Latent Structure Models for NLP

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deep-spin.github.io/tutorial

I. Introduction

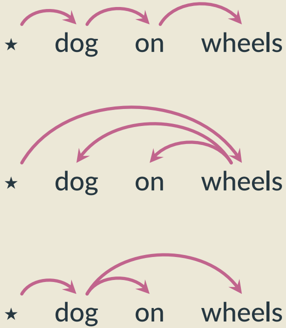
Structured prediction and NLP

- **Structured prediction**: a machine learning framework for predicting structured, constrained, and interdependent outputs
- **NLP** deals with *structured* and *ambiguous* textual data:
  - machine translation
  - speech recognition
  - syntactic parsing
  - semantic parsing
  - information extraction
  - ...

Examples of structure in NLP

Dependency parsing

...



...

Examples of structure in NLP

Dependency parsing

. . .

⋆ dog on wheels

Exponentially many parse trees!
Cannot enumerate.

⋆ dog on wheels

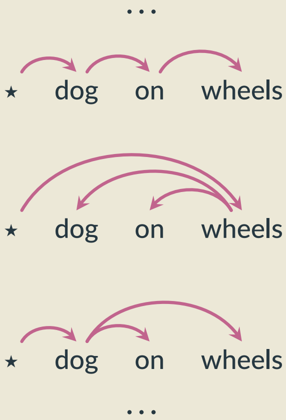
. . .

Examples of structure in NLP

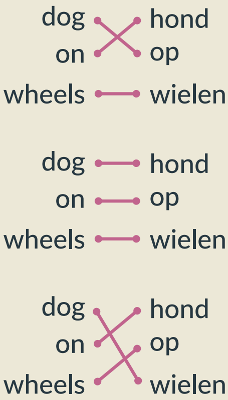
POS tagging

VERB	PREP	NOUN
dog	on	wheels
NOUN	PREP	NOUN
dog	on	wheels
NOUN	DET	NOUN
dog	on	wheels

Dependency parsing



Word alignments



NLP 5 years ago:

Structured prediction and pipelines

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- **Bigger disadvantage:** error propagates through the pipeline 💩

NLP today:

End-to-end training

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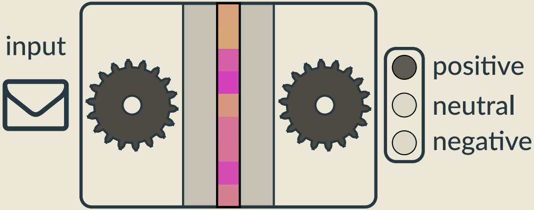
End-to-end training

- Forget pipelines—train everything from scratch!
- No more error propagation or linguistic annotations! 🎉
- Treat everything as *latent*! 🙌

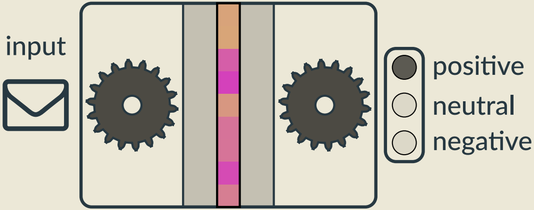
Representation learning

- Uncover hidden representations useful for the *downstream task*.
- Neural networks are well-suited for this: *deep computation graphs*.



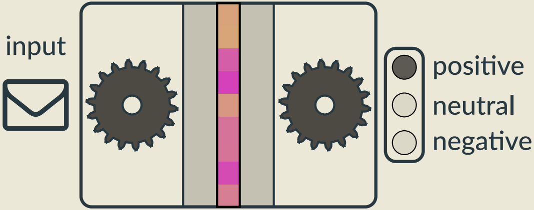
Representation learning

- Uncover hidden representations useful for the *downstream task*.
- Neural networks are well-suited for this: *deep computation graphs*.
- Neural representations are unstructured, inscrutable. Language data has underlying structure!



Latent structure models

- Seek *structured* hidden representations instead!



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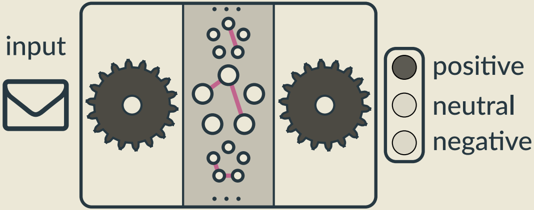

Latent structure models aren't so new!

- They have a very long history in NLP:
  - IBM Models for SMT (latent word alignments) [Brown et al., 1993]
  - HMMs [Rabiner, 1989]
  - CRFs with hidden variables [Quattoni et al., 2007]
  - Latent PCFGs [Petrov and Klein, 2008, Cohen et al., 2012]
- Trained with EM, spectral learning, method of moments, ...
- Often, very strict assumptions (e.g. strong factorizations)
- Today, neural networks opened up some new possibilities!

Why do we love latent structure models?

- The inferred latent variables can bring us some **interpretability**
- They offer a way of injecting prior knowledge as a **structured bias**
- Hopefully: Higher predictive power with fewer model parameters

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  - smaller carbon footprint!

What this tutorial is about:

- Discrete, combinatorial latent structures
- Often the structure is inspired by some linguistic intuition
- We'll cover both:
    - RL methods (structure built incrementally, reward coming from downstream task)
    - ... vs end-to-end differentiable approaches (global optimization, marginalization)
    - stochastic computation graphs
    - ... vs deterministic graphs.
- All plugged in *discriminative* neural models.

This tutorial is *not* about:

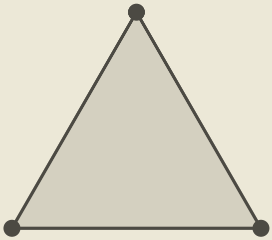
- It's not about continuous latent variables
- It's not about deep generative learning
- We won't cover GANs, VAEs, etc.
- There are (very good) recent tutorials on deep variational models for NLP:
    - "Variational Inference and Deep Generative Models" (Schulz and Aziz, ACL 2018)
    - "Deep Latent-Variable Models for Natural Language" (Kim, Wiseman, Rush, EMNLP 2018)

Background

Unstructured vs structured

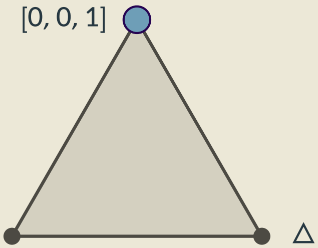
- To better explain the math, we'll often backtrack to *unstructured* models (where the latent variable is a categorical) before jumping to the *structured* ones

The unstructured case: Probability simplex



$\triangle$

The unstructured case: Probability simplex



- Each vertex is an *indicator vector*, representing one class:

$$\boldsymbol{z}_c = [0, \ldots, 0, \underbrace{1}_{c^{\text{th}} \text{ position}}, 0, \ldots, 0].$$

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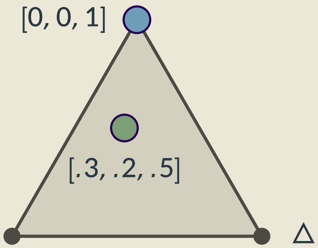

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- Points inside are *probability vectors*, a convex combination of classes:

$$\boldsymbol{p} \geq \boldsymbol{0}, \; \sum_c p_c = 1.$$

What's the analogous of $\triangle$ for a structure?

- A structured object $\boldsymbol{z}$ can be represented as a *bit vector*.

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- Example:
  - a dependency tree can be represented a $O(L^2)$ vector indexed by arcs
  - each entry is 1 iff the arc belongs to the tree
  - **structural constraints:** not all bit vectors represent valid trees!

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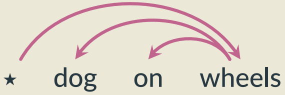
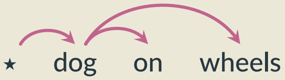
$\boldsymbol{z}_1 = [1, 0, 0, 0, 1, 0, 0, 0, 1]$

$\boldsymbol{z}_2 = [0, 0, 1, 0, 0, 1, 1, 0, 0]$

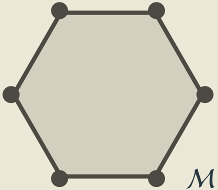


$\boldsymbol{z}_3 = [1, 0, 0, 0, 1, 0, 0, 1, 0]$



[Wainwright and Jordan, 2008]

The structured case: Marginal polytope



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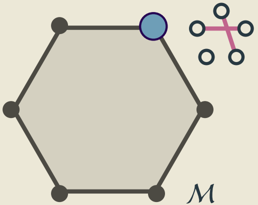
- Each vertex corresponds to one such *bit vector* $\boldsymbol{z}$



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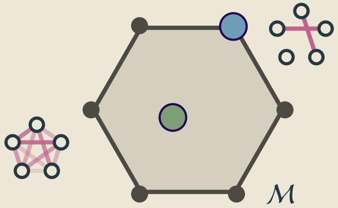
The structured case: Marginal polytope

- Each vertex corresponds to one such *bit vector* $\boldsymbol{z}$
- Points inside correspond to *marginal distributions*: convex combinations of structured objects

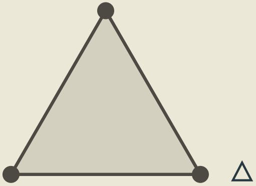


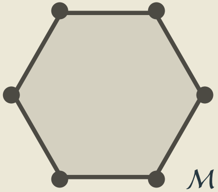
$$\boldsymbol{\mu} = \underbrace{p_1 \boldsymbol{z}_1 + \ldots + p_N \boldsymbol{z}_N}_{\text{exponentially many terms}}, \quad \boldsymbol{p} \in \Delta.$$

$$\begin{array}{ll} p_1 = 0.2, & \boldsymbol{z}_1 = [1, 0, 0, 0, 1, 0, 0, 0, 1] \\ p_2 = 0.7, & \boldsymbol{z}_2 = [0, 0, 1, 0, 0, 1, 1, 0, 0] \\ p_3 = 0.1, & \boldsymbol{z}_3 = [1, 0, 0, 0, 1, 0, 0, 1, 0] \end{array} \quad \Rightarrow \quad \boldsymbol{\mu} = [.3, 0, .7, 0, .3, .7, .7, .1, .2].$$

Unstructured vs Structured

- Unstructured case: simplex $\triangle$
- Structured case: marginal polytope $\mathcal{M}$





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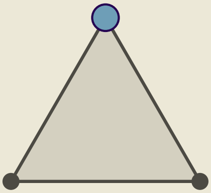

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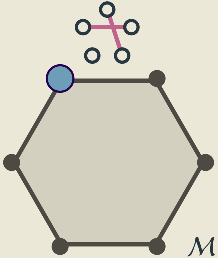

$\mathcal{M}$

Unstructured vs Structured

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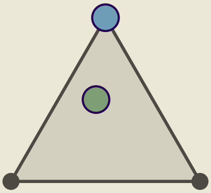

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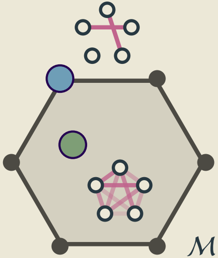
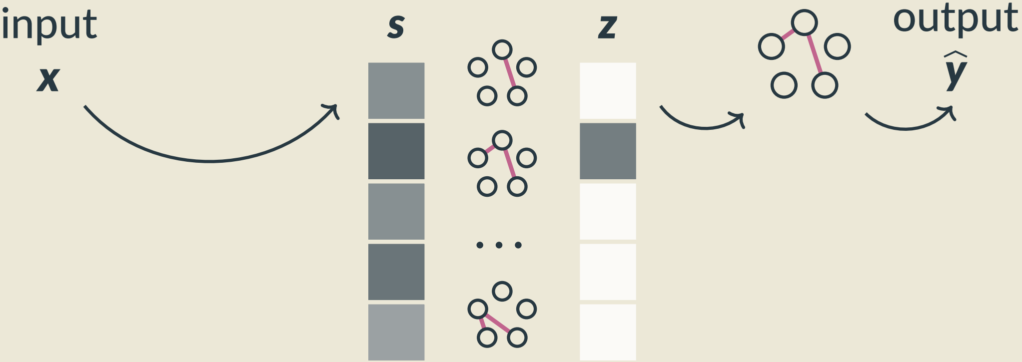


$\mathcal{M}$

Computing the most likely structure

is a very high-dimensional argmax



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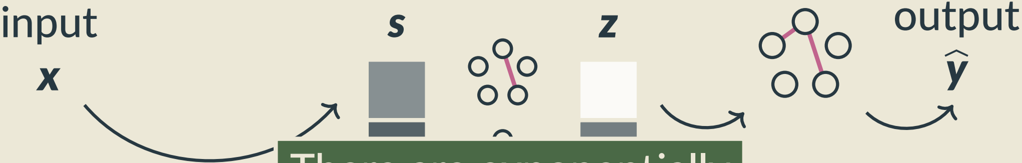
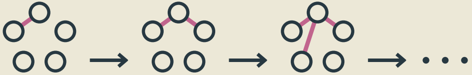


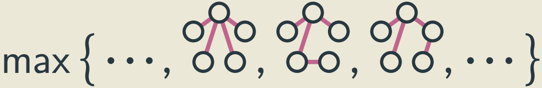
There are exponentially many structures

(s cannot fit in memory;

we cannot "loop" over s nor z)

Dealing with the combinatorial explosion





1. Incremental structures

- Build structure **greedily**, as sequence of discrete choices (e.g., shift-reduce).
- Scores (partial structure, action) tuples.
- **Advantages:** flexible, rich histories.
- **Disadvantages:** greedy, local decisions are suboptimal, error propagation.

2. Factorization into parts

- Optimizes **globally** (e.g. Viterbi, Chu-Liu-Edmonds, Kuhn-Munkres).
- Scores smaller parts.
- **Advantages:** optimal, elegant, can handle hard & global constraints.
- **Disadvantages:** strong assumptions.

The challenge of discrete choices.

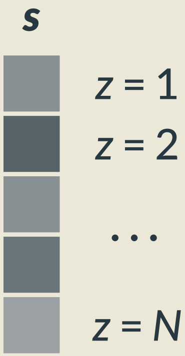
$$z = 1$$

$$z = 2$$

$$\dots$$

$$z = N$$

The challenge of discrete choices.



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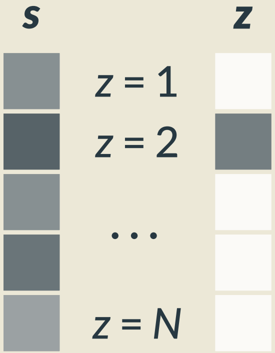

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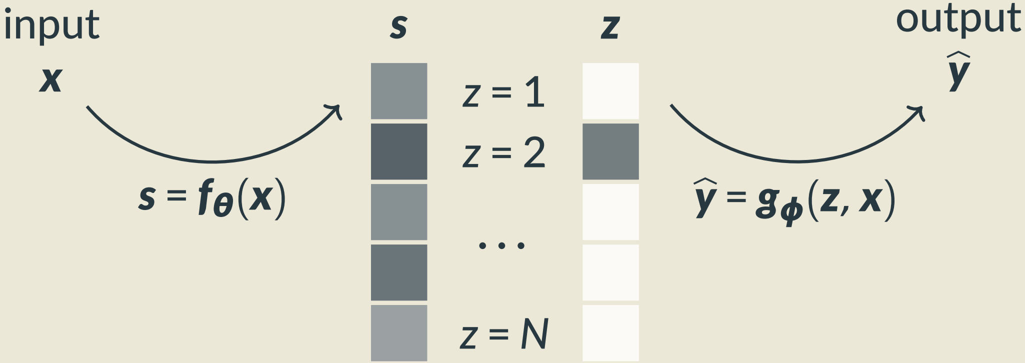

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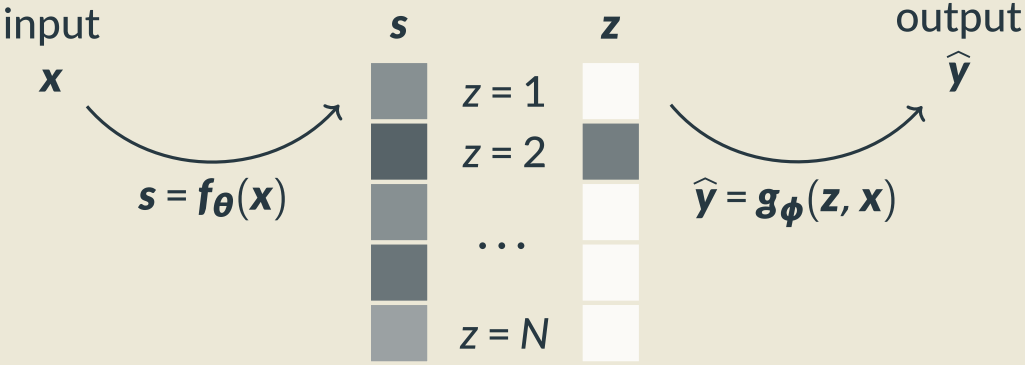
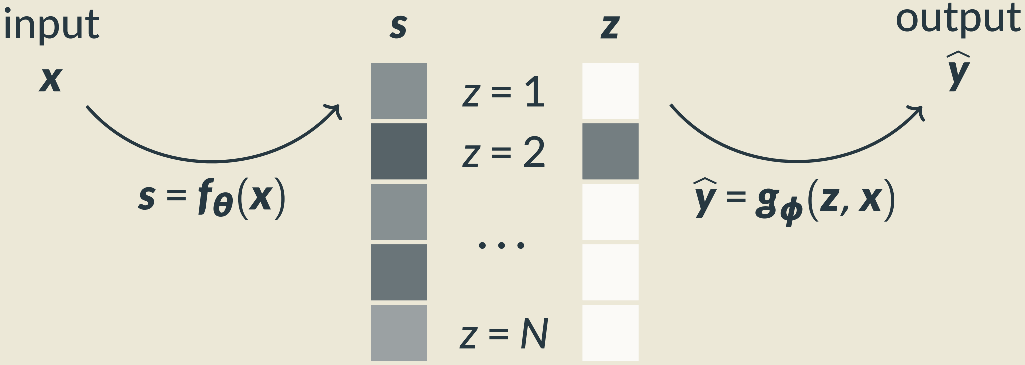


