GRAPH-BASED SEMANTIC PARSING, Compositional generalization AND LOSS FUNCTIONS

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SEMANTIC PARSING

Related publication

On graph-based reentrancy-free semantic parsing Alban Petit, Caio Corro TACL 2023

SEMANTIC PARSING

SQL parsing

- ► Input: sentence
- ► Output: SQL query

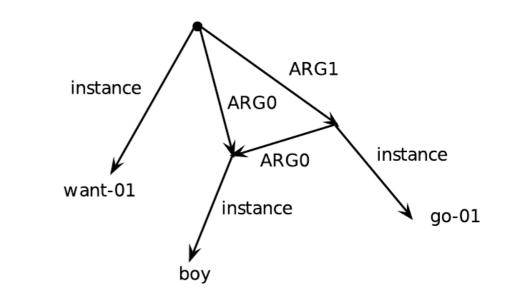
I want to book a flight from Paris to Rome.

SELECT * FROM flight WHERE from = "paris" AND to = "rome"

Abstract Meaning Representation (AMR) parsing

- ► Input: sentence
- ► Output: graph

The boy want to go.



REENTRANCY-FREE SEMANTIC PARSING

Reentrancy-free semantic structures

- ► Predicates and entities are typed (in the same sense than in "typed programming languages")
- ► An argument can only be used once

Semantic structures look like a simple instruction in a functional programming language.

```
What rivers do not run through Tennesse?

exclude ( river_all , traverse_2 ( stateid('Tennesse') ) )
```

Is this realistic?

"estimating that there are only 0.3% queries that would require a more general [..] representation." Task Oriented Parsing (TOP) dataset **[Gupta et al., 2018]**

COMPOSITIONAL GENERALIZATION

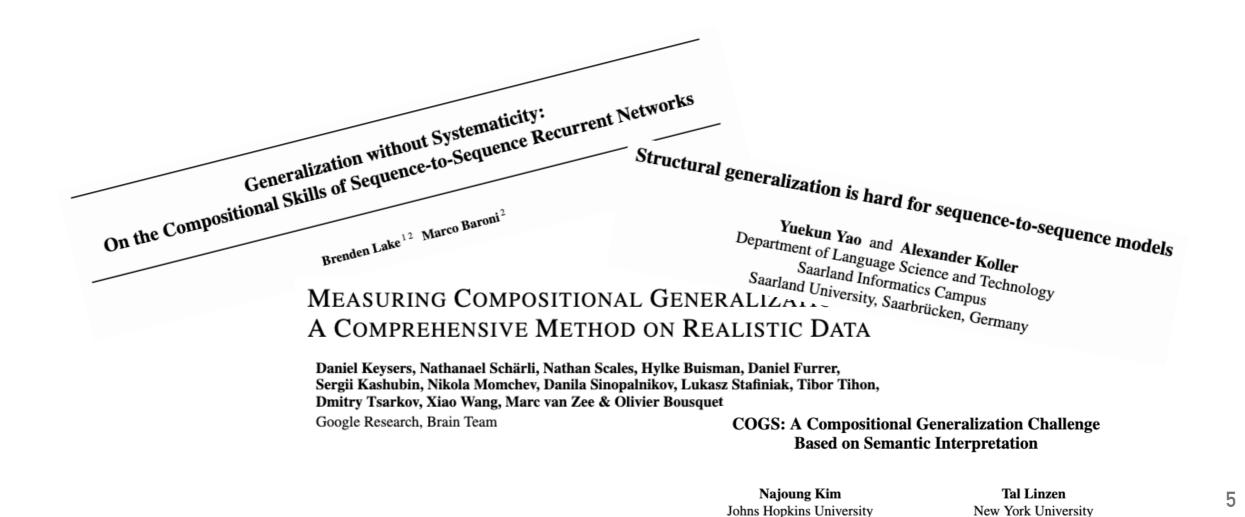
Compositionality: "the meaning of a complex expression is constructed from the meanings of its constituent parts" (Kim & Linzen, 2020)

Compositional generalization:

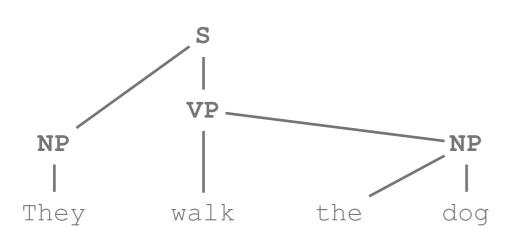
"Once a person learns the meaning of a new verb *dax*, he or she can immediately understand the meaning of *dax twice* or *sing and dax*." (Lake & Baroni, 2018)

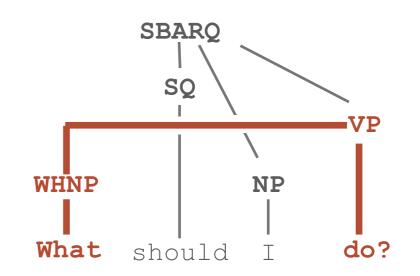
n.kim@jhu.edu

linzen@nyu.edu



SYNTACTIC PARSING: CONSTITUENCY PARSING

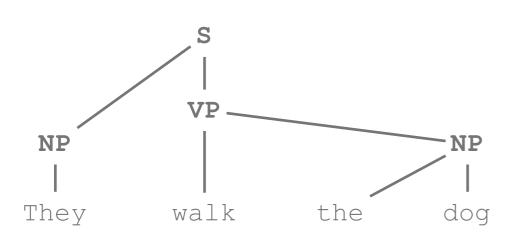


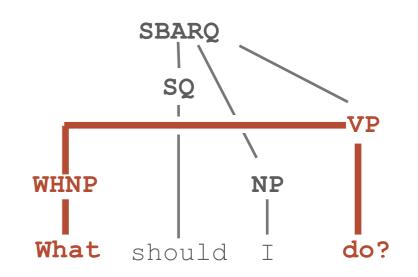


Constituency parsing complexity with formal grammars

e e	Context-free grammars	$\mathcal{O}(n^3)$	[Sakai, 1961]
easing th space	Well-nested LCFRS with a fan-out of 2	$\mathcal{O}(n^6)$	[Cómos Dodríguos et al 2010]
Increa search	Well-nested LCFRS with a fan-out of k, $k > 2$	$\mathcal{O}(n^{2k+2})$	[Gómez-Rodríguez et al., 2010]
I Se	LCFRS with bounded fan-out	NP-hard	[Satta, 1992]

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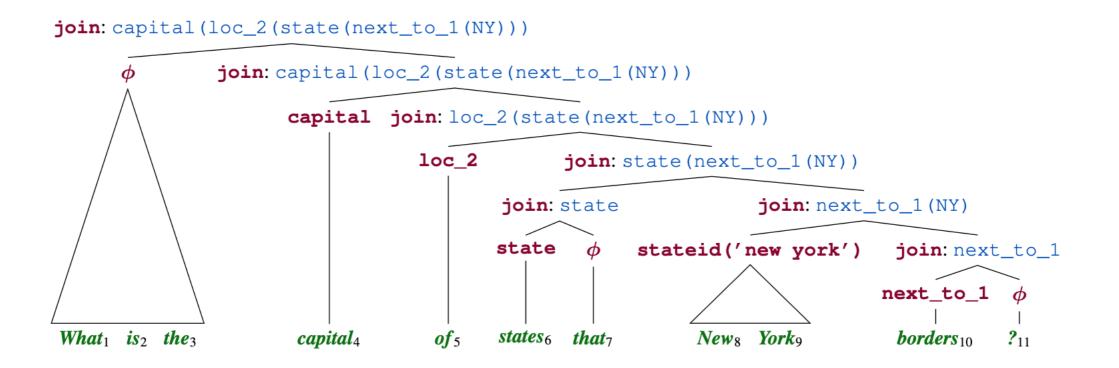
Constituency parsing complexity with span-based parsers

- Ensure the well-formedness of the resulting structure
- Do not enforce compliance of the syntactic content represented by the structure (e.g. a verbal phrase is not constrained to contain a verb)

Similar complexity than formal grammar parsers [Stern et al., 2017] [Corro, 2020]

Outline

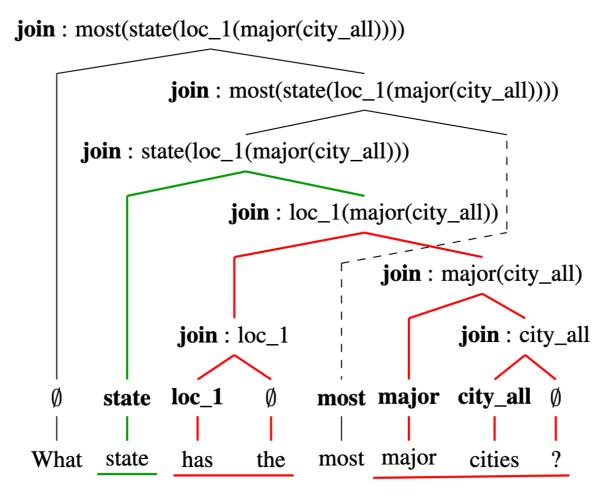
- Use a span-based constituency parser for semantic parsing (with extra valency constraints)
- ► Show that it is more robust to compositional generalization than seq-2-seq models



SPAN-BASED SEMANTIC PARSING

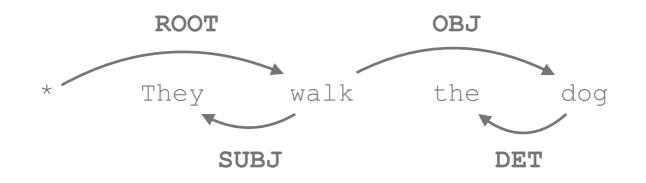
Limitation

The parser allows only a limited form of discontinuity that can be parsed in $\mathcal{O}(n^3)$ [Corro, 2020]



The constituent in red is discontinuous and also has a discontinuous parent (red+green) => outside the search space of the algorithm!

SYNTACTIC PARSING: DEPENDENCY PARSING



Dependency parsing complexity (among many other algorithms!)

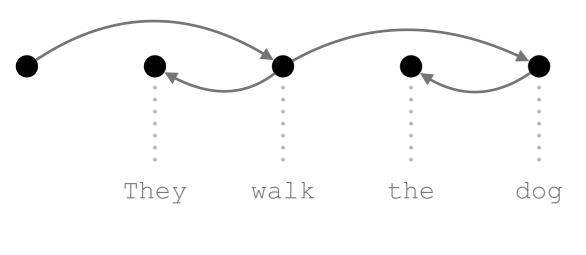
[Eisner, 2000]	$\mathcal{O}(n^3)$	Projective	
	$\mathcal{O}(n^7)$	Well-nested + 2-bounded block degree	ng ace
[Gómez-Rodríguez et al. 2009]	$\mathcal{O}(n^{3+2k})$	Well-nested + k-bounded block degree, $k > 2$	Increasing search space
[Satta, 1992]	NP-complete	k-bounded block degree, $k > 2$	Increa search
[McDonald et al., 2005]	$\mathcal{O}(n^2)$	Unrestricted (a.k.a. non-projective)	
[Tarjan, 1977]			•

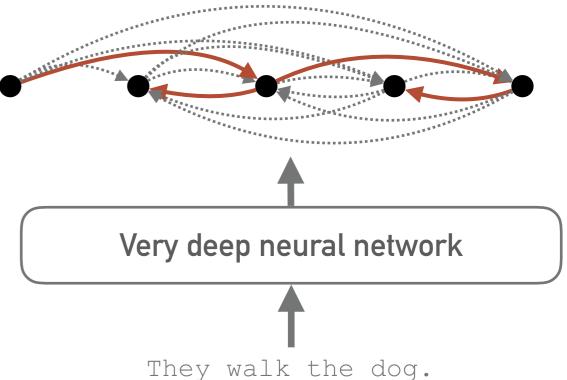
GRAPH-BASED PARSING

Prediction with a graph-based parser

Assume an input sentence with n words:

- 1. Create a complete directed graph with n vertices
- 2. Weight all arcs using a neural network
- 3. Compute the maximum spanning arborescence of the graph

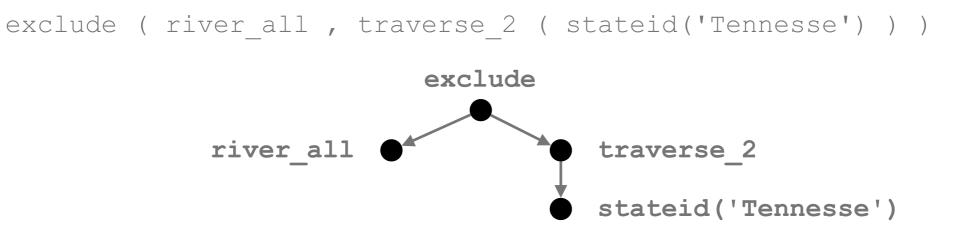




Intuition

The semantic program can be represented by its abstract syntax tree (AST)

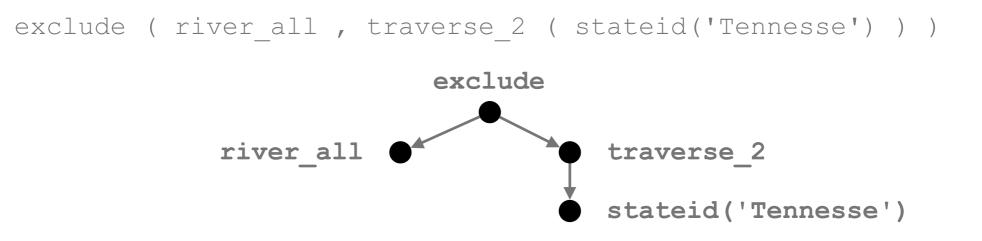
```
=> just predict the AST!
```



Intuition

The semantic program can be represented by its abstract syntax tree (AST)

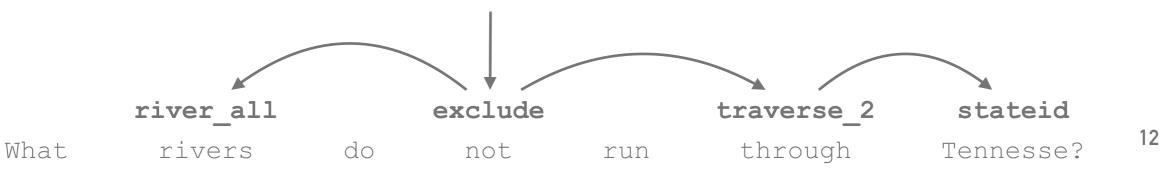
=> just predict the AST!



Graph-based prediction

Joint tagging (entity+predicate) and parsing (argument identification)

- Non-spanning structure (function words, etc)
- ► Valency constraints
- ► Non-projective structure



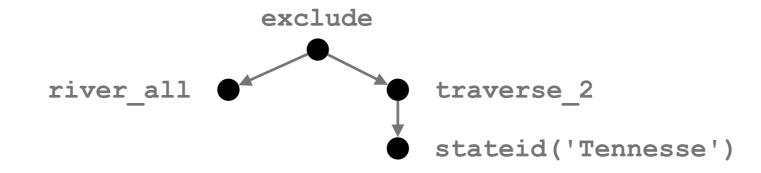
Semantic grammar

A semantic grammar is a tuple $\mathscr{G} = \langle E, T, f_{type}, f_{args} \rangle$ where:

- $\blacktriangleright E$ is a set of predicates and entities (set of tags)
- > T is a set of type
- ► $f_{type} : E \to T$ is a typing function that assigns a type to each tag
- ► $f_{args}: E \times T \to \mathbb{N}$ is a valency function that assigns the numbers of expected arguments of a given type

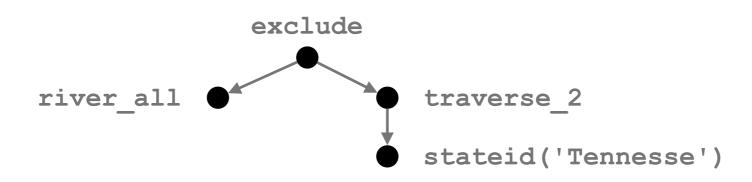
AST recognition

A labeled graph is a valid AST if and only if it can be recognized by the grammar \mathcal{G}



Example

 $E = \{exclude, river_all, traverse_1, traverse_2, state_id, ...\} \qquad T = \{river, state, ...\}$



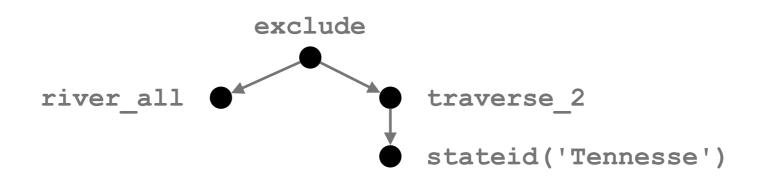
Example

 $E = \{exclude, river_all, traverse_1, traverse_2, state_id, ...\}$ $T = \{$

 $T = \{river, state, \dots\}$

ftype(river_all) = river
ftype(state_id) = state
ftype(traverse_2) = river
ftype(exclude) = river

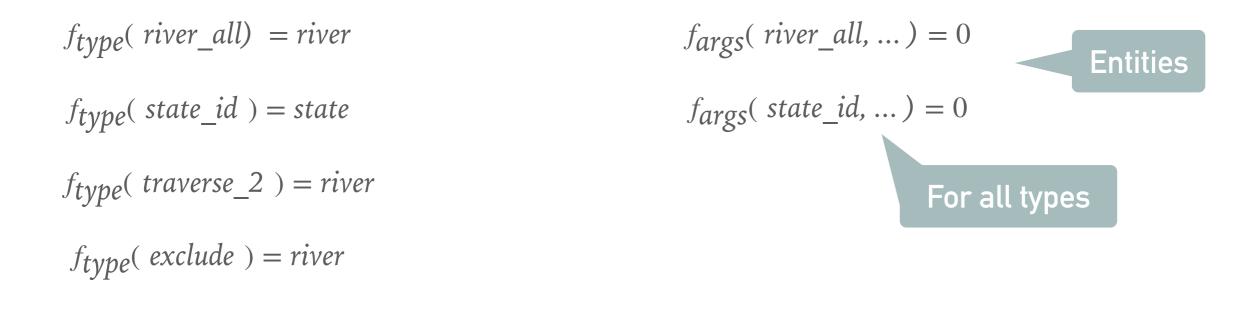
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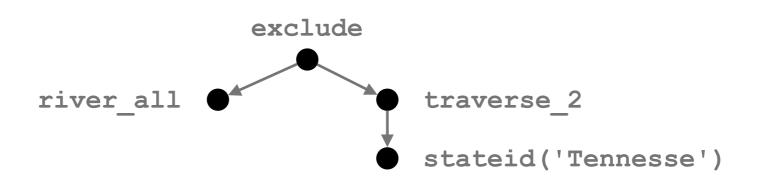


. . .

