Latent Structure Models for NLP

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work with:

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deep-spin.github.io/tutorial

I. Introduction

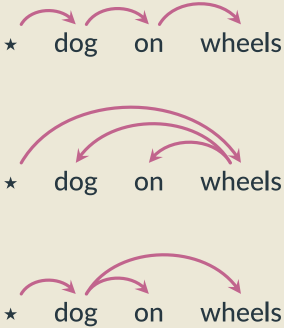
Structured prediction and NLP

- **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

…



★ dog on wheels

★ dog on wheels

★ dog on wheels

…

Examples of structure in NLP

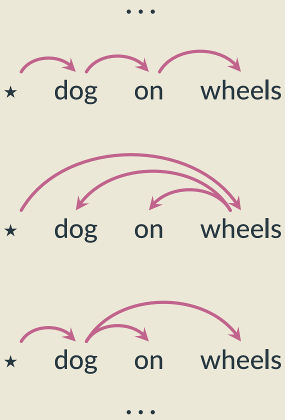
POS tagging

VERB PREP NOUN
dog on wheels

NOUN PREP NOUN
dog on wheels

NOUN DET NOUN
dog on wheels

Dependency parsing



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★ dog on wheels

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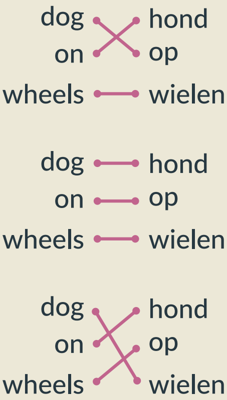
…

Word alignments



dog on wheels
hond op wielen

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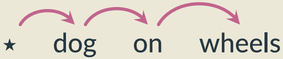
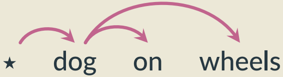


★ dog on wheels

Exponentially many structures!



★ dog on wheels

...

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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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- Forget pipelines—train everything from scratch!
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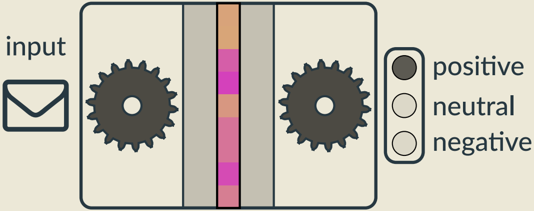
End-to-end training

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

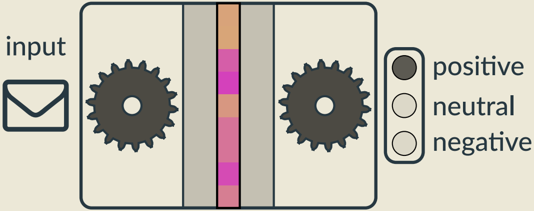
Representation learning

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



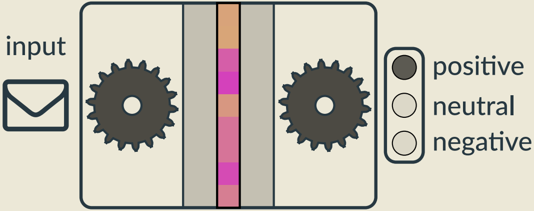
Representation learning

- 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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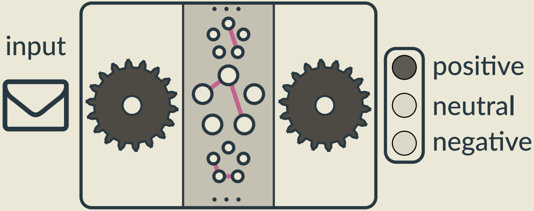

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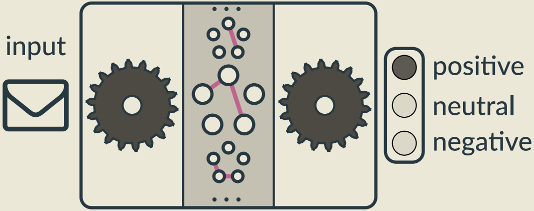
  - More interpretability;



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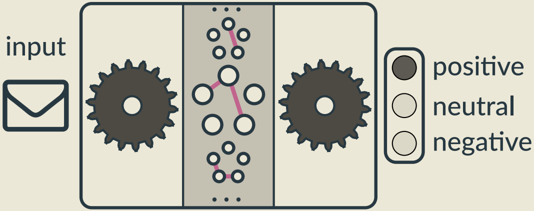
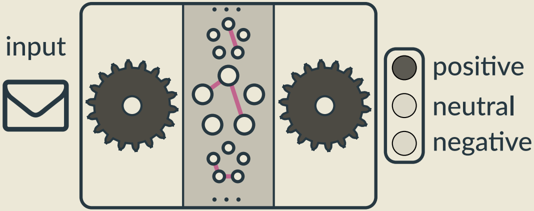


Latent structure models

- Seek *structured* hidden representations instead!
- They can bring us:
  - More interpretability;
  - Better inductive bias;
  - Hopefully: smaller models.



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!

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

- Simplest example of structure: Just a discrete choice among N categories.
- We call this *unstructured*.
- It will provide an important starting point.

The challenge of discrete choices

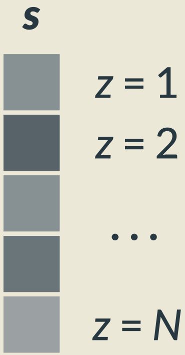
$$z = 1$$

$$z = 2$$

$$\dots$$

$$z = N$$

The challenge of discrete choices



s

$z = 1$

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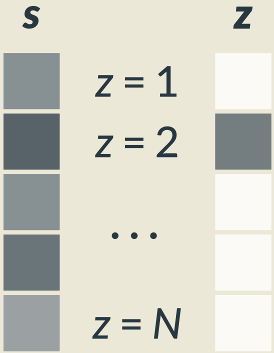
The challenge of discrete choices



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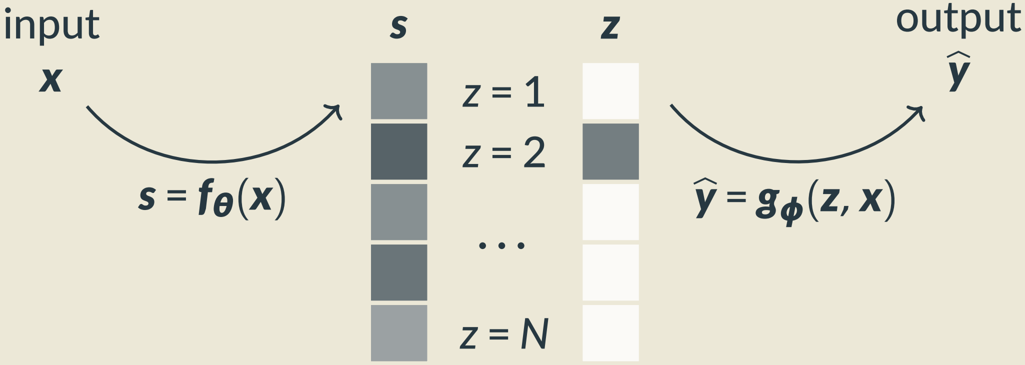

input

$\boldsymbol{x}$

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

$\boldsymbol{s}$

$z = 1$

$z = 2$

$\dots$

$z = N$

$\boldsymbol{z}$

output

$\widehat{\boldsymbol{y}}$

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

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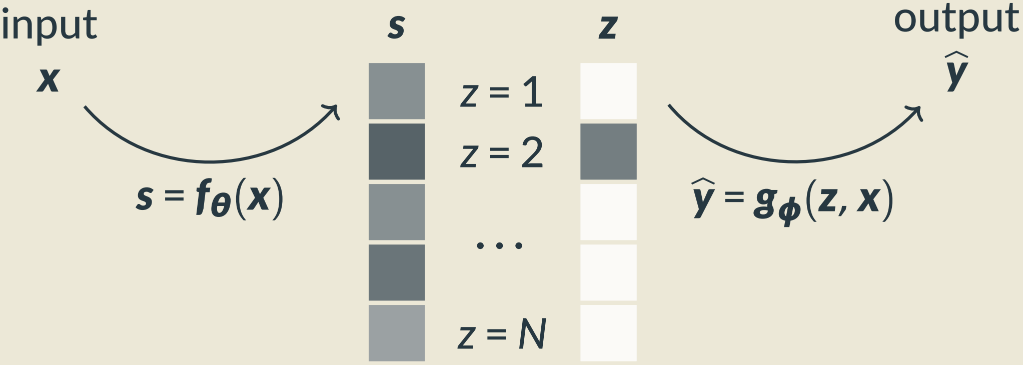
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$$\frac{\partial L(\widehat{\boldsymbol{y}}, \boldsymbol{y})}{\partial \boldsymbol{w}} = ?$$