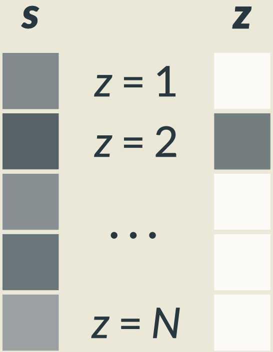
$$\frac{\partial L(\widehat{\boldsymbol{y}}, \boldsymbol{y})}{\partial \boldsymbol{w}} = ?$$

The challenge of discrete choices.



$$\frac{\partial L(\widehat{\boldsymbol{y}}, \boldsymbol{y})}{\partial \boldsymbol{w}} = ? \quad \text{or, essentially,} \quad \frac{\partial \boldsymbol{z}}{\partial \boldsymbol{s}} = ?$$

Discrete mappings are “flat”



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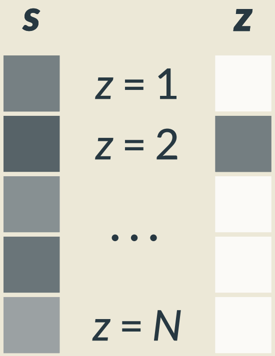

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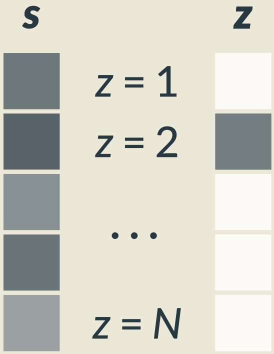

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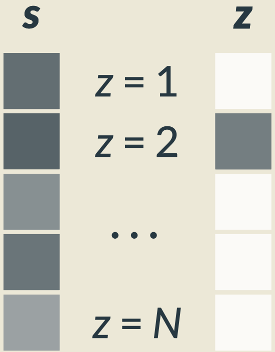

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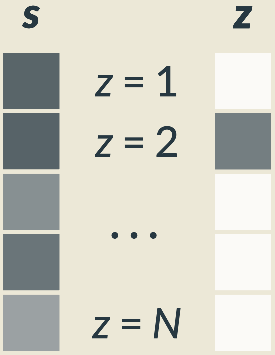

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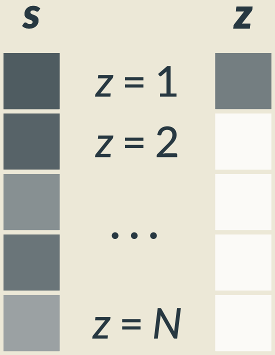

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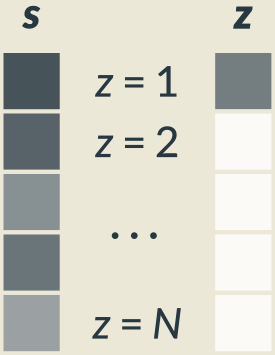

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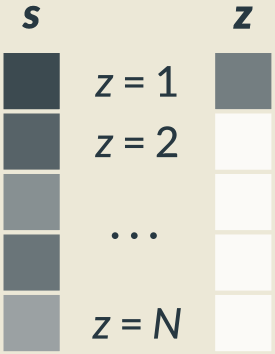

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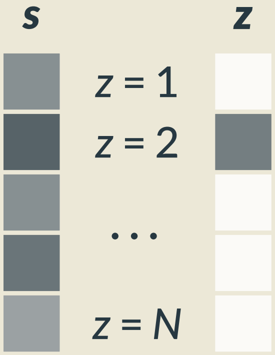
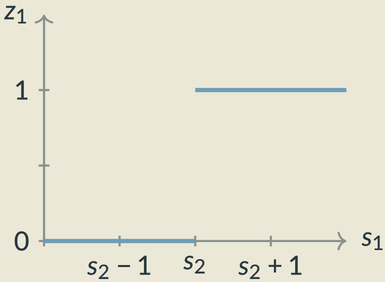
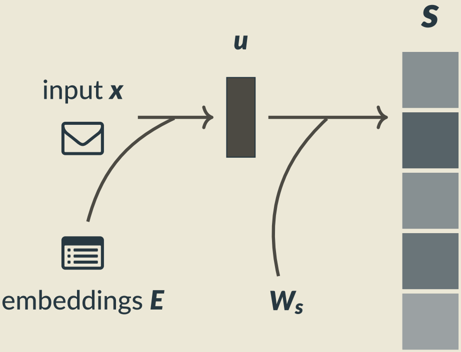
Argmax





$$\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{s}} = \boldsymbol{0}$$

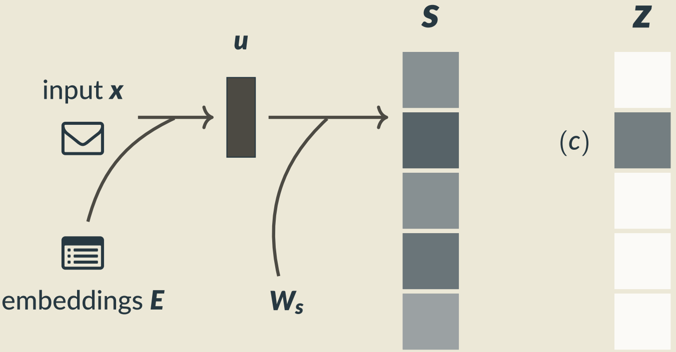
Example: Regression with latent categorization



$\mathbf{u} = \frac{1}{|\mathbf{x}|} \sum_j \mathbf{E}_{x_j}$

$\mathbf{s} = \mathbf{W_s} \mathbf{u}$

Example: Regression with latent categorization



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predict topic c ($\boldsymbol{z} = \boldsymbol{e}_c$)

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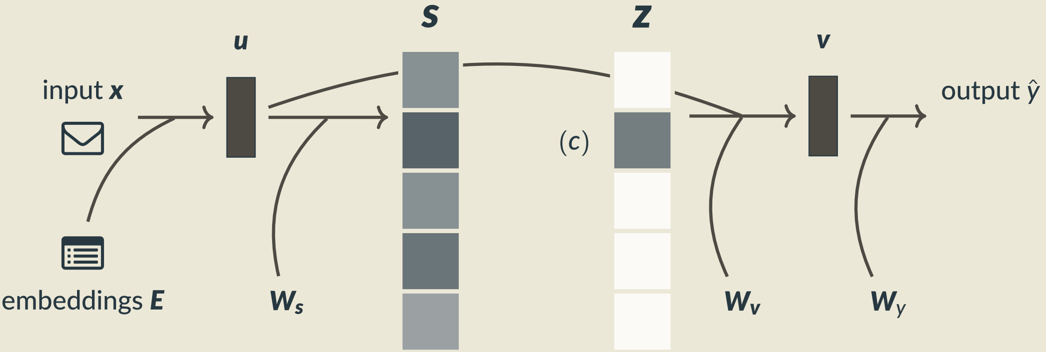

$\boldsymbol{u} = \frac{1}{|\boldsymbol{x}|}\sum_j \boldsymbol{E}_{x_j}$ $\quad$ $\boldsymbol{s} = \boldsymbol{W_s u}$ $\quad$ $\boldsymbol{v} = \tanh\left(\boldsymbol{W_v}[\boldsymbol{u}, \boldsymbol{z}]\right)$ $\quad$ $\hat{y} = \boldsymbol{W}_y\boldsymbol{v}$ $\quad$ $L = (\hat{y} - y)^2$

predict topic c ($\boldsymbol{z} = \boldsymbol{e}_c$)

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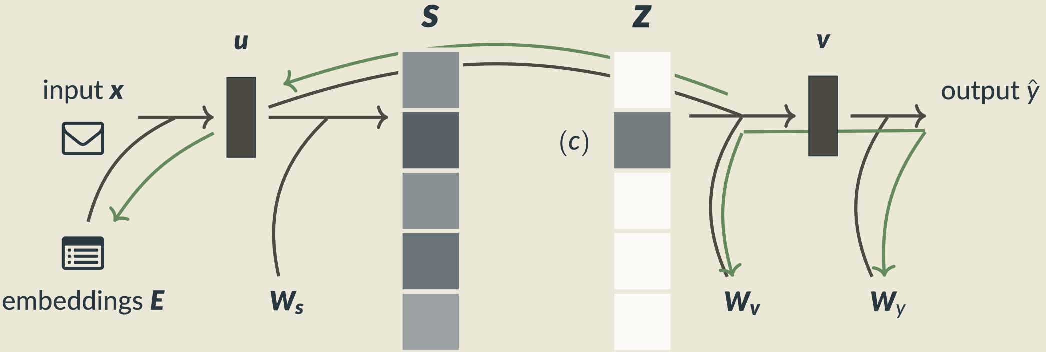

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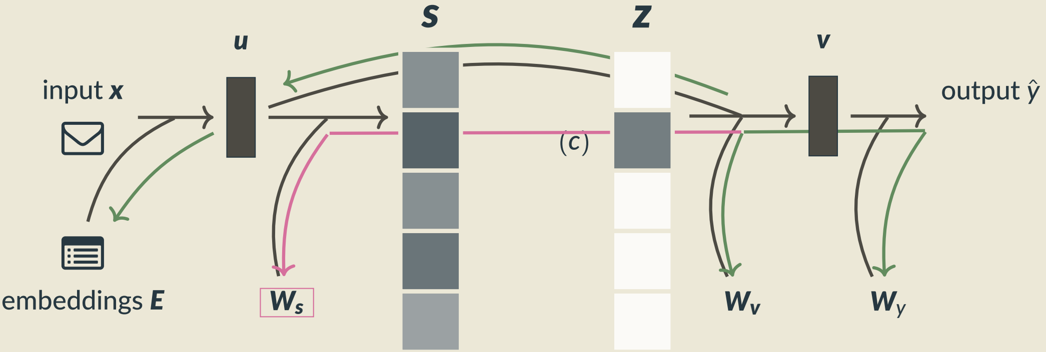

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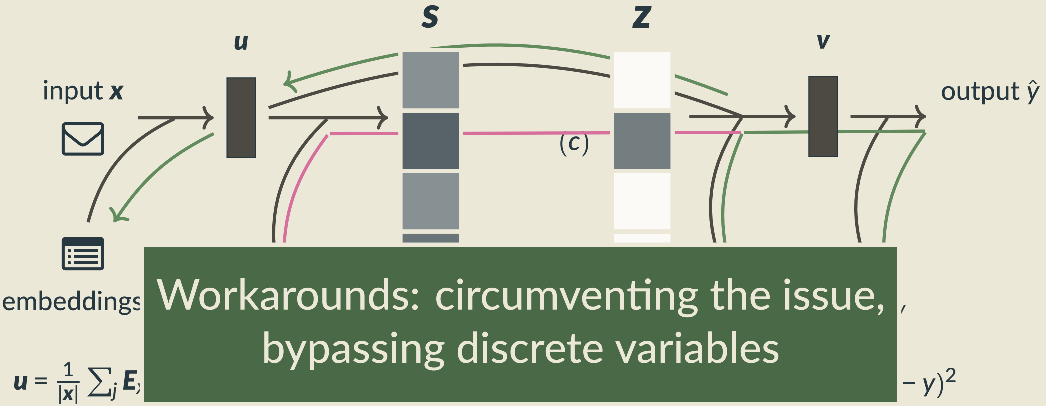
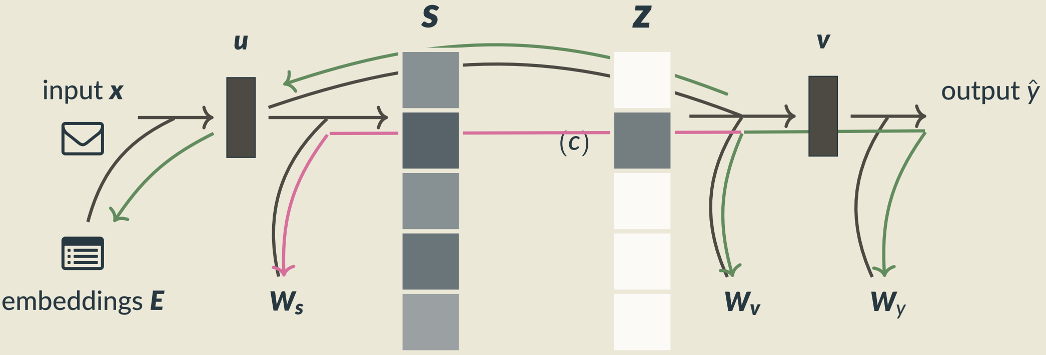
$$\frac{\partial L}{\partial \boldsymbol{W_s}} = \frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial \boldsymbol{v}} \frac{\partial \boldsymbol{v}}{\partial \boldsymbol{z}} \overbrace{\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{s}}}^{\equiv 0} \frac{\partial \boldsymbol{s}}{\partial \boldsymbol{W_s}}$$

Example: Regression with latent categorization



Workarounds: circumventing the issue,
bypassing discrete variables

Example: Regression with latent categorization



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Option 1. Pretrain latent classifier $\boldsymbol{W_s}$

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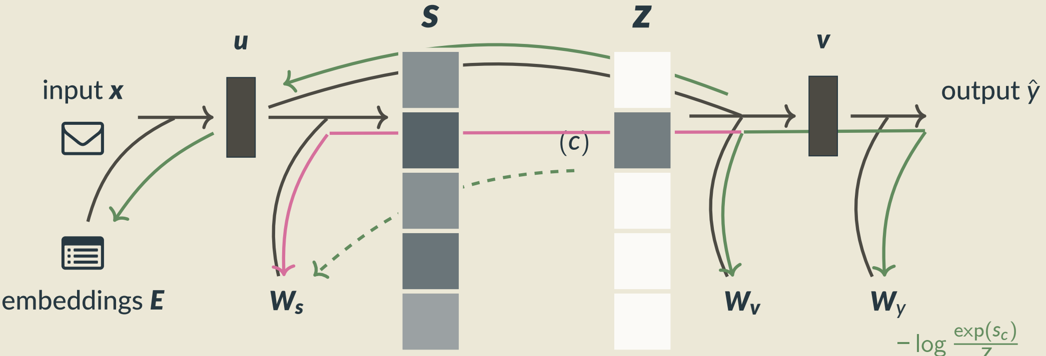

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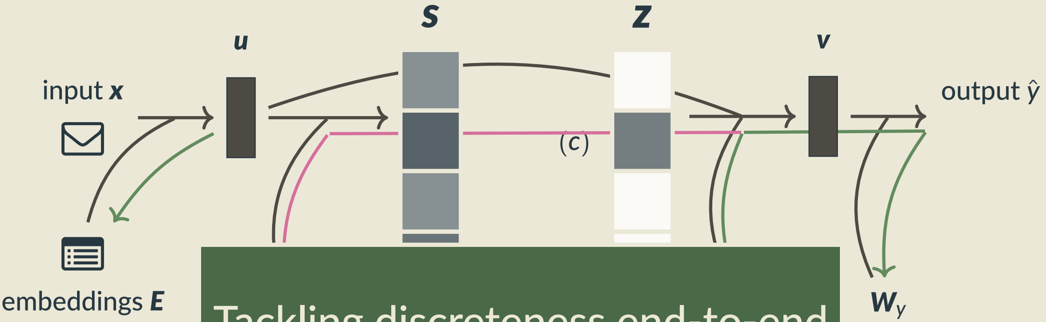
Option 2. Multi-task learning

Example: Regression with latent categorization



Tackling discreteness end-to-end

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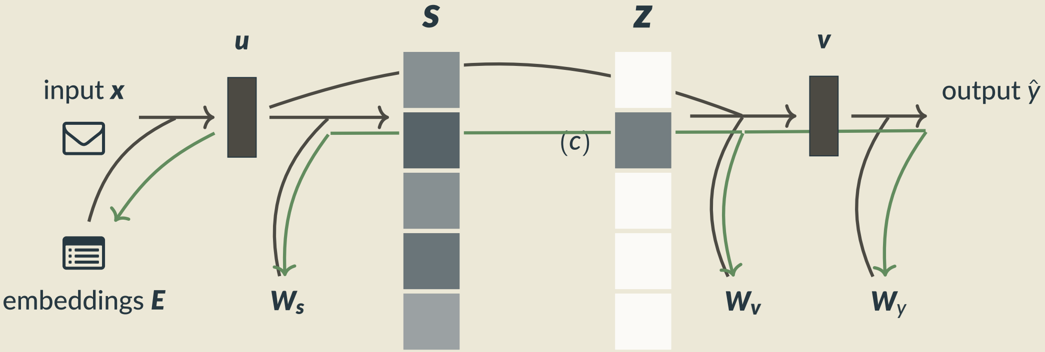

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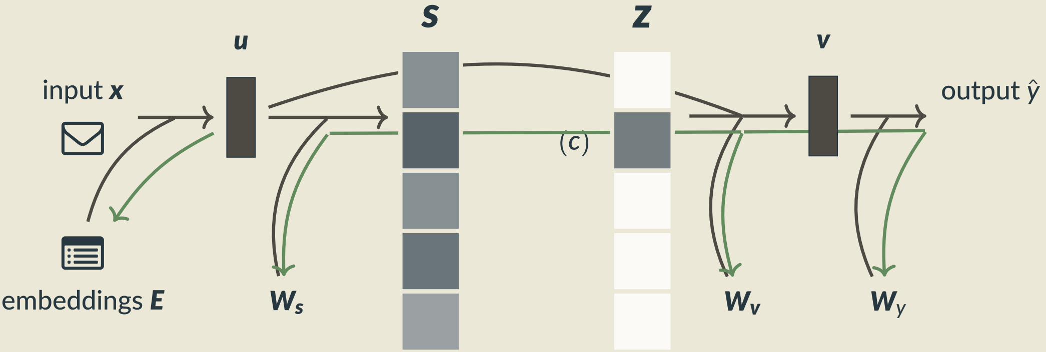
Option 3. Stochasticity! $\dfrac{\partial \mathbb{E}_{\boldsymbol{z}}(\hat{y}(\boldsymbol{z}) - y)^2}{\partial \boldsymbol{W}_s} \neq \boldsymbol{0}$