Example

 $E = \{exclude, river_all, traverse_1, traverse_2, state_id, \dots\} \qquad T = \{river, state, \dots\}$





Example

 $E = \{exclude, river_all, traverse_1, traverse_2, state_id, ...\} \qquad T = \{river, state, ...\}$

 $f_{type}(river_all) = river$ $f_{args}(river_all, ...) = 0$

 $f_{type}(state_id) = state$

 $f_{type}(traverse_2) = river$

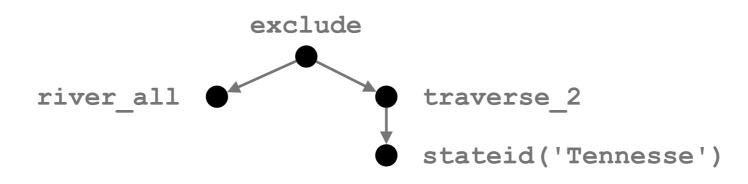
 $f_{type}(exclude) = river$

. . .

 $f_{args}(state_id, ...) = 0$

 $f_{args}(traverse_2, river) = 0$

 $f_{args}(traverse_2, state) = 1$



 $f_{type}(state_id) = state$

 $f_{type}(traverse_2) = river$

 $f_{type}(exclude) = river$

. . .

Example

 $E = \{exclude, river_all, traverse_1, traverse_2, state_id, ...\} \qquad T = \{river, state, ...\}$

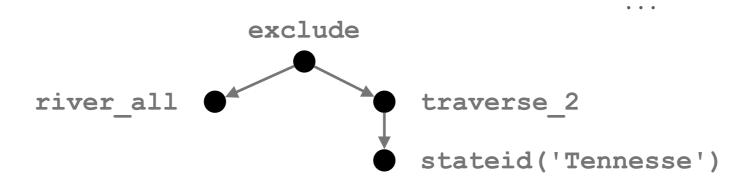
- $f_{type}(river_all) = river$ $f_{args}(river_all, ...) = 0$
 - $f_{args}(state_id, \dots) = 0$

 $f_{args}(traverse_2, river) = 0$

 $f_{args}(traverse_2, state) = 1$

 $f_{args}(exclude, river) = 2$

 $f_{args}(exclude, state) = 0$



 $f_{type}(state_id) = state$

 $f_{type}(traverse_2) = state$

 $f_{type}(exclude) = river$

. . .

Example

 $E = \{exclude, river_all, traverse_1, traverse_2, state_id, ...\} \qquad T = \{river, state, ...\}$

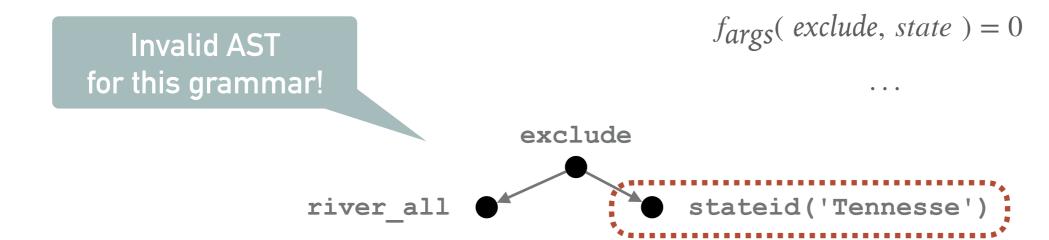
 $f_{type}(river_all) = river$ $f_{args}(river_all, ...) = 0$

 $f_{args}(state_id, ...) = 0$

 $f_{args}(traverse_2, river) = 0$

 $f_{args}(traverse_2, state) = 1$

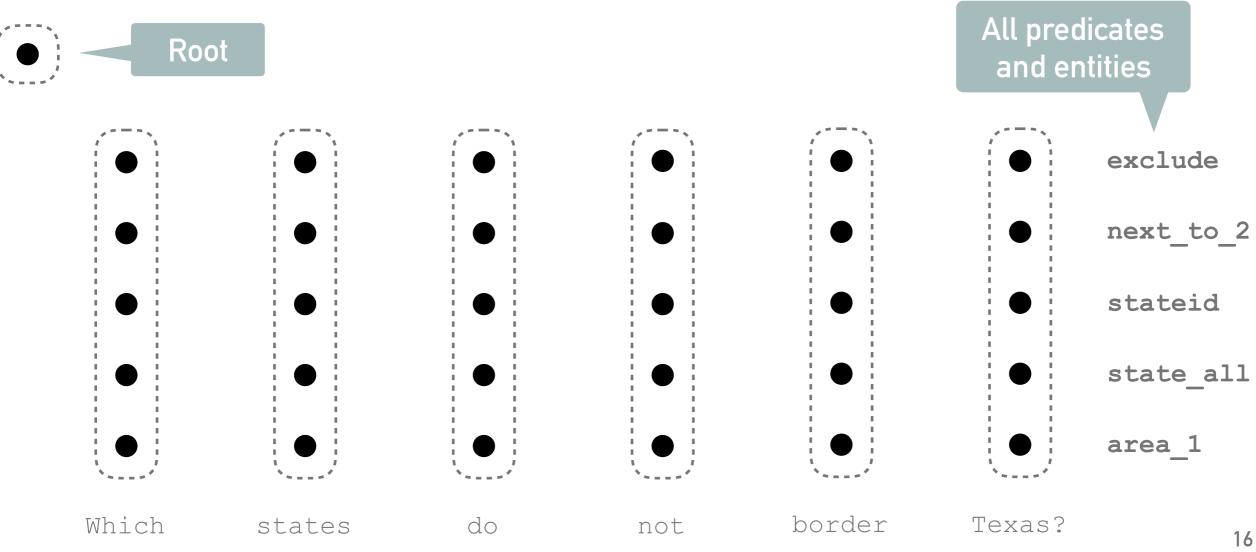
 $f_{args}(exclude, river) = 2$



REDUCTION TO A GRAPH PROBLEM

Graph construction

- 1. For each word, create a cluster
- 2. In each cluster, create one vertex per element of T
- 3. Add all possible arcs (with weights from the neural network)

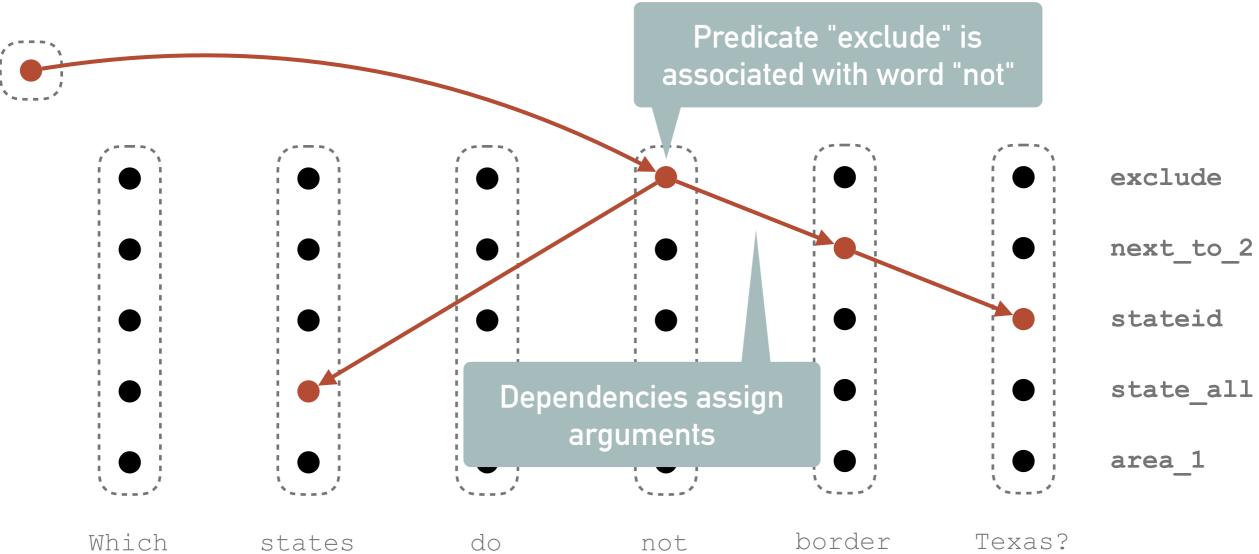


REDUCTION TO A GRAPH PROBLEM

AST parsing

Compute the rooted arborescence of maximum weight such that:

- ► There is at most one incident vertex per cluster
- ► Valency constraints are satisfied



NP-HARDNESS

AST parsing

Compute the rooted arborescence of maximum weight such that:

► There is at most one incident vertex per cluster

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Issue

This problem is NP hard! :(

(proof: by reduction of the maximum not-necessarily spanning arborescence problem)

NP-HARDNESS

AST parsing

Compute the rooted arborescence of maximum weight such that:

- ► There is at most one incident vertex per cluster
- ► Valency constraints are satisfied

Issue

This problem is NP hard! :(

(proof: by reduction of the maximum not-necessarily spanning arborescence problem)

Approximate solver

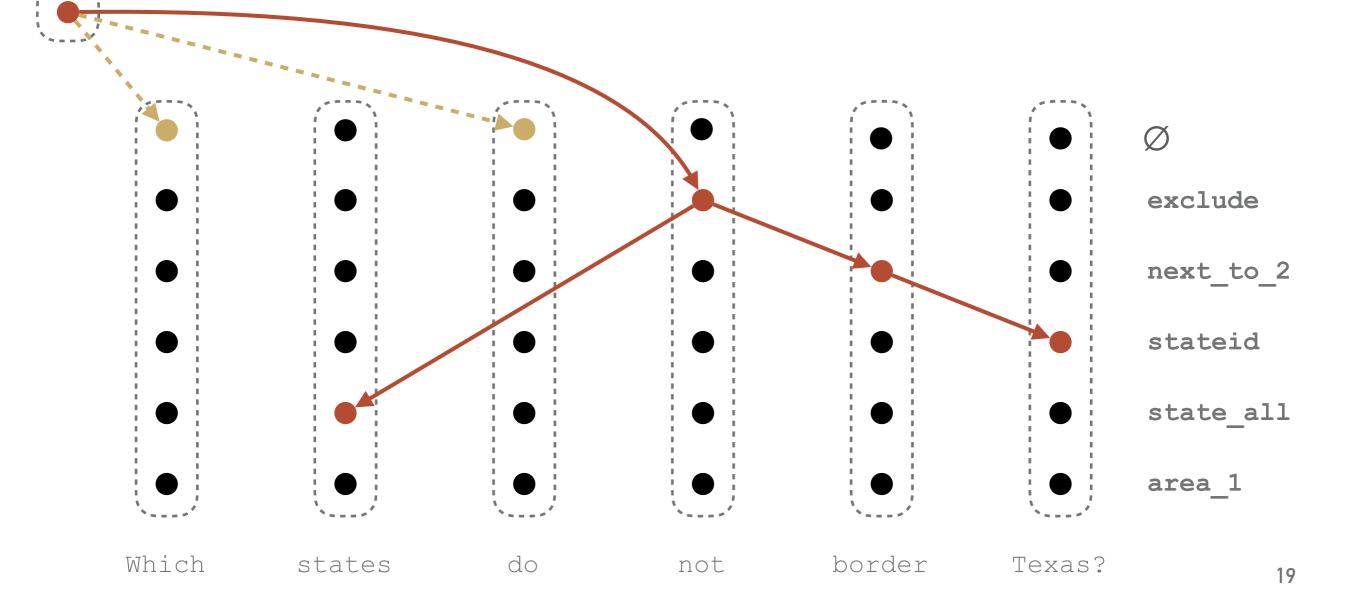
- 1. Formulation as a integer linear program
- 2. Relaxation of the integrality constraint
- 3. Identifying the difficult constraints and add them as penalties in the objective
- 4. Custom optimization algorithm based on the problem structure (indicator function smoothing + Frank-Wolfe)

$$\max_{\mathbf{z} \in [0,1]^d} \langle \mathbf{z}, \phi \rangle$$
s.t. $z \in \mathscr{C}^{(easy)}$
 $z \in \mathscr{C}^{(hard)}$
Valency constraints!

Problem reformulation

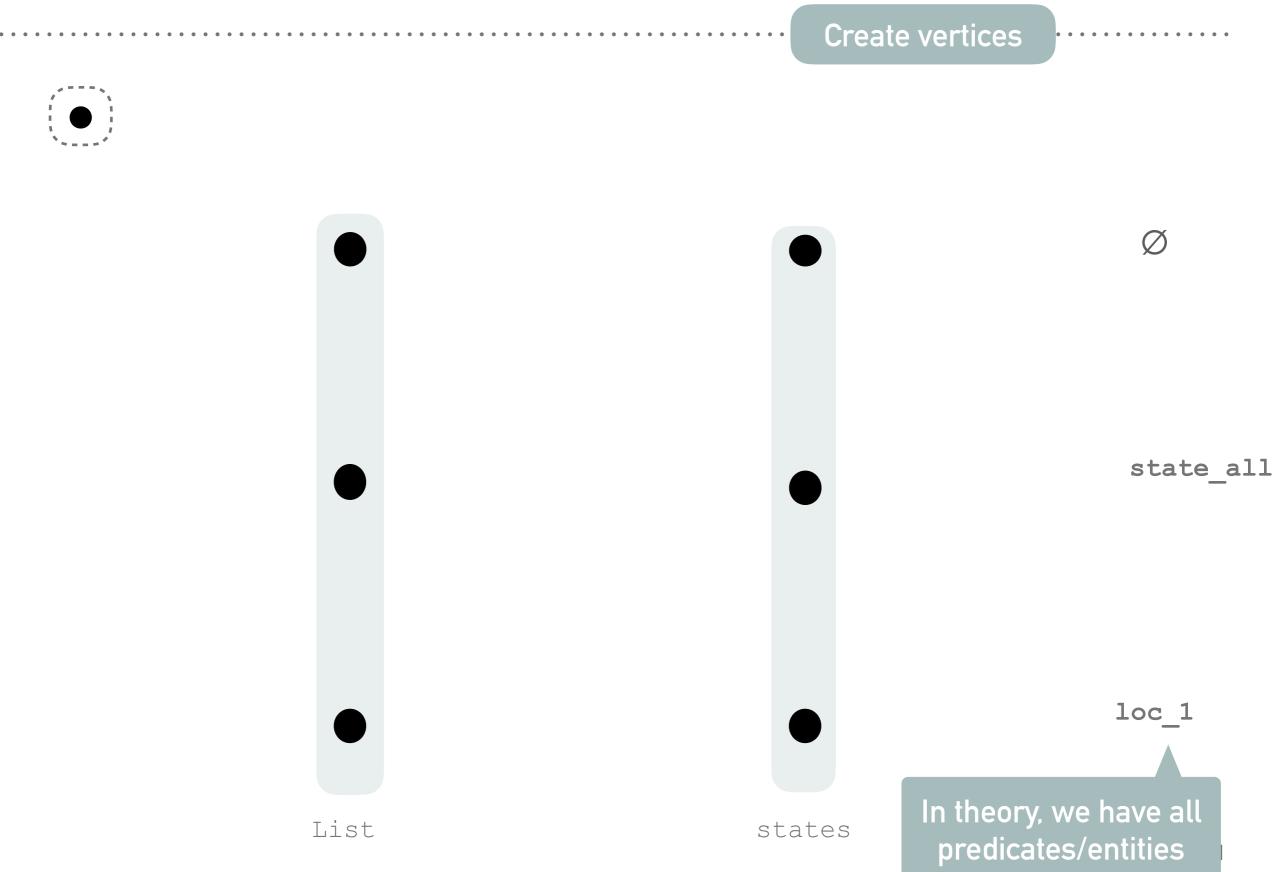
To simplify the algorithm, we add "empty entities":