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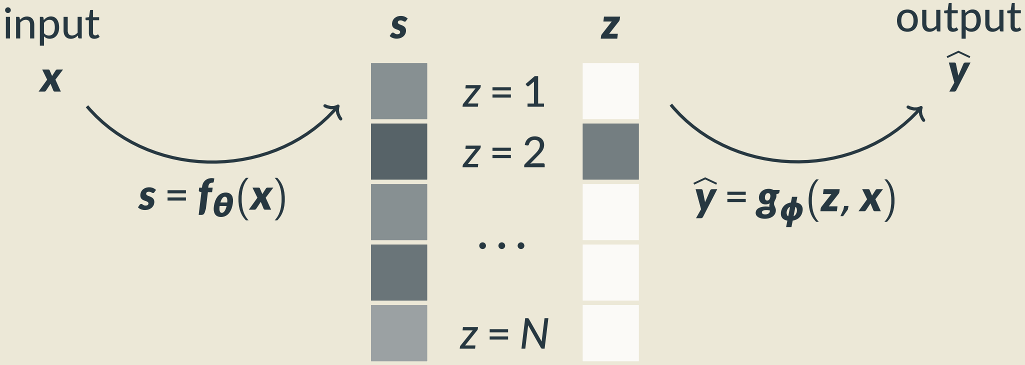

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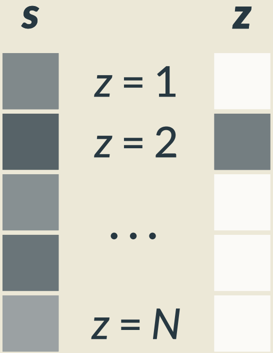
$\widehat{\boldsymbol{y}} = \boldsymbol{g}_{\boldsymbol{\phi}}(\boldsymbol{z}, \boldsymbol{x})$

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

Discrete mappings are “flat”



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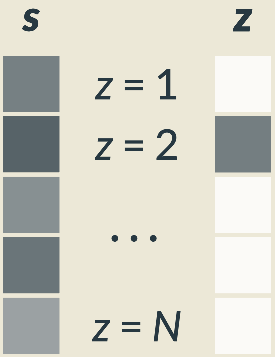

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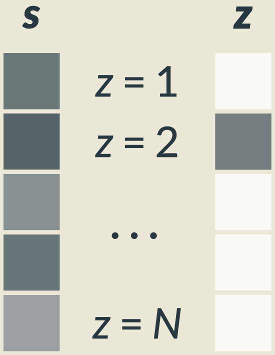

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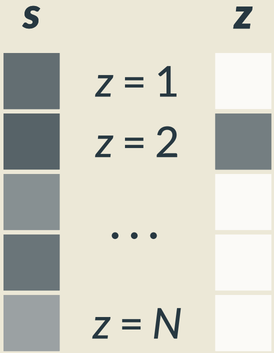

$\boldsymbol{s}$

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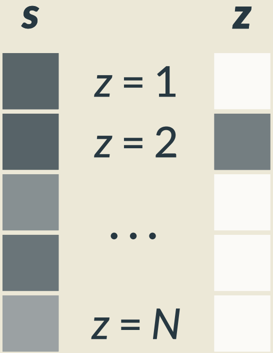

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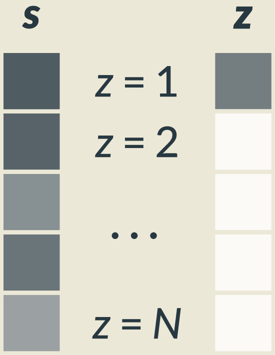

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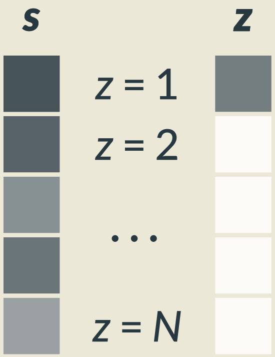

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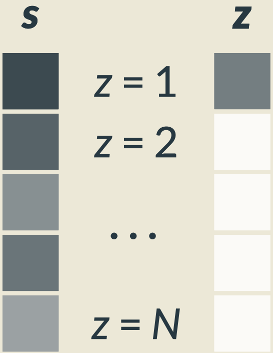

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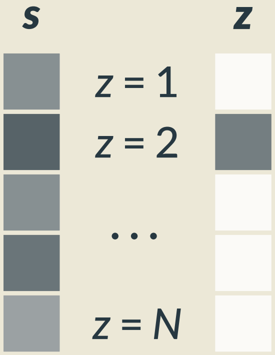
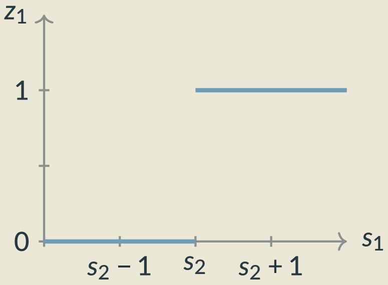
Argmax

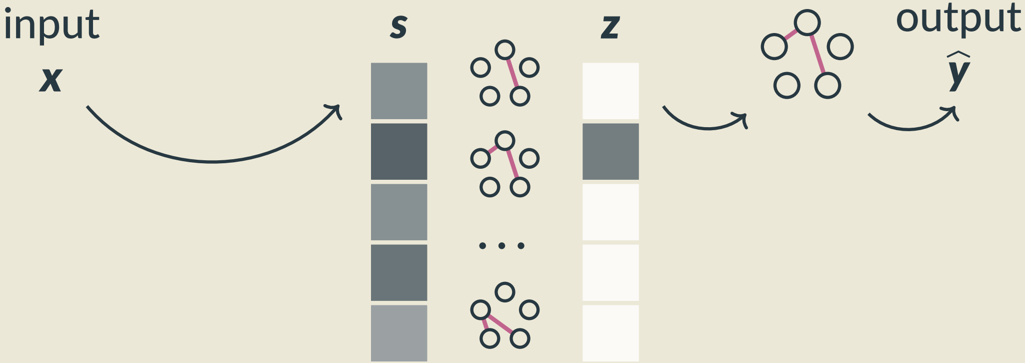




$$\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{s}} = \boldsymbol{0}$$

Computing the most likely structure

is a very high-dimensional argmax



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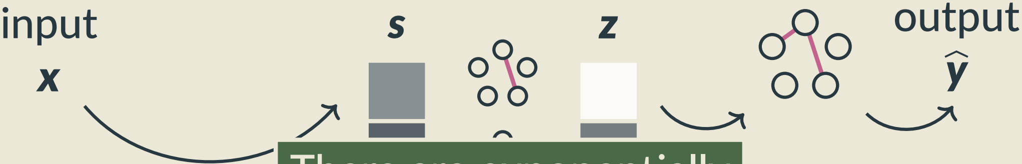


input $\boldsymbol{x}$

$\boldsymbol{s}$

$\boldsymbol{z}$

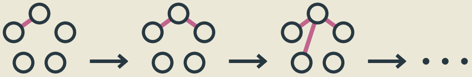
output $\hat{\boldsymbol{y}}$

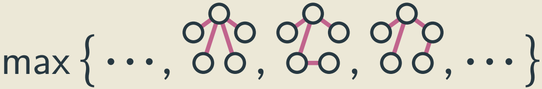
There are exponentially many structures

($\boldsymbol{s}$ cannot fit in memory;

we cannot “loop” over $\boldsymbol{s}$ nor $\boldsymbol{z}$)

