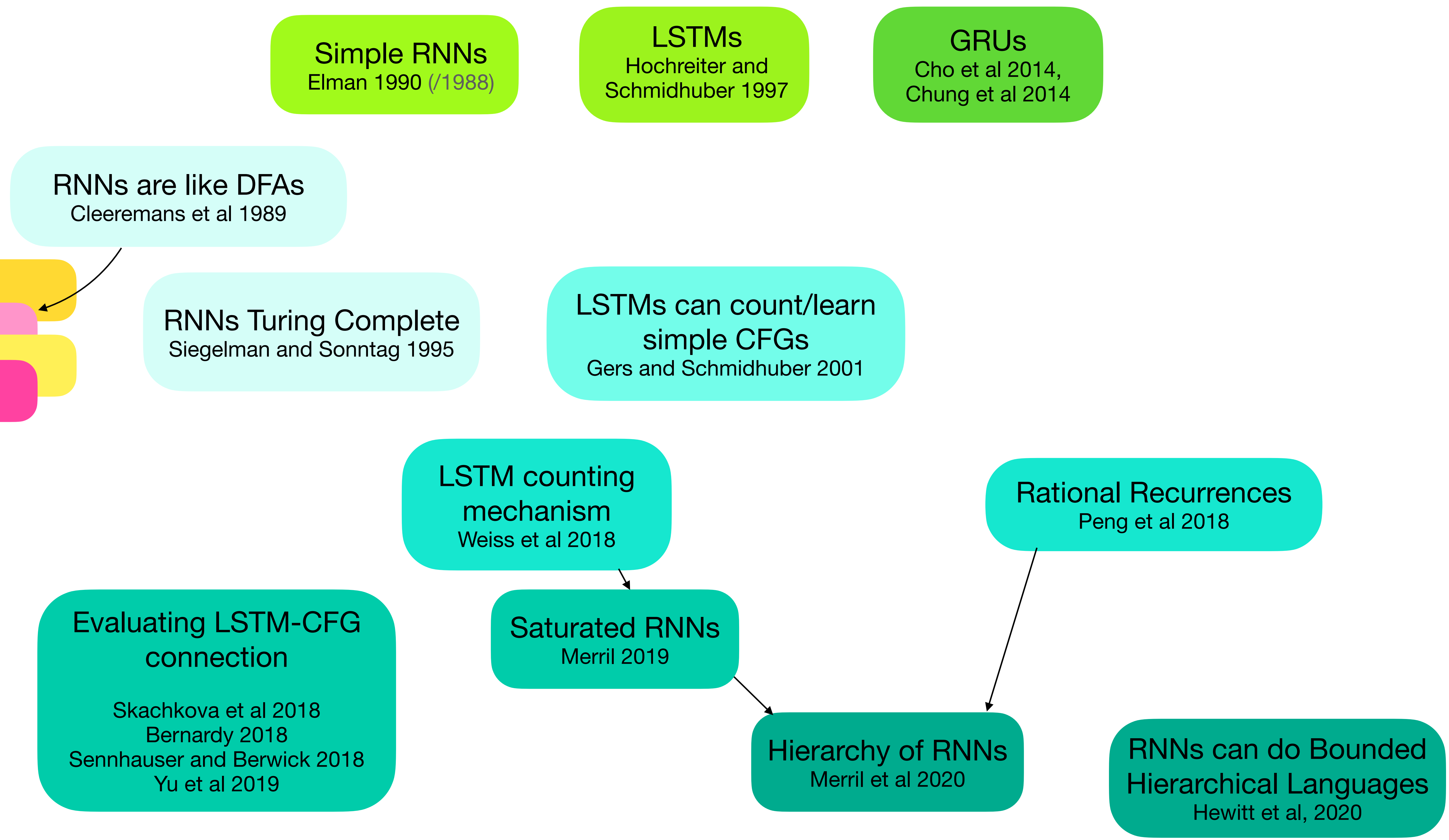
RNNs: Expressive Power



RNNs: Expressive Power