Example: Regression with latent categorization



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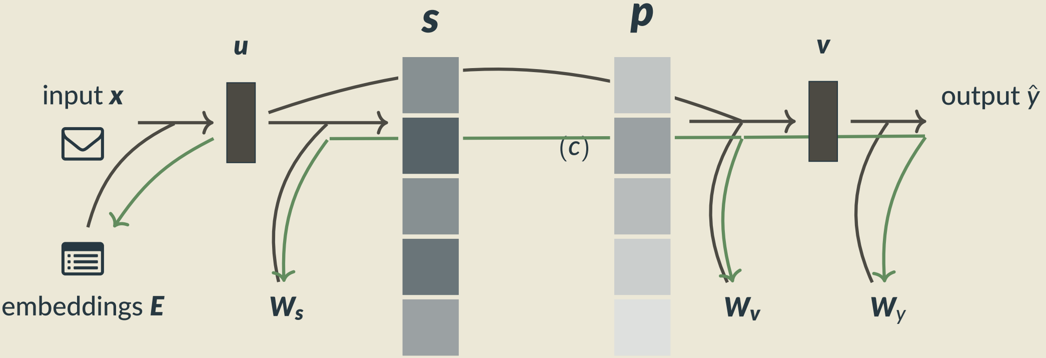
Option 4. Gradient surrogates (*e.g.* straight-through, $\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{s}} \leftarrow \boldsymbol{I}$)

Example: Regression with latent categorization



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Option 5. Continuous relaxation (*e.g.* softmax)

Dealing with discrete latent variables

1. Pre-train external classifier
2. Multi-task learning
3. Stochastic latent variables
4. Gradient surrogates
5. Continuous relaxation

Dealing with discrete latent variables

1. Pre-train external classifier
2. Multi-task learning
3. Stochastic latent variables (Part 2)
4. Gradient surrogates (Part 3)
5. Continuous relaxation (Part 4)

Roadmap of the tutorial

- Part 1: Introduction ✓
- Part 2: Reinforcement learning
- Part 3: Gradient surrogates

Coffee Break

- Part 4: End-to-end differentiable models
- Part 5: Conclusions

II. Reinforcement Learning Methods

Latent structure via marginalization

- Given a sentence-label pair (x, y) and its **known** parse tree $\boldsymbol{z}$,

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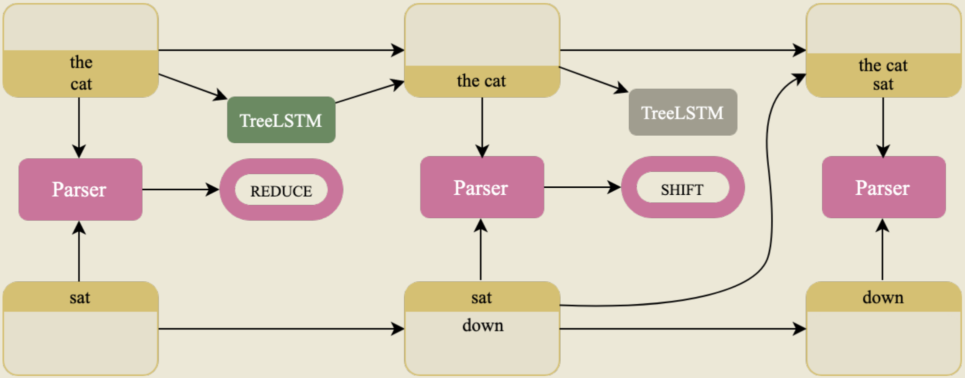
- But we don't know $\boldsymbol{z}$!
- In this section:
  we jointly learn a structured prediction model $\pi_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x)$
  by optimizing the **expected loss**,

$$\mathbb{E}_{\pi_{\boldsymbol{\theta}}(\boldsymbol{z}|x)}\left[L(\boldsymbol{z})\right]$$

But first, supervised SPINN

[Bowman et al., 2016]

Stack-augmented Parser-Interpreter Neural-Network



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- The parser, $f_{\boldsymbol{\theta}}(x)$ is a transition-based **shift-reduce** parser. It looks at top two elements of stack and top element of the buffer.
- **TreeLSTM** combines top two elements of the stack when the parser choses the REDUCE action.

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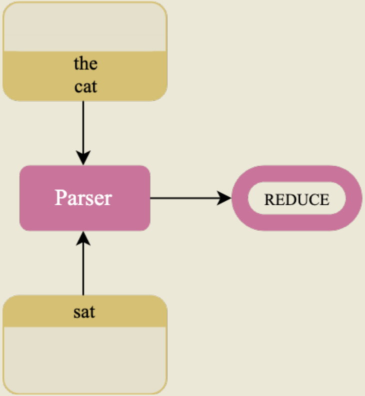

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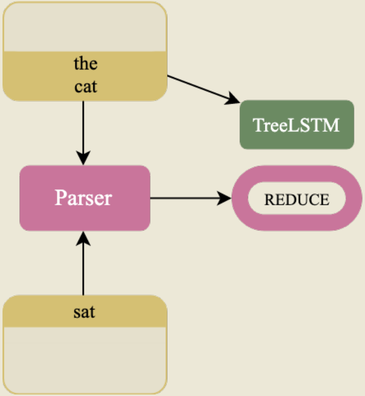

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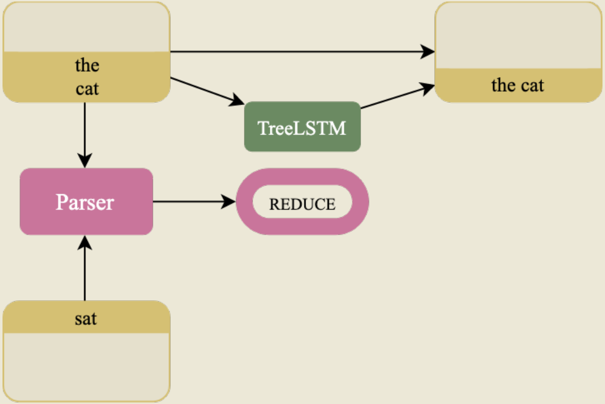

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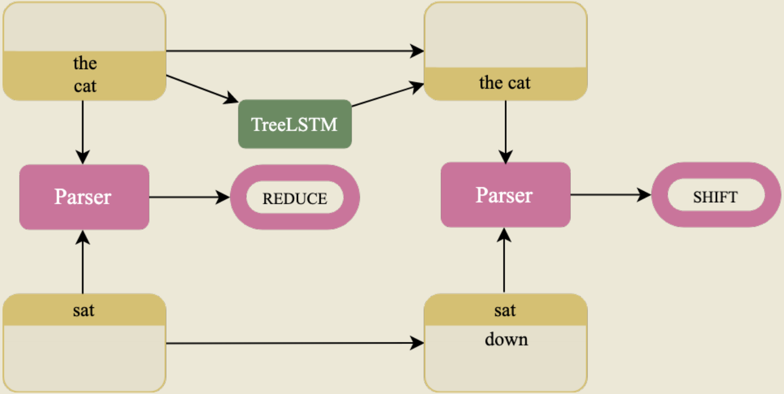

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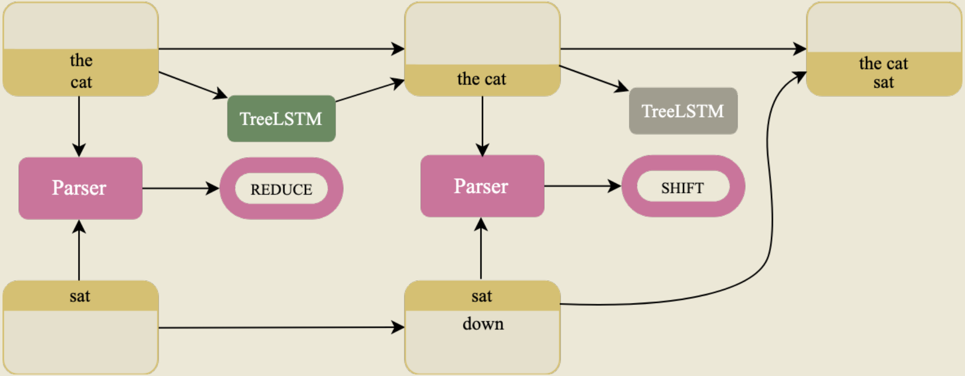

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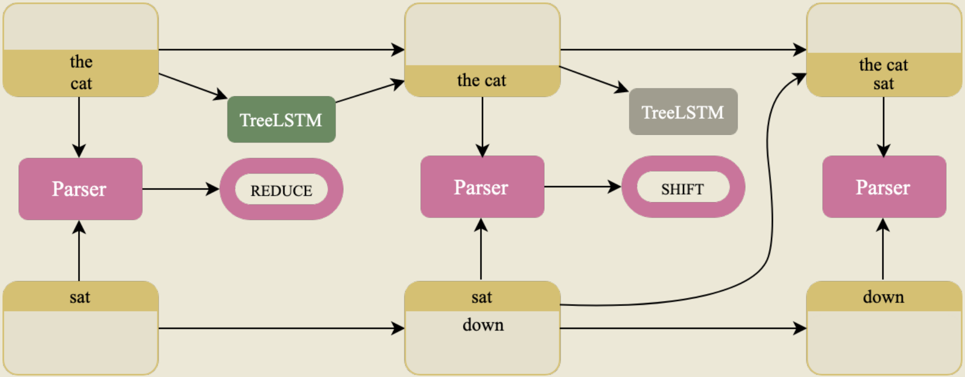


Shift-Reduce parsing

We can write a shift-reduce style parse as a sequence of Bernoulli random variables,

$$\boldsymbol{z} = \{z_1, \ldots, z_{2L-1}\}$$

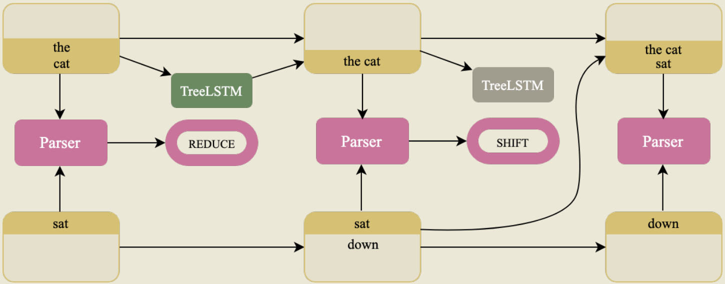
where, $z_j \in \{0, 1\}\ \forall j \in [1, 2L - 1]$

Shift-Reduce parsing

A sequence of Bernoulli trials but with conditional dependence,

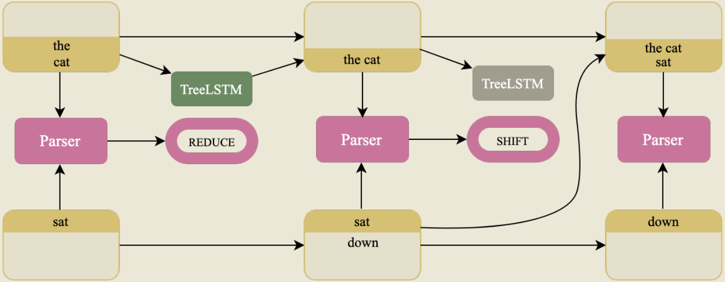
$$p(z_1, z_2, \ldots, z_{2L-1}) = \prod_{j=1}^{2L-1} p(z_j \mid z_{<j})$$

Latent structure learning with SPINN



Latent structure learning with SPINN

- But now, remove syntactic supervision from SPINN.



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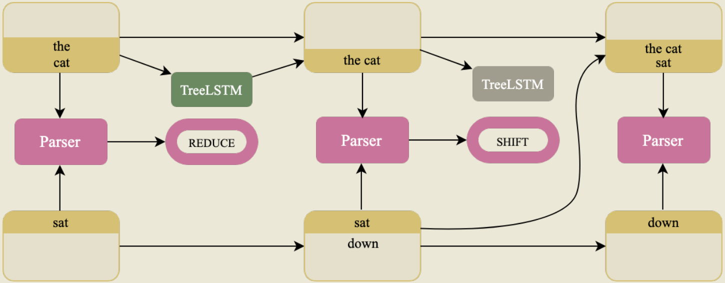

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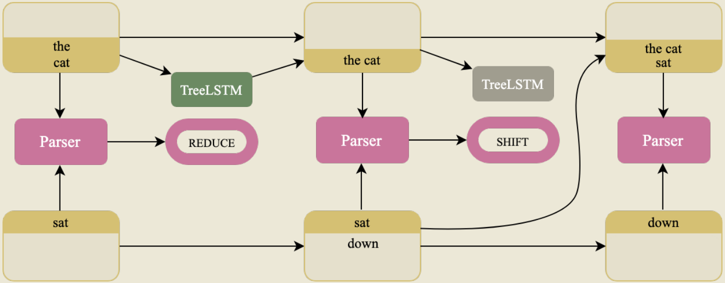

- We model the parse, $\boldsymbol{z}$, as a latent variable with our parser as the score function estimator, $f_{\boldsymbol{\theta}}(x)$.
- With shift-reduce parsing, we're making discrete decisions ⇒ REINFORCE as a "natural" solution.

Unsupervised SPINN

Unsupervised SPINN

No syntactic supervision.

Only reward is from the downstream task.

We only get this reward after parsing the full sentence.

SPINN with REINFORCE

Some basic terminology,

- The action space is $z_j \in \{\textsc{shift}, \textsc{reduce}\}$, and $\boldsymbol{z}$ is a sequence of actions.

SPINN with REINFORCE

[Williams, 1992]

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- Learning a policy network $\pi(\boldsymbol{z} \mid \boldsymbol{h}; \boldsymbol{\theta})$
- Maximize the reward, where $\mathcal{R}$ is performance on the downstream task like sentence classification.

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- Lear
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NOTE: Only a single reward at the end of parsing.

Through the looking glass of REINFORCE

$$\nabla_{\boldsymbol{\theta}} \mathbb{E}_{\boldsymbol{z} \sim \pi_{\boldsymbol{\theta}}(\boldsymbol{z}|x)}[L(\boldsymbol{z})]$$

Through the looking glass of REINFORCE

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(By definition of expectation. How to evaluate?)

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(By Leibniz integral rule for $\log$*)*

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SPINN with REINFORCE, aka RL-SPINN

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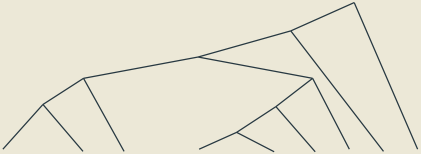
This model fails to solve a simple toy problem.

[Nangia and Bowman, 2018]

Toy problem: ListOps



[max 2 9 [min 4 7] 0]

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Toy problem: ListOps

Model	Accuracy $\mu(\sigma)$	Accuracy max	Self F1
LSTM	71.5 (1.5)	**74.4**	-
RL-SPINN	60.7 (2.6)	64.8	30.8
Random Trees	-	-	30.1

Model	F1 wrt. LB	F1 wrt. RB	F1 wrt. GT	Avg. Depth
48D RL-SPINN	**64.5**	**16.0**	32.1	**14.6**
128D RL-SPINN	43.5	13.0	**71.1**	10.4
GT Trees	41.6	8.8	100.0	9.6
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1. High variance of gradients
2. Coadaptation

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$$3 \text{ tokens} \Rightarrow 5 \text{ trees}$$
$$5 \text{ tokens} \Rightarrow 42 \text{ trees}$$
$$10 \text{ tokens} \Rightarrow 16796 \text{ trees}$$

High variance

- We have a single reward at the end of parsing.
- We are sampling parses from very large search space!
  Catalan number of binary trees.
- And the policy is stochastic.

High variance

So, sometimes the policy lands in a “rewarding state”:

[sm [sm [sm [max 5 6] 2] 0] 5 0 8 6]

Figure: Truth: 7; Pred: 7

High variance

Sometimes it doesn't:

Figure: Truth: 6; Pred: 5

High variance

Catalan number of parses means we need many many samples to lower variance!

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Possible solutions,

1. Gradient normalization
2. Control variates, aka baselines

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  Which we can do because,

$$\sum_{z} b(\boldsymbol{x}) \nabla \pi(\boldsymbol{z}) = b(\boldsymbol{x}) \sum_{z} \nabla \pi(\boldsymbol{z}) = b(\boldsymbol{x}) \nabla 1 = 0$$

Issues with SPINN with REINFORCE

This system faces two big problems,

1. High variance of gradients
2. Coadaptation

Coadaptation problem

Learning composition function parameters $\boldsymbol{\phi}$ with backpropagation, and parser parameters $\boldsymbol{\theta}$ with REINFORCE.

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Difference in variance of two gradient estimates.

Coadaptation problem

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Dif

Possible solution:
Proximal Policy Optimization (Schulman et al., 2017)

Making REINFORCE+SPINN work

Havrylov et al. [2019] use,

1. Input dependent control variate
2. Gradient normalization
3. Proximal Policy Optimization

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However, does not learn English grammars.

Should I? Shouldn't I?

- Unbiased!

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III. Gradient Surrogates

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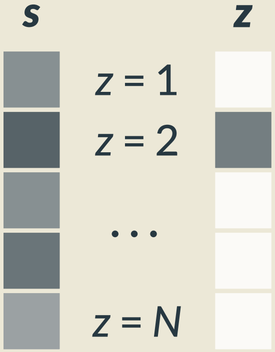
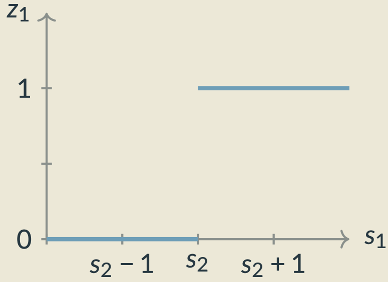
- 3A: try to optimize the deterministic loss directly
- 3B: use this strategy to reduce variance in the stochastic model.