Dealing with the combinatorial explosion





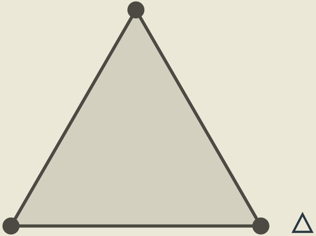
1. Incremental structures

- 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 unstructured case: Probability simplex



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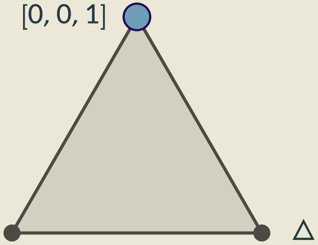

- Each vertex is an *indicator vector*, representing one class:

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

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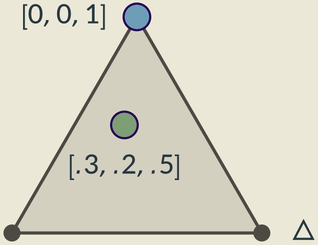

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$$\boldsymbol{z}_c = [0, \ldots, 0, \underbrace{1}_{c^{\text{th}} \text{ position}}, 0, \ldots, 0].$$

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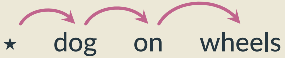
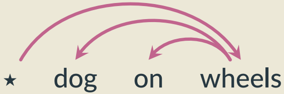
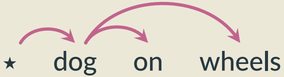
$\boldsymbol{z}_1 = [1, 0, 0, 0, 1, 0, 0, 0, 1]$



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

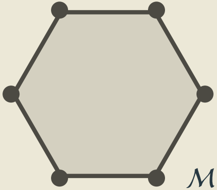


$\boldsymbol{z}_3 = [1, 0, 0, 0, 1, 0, 0, 1, 0]$



[Wainwright and Jordan, 2008]

The structured case: Marginal polytope



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The structured case: Marginal polytope

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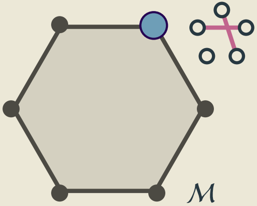
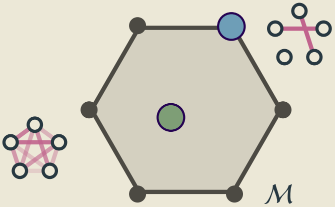


[Wainwright and Jordan, 2008]

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

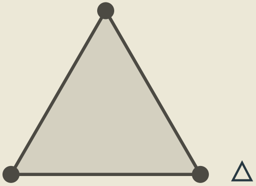


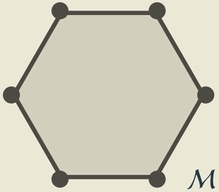
$$\boldsymbol{\mu} = \underbrace{p_1\boldsymbol{z}_1 + \ldots + p_N\boldsymbol{z}_N}_{\text{exponentially many terms}}, \quad \boldsymbol{p} \in \triangle.$$

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

Unstructured vs Structured

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





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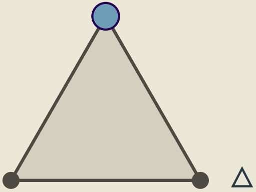

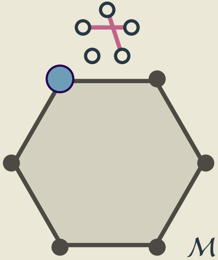

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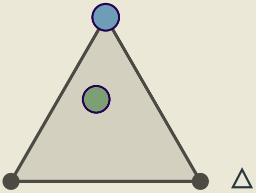
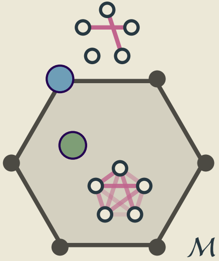
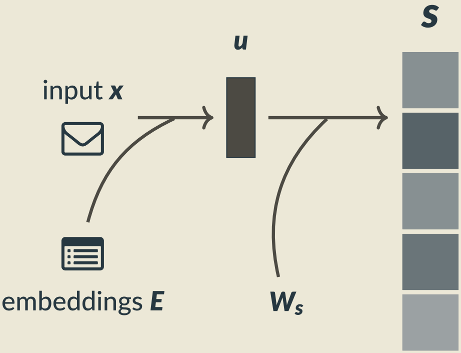




Example: Regression with latent categorization



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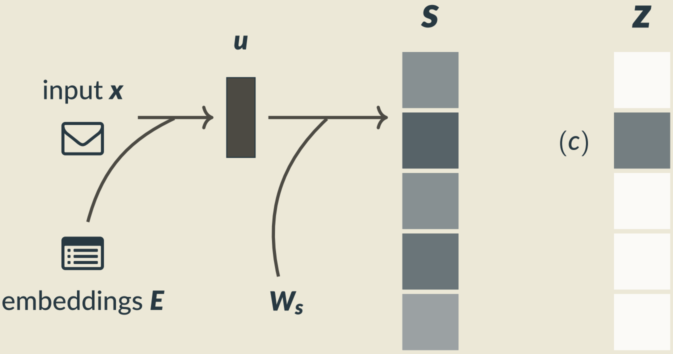

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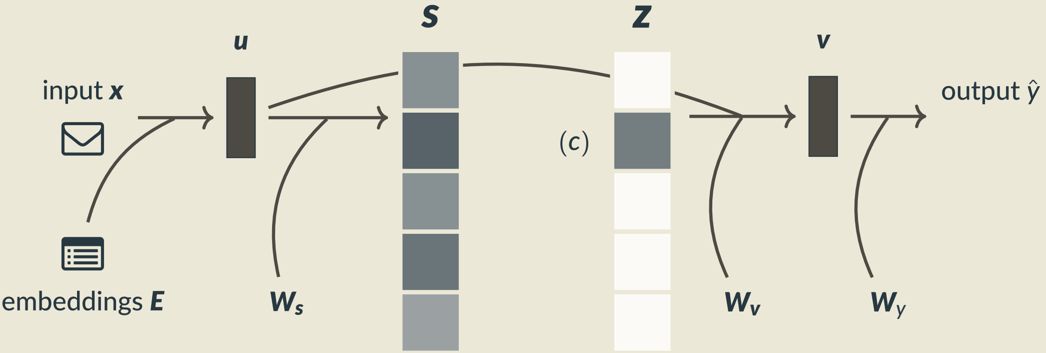

$\boldsymbol{u} = \frac{1}{|\boldsymbol{x}|} \sum_j \boldsymbol{E}_{x_j}$ $\boldsymbol{s} = \boldsymbol{W_s u}$ $\boldsymbol{v} = \tanh\left(\boldsymbol{W_v}[\boldsymbol{u}, \boldsymbol{z}]\right)$ $\hat{y} = \boldsymbol{W}_y \boldsymbol{v}$ $L = (\hat{y} - y)^2$