RNNs: Expressive Power



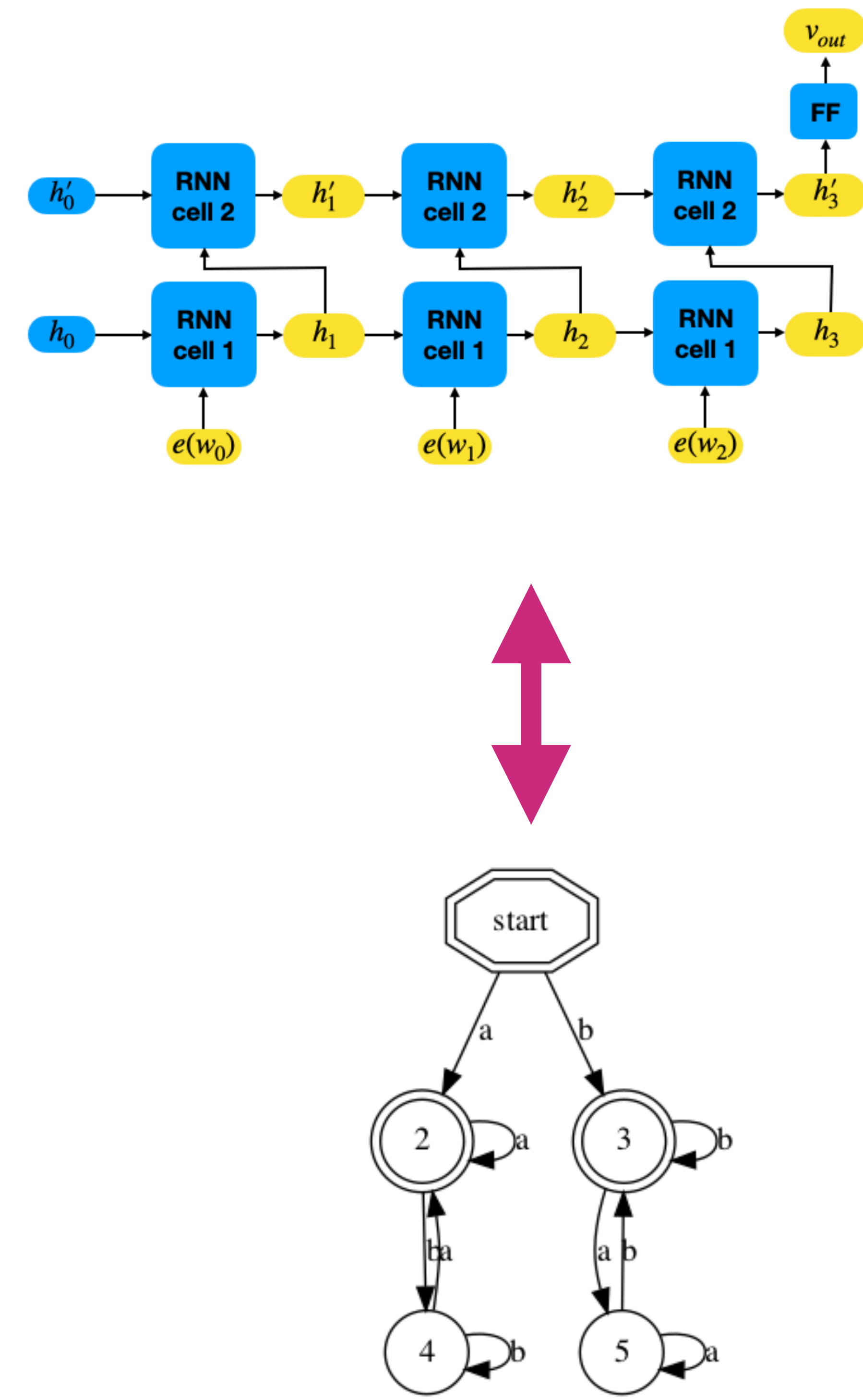
Overview

Recurrent Neural Networks (RNNs)