Recap: The argmax problem

$$\boldsymbol{z} = \arg\max(\boldsymbol{s})$$

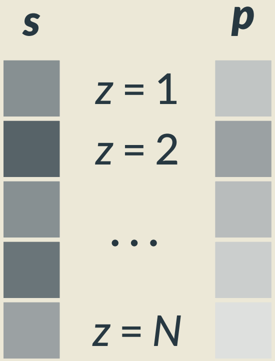


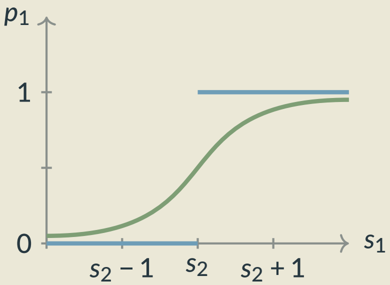


$$\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{s}} = \boldsymbol{0}$$

Softmax

$$p_j = \exp(s_j)/Z$$





$$\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{s}} = \mathrm{diag}(\boldsymbol{p}) - \boldsymbol{p}\boldsymbol{p}^\top$$

[Hinton, 2012, Bengio et al., 2013]

Straight-Through Estimator

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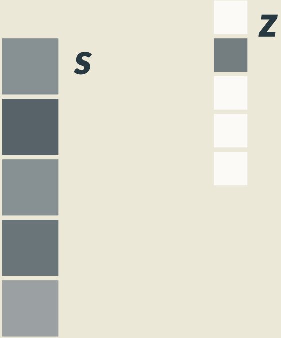

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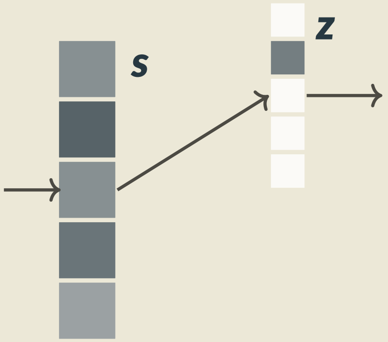

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- Forward: $\boldsymbol{z} = \arg\max(\boldsymbol{s})$
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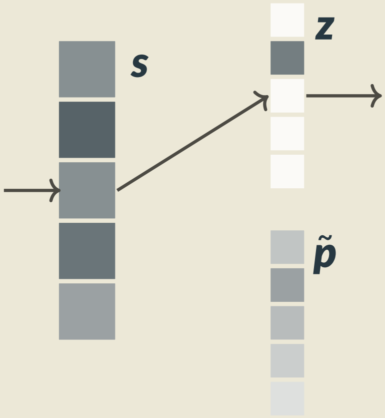

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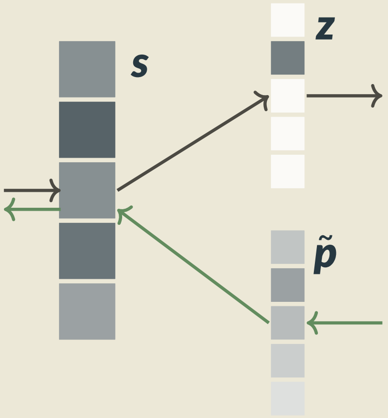

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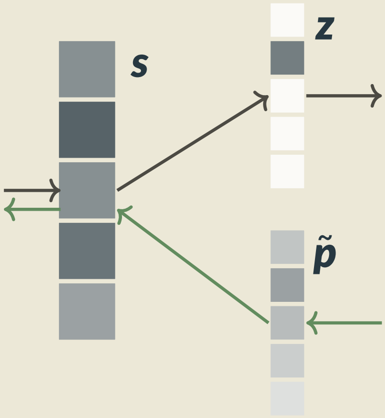

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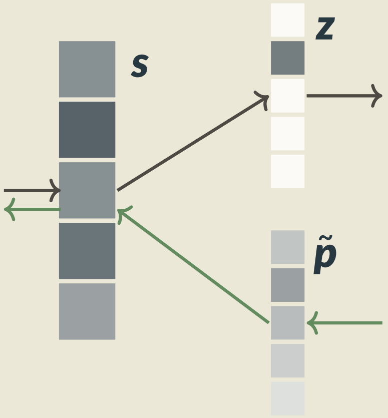

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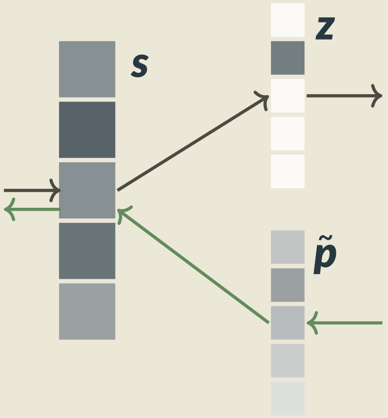
- More explanation in a while



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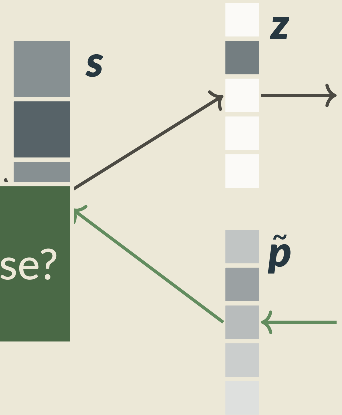
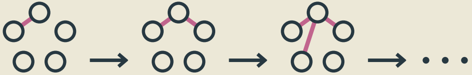
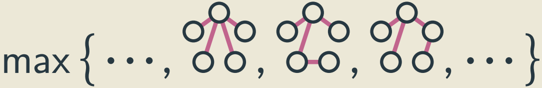
What about the structured case?



Dealing with the combinatorial explosion





1. Incremental structures

- Build structure **greedily**, as sequence of discrete choices (e.g., shift-reduce).
- Scores (partial structure, action) tuples.
- **Advantages:** flexible, rich histories.
- **Disadvantages:** greedy, local decisions are suboptimal, error propagation.

2. Factorization into parts

- Optimizes **globally** (e.g. Viterbi, Chu-Liu-Edmonds, Kuhn-Munkres).
- Scores smaller parts.
- **Advantages:** optimal, elegant, can handle hard & global constraints.
- **Disadvantages:** strong assumptions.

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  Example: Latent Tree Learning with Differentiable Parsers: Shift-Reduce Parsing and Chart Parsing [Maillard and Clark, 2018] (STE through beam search).

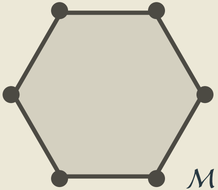
STE for the factorized approach

Requires a bit more work:

- Recap: marginal polytope
- Predicting structures globally: Maximum A Posteriori (MAP)
- Deriving Straight-Through and SPIGOT

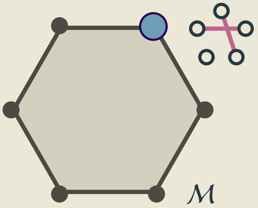
[Wainwright and Jordan, 2008]

The structured case: Marginal polytope



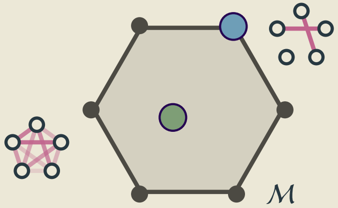
The structured case: Marginal polytope

- Each vertex corresponds to one such *bit vector* $\boldsymbol{z}$



The structured case: Marginal polytope

- Each vertex corresponds to one such *bit vector* $\boldsymbol{z}$
- Points inside correspond to *marginal distributions*: convex combinations of structured objects

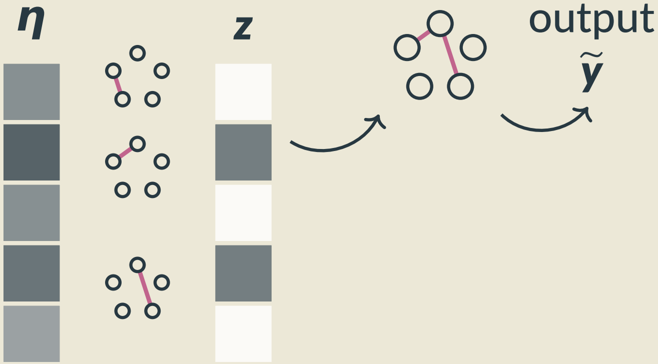


$$\boldsymbol{\mu} = \underbrace{p_1 \boldsymbol{z}_1 + \ldots + p_N \boldsymbol{z}_N}_{\text{exponentially many terms}}, \quad \boldsymbol{p} \in \Delta.$$

$$\begin{array}{ll} p_1 = 0.2, & \boldsymbol{z}_1 = [1,0,0,0,1,0,0,0,1] \\ p_2 = 0.7, & \boldsymbol{z}_2 = [0,0,1,0,0,1,1,0,0] \\ p_3 = 0.1, & \boldsymbol{z}_3 = [1,0,0,0,1,0,0,1,0] \end{array} \quad \Rightarrow \quad \boldsymbol{\mu} = [.3, 0, .7, 0, .3, .7, .7, .1, .2].$$

Predicting structures from scores of parts

- $\eta(i \to j)$: score of arc $i \to j$
- $z(i \to j)$: is arc $i \to j$ selected?



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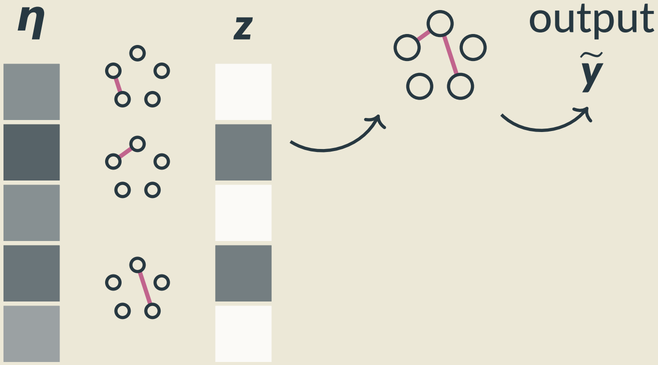
- Task-specific algorithm for the highest-scoring structure.

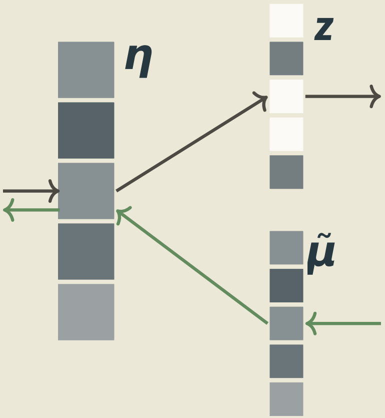


Algorithms for specific structures

	Best structure (MAP)
Sequence tagging	Viterbi [Rabiner, 1989]
Constituent trees	CKY [Kasami, 1966, Younger, 1967] [Cocke and Schwartz, 1970]
Temporal alignments	DTW [Sakoe and Chiba, 1978]
Dependency trees	Max. Spanning Arborescence [Chu and Liu, 1965, Edmonds, 1967]
Assignments	Kuhn-Munkres [Kuhn, 1955, Jonker and Volgenant, 1987]

Structured Straight-Through

- Forward pass:
  Find highest-scoring structure:
  $\boldsymbol{z} = \arg\max_{\boldsymbol{z} \in \mathcal{Z}} \boldsymbol{\eta}^\top \boldsymbol{z}$
- Backward pass:
  pretend we used $\tilde{\boldsymbol{\mu}} = \boldsymbol{\eta}$.



[Martins and Niculae, 2019]

Straight-Through Estimator

Revisited

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- if we had labels (multi-task learning), $L_{\text{MTL}} = L\big(\hat{y}(\boldsymbol{z}), y\big) + L_{\text{hid}}\big(\boldsymbol{s}, \boldsymbol{z}^{\text{true}}\big)$

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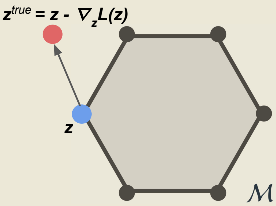
Straight-Through in the structured case

- Structured STE: perceptron update with induced annotation

$$\arg\min_{\boldsymbol{\mu}\in\mathbb{R}^D} L(\hat{y}(\boldsymbol{\mu}), y) \qquad \approx \boldsymbol{z} - \nabla_{\boldsymbol{z}} L(\boldsymbol{z}) \rightarrow \boldsymbol{z}^{\text{true}}$$

(one step of gradient descent)



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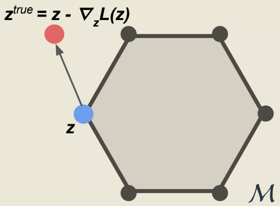
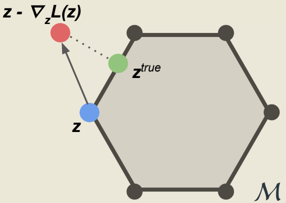


- SPIGOT takes into account the constraints; uses the induced annotation

$$\arg\min_{\boldsymbol{\mu}\in\mathcal{M}} L(\hat{y}(\boldsymbol{\mu}), y) \qquad \approx \mathrm{Proj}_{\mathcal{M}}\left(\boldsymbol{z} - \nabla_{\boldsymbol{z}} L(\boldsymbol{z})\right) \to \boldsymbol{z}^{\text{true}}$$

(one step of *projected* gradient descent!)



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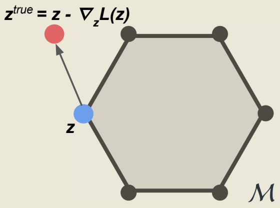
(one step of gradient descent)

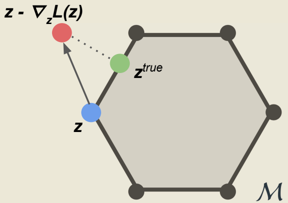
- SPIGOT takes into account the constraints; uses the induced annotation

$$\arg\min_{\boldsymbol{\mu}\in\mathcal{M}} L(\hat{y}(\boldsymbol{\mu}), y) \quad \approx \mathrm{Proj}_{\mathcal{M}}\left(\boldsymbol{z} - \nabla_{\boldsymbol{z}} L(\boldsymbol{z})\right) \to \boldsymbol{z}^{\text{true}}$$

(one step of *projected* gradient descent!)

- We discuss a generic way to compute the projection in part 4.





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Now we will see how to apply STE for stochastic graphs, as an alternative approach of REINFORCE.

Stochastic node in the computation graph

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Recall the stochastic objective:

$$\mathbb{E}_{\pi_{\boldsymbol{\theta}}(\boldsymbol{z}|x)}\left[L(\boldsymbol{z})\right]$$

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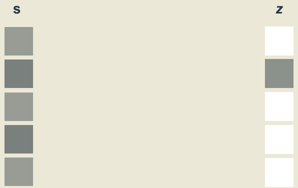
- REINFORCE (previous section). High variance. 😟
- An alternative is using the *reparameterization trick* [Kingma and Welling, 2014].

Categorical reparameterization

Categorical reparameterization

- Sampling from a categorical value in the middle of the computation graph.
  $\boldsymbol{z} \sim \pi_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x) \propto \exp \boldsymbol{s}_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x)$



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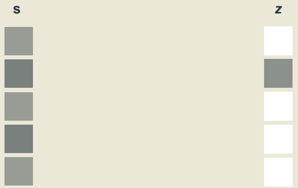

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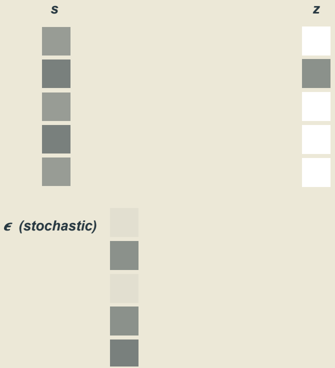

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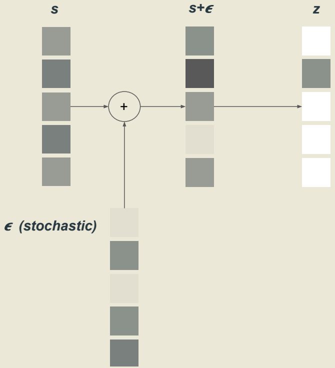

[Jang et al., 2017, Maddison et al., 2016]

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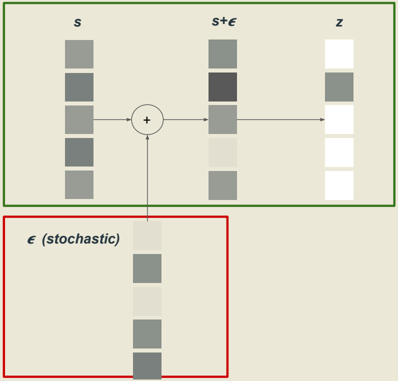

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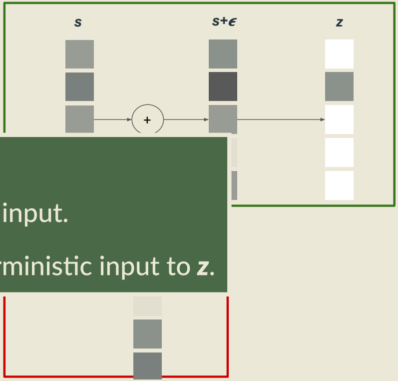


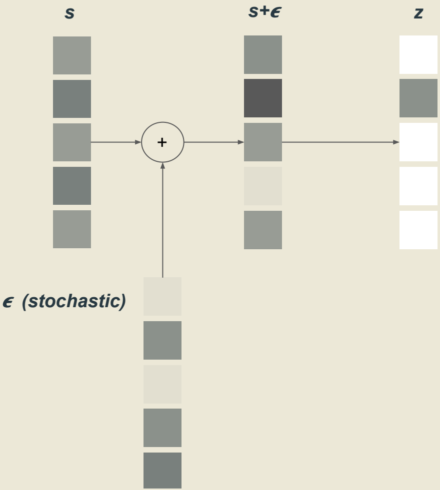
As a result:

Stochasticity is moved as an input.

We can backpropagate through the deterministic input to z.

[Jang et al., 2017, Maddison et al., 2016]

Categorical reparameterization



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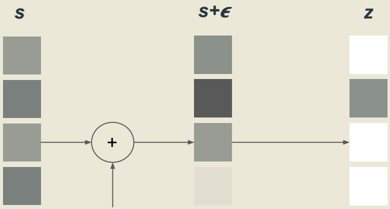

How do we sample from a categorical variable?