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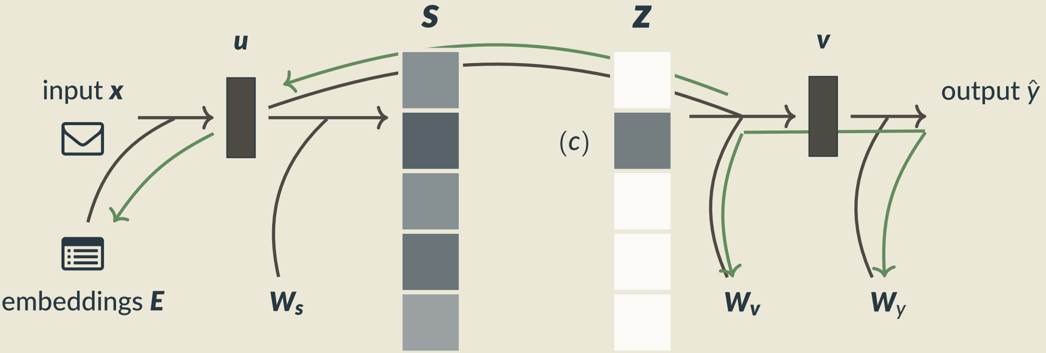

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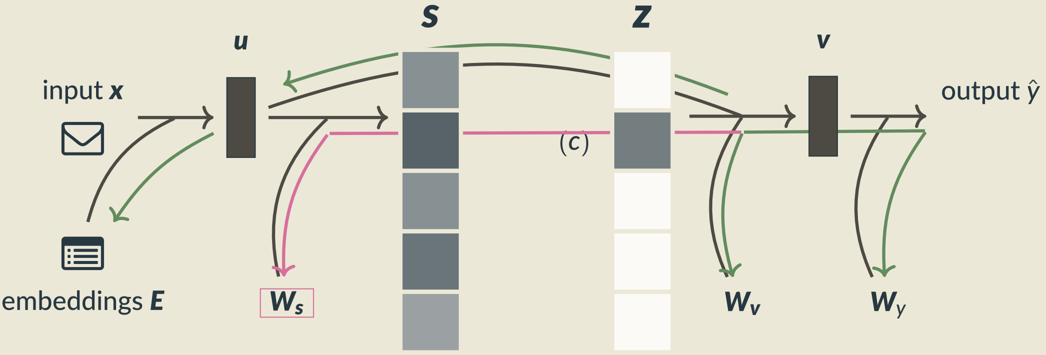

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$$\frac{\partial L}{\partial \boldsymbol{W}_s} = \frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial \boldsymbol{v}} \frac{\partial \boldsymbol{v}}{\partial \boldsymbol{z}} \overbrace{\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{s}}}^{\equiv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

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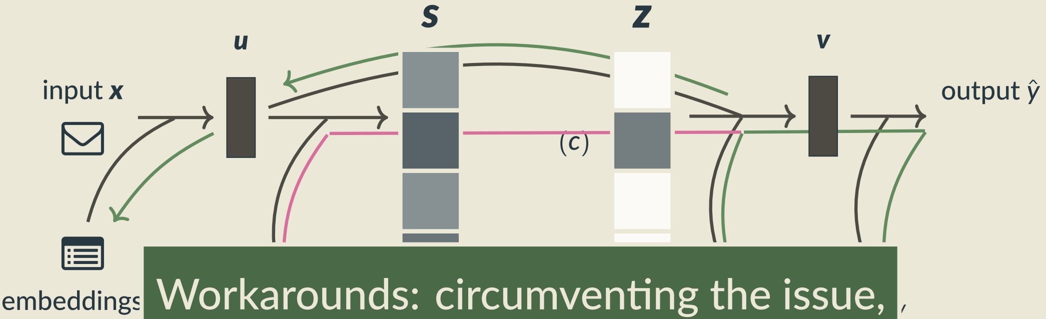


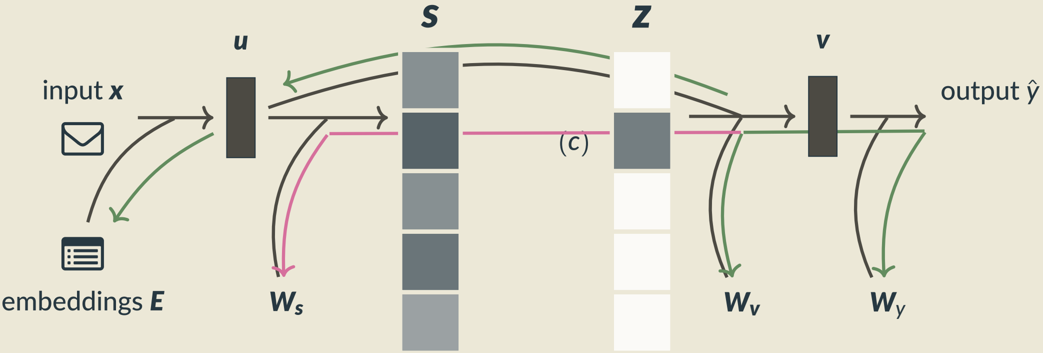
Workarounds: circumventing the issue, bypassing discrete variables

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

,

$- y)^2$

Example: Regression with latent categorization



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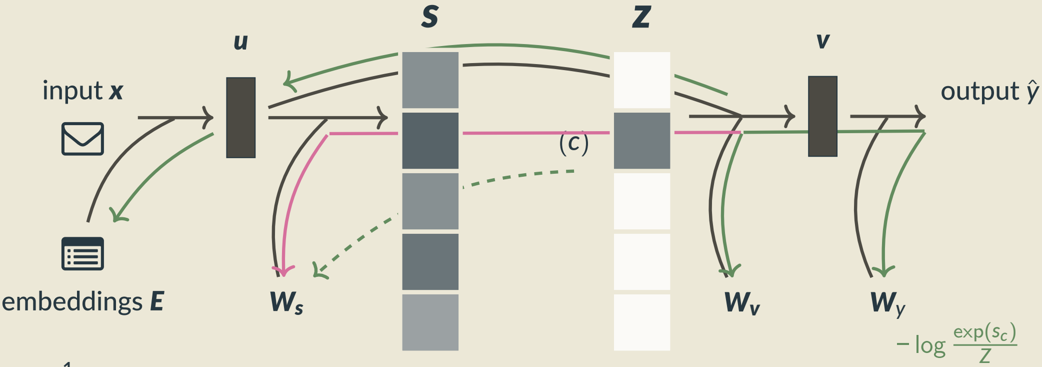
Option 1. Pretrain latent classifier $\boldsymbol{W_s}$

Example: Regression with latent categorization



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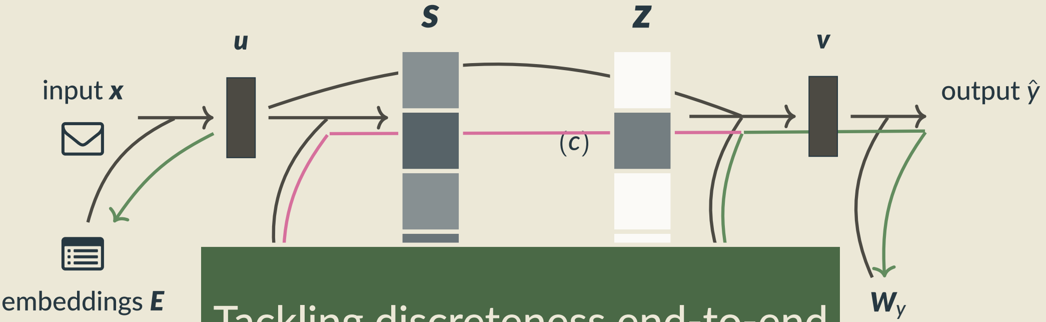
Option 2. Multi-task learning