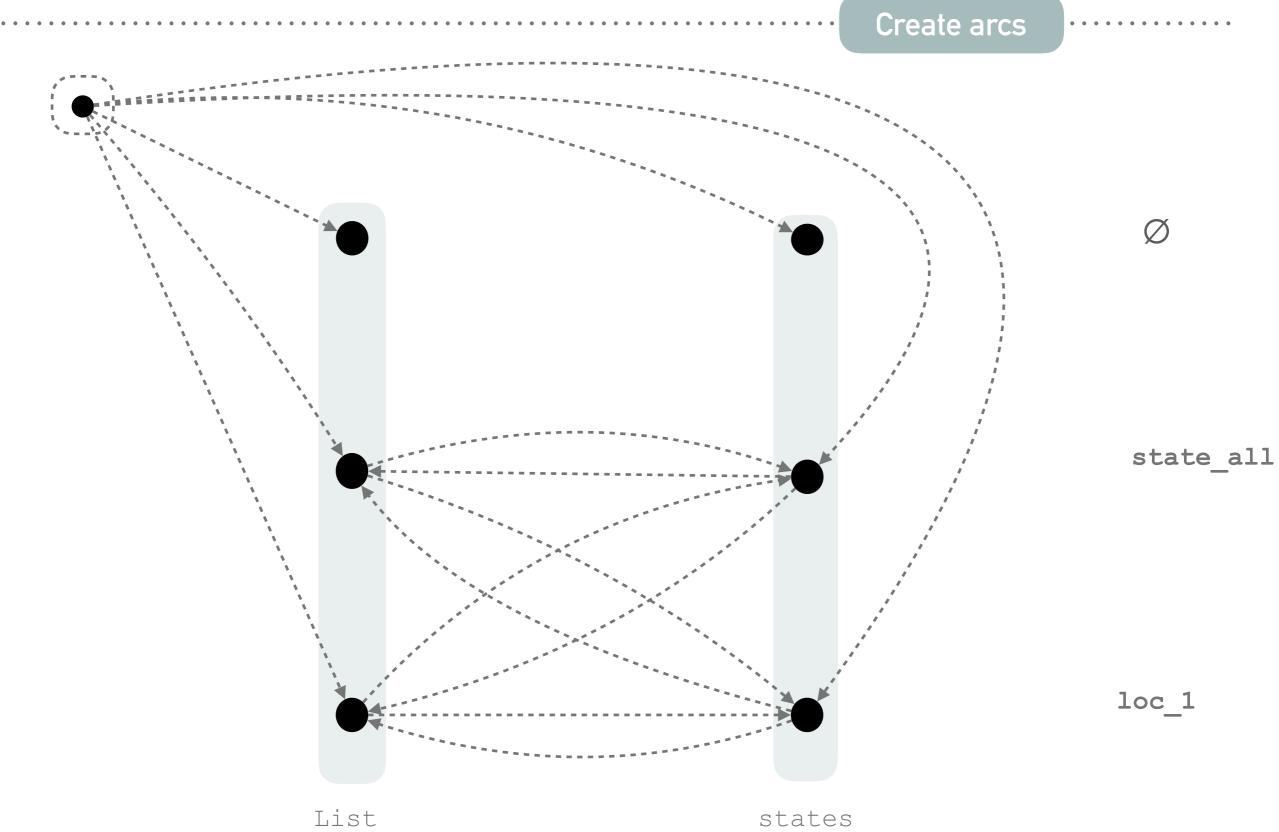
- ► The root must have exactly one outgoing arc to a non-empty entity/predicate
- ► The "empty entities" cannot have outgoing arcs in a solution

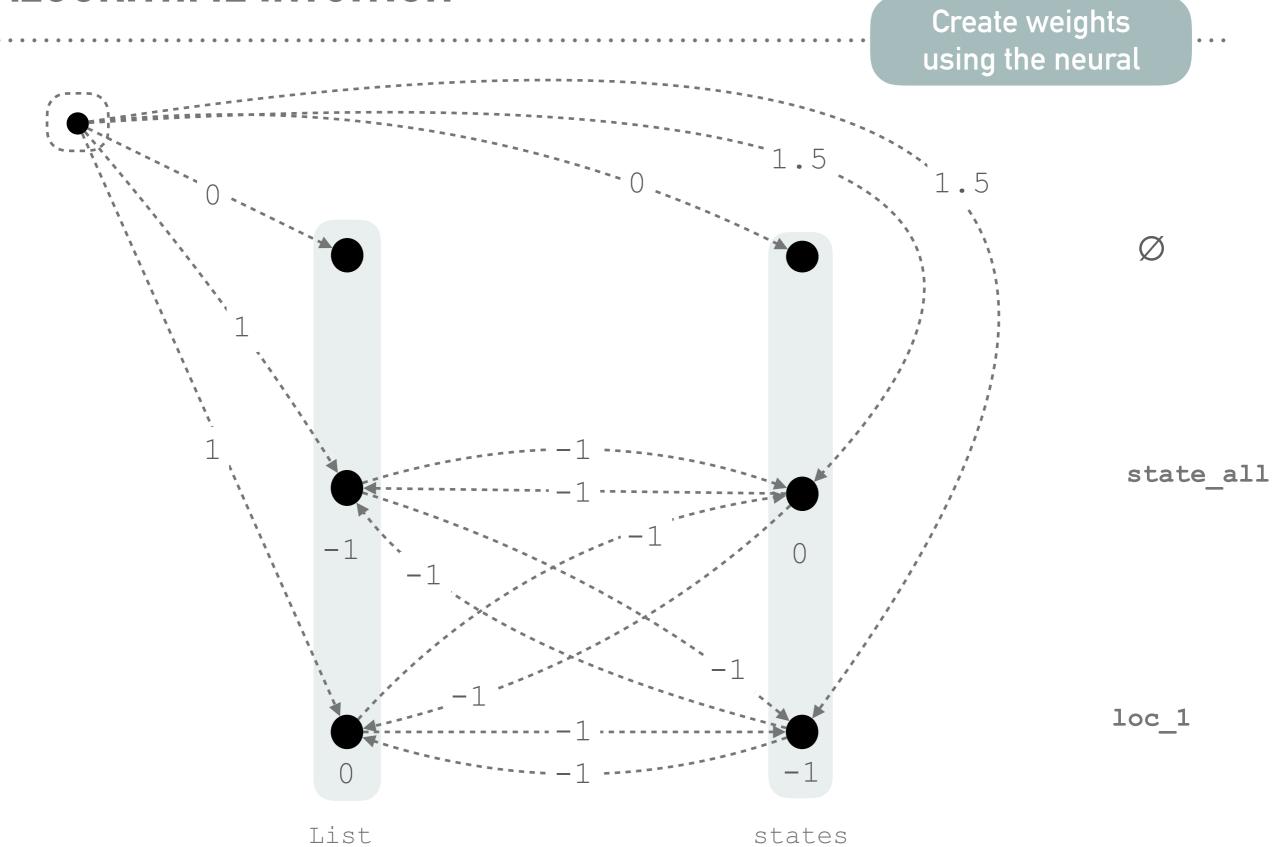


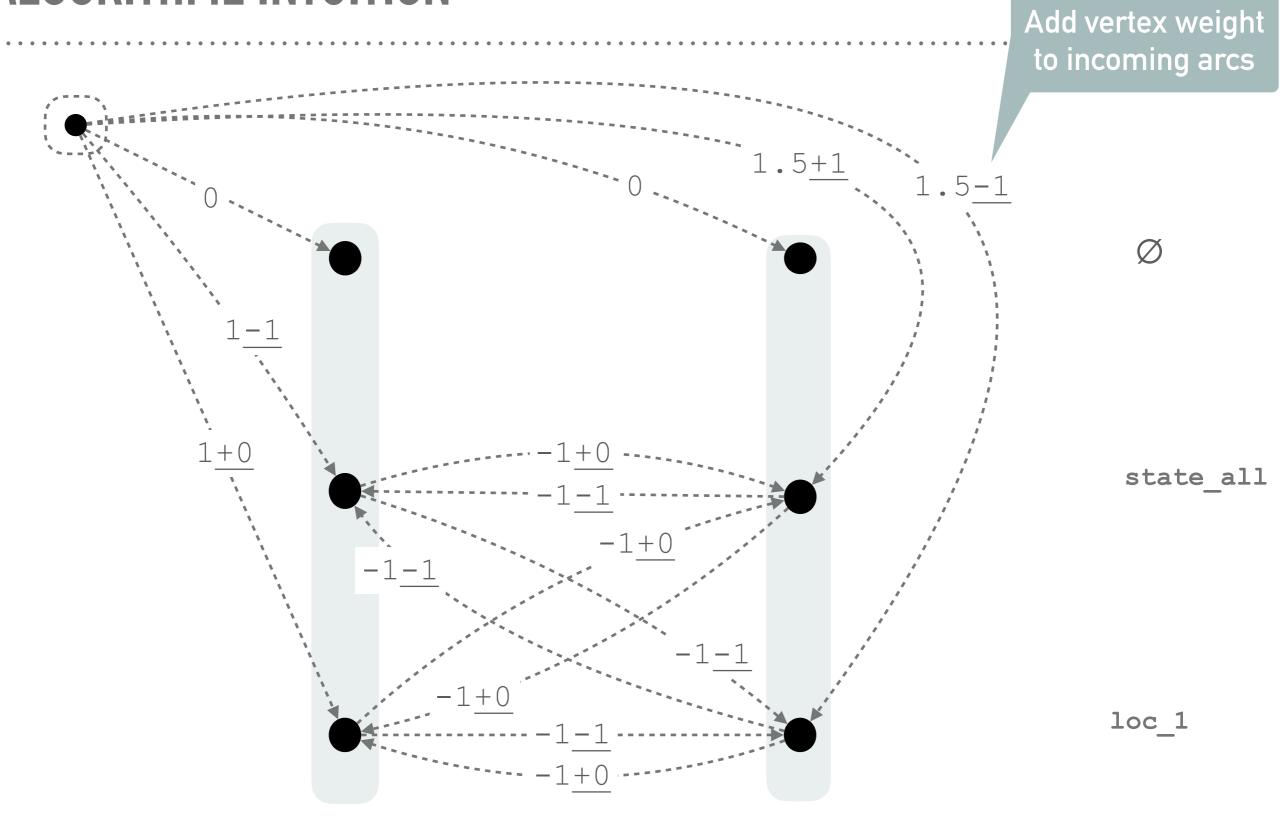
. .