Sampling from a categorical variable

We want to sample from a categorical variable with scores $\boldsymbol{s}$ (class i has a score s_i)

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Derivation & more info: [Adams, 2013, Vieira, 2014]

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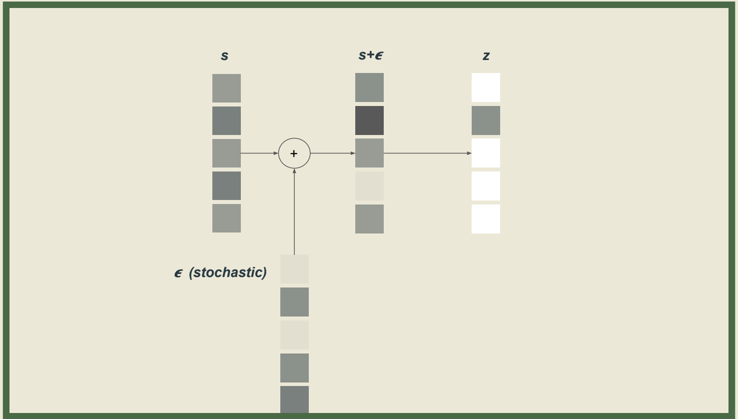

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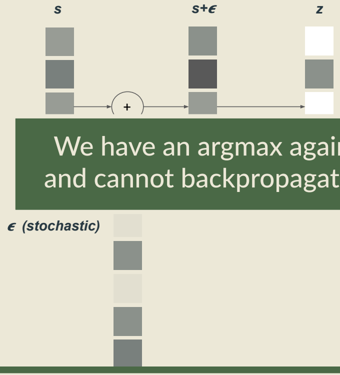

We have an argmax again and cannot backpropagate!

[Jang et al., 2017, Maddison et al., 2016]

Straight-Through Gumbel Estimator

Apply a variant of the Straight-Through Estimator to Gumbel-Max!

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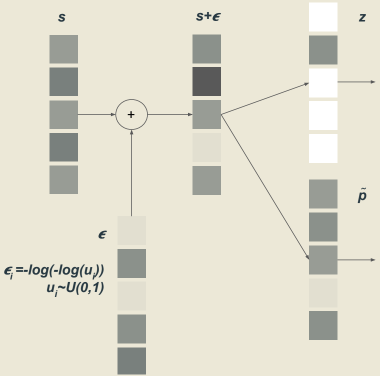

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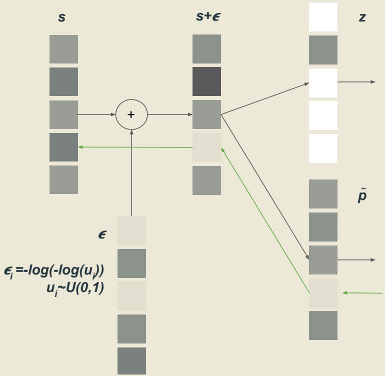

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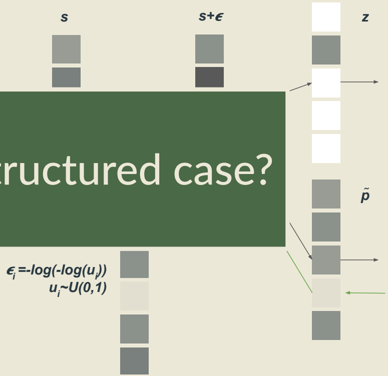
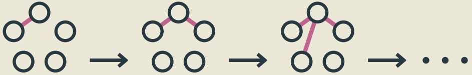
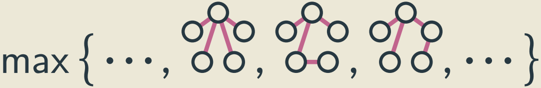


What about the structured case?

Dealing with the combinatorial explosion





1. Incremental structures

- Build structure **greedily**, as sequence of discrete choices (e.g., shift-reduce).
- Scores (partial structure, action) tuples.
- **Advantages:** flexible, rich histories.
- **Disadvantages:** greedy, local decisions are suboptimal, error propagation.

2. Factorization into parts

- Optimizes **globally** (e.g. Viterbi, Chu-Liu-Edmonds, Kuhn-Munkres).
- Scores smaller parts.
- **Advantages:** optimal, elegant, can handle hard & global constraints.
- **Disadvantages:** strong assumptions.

Sampling from incremental structures

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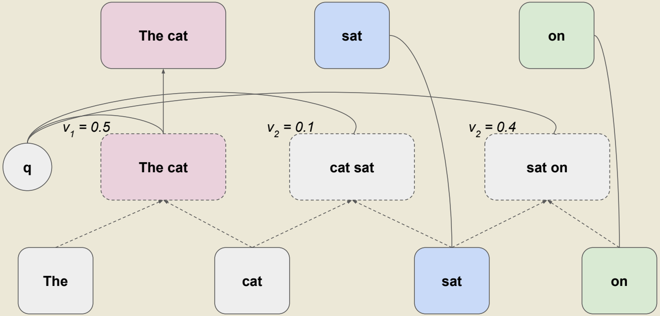
Example: Gumbel Tree-LSTM [Choi et al., 2018].

[Choi et al., 2018]

Example: Gumbel Tree-LSTM

- Building task-specific tree structures.
- Straight-Through Gumbel-Softmax at each step to select one arc.



[Papandreou and Yuille, 2011, Corro and Titov, 2019a,b]

Sampling from factorized models

Perturb-and-MAP

Reparameterize by **perturbing the arc scores.** (inexact!)

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Sampling from factorized models

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- Sample from the normal Gumbel distribution.
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- Compute MAP (task-specific algorithm).
- Backward: we could use Straight-Through with Identity.

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- $\tilde{\boldsymbol{\eta}} = \boldsymbol{\eta} + \boldsymbol{\epsilon}$
- $\arg\max_{\boldsymbol{z} \in \mathcal{Z}} \tilde{\boldsymbol{\eta}}^\top \boldsymbol{z}$

Summary: Gradient surrogates

- Based on the **Straight-Through Estimator**.
- Can be used for stochastic or deterministic computation graphs.
- **Forward pass**: Get an argmax (might be structured).
- **Backpropagation**: use a function, which we hope is close to argmax.
- Examples:
  - Argmax for iterative structures and factorization into parts
  - Sampling from iterative structures and factorization into parts

Gradient surrogates: Pros and cons

Pros

- Do not suffer from the high variance problem of REINFORCE.
- Allow for flexibility to select or sample a latent structured in the middle of the computation graph.
- Efficient computation.

Cons

- The Gumbel sampling with Perturb-and-MAP is an approximation.
- Bias, due to function mismatch on the backpropagation
  (next section will address this problem.)

Overview

$$\mathbb{E}_{\pi_{\boldsymbol{\theta}}(\boldsymbol{z}|x)}\left[L(\boldsymbol{z})\right] \qquad L\left(\arg\max_{z} \pi_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x)\right)$$

- REINFORCE
- Straight-Through Gumbel (Perturb & MAP)
- Straight-Through
- SPIGOT

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$$\mathbb{E}_{\pi_{\boldsymbol{\theta}}(\boldsymbol{z}|x)}\left[L(\boldsymbol{z})\right]$$

- REINFORCE
- Straight-Through Gumbel (Perturb & MAP)

$$L\left(\arg\max_{\boldsymbol{z}} \pi_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x)\right)$$

- Straight-Through
- SPIGOT

$$L\left(\mathbb{E}_{\pi_{\boldsymbol{\theta}}(\boldsymbol{z}|x)}[\boldsymbol{z}]\right)$$

- Structured Attn. Nets
- SparseMAP

And more, after the break!

IV. End-to-end Differentiable Relaxations

End-to-end differentiable relaxations

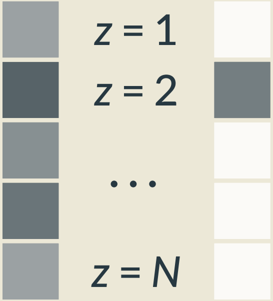
1. Digging into softmax
2. Alternatives to softmax
3. Generalizing to structured prediction
4. Stochasticity and global structures

Recall: Discrete choices & differentiability

input $\boldsymbol{x}$

$\boldsymbol{s}$ $\quad$ $\boldsymbol{z}$

output $\widehat{\boldsymbol{y}}$

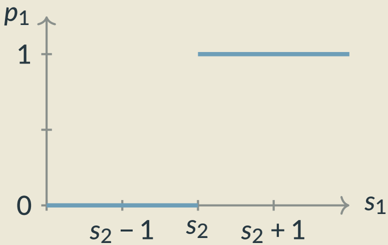


$\boldsymbol{s} = \boldsymbol{f_\theta}(\boldsymbol{x})$

$y = \boldsymbol{g_\phi}(\boldsymbol{z}, \boldsymbol{x})$

$\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{s}} = \boldsymbol{0}$ or n/a

(argmax)



One solution: smooth relaxation

input $\boldsymbol{x}$

$\boldsymbol{s} = \boldsymbol{f_\theta}(\boldsymbol{x})$

$\boldsymbol{s}$ $\boldsymbol{p}$

$z = 1$

$z = 2$

$\cdots$

$z = N$

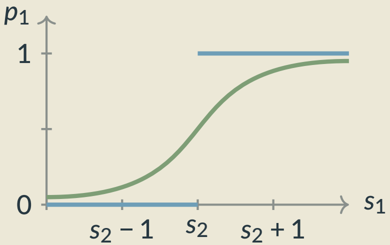
output $\widehat{\boldsymbol{y}}$

$y = \boldsymbol{g_\phi}(\boldsymbol{z}, \boldsymbol{x})$

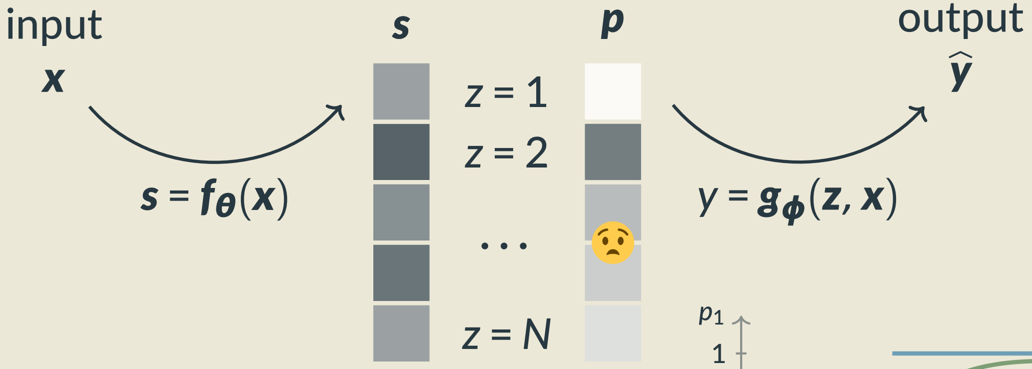
$\boldsymbol{p} = \mathrm{softmax}(\boldsymbol{s}) = \mathbb{E}[\boldsymbol{z}]$, i.e.
replace $\mathbb{E}\big[f(\boldsymbol{z})\big]$ with $f\big(\mathbb{E}[\boldsymbol{z}]\big)$

$\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{s}} =$

(softmax)



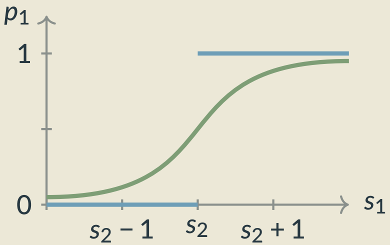
One solution: smooth relaxation



$\boldsymbol{p} = \text{softmax}(\boldsymbol{s}) = \mathbb{E}[\boldsymbol{z}]$, i.e.
replace $\mathbb{E}\big[f(\boldsymbol{z})\big]$ with $f\big(\mathbb{E}[\boldsymbol{z}]\big)$

$\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{s}} =$ 😊

(softmax)



Overview

$$\mathbb{E}_{\pi_{\boldsymbol{\theta}}(\boldsymbol{z}|x)}\big[L(\boldsymbol{z})\big] \qquad L\big(\arg\max_{z} \pi_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x)\big) \qquad L\big(\mathbb{E}_{\pi_{\boldsymbol{\theta}}(\boldsymbol{z}|x)}[\boldsymbol{z}]\big)$$

- REINFORCE
- Straight-Through Gumbel (Perturb & MAP)

- Straight-Through
- SPIGOT

What is softmax?

Often defined via $p_i = \dfrac{\exp s_i}{\sum_j \exp s_j}$, but where does it come from?

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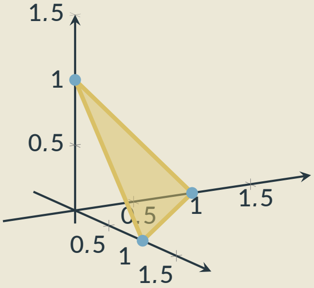

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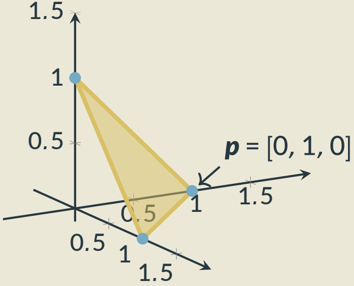

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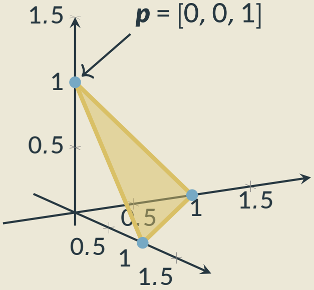

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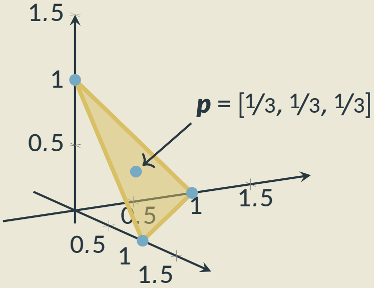

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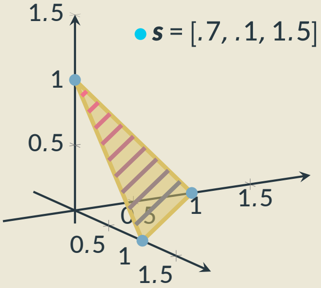

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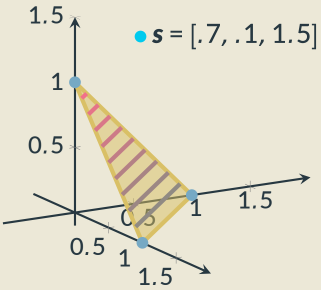

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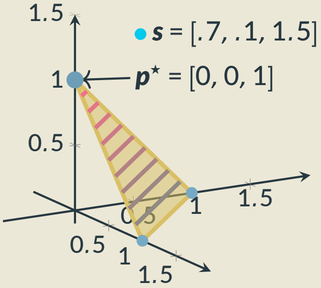

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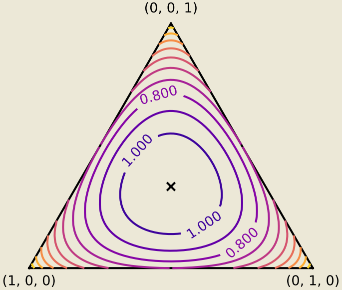

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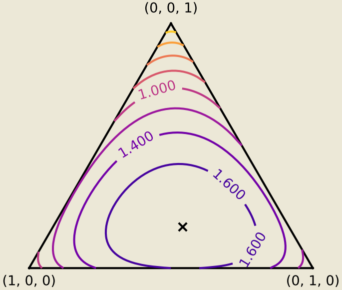
softmax maximizes **expected score** + **entropy**:



$$\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top \boldsymbol{s} + \mathrm{H}(\boldsymbol{p})$$

Variational form of softmax

Proposition. The unique solution to $\underset{\boldsymbol{p}\in\triangle}{\arg\max}\, \boldsymbol{p}^\top \boldsymbol{s} + \mathrm{H}(\boldsymbol{p})$ is given by $p_j = \frac{\exp s_j}{\sum_i \exp s_i}$.

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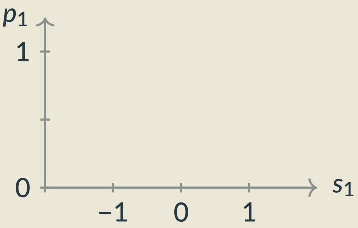
Answer: $Z = \sum_j \exp(s_j)$

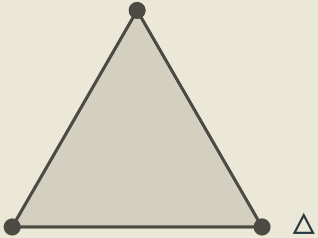
So, $p_i = \dfrac{\exp(s_i)}{\sum_j \exp(s_j)}$.