- Introduction
- RNN-Automata relation
- Extraction
    - DFAs
    - WFAs
    - More
- Analysis

Transformers

- Introduction
- A formal abstraction



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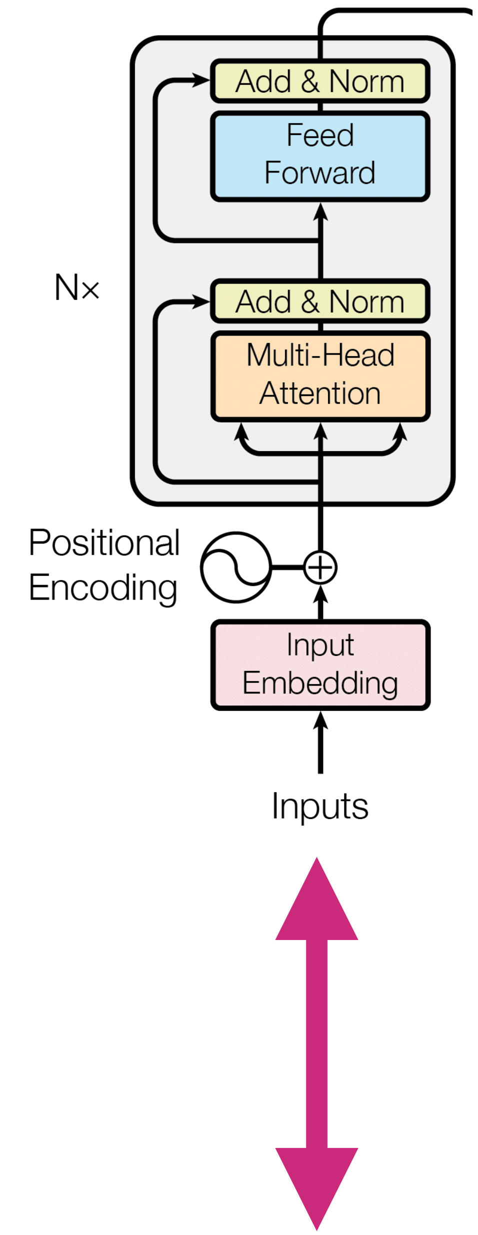

Code!?

Overview

Recurrent Neural Networks (RNNs)

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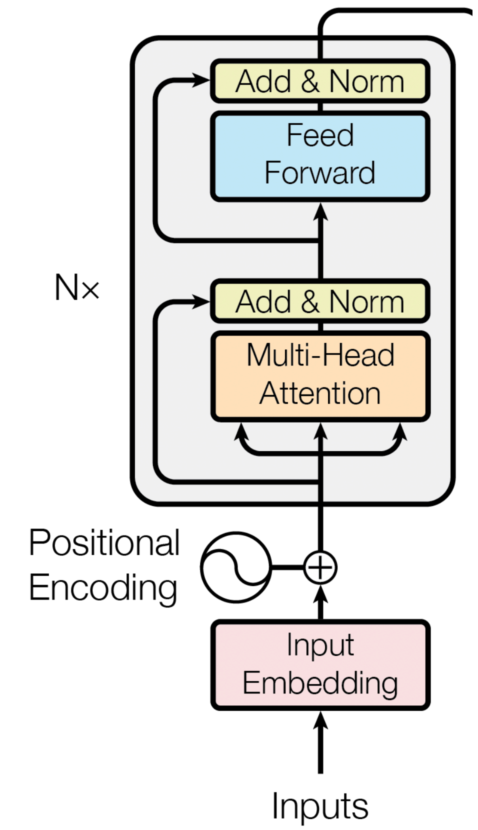
  - WFAs
  - More
- Analysis

Transformer Encoders

- Introduction
- A formal abstraction



Didn't make it! :(

But my website has links to talks on "Thinking Like Transformers", the work I wanted to introduce here:

https://sgailw.cswp.cs.technion.ac.il/publications/

The 1 hour talk includes an introduction on transformers, while the 5 minute talk assumes familiarity.