Input sentence



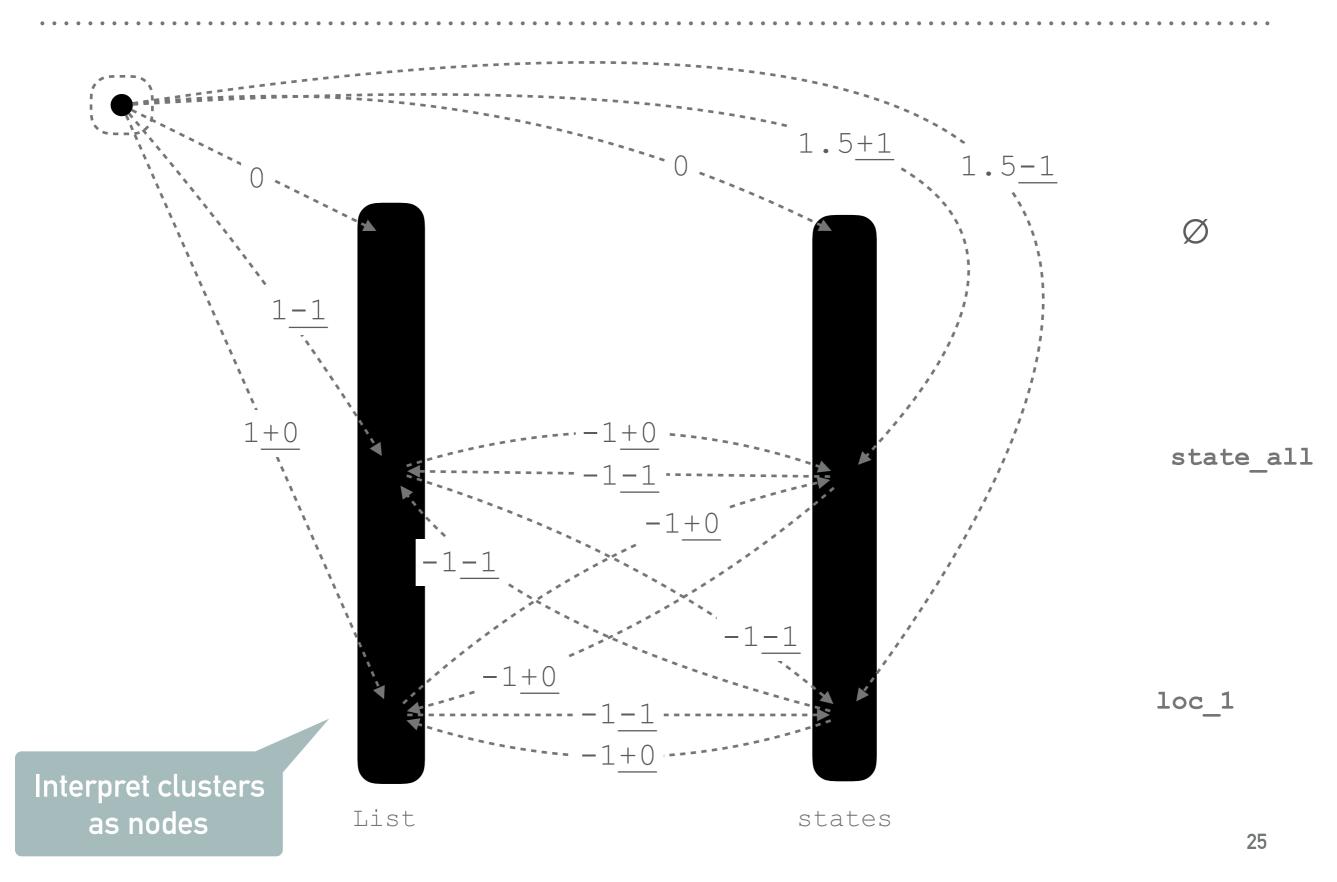


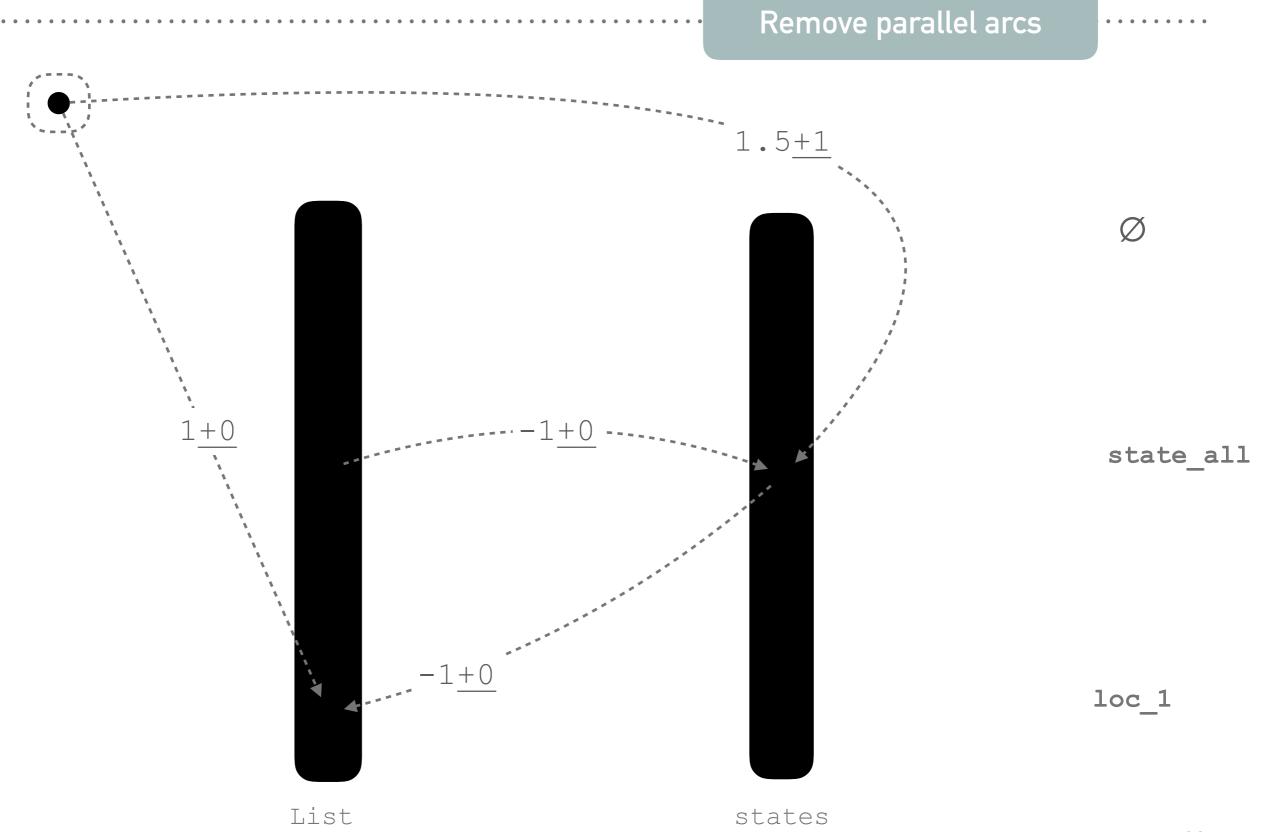




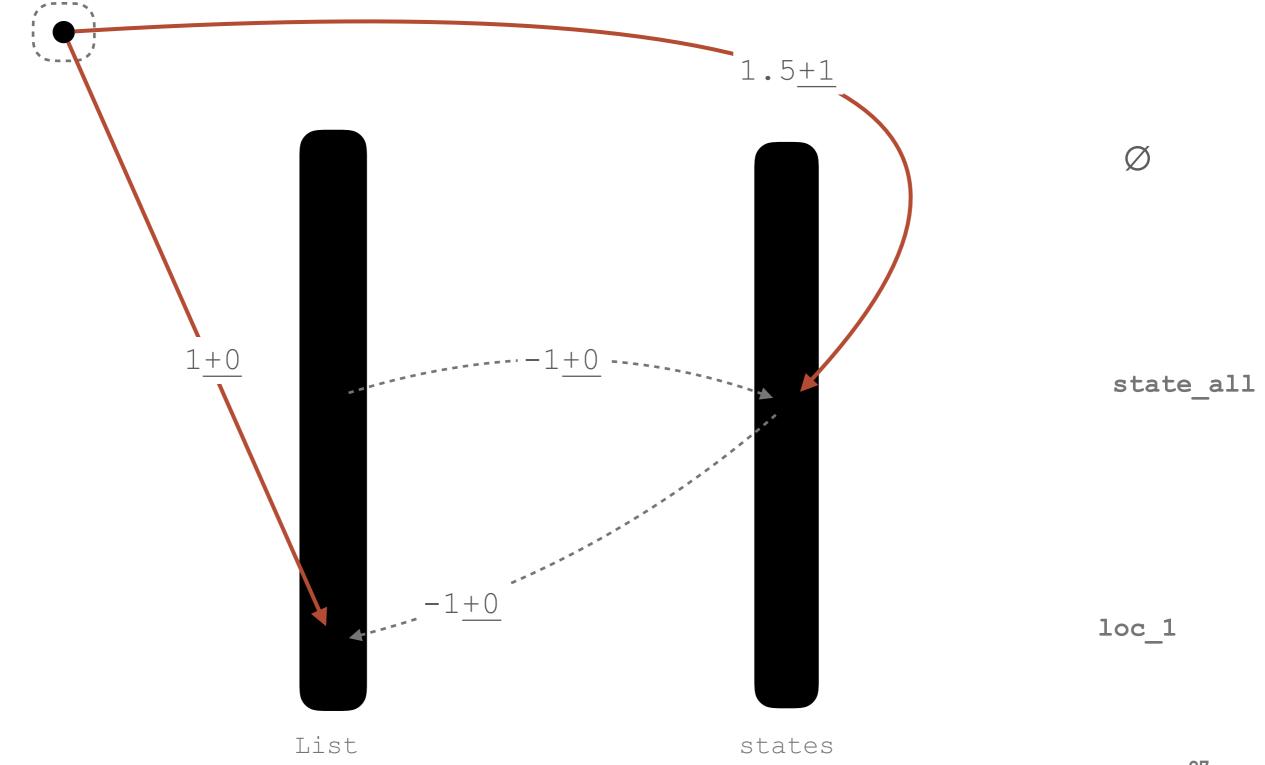


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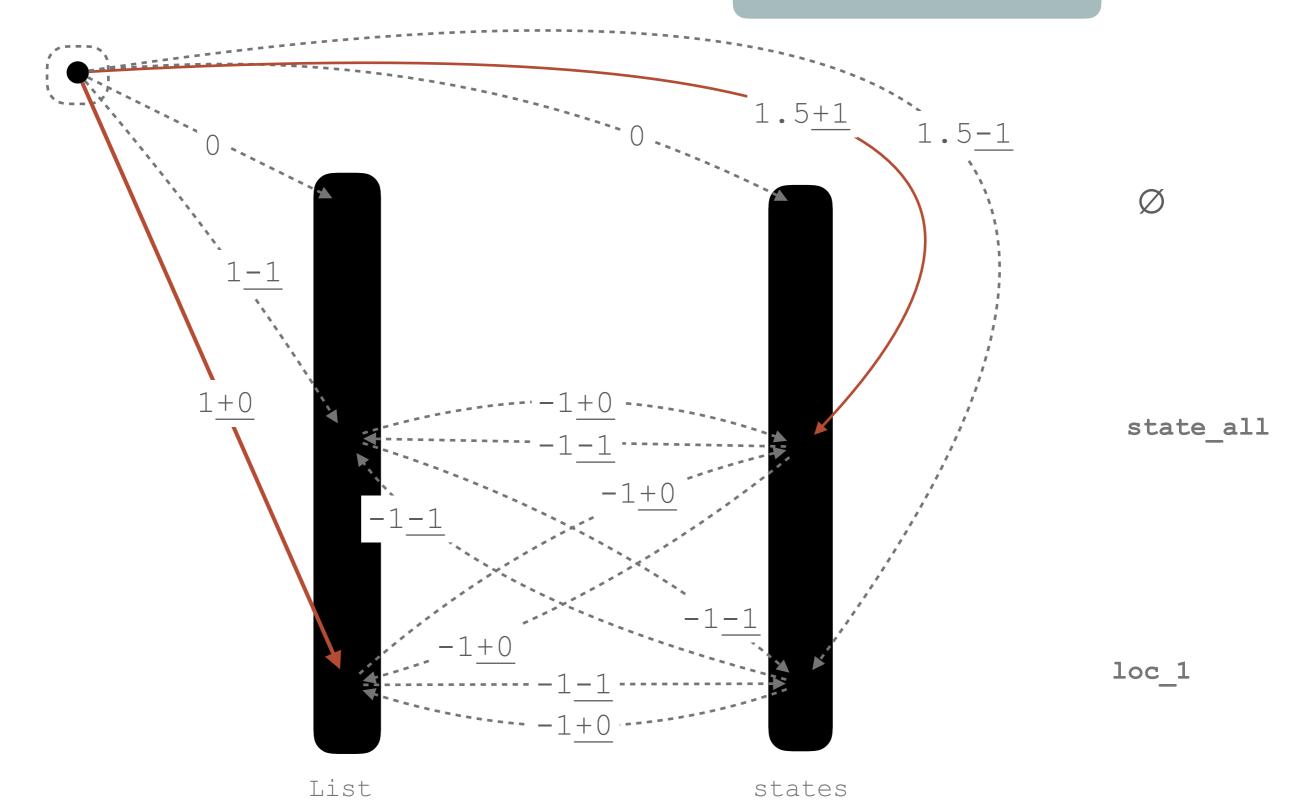


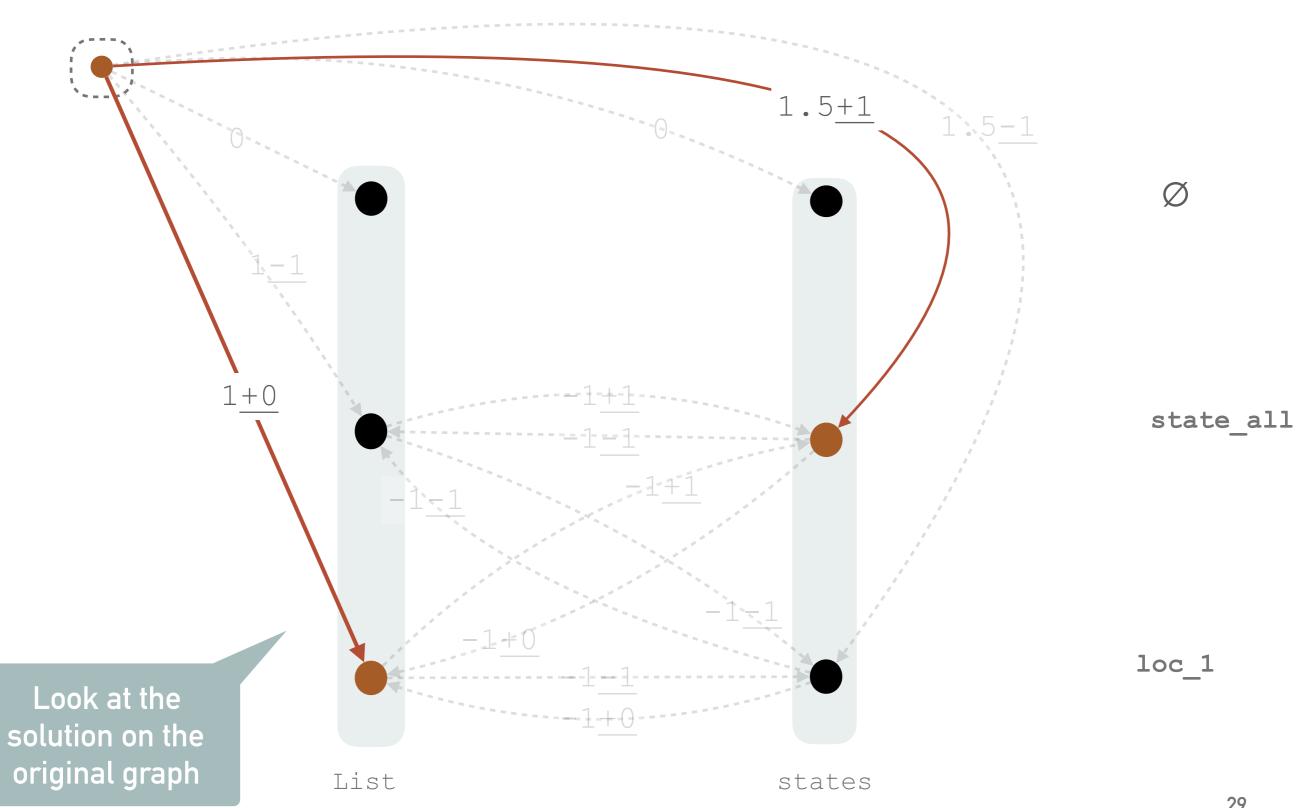


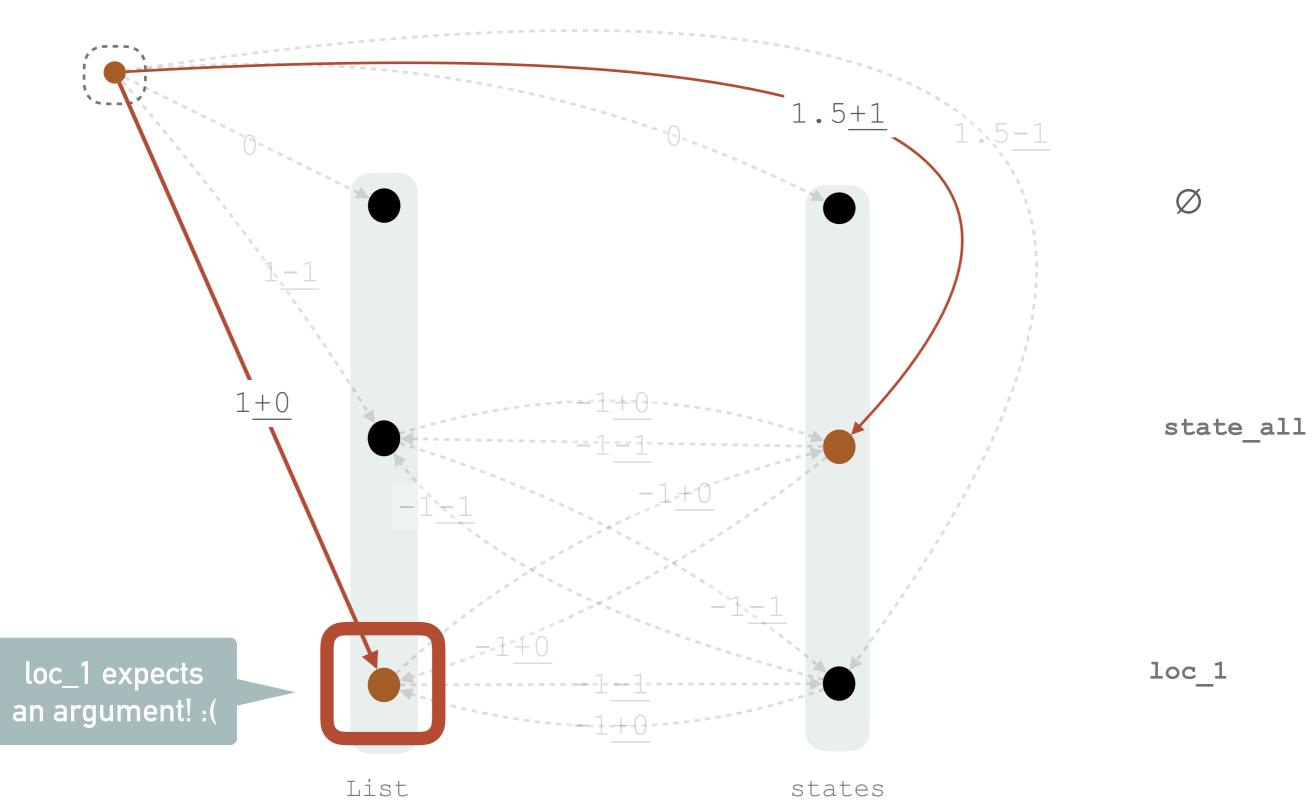
Compute the maximum spanning arborescence over clusters