Example: Regression with latent categorization

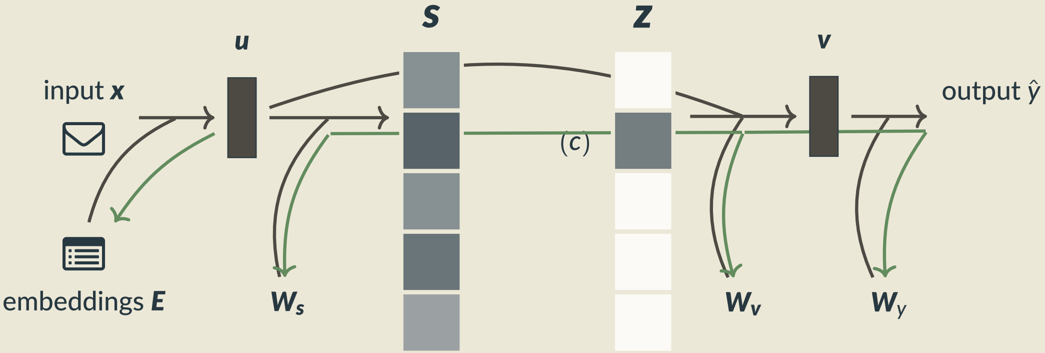


Tackling discreteness end-to-end

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

$. = (\hat{y} - y)^2$

Example: Regression with latent categorization



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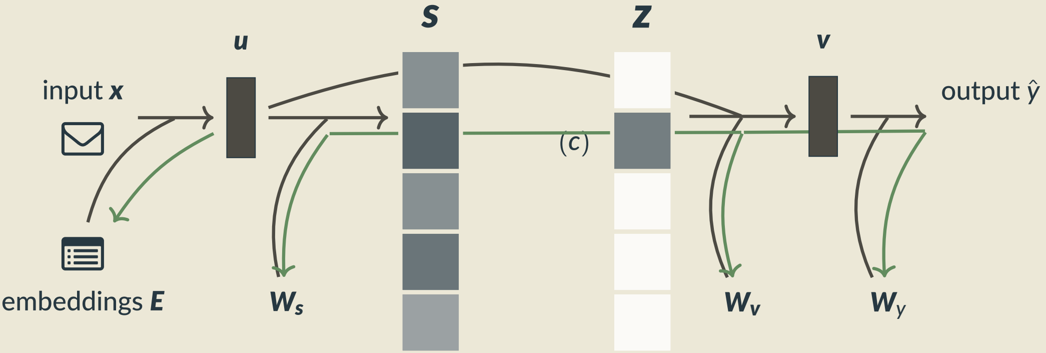
Option 3. Stochasticity! $\frac{\partial \mathbb{E}_{\boldsymbol{z}}(\hat{y}(\boldsymbol{z})-y)^2}{\partial \boldsymbol{W}_s} \neq \boldsymbol{0}$

Example: Regression with latent categorization



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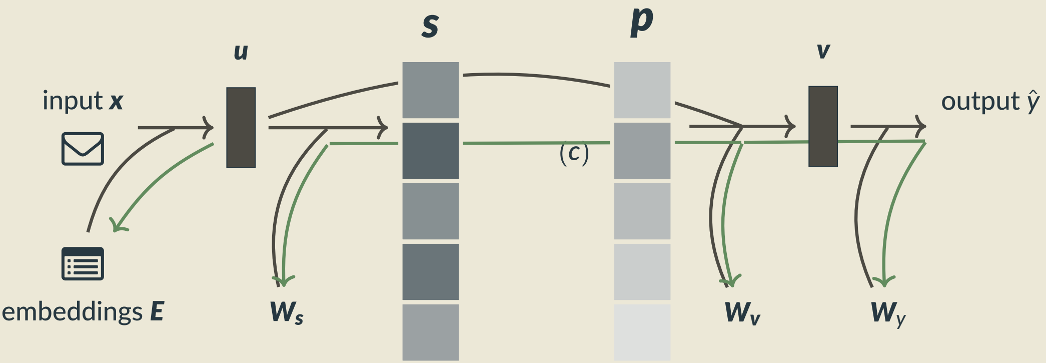
Option 4. Gradient surrogates (*e.g.* straight-through, $\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{s}} \leftarrow \boldsymbol{I}$)

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

Coffee Break

- Part 3: Gradient surrogates
- Part 4: End-to-end differentiable models (1/2)

Coffee Break

- Part 4: End-to-end differentiable models (2/2)
- Part 5: Conclusions

II. Reinforcement Learning Methods

Latent structure via marginalization

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- But we don't know $\boldsymbol{z}$!
- In this section:
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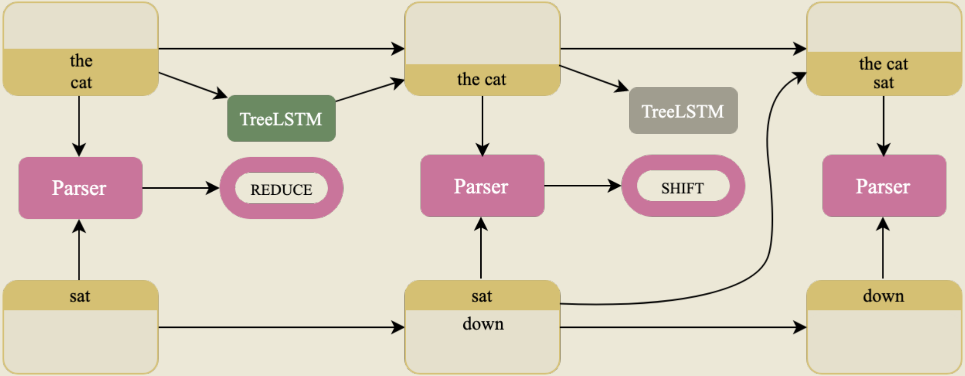
  by optimizing the **expected loss**,

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

But first, supervised SPINN

[Bowman et al., 2016]

Stack-augmented Parser-Interpreter Neural-Network



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- **TreeLSTM** combines top two elements of the stack when the parser chooses the REDUCE action.

[Bowman et al., 2016]

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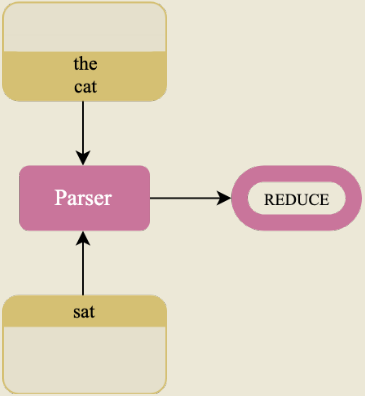

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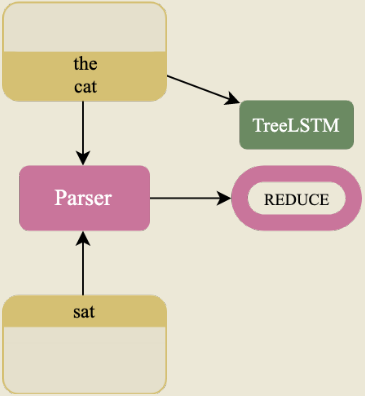