Classic result, e.g., [Boyd and Vandenberghe, 2004, Wainwright and Jordan, 2008]

Generalizing softmax: Smoothed argmaxes

$$\hat{\boldsymbol{p}}_\Omega(\boldsymbol{s}) = \arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s} - \Omega(\boldsymbol{p})$$





[Niculae and Blondel, 2017]

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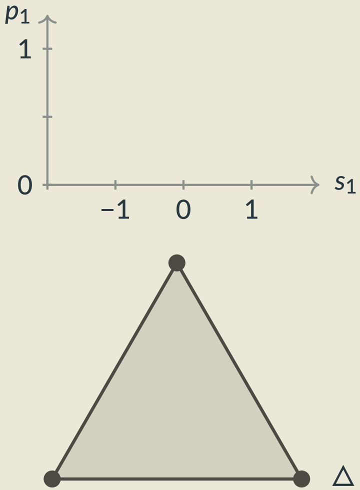

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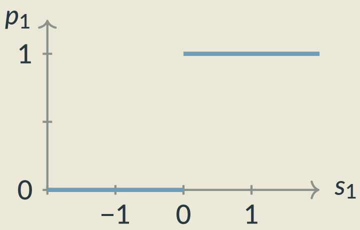

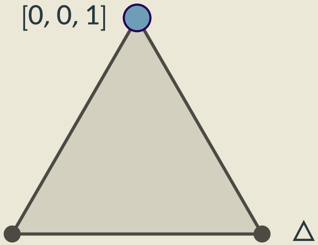

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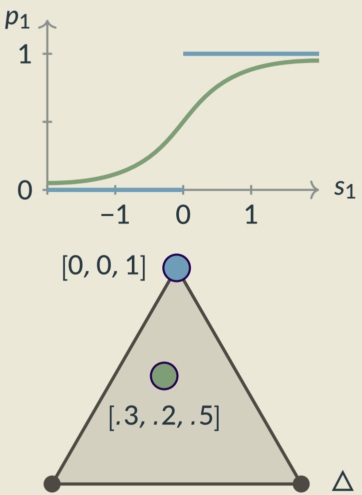

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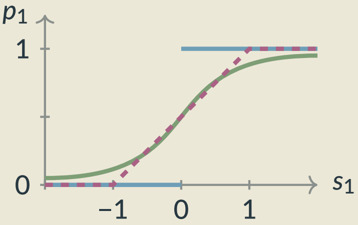

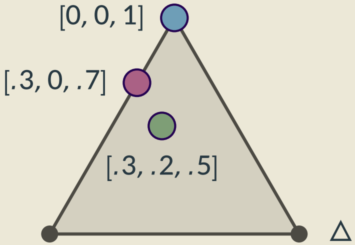

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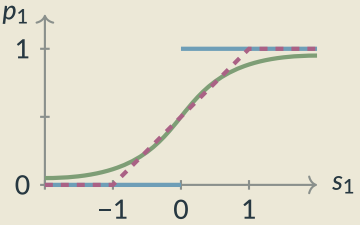

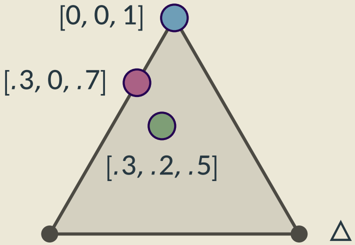

Generalized entropy interpolates in between [Tsallis, 1988]
Used in Sparse Seq2Seq: [Peters et al., 2019]
(Mon 13:50, poster session 2D)

[Niculae and Blondel, 2017, Martins and Kreutzer, 2017, Malaviya et al., 2018]

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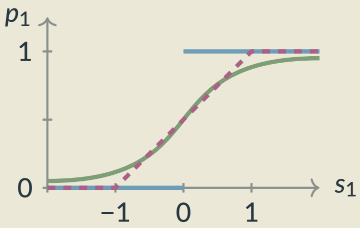
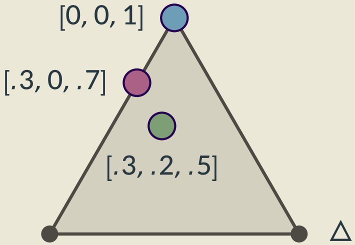
fusedmax: $\Omega(\boldsymbol{p}) = 1/2\|\boldsymbol{p}\|_2^2 + \sum_j |p_j - p_{j-1}|$

csparsemax: $\Omega(\boldsymbol{p}) = 1/2\|\boldsymbol{p}\|_2^2 + \iota(\boldsymbol{a} \leq \boldsymbol{p} \leq \boldsymbol{b})$

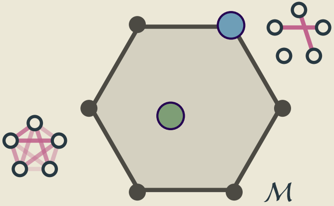
csoftmax: $\Omega(\boldsymbol{p}) = \sum_j p_j \log p_j + \iota(\boldsymbol{a} \leq \boldsymbol{p} \leq \boldsymbol{b})$





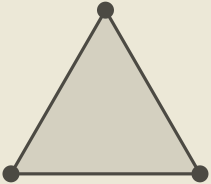
The structured case: Marginal polytope

- Each vertex corresponds to one such *bit vector* $\boldsymbol{z}$
- Points inside correspond to *marginal distributions*: convex combinations of structured objects



$$\boldsymbol{\mu} = \underbrace{p_1 \boldsymbol{z}_1 + \ldots + p_N \boldsymbol{z}_N}_{\text{exponentially many terms}}, \quad \boldsymbol{p} \in \Delta.$$

$$\begin{array}{ll} p_1 = 0.2, & \boldsymbol{z}_1 = [1, 0, 0, 0, 1, 0, 0, 0, 1] \\ p_2 = 0.7, & \boldsymbol{z}_2 = [0, 0, 1, 0, 0, 1, 1, 0, 0] \\ p_3 = 0.1, & \boldsymbol{z}_3 = [1, 0, 0, 0, 1, 0, 0, 1, 0] \end{array} \quad \Rightarrow \quad \boldsymbol{\mu} = [.3, 0, .7, 0, .3, .7, .7, .1, .2].$$



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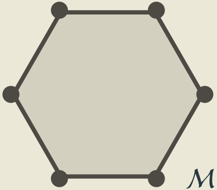
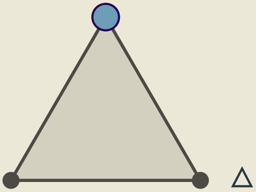
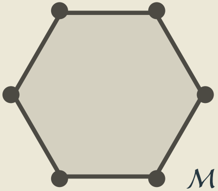


$\mathcal{M}$

- **argmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s}$





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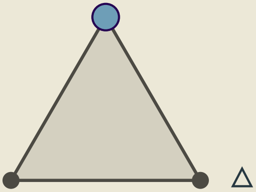

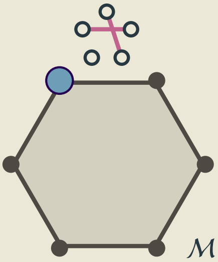

- **argmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s}$
- **softmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s} + \mathrm{H}(\boldsymbol{p})$

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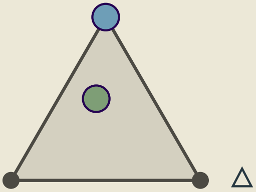

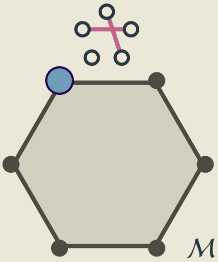

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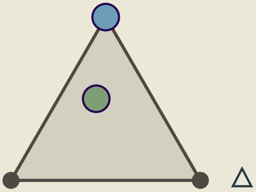

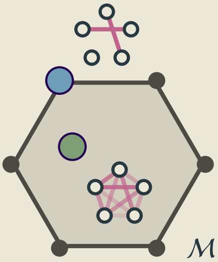

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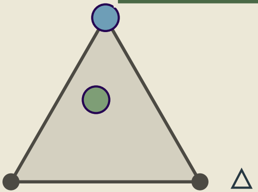
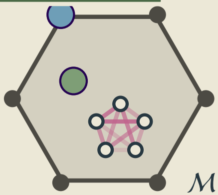
Just like softmax relaxes argmax,
marginals relax MAP **differentiably**!





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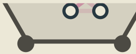
Unlike argmax/softmax, computation is not obvious!

$\triangle$



$\mathcal{M}$

Algorithms for specific structures

	Best structure (MAP)	Marginals
Sequence tagging	Viterbi [Rabiner, 1989]	Forward-Backward [Rabiner, 1989]
Constituent trees	CKY [Kasami, 1966, Younger, 1967] [Cocke and Schwartz, 1970]	Inside-Outside [Baker, 1979]
Temporal alignments	DTW [Sakoe and Chiba, 1978]	Soft-DTW [Cuturi and Blondel, 2017]
Dependency trees	Max. Spanning Arborescence [Chu and Liu, 1965, Edmonds, 1967]	Matrix-Tree [Kirchhoff, 1847]
Assignments	Kuhn-Munkres [Kuhn, 1955, Jonker and Volgenant, 1987]	#P-complete [Valiant, 1979, Taskar, 2004]

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Dynamic programming: marginals by **Forward-Backward**, **Inside-Outside**, etc.

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Marginals in a sequence tagging model.

input: d tags, n tokens, $\boldsymbol{\eta}_U \in \mathbb{R}^{n \times d}$, $\boldsymbol{\eta}_V \in \mathbb{R}^{d \times d}$
initialize $\boldsymbol{\alpha}_1 = \mathbf{0}$, $\boldsymbol{\beta}_n = \mathbf{0}$
for $i \in 2, \ldots, n$ **do** *# forward log-probabilities*
  $\alpha_{i,k} = \log \sum_{k'} \exp\left(\alpha_{i-1,k'} + (\boldsymbol{\eta}_U)_{i,k} + (\boldsymbol{\eta}_V)_{k',k}\right)$ for all k
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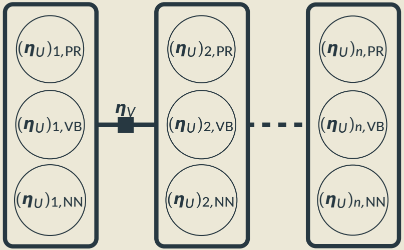

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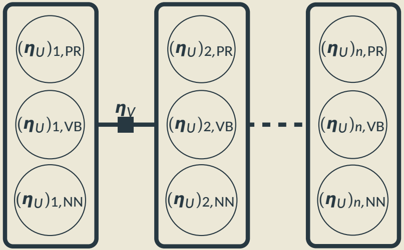

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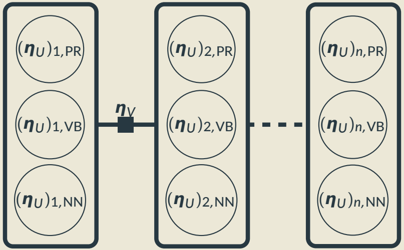

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- With circular dependencies, this breaks! Can get an approximation Stoyanov et al. [2011]

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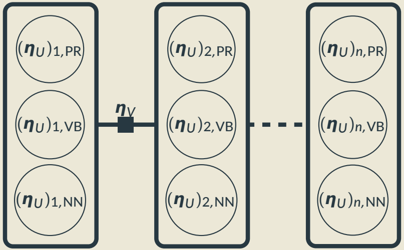


Derivatives of marginals 2: Matrix-Tree

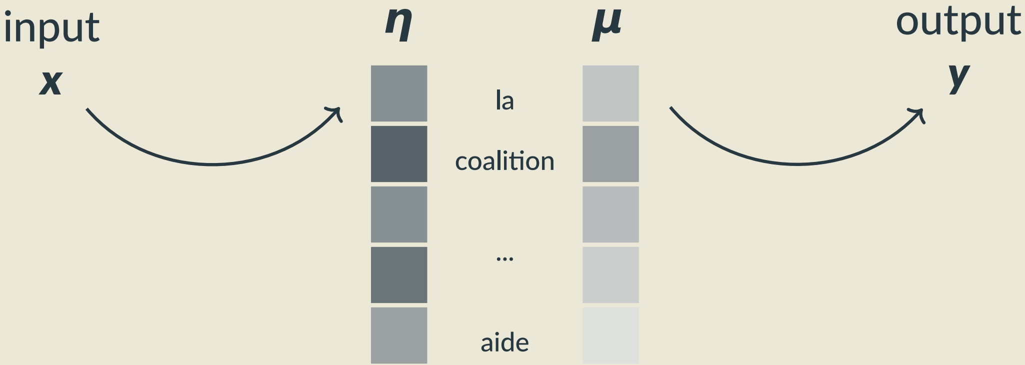
$\boldsymbol{L}(\boldsymbol{s})$: Laplacian of the edge score graph

$$Z = \det \boldsymbol{L}(\boldsymbol{s})$$

$$\boldsymbol{\mu} = \boldsymbol{L}(\boldsymbol{s})^{-1}$$

$$\nabla\boldsymbol{\mu} = \nabla\boldsymbol{L}^{-1} = \boldsymbol{L}^{-1}\left(\frac{\partial\boldsymbol{L}}{\partial\boldsymbol{\eta}}\right)\boldsymbol{L}^{-1}$$

Structured Attention Networks



[Kim et al., 2017]

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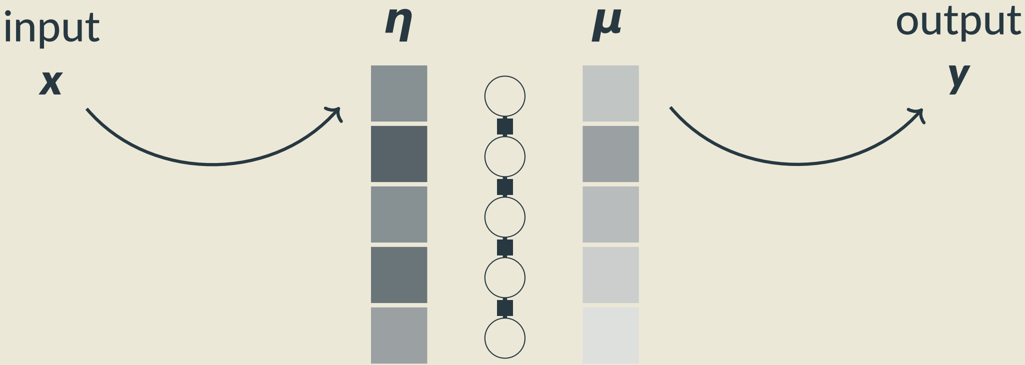

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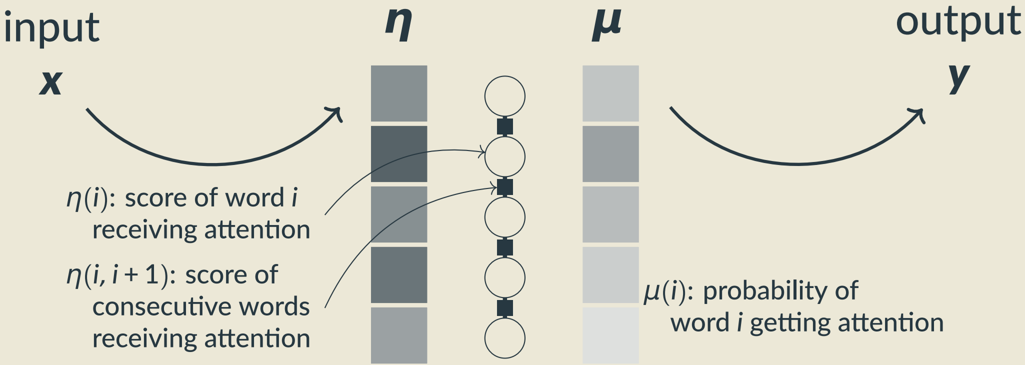

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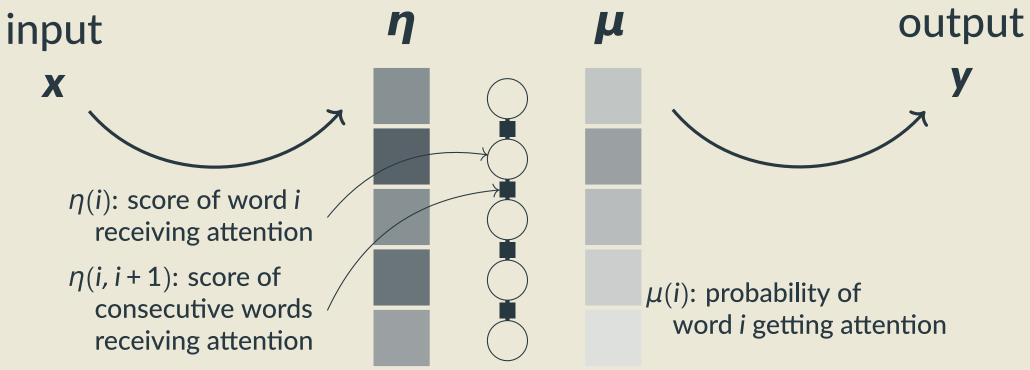

CRF marginals (from *forward–backward*) give attention weights $\in (0, 1)$

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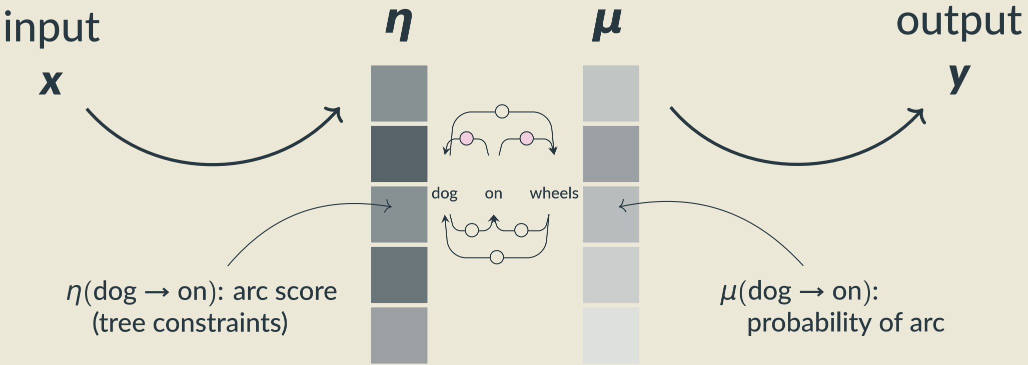

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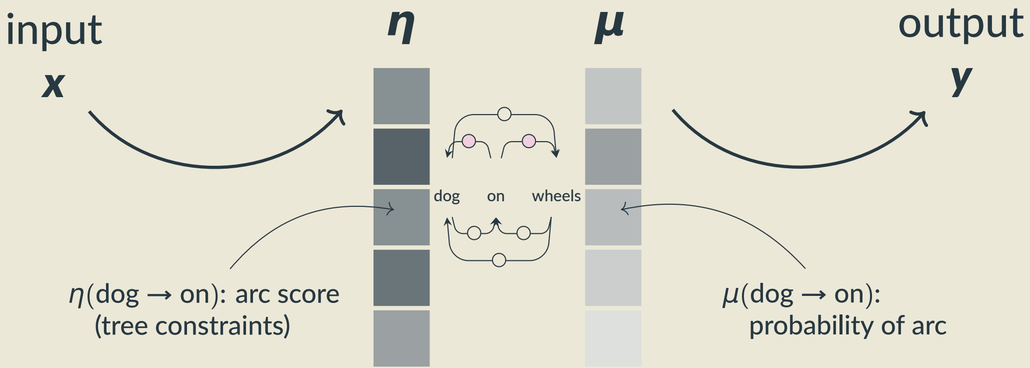

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Similar idea for projective dependency trees with *inside–outside*
and non-projective with the Matrix-Tree theorem [Liu and Lapata, 2018].