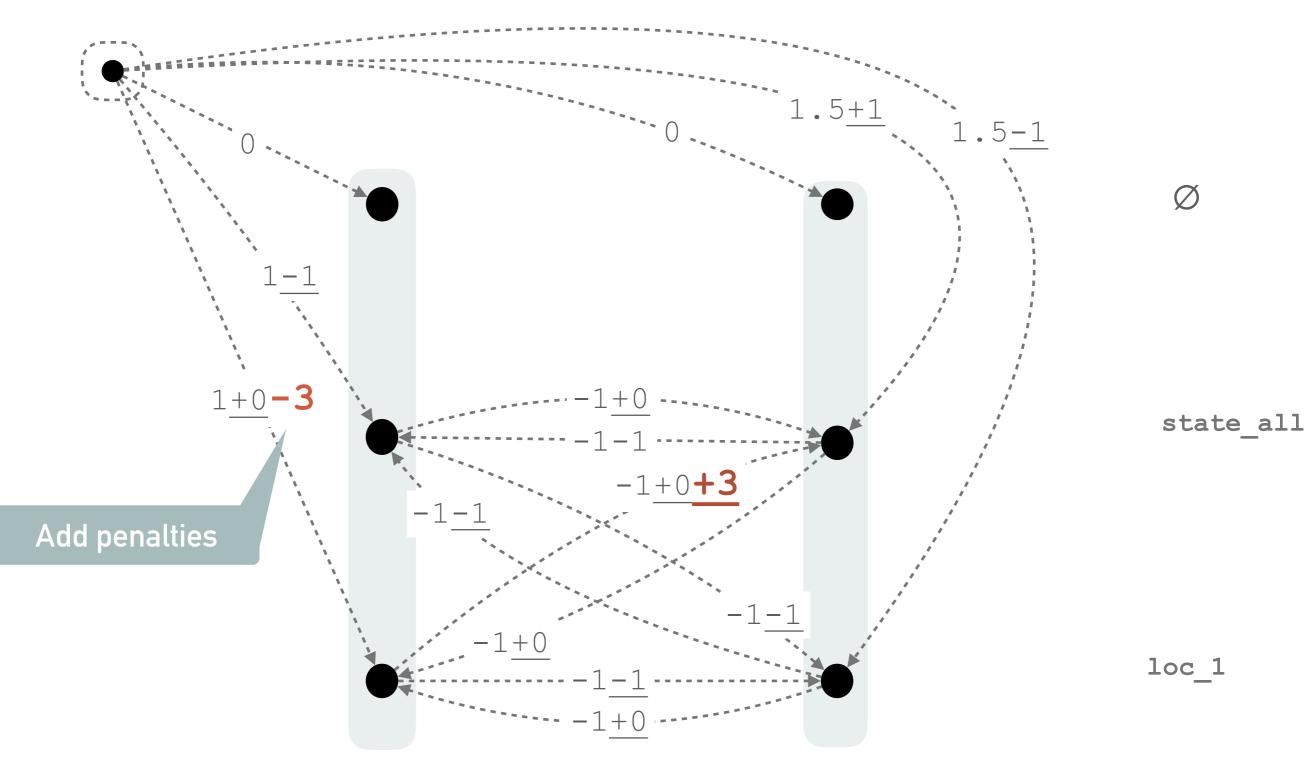


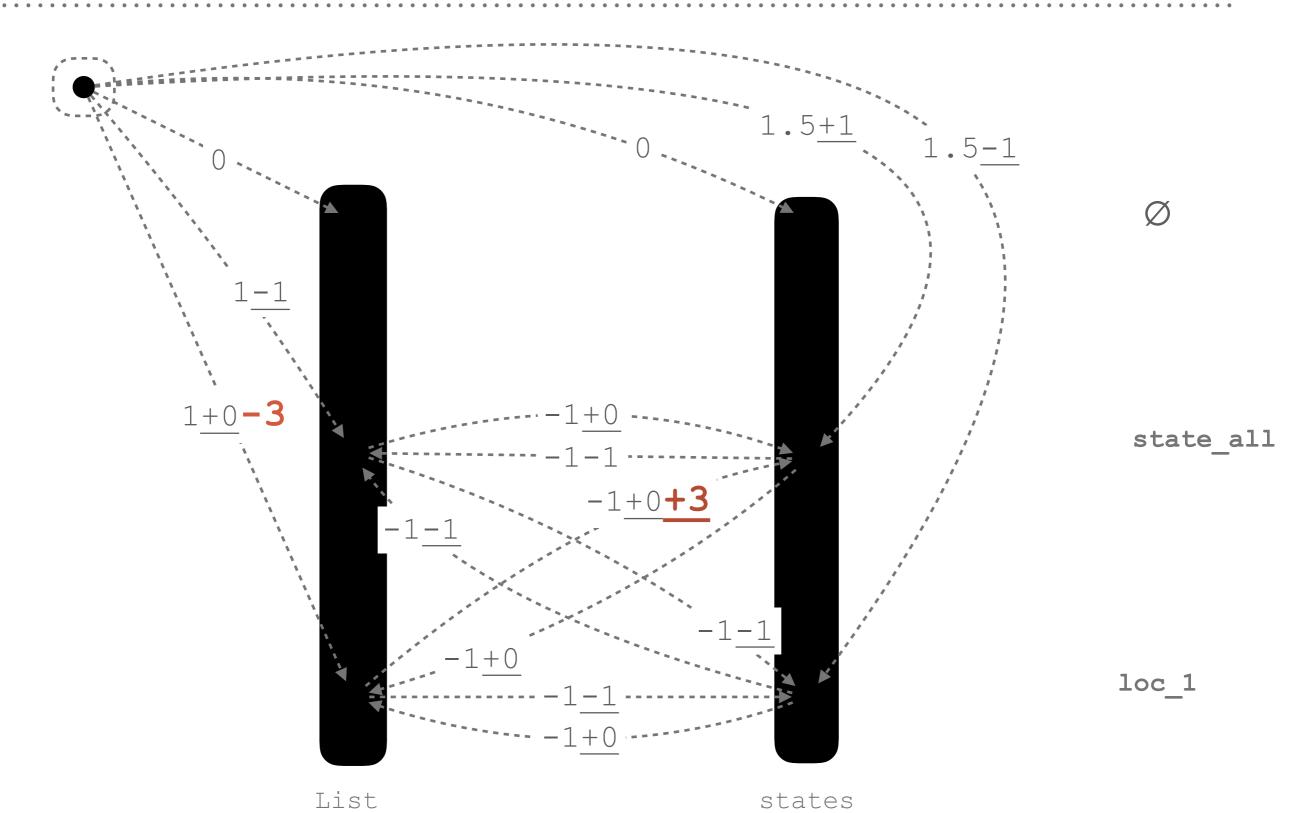
Reconstruct full graph

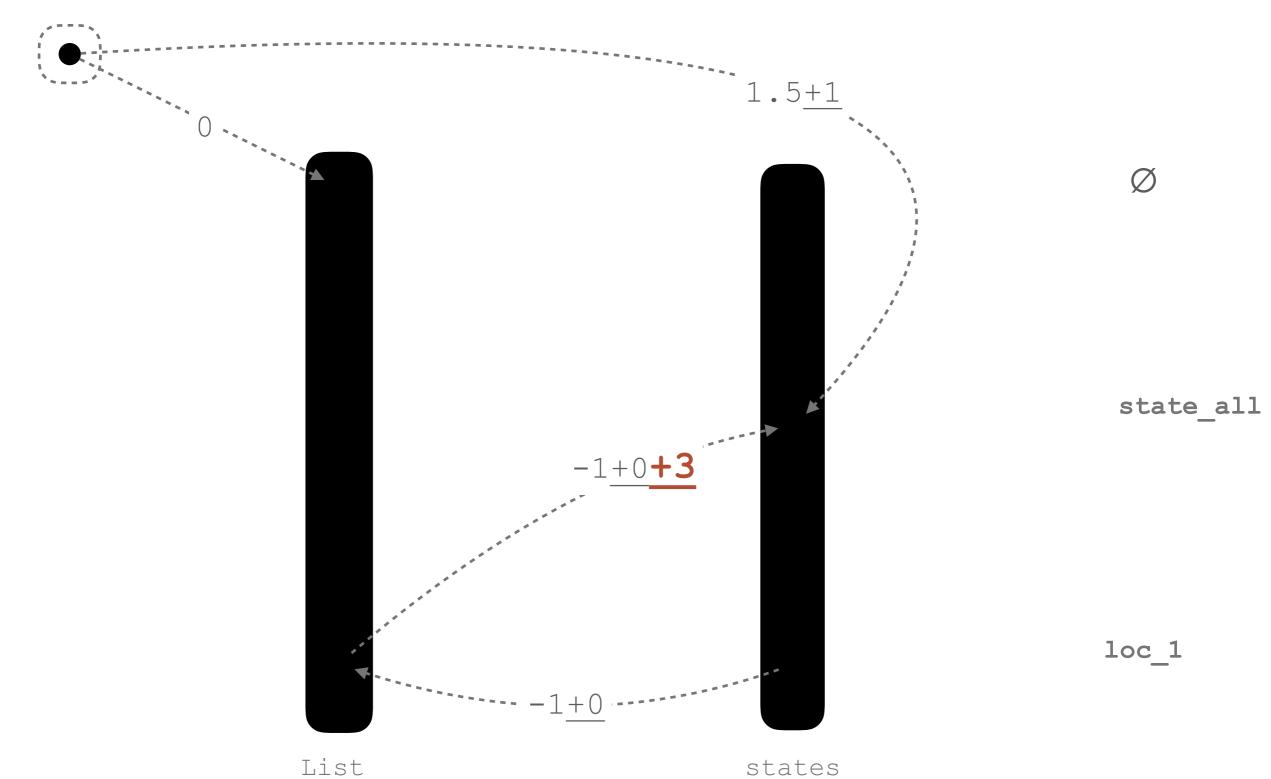


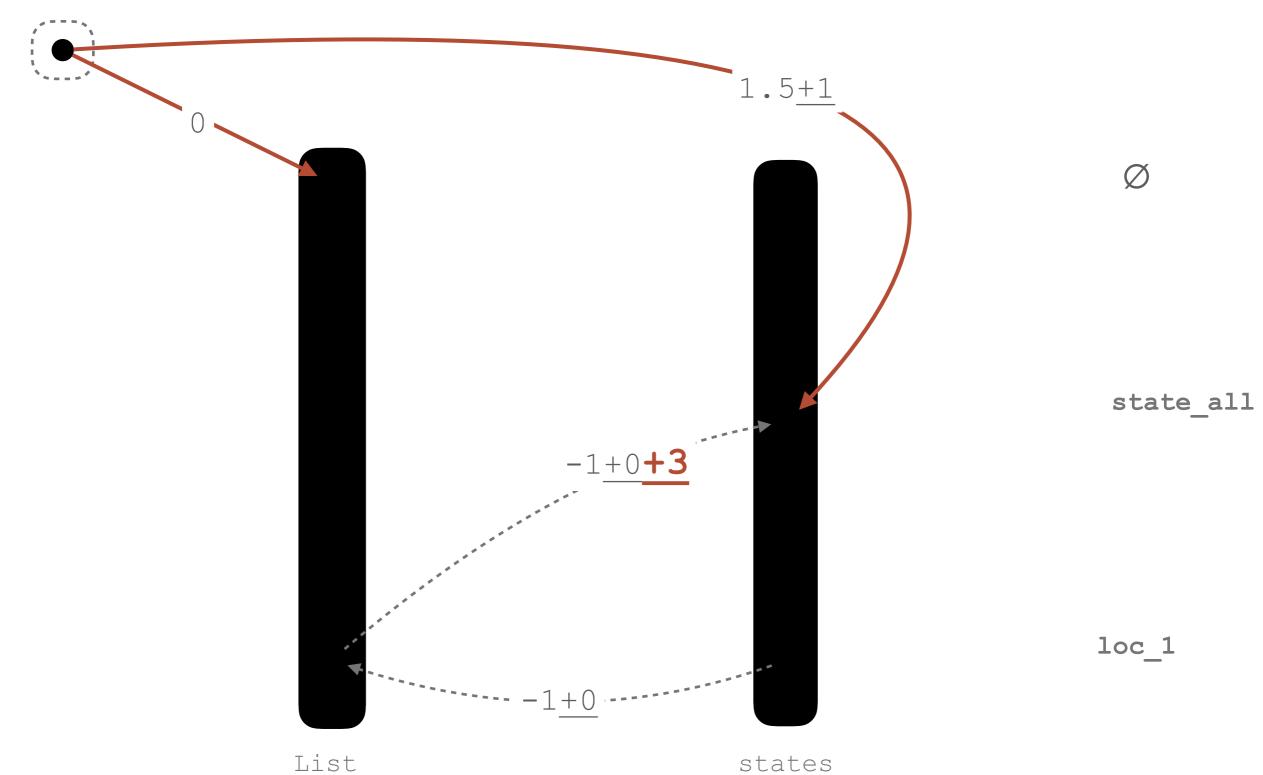


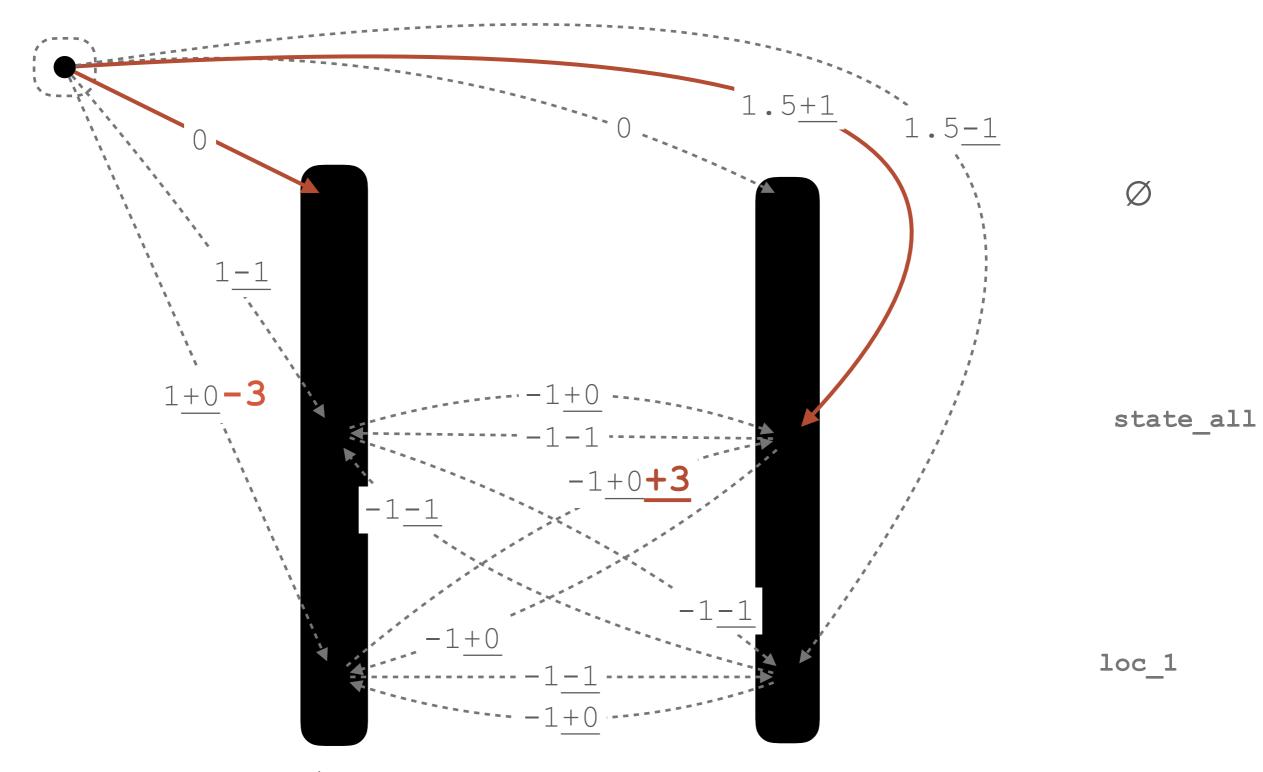


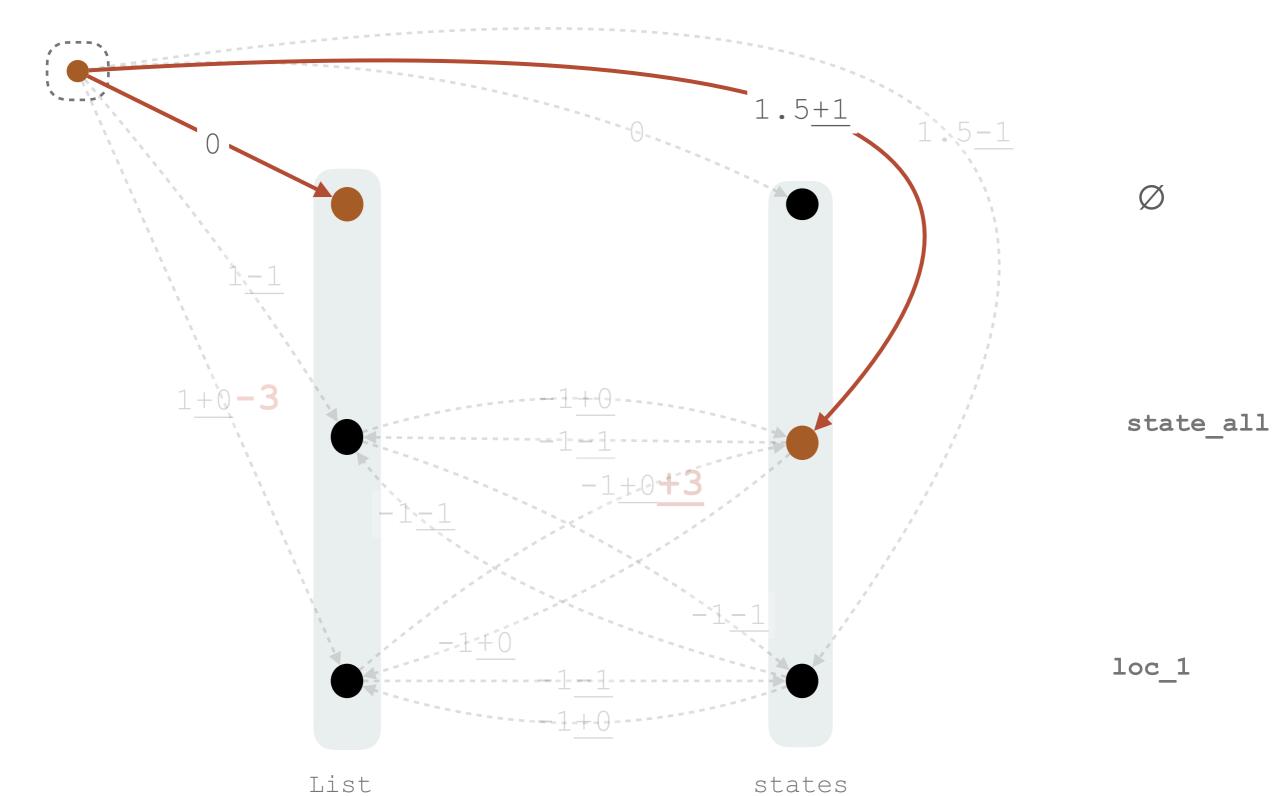


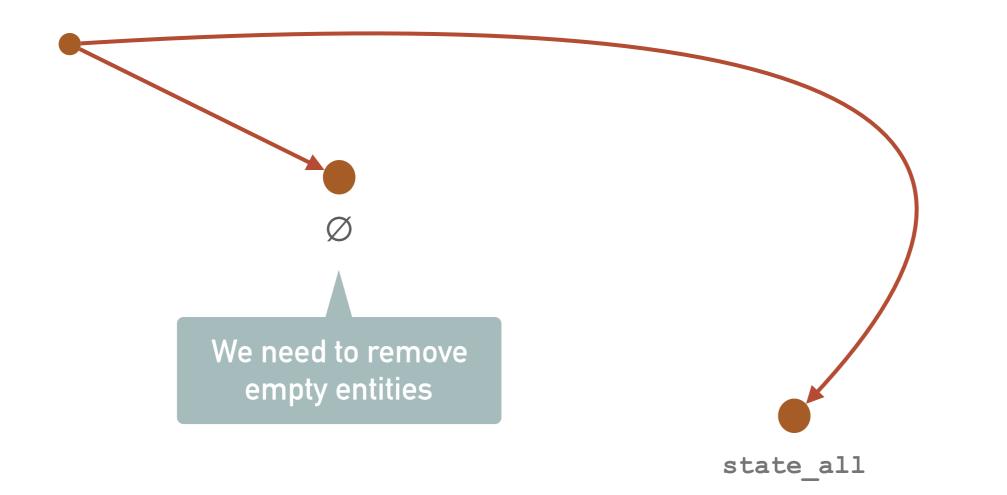


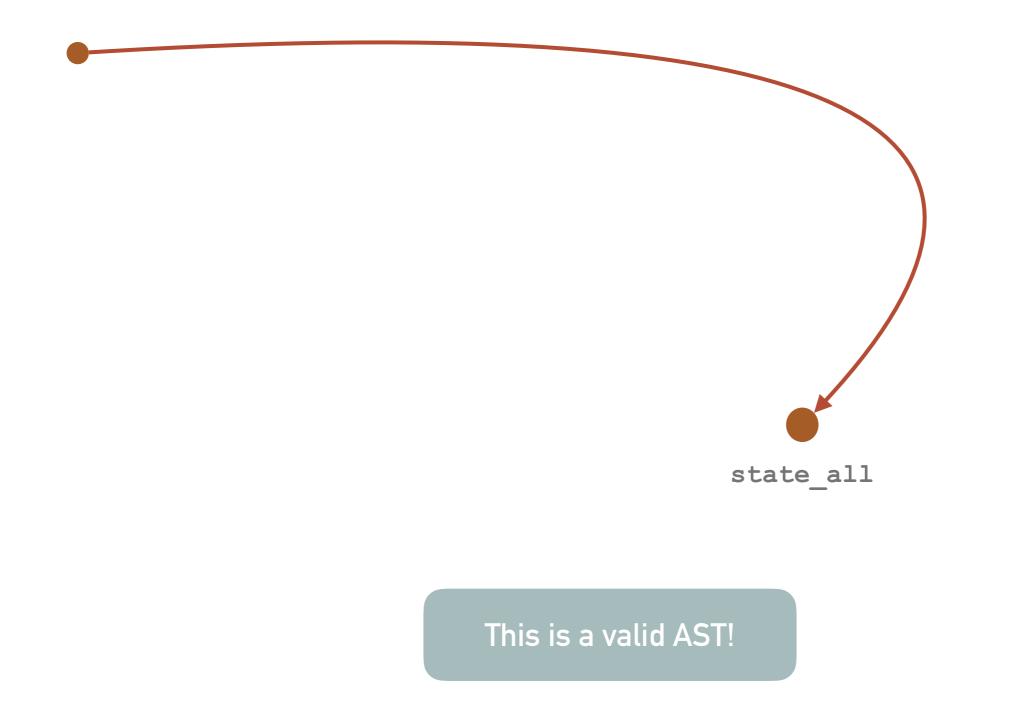












SUPERVISED LEARNING

NEGATIVE LOG-LIKELIHOOD

Notations

- Search space: directed graph G = (V, A) where V is the set of vertices and $A \subseteq V \times V$ is the set of arcs
- ► Vertex selection vector: $\mathbf{x} \in \{0,1\}^V$
- ► Arc selection vector: $\mathbf{y} \in \{0,1\}^A$
- ► Set of feasible solution (i.e. set of ASTs): $(\mathbf{x}, \mathbf{y}) \in \mathscr{C}$

Weight vectors

- ► Vertex weights: $\mu \in \mathbb{R}^V$
- ► Arc weights: $\phi \in \mathbb{R}^A$

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Boltzmann distribution over ASTs

Log-partition function

$$p_{\mu,\phi}(\mathbf{x},\mathbf{y}) = \begin{cases} \exp(\langle \mu, \mathbf{x} \rangle + \langle \phi, \mathbf{y} \rangle - c(\mu, \phi) \rangle) & \text{if } (\mathbf{x}, \mathbf{y}) \in \mathscr{C} \\ 0 & \text{otherwise,} \end{cases}$$

where

$$c(\mu, \phi) = \log \sum_{(\mathbf{x}', \mathbf{y}') \in \mathscr{C}} \exp\left(\langle \mu, \mathbf{x}' \rangle + \langle \phi, \mathbf{y}' \rangle\right)$$

NEGATIVE LOG-LIKELIHOOD

Boltzmann distribution over ASTs

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Negative log-likelihood loss

$$\begin{aligned} \ell(\mu, \phi; \mathbf{x}, \mathbf{y}) &= -\log p_{\mu, \phi}(\mathbf{x}, \mathbf{y}) \\ &= -\langle \mu, \mathbf{x} \rangle - \langle \phi, \mathbf{y} \rangle + c(\mu, \phi) \end{aligned}$$

(probably) intractable!