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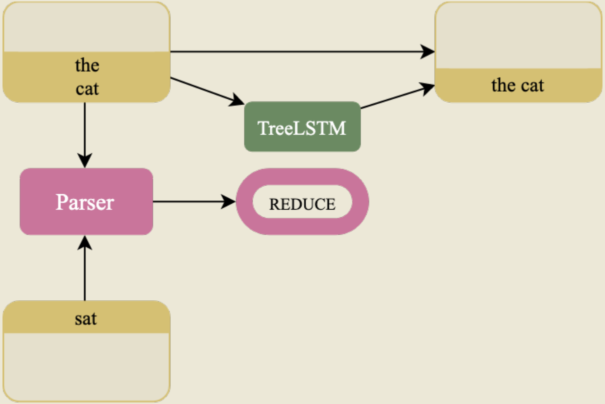

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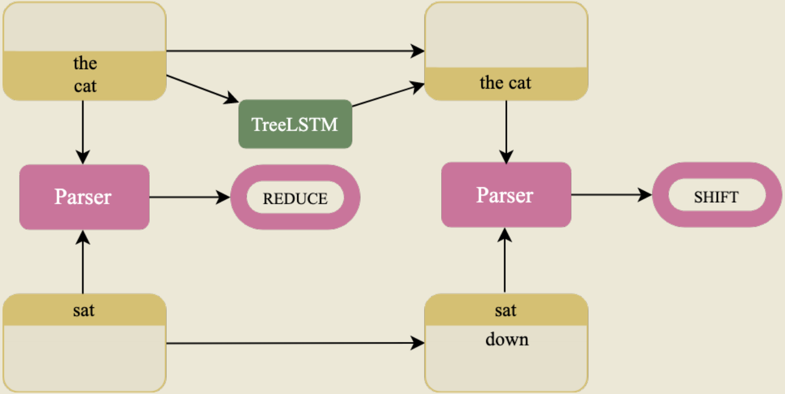

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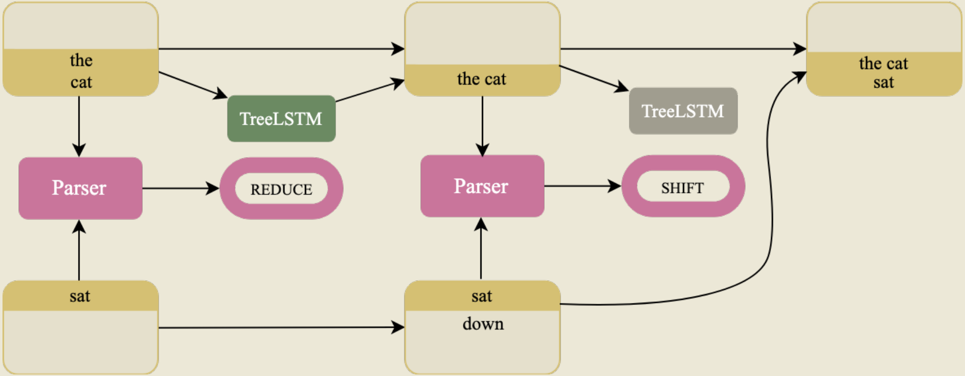

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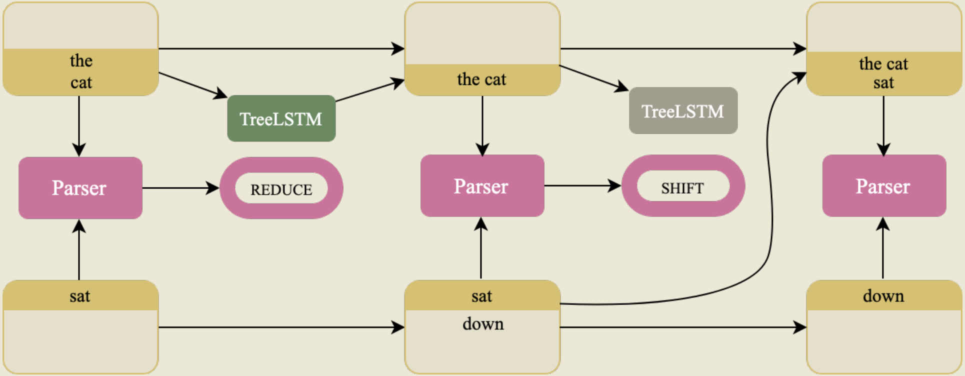


Shift-Reduce parsing

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

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

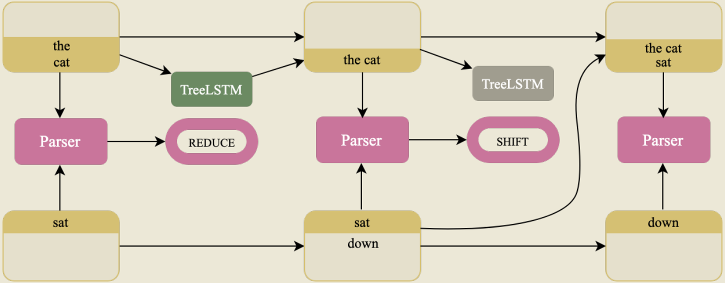
where, $z_j \in \{0, 1\}\ \forall j \in [1, 2L - 1]$

Shift-Reduce parsing

A sequence of Bernoulli trials but with conditional dependence,

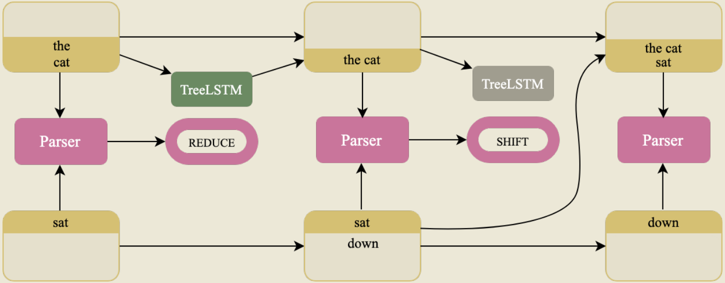
$$p(z_1, z_2, \dots, z_{2L-1}) = \prod_{j=1}^{2L-1} p(z_j \mid z_{<j})$$

Latent structure learning with SPINN



Latent structure learning with SPINN

- But now, remove syntactic supervision from SPINN.



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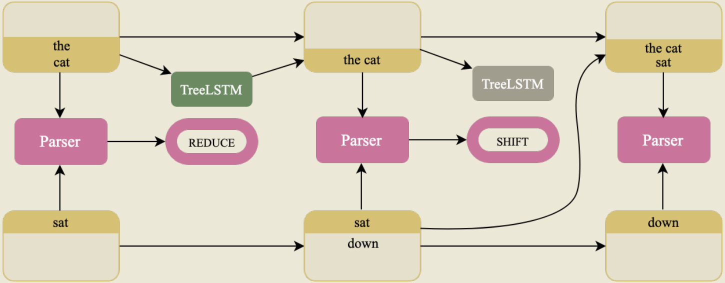

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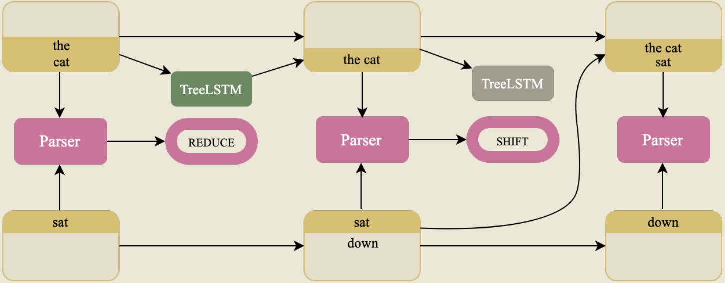

- We model the parse, $\boldsymbol{z}$, as a latent variable scored by $f_{\boldsymbol{\theta}}(x)$.
- With shift-reduce parsing, we're making discrete decisions

  $\Rightarrow$ 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.