[Corro and Titov, 2019a,b]

Differentiable Perturb & Parse

Extending Gumbel-Softmax to structured stochastic models

- Forward pass:

  sample structure $\boldsymbol{z}$ (approximately)

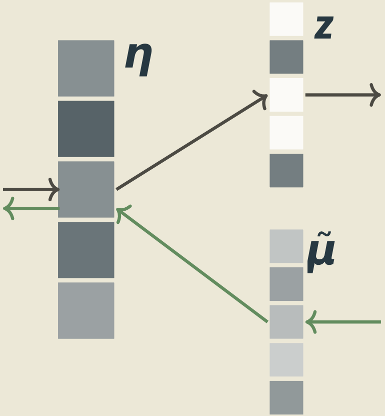
  $$\boldsymbol{z} = \arg\max_{\boldsymbol{z}\in\mathcal{Z}} (\boldsymbol{\eta} + \boldsymbol{\epsilon})^\top \boldsymbol{z}$$

- Backward pass:

  pretend we did marginal inference

  $$\tilde{\boldsymbol{\mu}} = \arg\max_{\boldsymbol{\mu}\in\mathcal{M}} (\boldsymbol{\eta} + \boldsymbol{\epsilon})^\top \boldsymbol{z} + \tilde{\mathrm{H}}(\boldsymbol{\mu})$$

  (or some similar relaxation)



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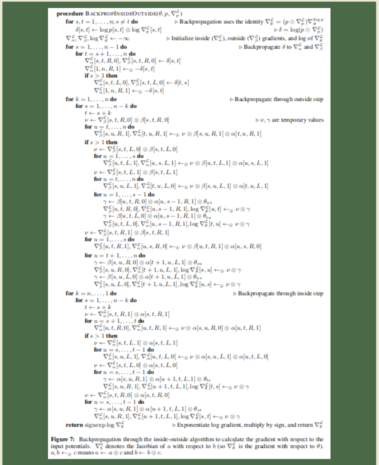

procedure $\textsc{BackpropInsideOutside}(\theta, p, \nabla^{\mathcal{L}}_p)$
  for $s, t = 1, \dots, n; s \neq t$ **do** ▷ Backpropagation uses the identity $\nabla^{\mathcal{L}}_\theta = (p \odot \nabla^{\mathcal{L}}_p)\nabla^{\log p}_\theta$
    $\delta[s,t] \leftarrow \log p[s,t] \otimes \log \nabla^{\mathcal{L}}_p[s,t]$ ▷ $\delta = \log(p \odot \nabla^{\mathcal{L}}_p)$
  $\nabla^{\mathcal{L}}_\alpha, \nabla^{\mathcal{L}}_\beta, \log \nabla^{\mathcal{L}}_\theta \leftarrow -\infty$ ▷ Initialize inside ($\nabla^{\mathcal{L}}_\alpha$), outside ($\nabla^{\mathcal{L}}_\beta$) gradients, and log of $\nabla^{\mathcal{L}}_\theta$
  for $s = 1, \dots, n-1$ **do** ▷ Backpropagate δ to $\nabla^{\mathcal{L}}_\alpha$ and $\nabla^{\mathcal{L}}_\beta$
    for $t = s+1, \dots, n$ **do**
      $\nabla^{\mathcal{L}}_\alpha[s,t,R,0], \nabla^{\mathcal{L}}_\beta[s,t,R,0] \leftarrow \delta[s,t]$
      $\nabla^{\mathcal{L}}_\alpha[1,n,R,1] \leftarrow_\oplus -\delta[s,t]$
      if $s > 1$ **then**
        $\nabla^{\mathcal{L}}_\alpha[s,t,L,0], \nabla^{\mathcal{L}}_\beta[s,t,L,0] \leftarrow \delta[t,s]$
        $\nabla^{\mathcal{L}}_\alpha[1,n,R,1] \leftarrow_\oplus -\delta[s,t]$
  for $k = 1, \dots, n$ **do** ▷ Backpropagate through outside step
    for $s = 1, \dots, n-k$ **do**
      $t \leftarrow s + k$
      $\nu \leftarrow \nabla^{\mathcal{L}}_\beta[s,t,R,0] \otimes \beta[s,t,R,0]$ ▷ ν, γ are temporary values
      for $u = t, \dots, n$ **do**
        $\nabla^{\mathcal{L}}_\beta[s,u,R,1], \nabla^{\mathcal{L}}_\alpha[t,u,R,1] \leftarrow_\oplus \nu \otimes \beta[s,u,R,1] \otimes \alpha[t,u,R,1]$
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        for $u = 1, \dots, s-1$ **do**
          $\gamma \leftarrow \beta[u,t,R,0] \otimes \alpha[u,s-1,R,1] \otimes \theta_{ut}$
          $\nabla^{\mathcal{L}}_\beta[u,t,R,0], \nabla^{\mathcal{L}}_\alpha[u,s-1,R,1], \log \nabla^{\mathcal{L}}_\theta[u,t] \leftarrow_\oplus \nu \otimes \gamma$
          $\gamma \leftarrow \beta[u,t,L,0] \otimes \alpha[u,s-1,R,1] \otimes \theta_{tu}$
          $\nabla^{\mathcal{L}}_\beta[u,t,L,0], \nabla^{\mathcal{L}}_\alpha[u,s-1,R,1], \log \nabla^{\mathcal{L}}_\theta[t,u] \leftarrow_\oplus \nu \otimes \gamma$
      $\nu \leftarrow \nabla^{\mathcal{L}}_\beta[s,t,R,1] \otimes \beta[s,t,R,1]$
      for $u = 1, \dots, s$ **do**
        $\nabla^{\mathcal{L}}_\beta[u,t,R,1], \nabla^{\mathcal{L}}_\alpha[u,s,R,0] \leftarrow_\oplus \nu \otimes \beta[u,t,R,1] \otimes \alpha[u,s,R,0]$
      for $u = t+1, \dots, n$ **do**
        $\gamma \leftarrow \beta[s,u,R,0] \otimes \alpha[t+1,u,L,1] \otimes \theta_{su}$
        $\nabla^{\mathcal{L}}_\beta[s,u,R,0], \nabla^{\mathcal{L}}_\alpha[t+1,u,L,1], \log \nabla^{\mathcal{L}}_\theta[s,u] \leftarrow_\oplus \nu \otimes \gamma$
        $\gamma \leftarrow \beta[s,u,L,0] \otimes \alpha[t+1,u,L,1] \otimes \theta_{us}$
        $\nabla^{\mathcal{L}}_\beta[s,u,L,0], \nabla^{\mathcal{L}}_\alpha[t+1,u,L,1], \log \nabla^{\mathcal{L}}_\theta[u,s] \leftarrow_\oplus \nu \otimes \gamma$
  for $k = n, \dots, 1$ **do** ▷ Backpropagate through inside step
    for $s = 1, \dots, n-k$ **do**
      $t \leftarrow s + k$
      $\nu \leftarrow \nabla^{\mathcal{L}}_\alpha[s,t,R,1] \otimes \alpha[s,t,R,1]$
      for $u = s+1, \dots, t$ **do**
        $\nabla^{\mathcal{L}}_\alpha[u,t,R,0], \nabla^{\mathcal{L}}_\alpha[u,t,R,1] \leftarrow_\oplus \nu \otimes \alpha[s,u,R,0] \otimes \alpha[u,t,R,1]$
      if $s > 1$ **then**
        $\nu \leftarrow \nabla^{\mathcal{L}}_\alpha[s,t,L,1] \otimes \alpha[s,t,L,1]$
        for $u = s, \dots, t-1$ **do**
          $\nabla^{\mathcal{L}}_\alpha[s,u,L,1], \nabla^{\mathcal{L}}_\alpha[u,t,L,0] \leftarrow_\oplus \nu \otimes \alpha[s,u,L,1] \otimes \alpha[u,t,L,0]$
        $\nu \leftarrow \nabla^{\mathcal{L}}_\alpha[s,t,L,0] \otimes \alpha[s,t,L,0]$
        for $u = s, \dots, t-1$ **do**
          $\gamma \leftarrow \alpha[s,u,R,1] \otimes \alpha[u+1,t,L,1] \otimes \theta_{ts}$
          $\nabla^{\mathcal{L}}_\alpha[s,u,R,1], \nabla^{\mathcal{L}}_\alpha[u+1,t,L,1], \log \nabla^{\mathcal{L}}_\theta[t,s] \leftarrow_\oplus \nu \otimes \gamma$
      $\nu \leftarrow \nabla^{\mathcal{L}}_\alpha[s,t,R,0] \otimes \alpha[s,t,R,0]$
      for $u = s, \dots, t-1$ **do**
        $\gamma \leftarrow \alpha[s,u,R,1] \otimes \alpha[u+1,t,L,1] \otimes \theta_{st}$
        $\nabla^{\mathcal{L}}_\alpha[s,u,R,1], \nabla^{\mathcal{L}}_\alpha[u+1,t,L,1], \log \nabla^{\mathcal{L}}_\theta[s,t] \leftarrow_\oplus \nu \otimes \gamma$
  return $\operatorname{signexp} \log \nabla^{\mathcal{L}}_\theta$ ▷ Exponentiate log gradient, multiply by sign, and return $\nabla^{\mathcal{L}}_\theta$

Figure 7: Backpropagation through the inside-outside algorithm to calculate the gradient with respect to the input potentials. ∇^a_b denotes the Jacobian of a with respect to b (so $\nabla^{\mathcal{L}}_\theta$ is the gradient with respect to θ). $a, b \leftarrow_\oplus c$ means $a \leftarrow a \oplus c$ and $b \leftarrow b \oplus c$.

Back-propagating through marginals

Pros:

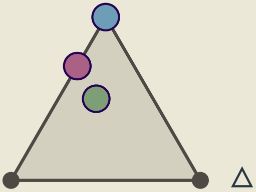
- Familiar algorithms for NLPers,
- (Structured Attention Networks:) All computations exact.

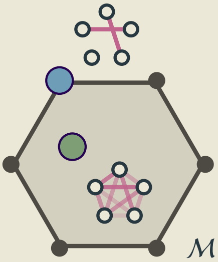
Cons:

- (Structured Attention Networks:) forward pass marginals are dense;
  (fixed by Perturb & MAP, at cost of rough approximation)
- Efficient & numerically stable back-propagation through DPs is tricky;
  (somewhat alleviated by Mensch and Blondel [2018])
- Not applicable when marginals are unavailable.
- Case-by-case algorithms required, can get tedious.

- **argmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s}$
- **softmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s} + \mathrm{H}(\boldsymbol{p})$
- **sparsemax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s} - 1/2\|\boldsymbol{p}\|^2$

- **MAP** $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta}$
- **marginals** $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta} + \widetilde{\mathrm{H}}(\boldsymbol{\mu})$

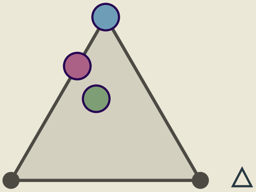


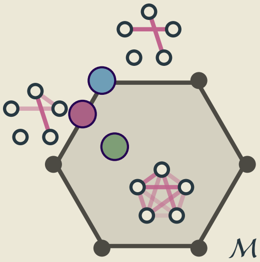


[Niculae et al., 2018a]

- **argmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s}$
- **softmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s} + \mathrm{H}(\boldsymbol{p})$
- **sparsemax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s} - 1/2\|\boldsymbol{p}\|^2$

- **MAP** $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta}$
- **marginals** $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta} + \widetilde{\mathrm{H}}(\boldsymbol{\mu})$
- **SparseMAP** $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta} - 1/2\|\boldsymbol{\mu}\|^2$





SparseMAP solution

$$\boldsymbol{\mu}^\star = \arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta} - 1/2\|\boldsymbol{\mu}\|^2$$

$=$  $= .6$  $+ .4$ 

($\boldsymbol{\mu}^\star$ is unique, but may have multiple decompositions $\boldsymbol{p}$. Active Set recovers a sparse one.)

Algorithms for SparseMAP

$$\boldsymbol{\mu}^\star = \underset{\boldsymbol{\mu}\in\mathcal{M}}{\arg\max}\, \boldsymbol{\mu}^\top \boldsymbol{\eta} - 1/2\|\boldsymbol{\mu}\|^2$$

Algorithms for SparseMAP

$$\boldsymbol{\mu}^{\star} = \underset{\boldsymbol{\mu} \in \mathcal{M}}{\arg\max}\, \boldsymbol{\mu}^{\top} \boldsymbol{\eta} - 1/2 \|\boldsymbol{\mu}\|^2$$

linear constraints
(alas, exponentially many!)

quadratic objective

Algorithms for SparseMAP

$$\boldsymbol{\mu}^\star = \underset{\boldsymbol{\mu} \in \mathcal{M}}{\arg\max}\, \boldsymbol{\mu}^\top \boldsymbol{\eta} - 1/2 \|\boldsymbol{\mu}\|^2$$

linear constraints
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quadratic objective

Conditional Gradient

[Frank and Wolfe, 1956, Lacoste-Julien and Jaggi, 2015]

Algorithms for SparseMAP

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Conditional Gradient

[Frank and Wolfe, 1956, Lacoste-Julien and Jaggi, 2015]

- select a new corner of $\mathcal{M}$

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quadratic objective

Conditional Gradient

[Frank and Wolfe, 1956, Lacoste-Julien and Jaggi, 2015]

- select a new corner of $\mathcal{M}$

$$\underset{\boldsymbol{\mu}\in\mathcal{M}}{\arg\max}\, \boldsymbol{\mu}^\top \underbrace{\left(\boldsymbol{\eta} - \boldsymbol{\mu}^{(t-1)}\right)}_{\tilde{\boldsymbol{\eta}}}$$

Algorithms for SparseMAP

$$\boldsymbol{\mu}^\star = \underset{\boldsymbol{\mu}\in\mathcal{M}}{\arg\max}\, \boldsymbol{\mu}^\top \boldsymbol{\eta} - 1/2\|\boldsymbol{\mu}\|^2$$

linear constraints
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Conditional Gradient

[Frank and Wolfe, 1956, Lacoste-Julien and Jaggi, 2015]

- select a new corner of $\mathcal{M}$
- update the (sparse) coefficients of $\boldsymbol{p}$
  - Update rules: vanilla, away-step, pairwise

Algorithms for SparseMAP

$$\boldsymbol{\mu}^{\star} = \underset{\boldsymbol{\mu} \in \mathcal{M}}{\arg\max}\, \boldsymbol{\mu}^{\top}\boldsymbol{\eta} - 1/2\|\boldsymbol{\mu}\|^2$$

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- update the (sparse) coefficients of $\boldsymbol{p}$
  - Update rules: vanilla, away-step, pairwise
  - Quadratic objective: **Active Set**
    a.k.a. Min-Norm Point, [Wolfe, 1976]
    [Martins et al., 2015, Nocedal and Wright, 1999,
    Vinyes and Obozinski, 2017]

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$$\boldsymbol{\mu}^\star = \arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta} - 1/2\|\boldsymbol{\mu}\|^2$$

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(alas, exponentially many!)

quadratic objective

Conditional Gradient

[Frank and Wolfe, 1956, Lacoste-Julien and Jaggi, 2015]

- select a new corne
- update the (sparse)
  - Update rules: vanilla
  - Quadratic objective:

Active Set achieves
finite & **linear** convergence!

a.k.a. Min-Norm Point, [Wolfe, 1976]

[Martins et al., 2015, Nocedal and Wright, 1999,

Vinyes and Obozinski, 2017]

Algorithms for SparseMAP

$$\boldsymbol{\mu}^\star = \arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta} - 1/2\|\boldsymbol{\mu}\|^2$$

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Backward pass

$\frac{\partial \boldsymbol{\mu}}{\partial \boldsymbol{\eta}}$ is sparse

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Backward pass

$\frac{\partial \boldsymbol{\mu}}{\partial \boldsymbol{\eta}}$ is sparse

computing $\left(\frac{\partial \boldsymbol{\mu}}{\partial \boldsymbol{\eta}}\right)^\top \boldsymbol{dy}$

takes $\mathcal{O}(\dim(\boldsymbol{\mu})\,\mathrm{nnz}(\boldsymbol{p}^\star))$

Algorithms for SparseMAP

$$\boldsymbol{\mu}^\star = \underset{\boldsymbol{\mu}\in\mathcal{M}}{\arg\max}\, \boldsymbol{\mu}^\top \boldsymbol{\eta} - 1/2\|\boldsymbol{\mu}\|^2$$

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[Frank and Wolfe, 1956

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    [Martins et al., 2015, Nocedal and Wright, 1999, Vinyes and Obozinski, 2017]

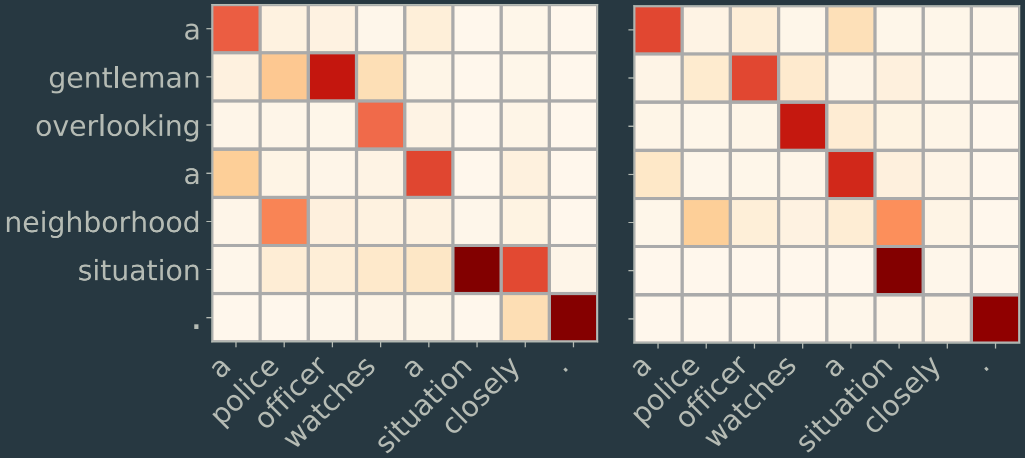
Completely modular: just add MAP

pass

rse

computing $\left(\frac{\partial \boldsymbol{\mu}}{\partial \boldsymbol{\eta}}\right)^\top \boldsymbol{dy}$
takes $\mathcal{O}(\dim(\boldsymbol{\mu})\,\mathrm{nnz}(\boldsymbol{p}^\star))$