We cannot compute the loss function! :(

Change of notation

$$\mathbf{z} = \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} \qquad \theta = \begin{bmatrix} \mu \\ \phi \end{bmatrix} \qquad \qquad \mathcal{Z} = \{ \mathbf{z}^{(1)}, \mathbf{z}^{(1)}, \dots, \mathbf{z}^{(k)} \}$$

Change of notation

$$\mathbf{z} = \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} \qquad \theta = \begin{bmatrix} \mu \\ \phi \end{bmatrix} \qquad \qquad \mathcal{Z} = \{ \mathbf{z}^{(1)}, \mathbf{z}^{(1)}, \dots, \mathbf{z}^{(k)} \}$$

Upper bound on the log-partition function

$$c(\theta) = \log \sum_{\mathbf{z} \in \mathcal{Z}} \exp \langle \theta, \mathbf{z} \rangle$$

Change of notation

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Upper bound on the log-partition function

 $\mathbf{U} = \begin{bmatrix} z_1^{(1)}, & z_1^{(1)}, & \dots, & z_d^{(1)} \\ z_1^{(2)}, & z_1^{(2)}, & \dots, & z_d^{(2)} \\ \vdots & & & \\ z_1^{(k)}, & z_1^{(k)}, & \dots, & z_d^{(k)} \end{bmatrix}$ $c(\theta) = \log \sum \exp \langle \theta, \mathbf{z} \rangle$ z∈£ $= \max_{\mathbf{p} \in \triangle^k} \langle \mathbf{p}, \mathbf{U}\theta \rangle - \sum_i p_i \log p_i$ $=H[\mathbf{p}]$ Fenchel bi-conjugate $\mathbf{U}\boldsymbol{\theta} = \begin{bmatrix} \langle \mathbf{z}^{(1)}, \boldsymbol{\theta} \rangle \\ \langle \mathbf{z}^{(2)}, \boldsymbol{\theta} \rangle \\ \vdots \\ \langle \mathbf{z}^{(k)}, \boldsymbol{\theta} \rangle \end{bmatrix}$ Weight of each AST 42

Set of feasible ASTs

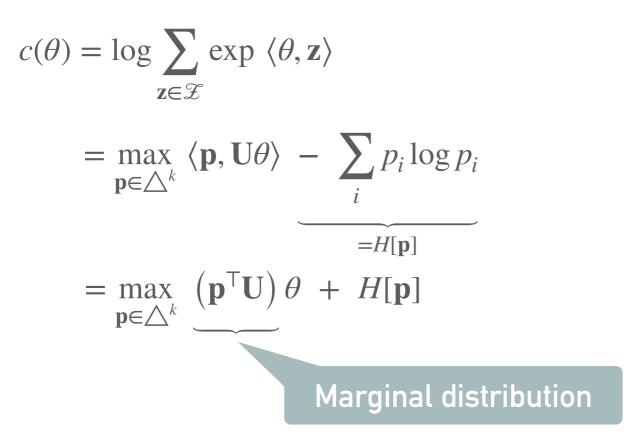
Each row is a

feasible AST

Change of notation

$$\mathbf{z} = \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \end{bmatrix} \qquad \theta = \begin{bmatrix} \mu \\ \phi \end{bmatrix} \qquad \qquad \mathcal{Z} = \{ \mathbf{z}^{(1)}, \mathbf{z}^{(1)}, \dots, \mathbf{z}^{(k)} \}$$

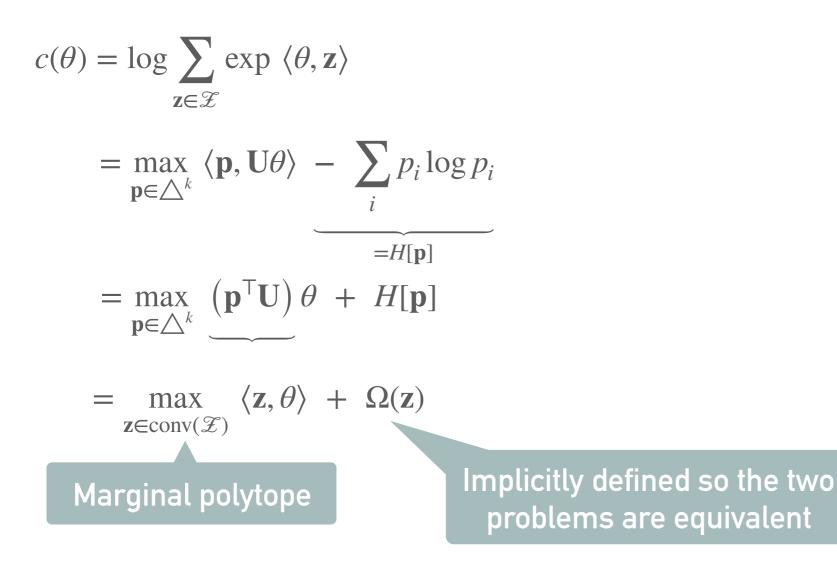
Upper bound on the log-partition function



Change of notation

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Upper bound on the log-partition function



Change of notation

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Upper bound on the log-partition function

$$c(\theta) = \log \sum_{\mathbf{z} \in \mathscr{X}} \exp \langle \theta, \mathbf{z} \rangle$$

$$= \max_{\mathbf{p} \in \Delta^{k}} \langle \mathbf{p}, \mathbf{U}\theta \rangle - \sum_{i} p_{i} \log p_{i}$$

$$= \max_{\mathbf{p} \in \Delta^{k}} (\mathbf{p}^{\mathsf{T}}\mathbf{U}) \theta + H[\mathbf{p}]$$

$$= \max_{\mathbf{z} \in \operatorname{conv}(\mathscr{X})} \langle \mathbf{z}, \theta \rangle + \Omega(\mathbf{z})$$

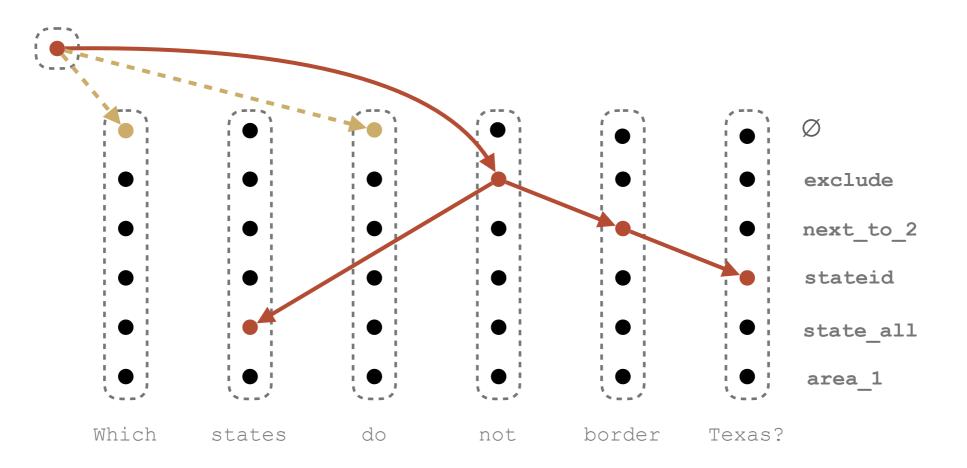
$$\leq \max_{\mathbf{z} \in \mathscr{X}} \langle \mathbf{z}, \theta \rangle + H(\mathbf{z})$$
Mean regularization
Outer approximation

Upper bound on the log-partition function

We need to choose \mathscr{L} such that the bound is easy to compute.

Note that each feasible solution in \mathscr{C} satisfies the following conditions:

- 1. Each cluster has exactly one selected vertex
- 2. Each cluster (except the root) has exactly one incoming arc



 $c(\theta) \le \max_{\mathbf{z} \in \mathscr{L}} \langle \mathbf{z}, \theta \rangle + H(\mathbf{z}) = \widetilde{c}(\theta)$

Upper bound on the log-partition function

We need to choose \mathscr{L} such that the bound is easy to compute.

Note that each feasible solution in \mathscr{C} satisfies the following conditions:

- 1. Each cluster has exactly one selected vertex
- 2. Each cluster (except the root) has exactly one incoming arc

Token-separable negative log-likelihood

Define \mathscr{L} as the convex hull of structures that satisfy (1) and (2), Then:

$$\ell(\mu,\phi;\mathbf{x},\mathbf{y}) \leq -\langle \mu,\mathbf{x}\rangle - \langle \phi,\mathbf{y}\rangle + \widetilde{c}(\mu,\phi)$$

is simply a sum of negative log-likelihood losses. For each cluster:

- ► One NLL over all vertices in the cluster
- ► One NLL over all incoming arcs in the cluster

 $c(\theta) \le \max_{\mathbf{z} \in \mathscr{L}} \langle \mathbf{z}, \theta \rangle + H(\mathbf{z}) = \widetilde{c}(\theta)$

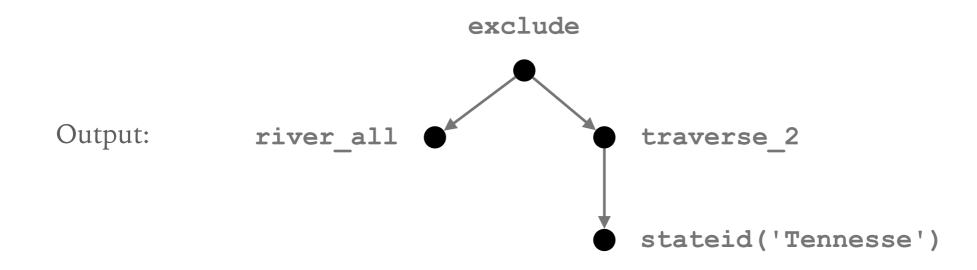
WEAKLY-SUPERVISED LEARNING

Annotation issue

In most dataset, the entities and predicates are not anchored!

Example

Input: What rivers do not run through Tennesse?



$$\begin{split} \widetilde{\ell}(\mu,\phi;\mathscr{C}^*) &= -\log\sum_{(\mathbf{x},\mathbf{y})\in\mathscr{C}^*} p_{\mu,\phi}(\mathbf{x},\mathbf{y}) = -\log\sum_{(\mathbf{x},\mathbf{y})\in\mathscr{C}^*} \exp\left(\langle \mu,\mathbf{x}\rangle + \langle \phi,\mathbf{y}\rangle - c(\mu,\phi)\right) \\ &= -\log\sum_{(\mathbf{x},\mathbf{y})\in\mathscr{C}^*} \exp\left(\langle \mu,\mathbf{x}\rangle + \langle \phi,\mathbf{y}\rangle\right) + c(\mu,\phi) \end{split}$$

. .

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$$\begin{split} \widetilde{\ell}(\mu,\phi;\mathscr{C}^*) &= -\log\sum_{(\mathbf{x},\mathbf{y})\in\mathscr{C}^*} p_{\mu,\phi}(\mathbf{x},\mathbf{y}) = -\log\sum_{(\mathbf{x},\mathbf{y})\in\mathscr{C}^*} \exp\left(\langle \mu,\mathbf{x}\rangle + \langle \phi,\mathbf{y}\rangle - c(\mu,\phi)\right) \\ &= -\log\sum_{(\mathbf{x},\mathbf{y})\in\mathscr{C}^*} \exp\left(\langle \mu,\mathbf{x}\rangle + \langle \phi,\mathbf{y}\rangle\right) + c(\mu,\phi) \end{split}$$

.

Lower bound on the first term

$$\log \sum_{(\mathbf{x},\mathbf{y})\in\mathscr{C}^*} \exp(\langle \mu,\mathbf{x}\rangle + \langle \phi,\mathbf{y}\rangle) = \log \sum_{(\mathbf{x},\mathbf{y})\in\mathscr{C}^*} \frac{q(\mathbf{x},\mathbf{y})}{q(\mathbf{x},\mathbf{y})} \exp(\langle \mu,\mathbf{x}\rangle + \langle \phi,\mathbf{y}\rangle)$$
Proposal distribution

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$$\begin{split} \widetilde{\ell}(\mu,\phi;\mathscr{C}^*) &= -\log\sum_{(\mathbf{x},\mathbf{y})\in\mathscr{C}^*} p_{\mu,\phi}(\mathbf{x},\mathbf{y}) = -\log\sum_{(\mathbf{x},\mathbf{y})\in\mathscr{C}^*} \exp\left(\langle \mu,\mathbf{x}\rangle + \langle \phi,\mathbf{y}\rangle - c(\mu,\phi)\right) \\ &= -\log\sum_{(\mathbf{x},\mathbf{y})\in\mathscr{C}^*} \exp\left(\langle \mu,\mathbf{x}\rangle + \langle \phi,\mathbf{y}\rangle\right) + c(\mu,\phi) \end{split}$$

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$$\geq \sum_{(\mathbf{x},\mathbf{y})\in\mathscr{C}^{*}} q(\mathbf{x},\mathbf{y}) \log \frac{\exp\left(\langle \mu, \mathbf{x} \rangle + \langle \phi, \mathbf{y} \rangle \right)}{q(\mathbf{x},\mathbf{y})}$$
Jensen's inequality

$$\begin{split} \widetilde{\ell}(\mu,\phi;\mathscr{C}^*) &= -\log\sum_{(\mathbf{x},\mathbf{y})\in\mathscr{C}^*} p_{\mu,\phi}(\mathbf{x},\mathbf{y}) = -\log\sum_{(\mathbf{x},\mathbf{y})\in\mathscr{C}^*} \exp\left(\langle \mu,\mathbf{x}\rangle + \langle \phi,\mathbf{y}\rangle - c(\mu,\phi)\right) \\ &= -\log\sum_{(\mathbf{x},\mathbf{y})\in\mathscr{C}^*} \exp\left(\langle \mu,\mathbf{x}\rangle + \langle \phi,\mathbf{y}\rangle\right) + c(\mu,\phi) \end{split}$$

Lower bound on the first term

$$\log \sum_{(\mathbf{x}, \mathbf{y}) \in \mathscr{C}^*} \exp\left(\langle \mu, \mathbf{x} \rangle + \langle \phi, \mathbf{y} \rangle\right) = \log \sum_{(\mathbf{x}, \mathbf{y}) \in \mathscr{C}^*} \frac{q(\mathbf{x}, \mathbf{y})}{q(\mathbf{x}, \mathbf{y})} \exp\left(\langle \mu, \mathbf{x} \rangle + \langle \phi, \mathbf{y} \rangle\right)$$
$$\geq \sum_{(\mathbf{x}, \mathbf{y}) \in \mathscr{C}^*} q(\mathbf{x}, \mathbf{y}) \log \frac{\exp\left(\langle \mu, \mathbf{x} \rangle + \langle \phi, \mathbf{y} \rangle\right)}{q(\mathbf{x}, \mathbf{y})}$$
$$= \mathbb{E}_q \left[\langle \mu, \mathbf{x} \rangle + \langle \phi, \mathbf{y} \rangle\right] + H[q]$$

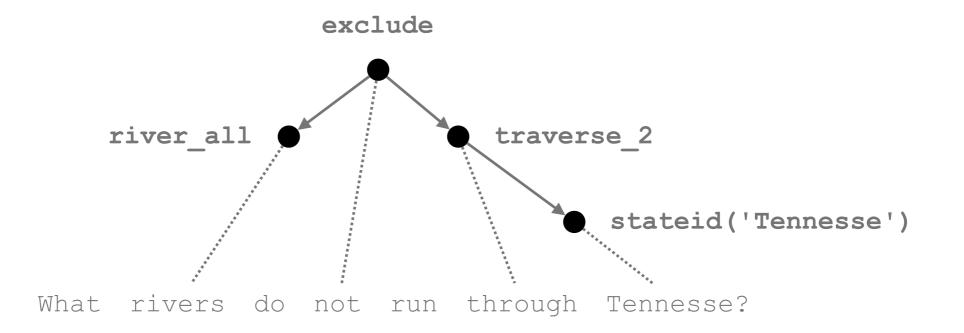
As usual:

- ► The bound is tight if q is equal to the posterior distribution, "à la" EM
- ► We can instead use a proposal that put all the mass on single value, "à la" hard EM

$$\widetilde{\mathscr{\ell}}(\mu,\phi;\mathscr{C}^*) = -\log \sum_{(\mathbf{x},\mathbf{y})\in\mathscr{C}^*} p_{\mu,\phi}(\mathbf{x},\mathbf{y}) \leq \mathbb{E}_q\left[\langle \mu,\mathbf{x} \rangle + \langle \phi,\mathbf{y} \rangle \right] + H[q] + \widetilde{c}(\mu,\phi)$$

Hard-EM like optimization

- ► (E step) Compute the best alignment between vertices in the AST and words in the sentence
- ► (M step) One gradient step on the neural network parameters



NP-hardness

The E step is a NP-hard problem => approximate solver based on constraint relaxation + dynamic programming

EXPERIMENTAL RESULTS

SCAN: Simplified version of the CommAI Navigation tasks [Lake & Baroni, 2018]

- ► Input : command
- ► Output : action sequence

```
jump ⇒ JUMP
jump left ⇒ LTURN JUMP
jump around right ⇒ RTURN JUMP RTURN JUMP RTURN JUMP RTURN JUMP
turn left twice ⇒ LTURN LTURN
jump thrice ⇒ JUMP JUMP
jump opposite left and walk thrice ⇒ LTURN LTURN JUMP WALK WALK WALK
jump opposite left after walk around left
⇒ LTURN WALK LTURN WALK LTURN WALK LTURN WALK LTURN JUMP
```

SCAN-SP

[Herzig & Berant, 2021]

Variant of scan where outputs are reformulated as functional programs

run around left twice and jump left
⇒ i_and (i_twice (i_run (i_left , i_around)) , i_jump (i_left))

SCAN : IID

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Random split of the data

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SCAN : IID

Random split of the data

SCAN : Right

- ➤ The term "right" is never seen without a manner adverbs (around, opposite) during training
- The model must learn to generalize to the simplest usage of right (as seen during training for "left")

Train		Test		
jump	left	jump	right	
turn	left	turn	right	
jump	around left	• • •		
jump	around right			
turn	opposite right			
turn	around left			

.