[Williams, 1992]

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.

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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.

[Williams, 1992]

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- Max ke sentence classification.

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

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

(Need to turn it into $\mathbb{E}[\cdot]$ so we can MC-estimate)

Through the looking glass of REINFORCE

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$$\nabla \log f = \frac{\nabla f}{f}, \text{ so } \nabla f = f \, \nabla \log f.$$

Through the looking glass of REINFORCE

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SPINN with REINFORCE, aka RL-SPINN

Yogatama et al. [2017] uses REINFORCE to train SPINN!

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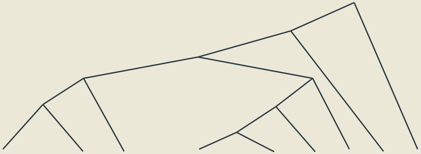
However, this vanilla implementation isn't very effective at learning syntax.

This model fails to solve a simple toy problem.

[Nangia and Bowman, 2018]

Toy problem: ListOps



[max 2 9 [min 4 7] 0]

[Nangia and Bowman, 2018]

Toy problem: ListOps

Model	**Accuracy**
LSTM	**74.4**
RL-SPINN	64.8
TreeLSTM with ground-truth trees	98.7

[Nangia and Bowman, 2018]

Toy problem: ListOps

Model	Accuracy
LSTM	**74.4**
RL-SPIN	4.8
TreeLST	8.7

But why?

RL-SPINN’s Troubles

This system faces at least two big problems,

RL-SPINN’s Troubles

This system faces at least two big problems,

1. High variance of gradients
2. Coadaptation

High variance

- We have a single reward at the end of parsing.

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  Catalan number of binary trees.

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- We are sampling parses from very large search space! **Catalan number** of binary trees.

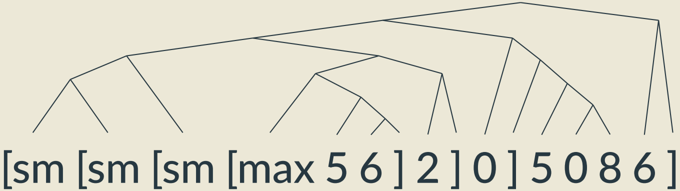
$$\begin{aligned} 3 \text{ tokens} &\Rightarrow 5 \text{ trees} \\ 5 \text{ tokens} &\Rightarrow 42 \text{ trees} \\ 10 \text{ tokens} &\Rightarrow 16796 \text{ trees} \end{aligned}$$

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”:

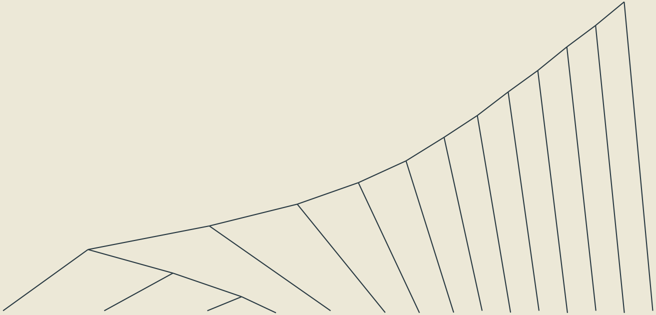


[sm [sm [sm [max 5 6] 2] 0] 5 0 8 6]

Figure: Truth: 7; Pred: 7

High variance

Sometimes it doesn't:



[max [med [med 1 [sm 3 1 3] 9] 6] 5]

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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  So,

$$\nabla \mathbb{E}_{\boldsymbol{z} \sim \pi(\boldsymbol{z})} = \mathbb{E}_{\boldsymbol{z} \sim \pi(\boldsymbol{z})}[(L(\boldsymbol{z}) - b(\boldsymbol{x}))\, \nabla \pi(\boldsymbol{z})]$$

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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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?

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- High variance 😟
- Has not yet been very effective at learning English syntax.

Roadmap of the tutorial

- Part 1: Introduction ✓
- Part 2: Reinforcement learning ✓

Coffee Break

- Part 3: Gradient surrogates
- Part 4: End-to-end differentiable models (1/2)

Coffee Break

- Part 4: End-to-end differentiable models (2/2)
- Part 5: Conclusions

III. Gradient Surrogates

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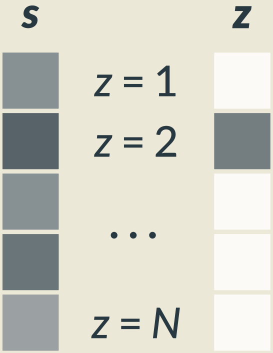
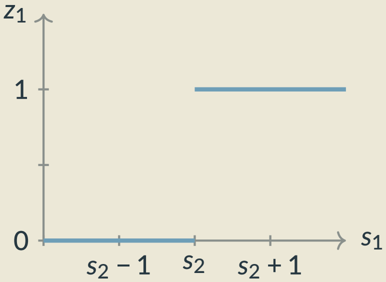
- 3A: try to optimize the deterministic loss directly
- 3B: use this strategy to reduce variance in the stochastic model.

Recap: The argmax problem

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

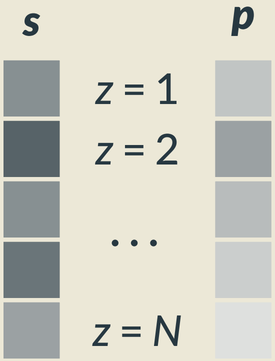


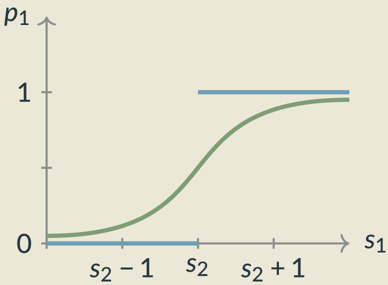


$$\frac{\partial \boldsymbol{z}}{\partial \boldsymbol{s}} = \boldsymbol{0}$$

Softmax

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





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

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

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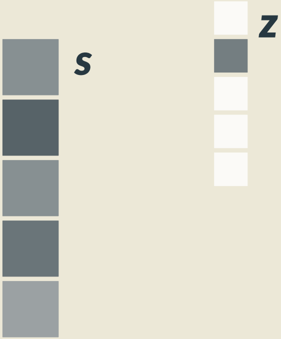

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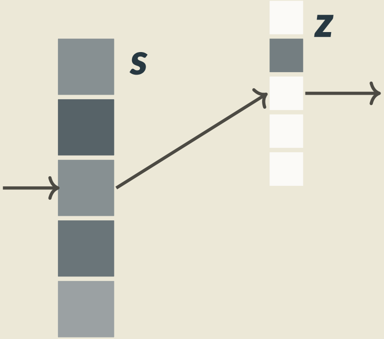

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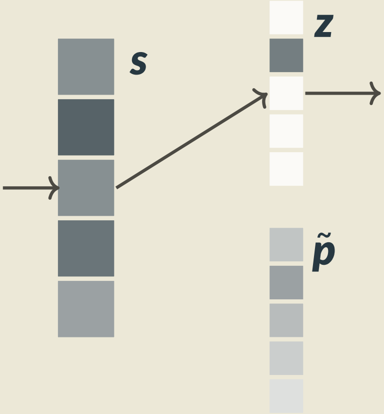

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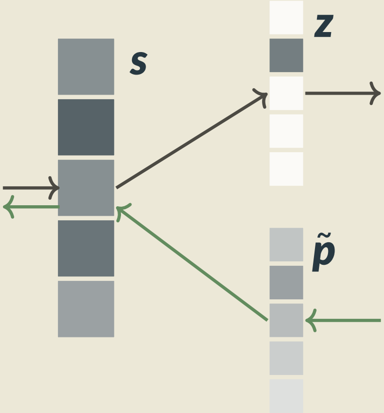