[Chen et al., 2017]



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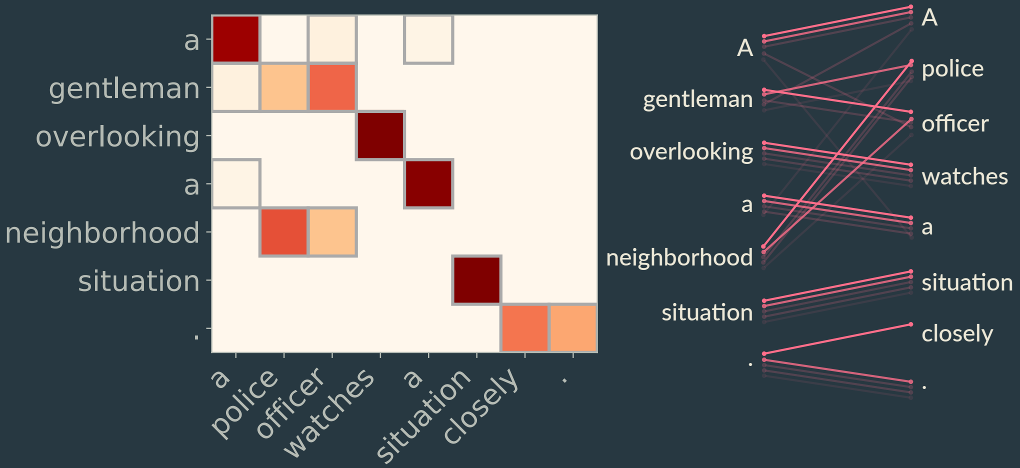

Overview

$$\mathbb{E}_{\pi_{\boldsymbol{\theta}}(\boldsymbol{z}|x)}\Big[L(\boldsymbol{z})\Big]$$

- REINFORCE
- Straight-Through Gumbel (Perturb & MAP)

$$L\Big(\arg\max_{\boldsymbol{z}} \pi_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x)\Big)$$

- Straight-Through
- SPIGOT

$$L\Big(\mathbb{E}_{\pi_{\boldsymbol{\theta}}(\boldsymbol{z}|x)}[\boldsymbol{z}]\Big)$$

- Structured Attn. Nets
- SparseMAP

Model restrictions:

- $\operatorname{dom} L$ may be only $\mathcal{Z}$,
- $\nabla_{\boldsymbol{z}} L$ need not exist!

- $L(\boldsymbol{z})$ with $\boldsymbol{z} \in \mathcal{Z}$ in forward
- needs (relaxed) $\nabla_{\boldsymbol{z}} L$ in backward.

- $L(\boldsymbol{z})$ must be relaxed and differentiable.
- (sparsity gets us closer to $\mathcal{Z}$).

Structured latent variables without sampling

$$\mathbb{E}_{\boldsymbol{z}}\left[L(\boldsymbol{z})\right] = \sum_{\boldsymbol{z}\in\mathcal{Z}} L\big(\hat{y}\ \ (\boldsymbol{z})\big)\,\pi\ \ (\boldsymbol{z}\mid x)$$

Structured latent variables without sampling

$$\mathbb{E}_{\boldsymbol{z}}\left[L(\boldsymbol{z})\right] = \sum_{\boldsymbol{z}\in\mathcal{Z}} L\left(\hat{y}_{\boldsymbol{\phi}}(\boldsymbol{z})\right)\, \pi_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x)$$

Structured latent variables without sampling

e.g., a TreeLSTM defined by $\boldsymbol{z}$

$$\mathbb{E}_{\boldsymbol{z}}\left[L(\boldsymbol{z})\right] = \sum_{\boldsymbol{z}\in\mathcal{Z}} L\left(\hat{y}_{\boldsymbol{\phi}}(\boldsymbol{z})\right)\, \pi_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x)$$

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$$\mathbb{E}_{\boldsymbol{z}}\big[L(\boldsymbol{z})\big] = \sum_{\boldsymbol{z}\in\mathcal{Z}} L\big(\hat{y}_{\boldsymbol{\phi}}(\boldsymbol{z})\big)\ \pi_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x)$$

parsing model,
using some scorer $f_{\boldsymbol{\theta}}(\boldsymbol{z}; x)$

Structured latent variables without sampling

sum over
all possible trees

e.g., a TreeLSTM defined by $\boldsymbol{z}$

$$\mathbb{E}_{\boldsymbol{z}}\left[L(\boldsymbol{z})\right] = \sum_{\boldsymbol{z}\in\mathcal{Z}} L\left(\hat{y}_{\boldsymbol{\phi}}(\boldsymbol{z})\right)\, \pi_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x)$$

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Exponentially large sum!

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$$\mathbb{E}_{\boldsymbol{z}}\big[L(\boldsymbol{z})\big] = \sum_{\boldsymbol{z}\in\mathcal{Z}} L\big(\hat{y}_{\boldsymbol{\phi}}(\boldsymbol{z})\big)\ \pi_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x)$$

parsing model,
using some scorer $f_{\boldsymbol{\theta}}(\boldsymbol{z}; x)$

How to define $\pi_{\boldsymbol{\theta}}$?

idea 1

idea 2

idea 3

Structured latent variables without sampling

sum over
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e.g., a TreeLSTM defined by $\boldsymbol{z}$

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$$\sum_{h\in\mathcal{H}}$$

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parsing model,
using some scorer $f_{\boldsymbol{\theta}}(\boldsymbol{z}; x)$

How to define $\pi_{\boldsymbol{\theta}}$?

$$\sum_{h\in\mathcal{H}} \quad \frac{\partial\mathbb{E}\big[L(\boldsymbol{z})\big]}{\partial\boldsymbol{\theta}}$$

idea 1

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idea 3

Structured latent variables without sampling

sum over
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$$\mathbb{E}_{\boldsymbol{z}}\big[L(\boldsymbol{z})\big] = \sum_{\boldsymbol{z}\in\mathcal{Z}} L\big(\hat{y}_{\boldsymbol{\phi}}(\boldsymbol{z})\big)\ \pi_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x)$$

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$$\sum_{h\in\mathcal{H}} \quad \frac{\partial\mathbb{E}\big[L(\boldsymbol{z})\big]}{\partial\boldsymbol{\theta}}$$

idea 1 $\quad \pi_{\boldsymbol{\theta}}(\boldsymbol{z}) \propto \exp\big(f_{\boldsymbol{\theta}}(\boldsymbol{z})\big)$ softmax

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How to define $\pi_{\boldsymbol{\theta}}$?

			$\sum_{h\in\mathcal{H}}$	$\frac{\partial\mathbb{E}\left[L(\boldsymbol{z})\right]}{\partial\boldsymbol{\theta}}$
idea 1	$\pi_{\boldsymbol{\theta}}(\boldsymbol{z}) \propto \exp\left(f_{\boldsymbol{\theta}}(\boldsymbol{z})\right)$	softmax	😱	😊
idea 2				
idea 3				

Structured latent variables without sampling

sum over
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e.g., a TreeLSTM defined by $\boldsymbol{z}$

$$\mathbb{E}_{\boldsymbol{z}}\big[L(\boldsymbol{z})\big] = \sum_{\boldsymbol{z}\in\mathcal{Z}} L\big(\hat{y}_{\boldsymbol{\phi}}(\boldsymbol{z})\big)\, \pi_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x)$$

parsing model,
using some scorer $f_{\boldsymbol{\theta}}(\boldsymbol{z}; x)$

How to define $\pi_{\boldsymbol{\theta}}$?

All methods we've seen require sampling; hard in general.

idea 2

idea 3

Structured latent variables without sampling

sum over
all possible trees

e.g., a TreeLSTM defined by $\boldsymbol{z}$

$$\mathbb{E}_{\boldsymbol{z}}\big[L(\boldsymbol{z})\big] = \sum_{\boldsymbol{z}\in\mathcal{Z}} L\big(\hat{y}_{\boldsymbol{\phi}}(\boldsymbol{z})\big)\ \pi_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x)$$

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How to define $\pi_{\boldsymbol{\theta}}$?

$$\sum_{h\in\mathcal{H}} \qquad \frac{\partial\mathbb{E}\big[L(\boldsymbol{z})\big]}{\partial\boldsymbol{\theta}}$$

idea 1	$\pi_{\boldsymbol{\theta}}(\boldsymbol{z}) \propto \exp\big(f_{\boldsymbol{\theta}}(\boldsymbol{z})\big)$	softmax	😱	😊
idea 2	$\pi_{\boldsymbol{\theta}}(\boldsymbol{z}) = 1$ if $\boldsymbol{z} = \mathrm{MAP}(f_{\boldsymbol{\theta}}(\cdot))$ else 0	argmax		
idea 3				

Structured latent variables without sampling

sum over
all possible trees

e.g., a TreeLSTM defined by $\boldsymbol{z}$

$$\mathbb{E}_{\boldsymbol{z}}\left[L(\boldsymbol{z})\right] = \sum_{\boldsymbol{z}\in\mathcal{Z}} L\left(\hat{y}_{\boldsymbol{\phi}}(\boldsymbol{z})\right)\, \pi_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x)$$

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using some scorer $f_{\boldsymbol{\theta}}(\boldsymbol{z}; x)$

How to define $\pi_{\boldsymbol{\theta}}$?

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idea 2	$\pi_{\boldsymbol{\theta}}(\boldsymbol{z}) = 1$ if $\boldsymbol{z} = \mathrm{MAP}(f_{\boldsymbol{\theta}}(\cdot))$ else 0	argmax	😊	
idea 3				

Structured latent variables without sampling

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parsing model,
using some scorer $f_{\boldsymbol{\theta}}(\boldsymbol{z}; x)$

How to define $\pi_{\boldsymbol{\theta}}$?

			$\sum_{h\in\mathcal{H}}$	$\frac{\partial \mathbb{E}[L(\boldsymbol{z})]}{\partial \boldsymbol{\theta}}$
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idea 2	$\pi_{\boldsymbol{\theta}}(\boldsymbol{z}) = 1$ if $\boldsymbol{z} = \mathrm{MAP}(f_{\boldsymbol{\theta}}(\cdot))$ else 0	argmax	😊	😟
idea 3				

Structured latent variables without sampling

sum over
all possible trees

e.g., a TreeLSTM defined by $\boldsymbol{z}$

$$\mathbb{E}_{\boldsymbol{z}}\left[L(\boldsymbol{z})\right] = \sum_{\boldsymbol{z} \in \mathcal{Z}} L\left(\hat{y}_{\boldsymbol{\phi}}(\boldsymbol{z})\right) \pi_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x)$$

parsing model,
using some scorer $f_{\boldsymbol{\theta}}(\boldsymbol{z}; x)$

How to define $\pi_{\boldsymbol{\theta}}$?

$\dfrac{\partial \mathbb{E}\left[L(\boldsymbol{z})\right]}{\partial \boldsymbol{\theta}}$

STE / SPIGOT relax $\hat{y}$ in backward.

idea 1 $\pi_{\boldsymbol{\theta}}($ 😊

idea 2 $\pi_{\boldsymbol{\theta}}(\boldsymbol{z}) = 1$ if $\boldsymbol{z} = \mathrm{MAP}(f_{\boldsymbol{\theta}}(\cdot))$ else 0 argmax 😊 😟

idea 3

Structured latent variables without sampling

sum over
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e.g., a TreeLSTM defined by $\boldsymbol{z}$

$$\mathbb{E}_{\boldsymbol{z}}\big[L(\boldsymbol{z})\big] = \sum_{\boldsymbol{z}\in\mathcal{Z}} L\big(\hat{y}_{\boldsymbol{\phi}}(\boldsymbol{z})\big)\ \pi_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x)$$

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idea 2	$\pi_{\boldsymbol{\theta}}(\boldsymbol{z}) = 1$ if $\boldsymbol{z} = \mathrm{MAP}(f_{\boldsymbol{\theta}}(\cdot))$ else 0	argmax	😊	😟
idea 3		SparseMAP	😊	😊

Structured latent variables without sampling

 = .7×  + .3× 

recall our shorthand $L(\boldsymbol{z}) = L(\hat{y}_{\boldsymbol{\phi}}(\boldsymbol{z}), y)$

Structured latent variables without sampling

 = .7×  + .3×  +0×  + ...

recall our shorthand $L(\boldsymbol{z}) = L(\hat{y}_{\boldsymbol{\phi}}(\boldsymbol{z}), y)$

Structured latent variables without sampling

 $= .7\times$  $+ .3\times$  $+0\times$  $+ \ldots$

$\mathbb{E}[L(\boldsymbol{z})] = .7\times L($  $) + .3\times L($  $)$

recall our shorthand $L(\boldsymbol{z}) = L(\hat{y}_{\boldsymbol{\phi}}(\boldsymbol{z}), y)$

Stanford Sentiment (Accuracy)

Socher et al	
Bigram Naive Bayes	83.1
[Niculae et al., 2018b]	
TreeLSTM w/ CoreNLP	83.2
TreeLSTM w/ SparseMAP	84.7
[Corro and Titov, 2019b]	
GCN w/ CoreNLP	83.8
GCN w/ Perturb-and-MAP	84.6

Stanford Natural Language Inference (Accuracy)

[Kim et al., 2017]	
Simple Attention	86.2
Structured Attention	86.8
[Liu and Lapata, 2018]	
100D SAN -	86.8
Yogatama et al	
100D RL-SPINN	80.5
[Choi et al., 2018]	
100D ST Gumbel-Tree	82.6
300D -	85.6
600D -	86.0
[Corro and Titov, 2019b]	
Latent Tree + 1 GCN -	85.2
Latent Tree + 2 GCN -	86.2

V. Conclusions

Is it syntax?!

- Unlike e.g. unsupervised parsing, the structures we learn are guided by **a downstream objective** (typically discriminative).
- They don't typically resemble grammatical structure (yet) [Williams et al., 2018]

  (future work: more inductive biases and constraints?)

Is it syntax?!

- Unlike e.g. unsupervised parsing, the structures we learn are guided by **a downstream objective** (typically discriminative).
- They don't typically resemble grammatical structure (yet) [Williams et al., 2018]
  (future work: more inductive biases and constraints?)
- Common to compare latent structures with parser outputs.
  But is this always a meaningful comparison?

[Niculae et al., 2018b]

Syntax vs. Composition Order

CoreNLP parse, $p = 21.4\%$

⋆ lovely and poignant .

Syntax vs. Composition Order

$p = 22.6\%$

CoreNLP parse, $p = 21.4\%$

. . .

Syntax vs. Composition Order

$p = 22.6\%$

⋆ lovely and poignant .

CoreNLP parse, $p = 21.4\%$

⋆ lovely and poignant .

…

$p = 15.33\%$

⋆ a deep and meaningful film .

$p = 15.27\%$

⋆ a deep and meaningful film .

…

CoreNLP parse, $p = 0\%$

⋆ a deep and meaningful film .

Overview

$$\mathbb{E}_{\pi_{\boldsymbol{\theta}}(\mathbf{z}|x)}\Big[L(\mathbf{z})\Big]$$

- REINFORCE
- Straight-Through Gumbel (Perturb & MAP)
- SparseMAP

$$L\Big(\arg\max_{\mathbf{z}} \pi_{\boldsymbol{\theta}}(\mathbf{z} \mid x)\Big)$$

- Straight-Through
- SPIGOT

$$L\Big(\mathbb{E}_{\pi_{\boldsymbol{\theta}}(\mathbf{z}|x)}[\mathbf{z}]\Big)$$

- Structured Attn. Nets
- SparseMAP

Model restrictions:

- $\operatorname{dom} L$ may be only $\mathcal{Z}$,
- $\nabla_{\mathbf{z}} L$ need not exist!

- $L(\mathbf{z})$ with $\mathbf{z} \in \mathcal{Z}$ in forward
- needs (relaxed) $\nabla_{\mathbf{z}} L$ in backward.

- $L(\mathbf{z})$ must be relaxed and differentiable.
- (sparsity gets us closer to $\mathcal{Z}$).

Overview

$$\mathbb{E}_{\pi_{\boldsymbol{\theta}}(\boldsymbol{z}|x)}\Big[L(\boldsymbol{z})\Big] \qquad L\Big(\arg\max_{\boldsymbol{z}} \pi_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x)\Big) \qquad L\Big(\mathbb{E}_{\pi_{\boldsymbol{\theta}}(\boldsymbol{z}|x)}[\boldsymbol{z}]\Big)$$

- REINFORCE[SPL]
- Straight-Through Gumbel (Perturb & MAP)[SPL,MRG]
- SparseMAP[MAP+]

- Straight-Through[MAP,MRG]
- SPIGOT[MAP+]

- Structured Attn. Nets[MRG]
- SparseMAP[MAP+]

Computation:

SPL: Sampling. (Simple in incremental/unstructured, hard for most global structures.)

MAP: Finding the highest-scoring structure.

MRG: Marginal inference.

Conclusions

- Latent structure models are desirable for interpretability, structural bias, and higher predictive power with fewer parameters.
- Stochastic latent variables can be dealt with RL or straight-through gradients.
- Deterministic argmax requires surrogate gradients (e.g. SPIGOT).
- Continuous relaxations of argmax include SANs and SparseMAP.
- Intuitively, some of these different methods are trying to do similar things or require the same building blocks (e.g. SPIGOT and SparseMAP).
- ... we didn't even get into deep *generative* models! These tools apply, but there are new challenges. [Corro and Titov, 2019a, Kim et al., 2019a,b, Kawakami et al., 2019]

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