SCAN : IID

Random split of the data

SCAN : Right

- ➤ The term "right" is never seen without a manner adverbs (around, opposite) during training
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SCAN : Around right

- ➤ Test test set contains all exemple with "around right"
- ► The train set contains all other examples

	Train		Test	
jump	left	jump	around	right
jump	right	turn	around	right
jump	around left	• • •		
jump	opposite right			
turn	opposite right			
turn	around left			

.

SCAN : IID

Random split of the data

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- ➤ Test test set contains all exemple with "around right"
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	train	dev	test
IID	13 383	3 345	4 182
Right	12 180	3 045	4 476
ARight	12 180	3 045	4 476

GeoQuery

- Input: question related to USA geography
- Output: query that can be executed against a database

```
what state has the largest city? → answer(state(loc_1(largest(city(all)))))
how many square kilometers in the us? → answer(area_1(countryid('usa')))
```

GeoQuery

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• • •

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```

SCAN : IID

Random split of the data

SCAN : Template

All sentences that shares the same semantic template are used only for training or only for testing.

name the rivers in arkansas name all the rivers in colorado name all the rivers in colorado rivers in new york ? what are all the rivers in texas ?

GeoQuery

- ► Input: question related to USA geography
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```

SCAN : IID

Random split of the data

SCAN : Template

All sentences that shares the same semantic template are used only for training or only for testing.

SCAN : Length

Test sentences are (in average) longer than train sentences

Train

- ► sentence length: min=4 / max=13 / mean=7.5
- ► program length: min=1 / max=4 / mean=3.1

Test

- sentence length: min=7 / max=18 / mean=10.5
- program length: min=2 / max=9 / mean=5.2

GeoQuery

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SCAN : IID

Random split of the data

SCAN : Template

All sentences that shares the same semantic template are used only for training or only for testing.

SCAN : Length

Test sentences are (in average) longer than train sentences

	train	dev	test
IID	540	60	280
Template	544	60	276
Length	540	60	280

Clevr

- ► Input: question related to objects in a picture
- Output: query that can be executed against a database

Are there any shiny objects that have the same color as the matte block?

⇒ exist(filter(metal,relate_att_eq(color,filter(rubber,cube,scene()))))

Clevr

- ► Input: question related to objects in a picture
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SCAN : IID

Random split of the data

SCAN : Closure

- ► Questions in Clevr are generated from 80 templates
- ► Questions in Closure are generated from 7 new templates

Clevr

- ► Input: question related to objects in a picture
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Random split of the data

SCAN : Closure

- ► Questions in Clevr are generated from 80 templates
- ► Questions in Closure are generated from 7 new templates

	train	dev	test	
IID	694 689	5 000	149 991	
Closure	694 689	5 000	25 200	

EXPERIMENTAL RESULTS

		SCAN		GeoQuery		CLEVR		
	Iid	RIGHT	ARIGHT	IID	TEMPLATE	Length	IID	CLOSURE
Baselines (denotation	n accuracy	only)						
SEQ2SEQ	99.9	11.6	0	78.5	46.0	24.3	100	59.5
+ ELMO	100	54.9	41.6	79.3	50.0	25.7	100	64.2
BERT2SEQ	100	77.7	95.3	81.1	49.6	26.1	100	56.4
GRAMMAR	100	0.0	4.2	72.1	54.0	24.6	100	51.3
BART	100	50.5	100	87.1	67.0	19.3	100	51.5
S PAN B ASED S P	100	100	100	86.1	82.2	63.6	96.7	98.8

All baselines are from [Herzig & Berant, 2021]

EXPERIMENTAL RESULTS

		SCAN		GEOQUERY		CLEVR		
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BART	100	50.5	100	87.1	67.0	19.3	100	51.5
SPANBASEDSP	100	100	100	86.1	82.2	63.6	96.7	98.8
Our approach								
Denotation accuracy	100	100	100	92.9	89.9	74.9	100	99.6
└ Corrected executor				91.8	88.7	74.5		
Exact match	100	100	100	90.7	86.2	69.3	100	99.6
↓ w/o CPLEX heuristic	100	100	100	90.0	83.0	67.5	100	98.0

Neural network

BERT-base + BiLSTM + Biaffine (details in the appendix of the paper)

Related publication

On the inconsistency of separable losses for structured prediction

Caio Corro

EACL 2023

LOSS FUNCTIONS AND BAYES CONSISTENCY

Motivations

We approximate the log-partition function in the loss,

.

how does this impact the solution of the training problem?

LOSS FUNCTIONS AND BAYES CONSISTENCY

Motivations

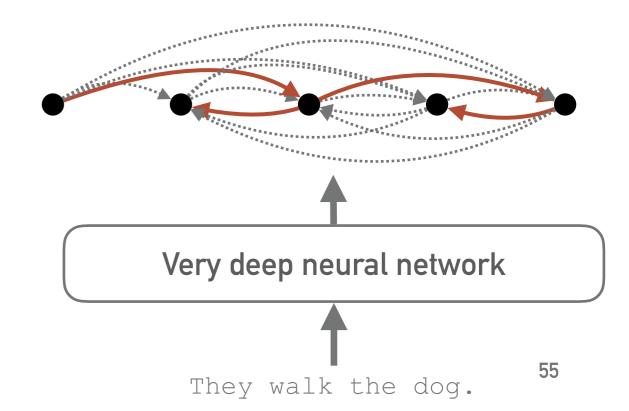
We approximate the log-partition function in the loss,

how does this impact the solution of the training problem?

Simpler example: syntactic dependency parsing

- > Compute the maximum spanning arborescence : $\mathcal{O}(n^2)$ [Tarjan, 1977]
- Summing over all arborescences : $\mathcal{O}(n^3)$ (via the matrix tree theorem, MTT)
 - Numerically instable (matrix inversion)
 - ► Not very fast on GPU compared to simpler losses
 - ► Non-trivial to implement

[Koo et al., 2007] [McDonald & Satta, 2007] [Smith & Smith, 2007]



LOSS FUNCTIONS AND BAYES CONSISTENCY

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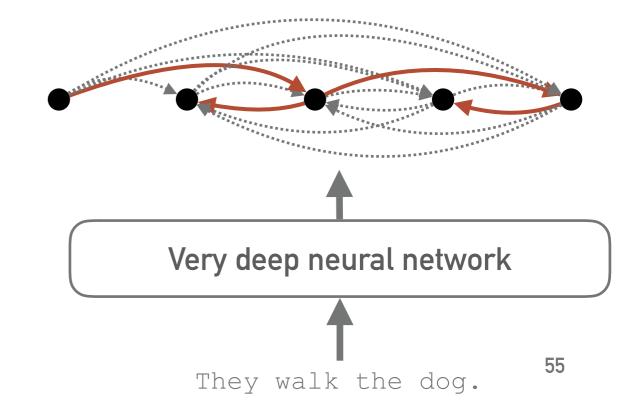
Head selection loss [Zhang et al., 2017]

As each word has exactly one head

=> one multi-class classification loss per word





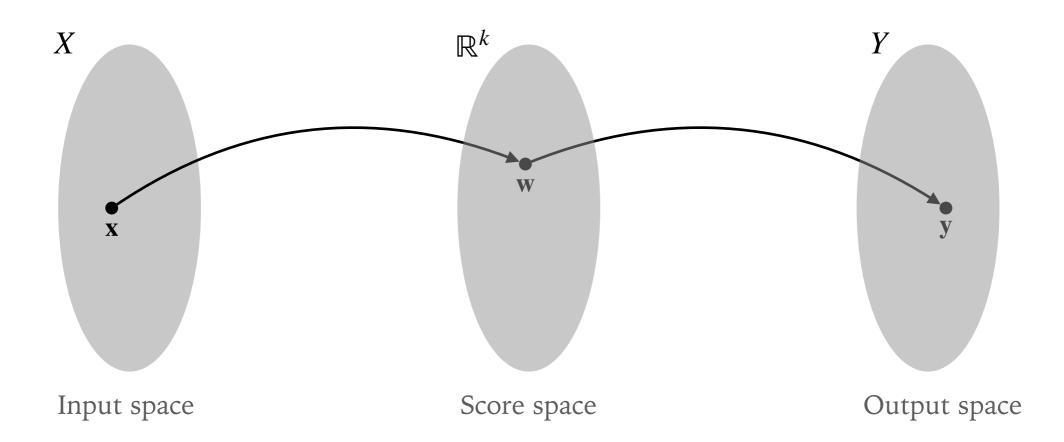


MULTICLASS CLASSIFICATION

Notations

► Y

- $\succ k$: number of classes
- $\succ X$: input space
 - : output space, set of one-hot vectors of dimension k
- ► $f: X \to \mathbb{R}^k$: scoring function
- ► $\hat{\mathbf{y}} : \mathbb{R}^k \to Y$: prediction function, $\hat{\mathbf{y}}(\mathbf{w}) = \arg \max_{\mathbf{y} \in Y} \langle \mathbf{w}, \mathbf{y} \rangle$



0-1 loss function

Returns 1 if the output will be incorrect for a given score vector

$$\mathscr{E}: \mathbb{R}^k \times Y \to \mathbb{R}_+ \qquad \qquad \mathscr{E}(\mathbf{w}, \mathbf{y}) = \begin{cases} 0 & \text{if } \mathbf{y} \in \arg\max_{\mathbf{y}' \in Y} \langle \mathbf{y}', \mathbf{w} \rangle, \\ 1 & \text{otherwise.} \end{cases}$$

0-1 loss function

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Optimal Bayes risk

$$r^{*} = \inf_{f \in F} r(f) = \inf_{f \in F} \mathbb{E}_{\mathbf{x}, \mathbf{y}} [\ell(f(\mathbf{x}), \mathbf{y})] = \mathbb{E}_{\mathbf{x}} [1 - \max_{\mathbf{y} \in Y} p(\mathbf{y} | \mathbf{x})]$$

Optimal Bayes risk

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$$\ell: \mathbb{R}^k \times Y \to \mathbb{R}_+ \qquad \qquad \ell(\mathbf{w}, \mathbf{y}) = \begin{cases} 0 & \text{if } \mathbf{y} \in \arg\max_{\mathbf{y}' \in Y} \langle \mathbf{y}', \mathbf{w} \rangle, \\ 1 & \text{otherwise.} \end{cases}$$

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Bayes risk of f

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Training objective!

0-1 loss function

Returns 1 if the output will be incorrect for a given score vector

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Bayes risk when we predict the most probable output for each input

0-1 loss function

Returns 1 if the output will be incorrect for a given score vector

$$\ell: \mathbb{R}^k \times Y \to \mathbb{R}_+ \qquad \qquad \ell(\mathbf{w}, \mathbf{y}) = \begin{cases} 0 & \text{if } \mathbf{y} \in \arg\max_{\mathbf{y}' \in Y} \langle \mathbf{y}', \mathbf{w} \rangle, \\ 1 & \text{otherwise.} \end{cases}$$

Optimal Bayes risk

Given a set of scoring function F, what is minimum average number of error we can obtain?

$$r^* = \inf_{\mathbf{f} \in F} r(f) = \inf_{f \in F} \mathbb{E}_{\mathbf{x}, \mathbf{y}} [\ell(f(\mathbf{x}), \mathbf{y})] = \mathbb{E}_{\mathbf{x}} [1 - \max_{\mathbf{y} \in Y} p(\mathbf{y} | \mathbf{x})]$$

Bayes risk minimization

- ► The 0-1 loss function is not convex in **W**
- ► The derivatives of the objective are null a.e.
- ► The problem is know to be intractable even in simple cases

SURROGATE LOSSES

Motivations

We can not use the 0-1 loss ℓ for training, therefore we want to use a surrogate loss ℓ , are solutions of the surrogate training problem <u>optimal Bayes classifiers</u>?

SURROGATE LOSSES

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Surrogate risk

$$\widetilde{r}^* = \inf_{\mathbf{f} \in F} \widetilde{r}(f) = \inf_{f \in F} \mathbb{E}_{\mathbf{x},\mathbf{y}} [\widetilde{\ell}(f(\mathbf{x}),\mathbf{y})]$$

SURROGATE LOSSES

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$$\widetilde{r}^* = \inf_{\mathbf{f} \in F} \widetilde{r}(f) = \inf_{f \in F} \mathbb{E}_{\mathbf{x},\mathbf{y}}[\widetilde{\ell}(f(\mathbf{x}),\mathbf{y})]$$

Bayes consistency

A surrogate loss $\widetilde{\ell}$ is said to be Bayes consistent / Fisher consistent / classification calibrated if:

$$f^* \in \arg\min_{f \in F} \widetilde{r}(f) \implies r(f^*) = r^*$$

POINTWISE CONSISTENCY

Standard assumptions

- ► F is the set of all measurable mappings
- ► Infinite number of training datapoints (i.e. expectation over the "true" data distribution)

Pointwise setting

- ► Choose a datapoint $\mathbf{x} \in X$ such that $p(\mathbf{x}) > 0$
- > Redefine the Bayes and surrogate risks as expectation over the conditional distribution $p(\mathbf{y} | \mathbf{x})$
- ► Minimize over the score vector $\mathbf{w} \in \mathbb{R}^k$ instead of over function set F, where $\mathbf{w} = f(\mathbf{x})$

$$r^* = \inf_{\mathbf{w} \in \mathbb{R}^k} r(\mathbf{w}) = \inf_{\mathbf{w} \in \mathbb{R}^k} \mathbb{E}_{\mathbf{y} \mid \mathbf{x}} [\ell(\mathbf{w}, \mathbf{y})] = 1 - \max_{\mathbf{y} \in Y} p(\mathbf{y} \mid \mathbf{x})$$

$$\widetilde{r}^* = \inf_{\mathbf{w}\in\mathbb{R}^k} \widetilde{r}(\mathbf{w}) = \inf_{\mathbf{w}\in\mathbb{R}^k} \mathbb{E}_{\mathbf{y}|\mathbf{x}} [\widetilde{\ell}(\mathbf{w},\mathbf{y})]$$

Negative log-likelihood loss

.

$$\widetilde{\ell}(\mathbf{w}, \mathbf{y}) = -\langle \mathbf{w}, \mathbf{y} \rangle + \log \sum_{\mathbf{y}' \in Y} \exp\langle \mathbf{w}, \mathbf{y}' \rangle = -\langle \mathbf{w}, \mathbf{y} \rangle + c(\mathbf{w})$$

Negative log-likelihood loss

$$\widetilde{\ell}(\mathbf{w}, \mathbf{y}) = -\langle \mathbf{w}, \mathbf{y} \rangle + \log \sum_{\mathbf{y}' \in Y} \exp\langle \mathbf{w}, \mathbf{y}' \rangle = -\langle \mathbf{w}, \mathbf{y} \rangle + c(\mathbf{w})$$

Surrogate risk

.

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$$= \inf_{\mathbf{w}\in\mathbb{R}^{k}} \mathbb{E}_{\mathbf{y}|\mathbf{x}} [-\langle \mathbf{w}, \mathbf{y} \rangle + c(\mathbf{w})]$$
$$= \inf_{\mathbf{w}\in\mathbb{R}^{k}} -\langle \mathbf{w}, E_{\mathbf{y}|\mathbf{x}}[\mathbf{y}] \rangle + c(\mathbf{w})$$

Negative log-likelihood loss

$$\widetilde{\ell}(\mathbf{w}, \mathbf{y}) = -\langle \mathbf{w}, \mathbf{y} \rangle + \log \sum_{\mathbf{y}' \in Y} \exp\langle \mathbf{w}, \mathbf{y}' \rangle = -\langle \mathbf{w}, \mathbf{y} \rangle + c(\mathbf{w})$$

Surrogate risk

$$\inf_{\mathbf{w}\in\mathbb{R}^{k}} \widetilde{r}(\mathbf{w}) = \inf_{\mathbf{w}\in\mathbb{R}^{k}} \mathbb{E}_{\mathbf{y}|\mathbf{x}} [\widetilde{\ell}(\mathbf{w}, \mathbf{y})]$$
$$= \inf_{\mathbf{w}\in\mathbb{R}^{k}} \mathbb{E}_{\mathbf{y}|\mathbf{x}} [-\langle \mathbf{w}, \mathbf{y} \rangle + c(\mathbf{w})]$$
$$= \inf_{\mathbf{w}\in\mathbb{R}^{k}} -\langle \mathbf{w}, E_{\mathbf{y}|\mathbf{x}}[\mathbf{y}] \rangle + c(\mathbf{w})$$

Optimality conditions

- Let: $\succ \widehat{\mathbf{W}}$ be a minimizer of the problem above
 - ► $\mathbf{y}^{(i)}$ the one-hot vector for which $\mathbf{y}_i^{(i)} = 1$

By first order optimality conditions:

$$\frac{\partial}{\partial \widehat{w}_{i}} \left(-\langle \widehat{\mathbf{w}}, E_{\mathbf{y}|\mathbf{x}}[\mathbf{y}] \rangle + c(\widehat{\mathbf{w}}) \right) = 0$$

Negative log-likelihood loss

$$\widetilde{\ell}(\mathbf{w}, \mathbf{y}) = -\langle \mathbf{w}, \mathbf{y} \rangle + \log \sum_{\mathbf{y}' \in Y} \exp\langle \mathbf{w}, \mathbf{y}' \rangle = -\langle \mathbf{w}, \mathbf{y} \rangle + c(\mathbf{w})$$

Surrogate risk

$$\inf_{\mathbf{w}\in\mathbb{R}^{k}} \widetilde{r}(\mathbf{w}) = \inf_{\mathbf{w}\in\mathbb{R}^{k}} \mathbb{E}_{\mathbf{y}|\mathbf{x}} [\widetilde{\ell}(\mathbf{w}, \mathbf{y})]$$
$$= \inf_{\mathbf{w}\in\mathbb{R}^{k}} \mathbb{E}_{\mathbf{y}|\mathbf{x}} [-\langle \mathbf{w}, \mathbf{y} \rangle + c(\mathbf{w})]$$
$$= \inf_{\mathbf{w}\in\mathbb{R}^{k}} -\langle \mathbf{w}, E_{\mathbf{y}|\mathbf{x}}[\mathbf{y}] \rangle + c(\mathbf{w})$$

Optimality conditions

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By first order optimality conditions:

$$\frac{\partial}{\partial \widehat{w}_i} \left(-\langle \widehat{\mathbf{w}}, E_{\mathbf{y}|\mathbf{x}}[\mathbf{y}] \rangle + c(\widehat{\mathbf{w}}) \right) = 0 \quad \Longrightarrow \quad \frac{\exp \widehat{w}_i}{\sum_j \exp \widehat{w}_j} = p(\mathbf{y}^{(i)} | \mathbf{x})$$

Bayes consistent!

EXAMPLE

. . .

Optimality conditions

$$\frac{\partial}{\partial \widehat{w}_{i}} \left(-\langle \widehat{\mathbf{w}}, E_{\mathbf{y}|\mathbf{x}}[\mathbf{y}] \rangle + c(\widehat{\mathbf{w}}) \right) = 0 \qquad \Longrightarrow \qquad \frac{\exp \widehat{w}_{i}}{\sum_{j} \exp \widehat{w}_{j}} = p(\mathbf{y}^{(i)} | \mathbf{x})$$
$$\implies \qquad \widehat{w}_{i} = \log p(\mathbf{y}^{(i)} | \mathbf{x})$$

Example

$$p(\mathbf{y}^{(1)} | \mathbf{x}) = 0.7$$

 $p(\mathbf{y}^{(2)} | \mathbf{x}) = 0.1$
 $p(\mathbf{y}^{(3)} | \mathbf{x}) = 0.2$

	Ŵ
1	log 0.7
2	log 0.1
3	log 0.2

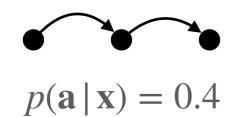
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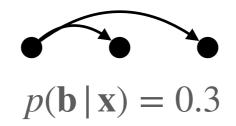
. .

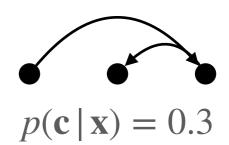
Distribution over dependency trees

► Sentence length: 2

► No single root constraint





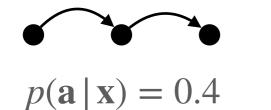


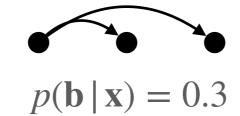
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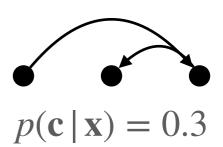
Distribution over dependency trees

► Sentence length: 2

► No single root constraint







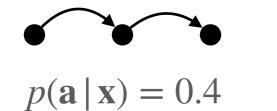
Arc factored scoring function

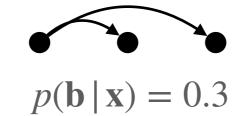
$$\mathbf{w}(\mathbf{a}) = w_{0 \to 1} + w_{1 \to 2}$$
 $\mathbf{w}(\mathbf{b}) = w_{0 \to 1} + w_{0 \to 2}$ $\mathbf{w}(\mathbf{c}) = w_{0 \to 2} + w_{2 \to 1}$

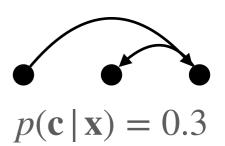
Distribution over dependency trees

► Sentence length: 2

► No single root constraint







Arc factored scoring function

$$\mathbf{w}(\mathbf{a}) = w_{0 \to 1} + w_{1 \to 2}$$
 $\mathbf{w}(\mathbf{b}) = w_{0 \to 1} + w_{0 \to 2}$ $\mathbf{w}(\mathbf{c}) = w_{0 \to 2} + w_{2 \to 1}$

Optimality conditions

 $\widehat{\mathbf{w}}(\mathbf{a}) = \log p(\mathbf{a} \mid \mathbf{x})$

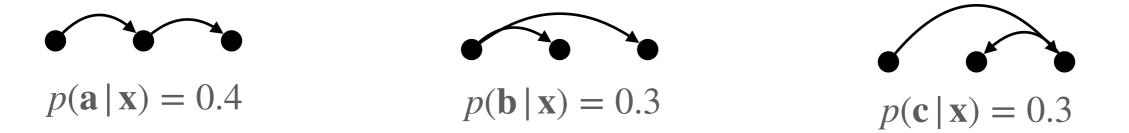
 $\widehat{\mathbf{w}}(\mathbf{b}) = \log p(\mathbf{b} | \mathbf{x})$

 $\widehat{\mathbf{w}}(\mathbf{c}) = \log p(\mathbf{c} \mid \mathbf{x})$

Distribution over dependency trees

► Sentence length: 2

► No single root constraint



Arc factored scoring function

 $\mathbf{w}(\mathbf{a}) = w_{0 \to 1} + w_{1 \to 2}$ $\mathbf{w}(\mathbf{b}) = w_{0 \to 1} + w_{0 \to 2}$ $\mathbf{w}(\mathbf{c}) = w_{0 \to 2} + w_{2 \to 1}$

Optimality conditions

- $\widehat{\mathbf{w}}(\mathbf{a}) = \log p(\mathbf{a} | \mathbf{x})$ $\widehat{w}_{0 \to 1} + \widehat{w}_{1 \to 2} = \log p(\mathbf{a} | \mathbf{x})$
- $\widehat{\mathbf{w}}(\mathbf{b}) = \log p(\mathbf{b} \,|\, \mathbf{x})$

 $\widehat{\mathbf{w}}(\mathbf{c}) = \log p(\mathbf{c} \mid \mathbf{x})$

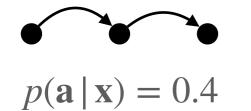
 $\widehat{w}_{0 \to 2} + \widehat{w}_{2 \to 1} = \log p(\mathbf{c} | \mathbf{x})$

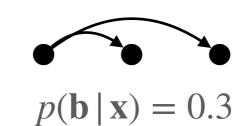
 $\widehat{w}_{0 \to 1} + \widehat{w}_{0 \to 2} = \log p(\mathbf{b} \mid \mathbf{x})$

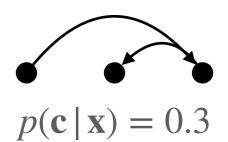
Distribution over dependency trees

► Sentence length: 2

► Single root







Optimality conditions

$$\widehat{w}_{0 \to 1} + \widehat{w}_{1 \to 2} = \log p(\mathbf{a} \mid \mathbf{x})$$

$$\widehat{w}_{0 \to 1} + \widehat{w}_{0 \to 2} = \log p(\mathbf{b} | \mathbf{x})$$

$$\widehat{w}_{0\to 2} + \widehat{w}_{2\to 1} = \log p(\mathbf{c} | \mathbf{x})$$

 ŵ
 0
 1
 2

 0
 /
 0
 log 0.3

 1
 /
 log 0.4

 2
 /
 0
 /

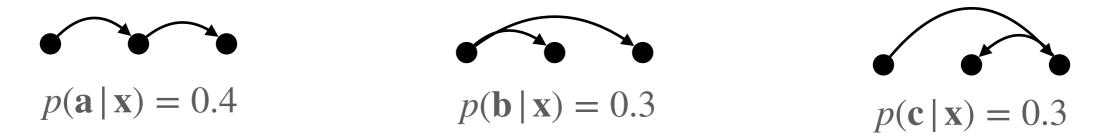
Head index

Modifier index

Distribution over dependency trees

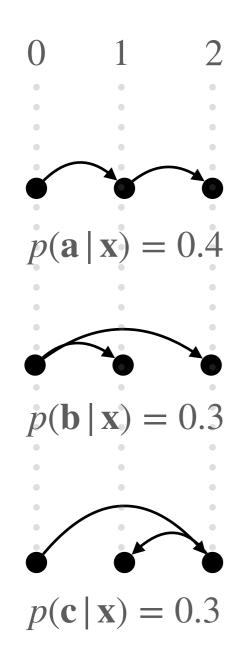
► Sentence length: 2

► Single root

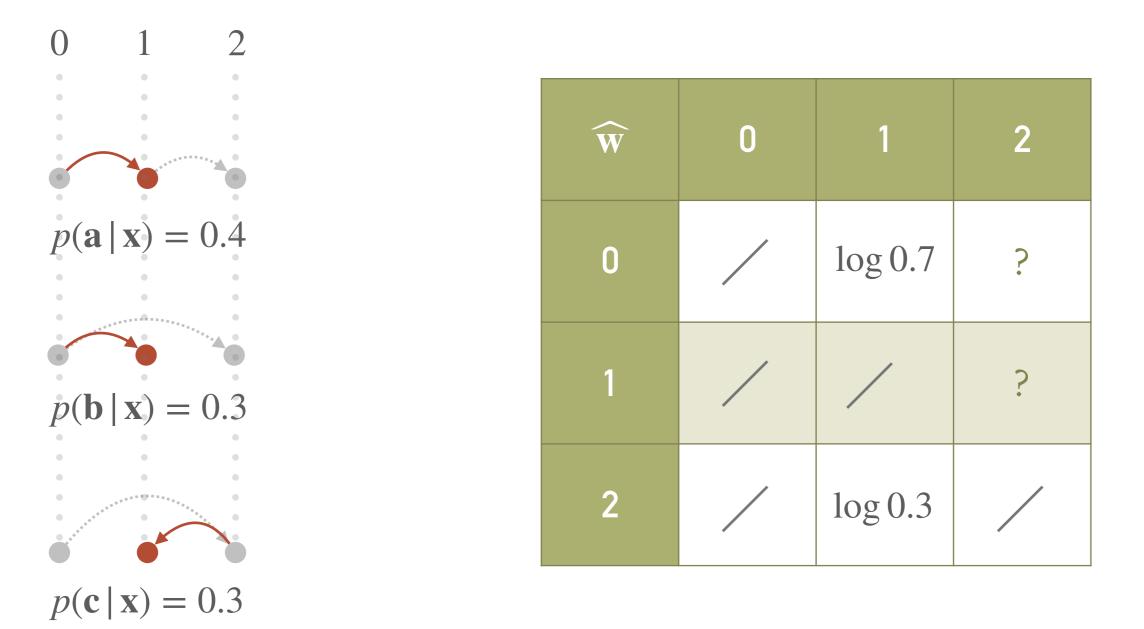


Main idea

As each word has exactly one head, instead of minimizing the NLL over the dependency tree distribution, we can minimize one multiclass classification NLL per word

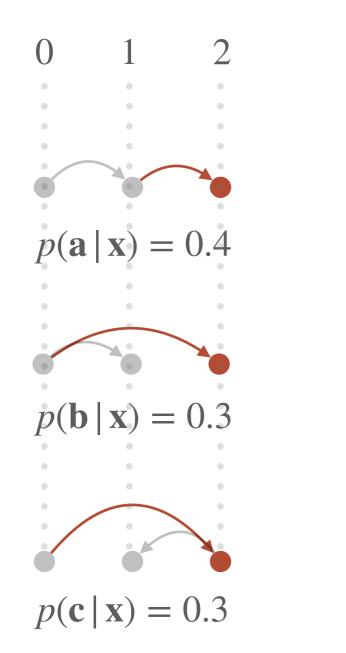


Ŵ	0	1	2
0		?	?
1			?
2		?	



Focus on vertex 1

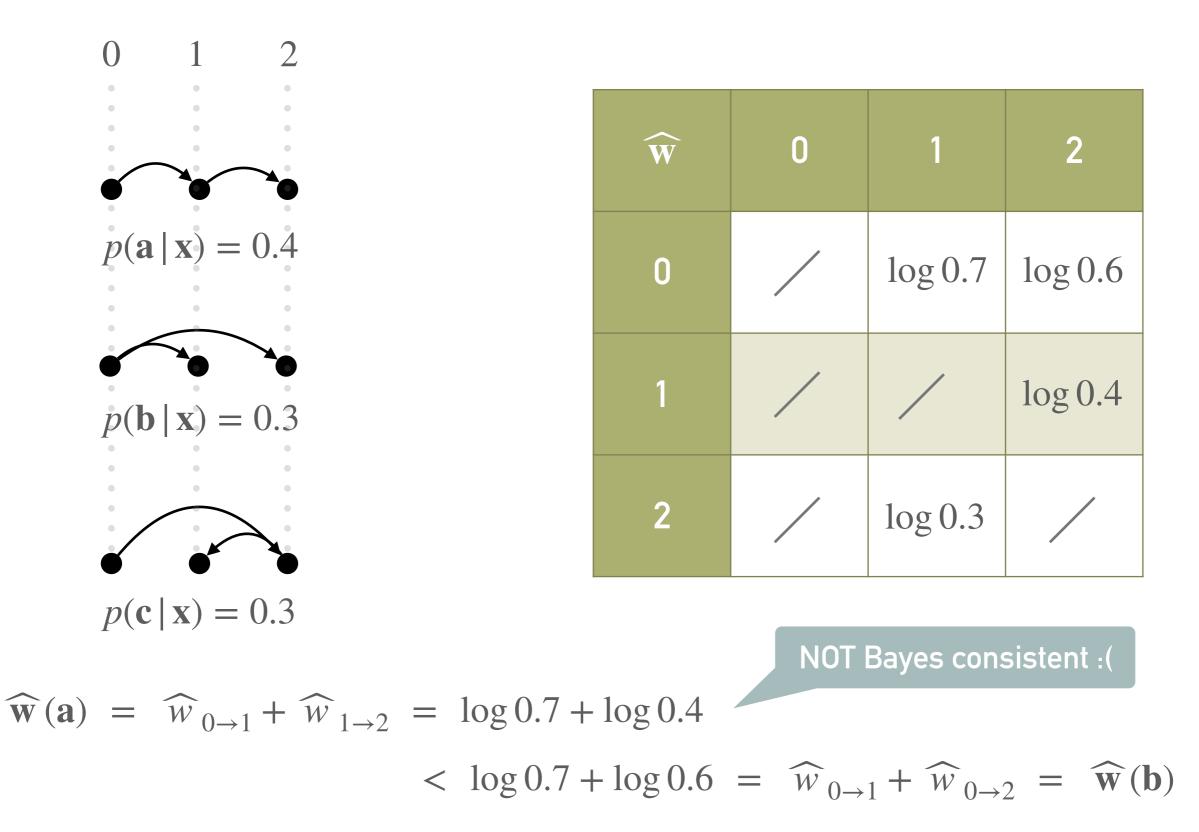
- > Probability to have vertex 0 as head: $p(\mathbf{a} | \mathbf{x}) + p(\mathbf{b} | \mathbf{x}) = 0.4 + 0.3 = 0.7$
- ► Probability to have vertex 2 as head: $p(\mathbf{c} | \mathbf{x}) = 0.3$



Ŵ	0	1	2
0		log 0.7	log 0.6
1			log 0.4
2		log 0.3	

Focus on vertex 2

- ► Probability to have vertex 0 as head: $p(\mathbf{b} | \mathbf{x}) + p(\mathbf{c} | \mathbf{x}) = 0.3 + 0.3 = 0.6$
- ► Probability to have vertex 1 as head: $p(\mathbf{a} | \mathbf{x}) = 0.4$



INTERMEDIATE CONCLUSION

Take home message

Token-separable losses are not necessarily Bayes consistent.

Other examples of separable losses

- ➤ Token level NLL for BIO tagging (ignores the fact that a I tag can not follow a O tag)
- Semantic parsing [Panupong et al., 2019]
- ► Discontinuous constituency parsing [Corro, 2020]

Should we care about loss function properties?

Machine learning is at the core of modern NLP models, so yes.

Should we care about Bayes consistency?

Clearly, separable losses work in practice, but:

- ► We need theory, "it works" is not good enough
- Previous work showed that Bayes consistency may be misleading as it ignore the structure of the scoring function [Long and Servedio, 2013]

CONCLUSION

CONCLUSION

Take home message 1

Structured prediction is not dead:

- ► seq-2-seq models are know to fail in several generalization settings (compositional, structural, ...)
- Beside syntactic parsing and alignment models for MT, there are many NLP problems for which combinatorial algorithms have been understudied. See for example [Corro, 2022] for NER
- ► Open question: how to embed "structural knowledge" in seq-2-seq models?

obvious exaggeration :)

Take home message 2

- ► Loss functions are the cornestone of machine learning
- NLP has a lot of interesting learning problems were theory is missing
 For other examples in NLP, check: [Ma & Collins, 2018] [Effland & Collins, 2021]

(advertising) Book on discrete latent structure in neural networks

https://arxiv.org/abs/2301.07473

Discrete Latent Structure in Neural Networks

Vlad Niculae¹, Caio F. Corro², Nikita Nangia³, Tsvetomila Mihaylova^{4,5} and André F. T. Martins^{4,5,6}