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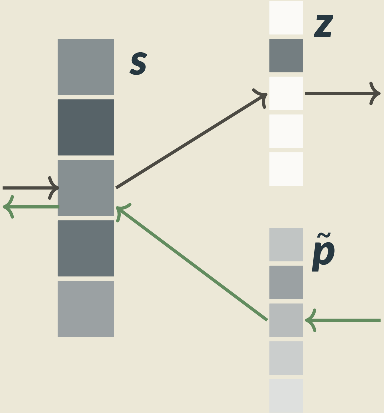

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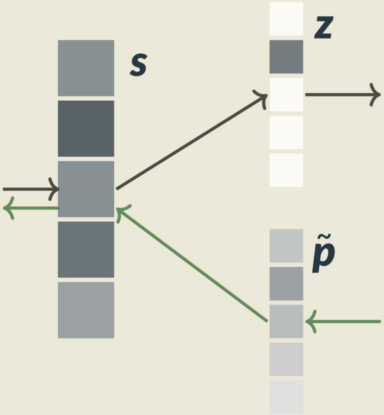

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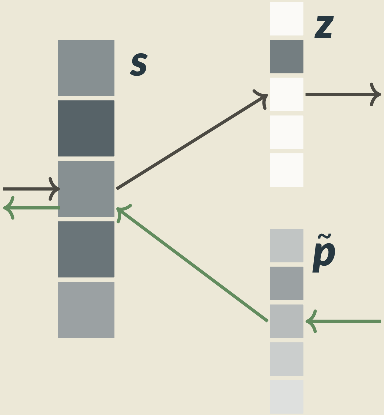
- More explanation in a while



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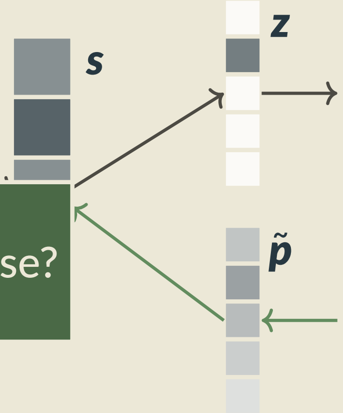
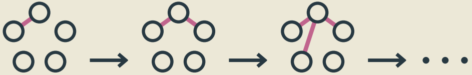
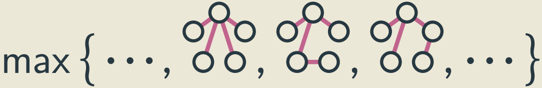
What about the structured case?



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).

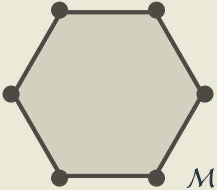
STE for the factorized approach

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



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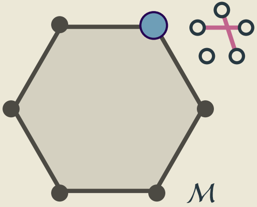
The structured case: Marginal polytope

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



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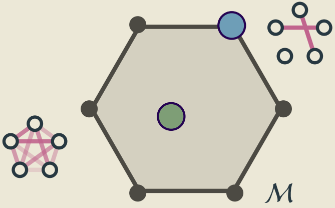
The structured case: Marginal polytope

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

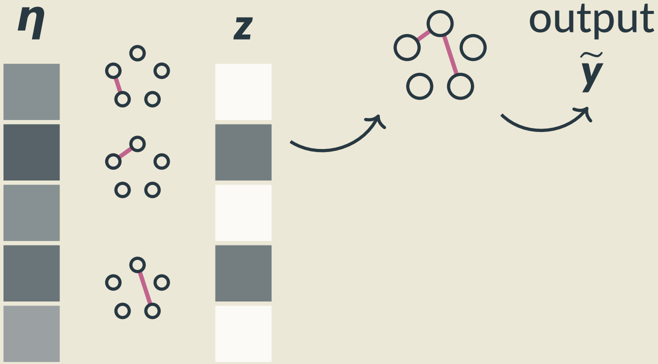


$$\boldsymbol{\mu} = \underbrace{p_1\boldsymbol{z}_1 + \ldots + p_N\boldsymbol{z}_N}_{\text{exponentially many terms}}, \ \boldsymbol{p} \in \triangle.$$

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

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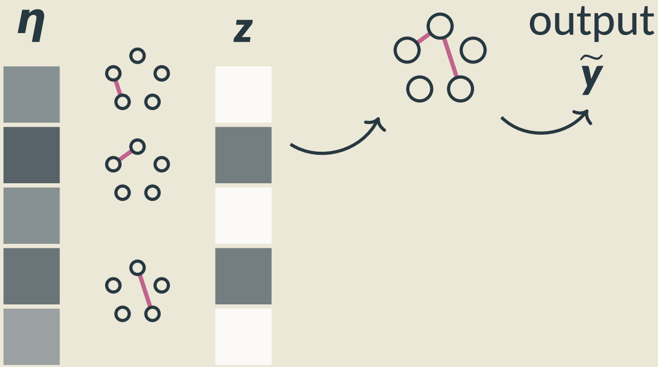
- Task-specific algorithm for the highest-scoring structure.



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

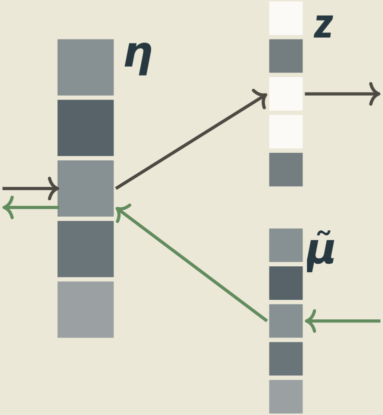
- Forward pass:

  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]

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Revisited

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

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Revisited

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- if we had labels (multi-task learning), $L_{\text{MTL}} = L\big(\hat{y}(\boldsymbol{z}), y\big) + L_{\text{hid}}\big(\boldsymbol{s}, \boldsymbol{z}^{\text{true}}\big)$
- One choice: perceptron loss $L_{\text{hid}}(\boldsymbol{s}, \boldsymbol{z}^{\text{true}}) = \boldsymbol{s}^\top \boldsymbol{z} - \boldsymbol{s}^\top \boldsymbol{z}^{\text{true}}$; $\frac{\partial L_{\text{hid}}}{\partial \boldsymbol{s}} = \boldsymbol{z} - \boldsymbol{z}^{\text{true}}$.
- We don't have labels! Induce labels by "pulling back" the downstream target: the "best" (unconstrained) latent value would be: $\arg\min_{\tilde{\boldsymbol{z}} \in \mathbb{R}^D} L\big(\hat{y}(\tilde{\boldsymbol{z}}), y\big)$
- One gradient descent step starting from $\boldsymbol{z}$: $\boldsymbol{z}^{\text{true}} \leftarrow \boldsymbol{z} - \frac{\partial L}{\partial \boldsymbol{z}}$

$$\frac{\partial L_{\text{MTL}}}{\partial \boldsymbol{s}} = \underbrace{\frac{\partial L}{\partial \boldsymbol{s}}}_{=\mathbf{0}} + \frac{\partial L_{\text{hid}}}{\partial \boldsymbol{s}} = \boldsymbol{z} - \left(\boldsymbol{z} - \frac{\partial L}{\partial \boldsymbol{z}}\right) = \frac{\partial L}{\partial \boldsymbol{z}}$$

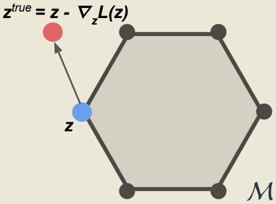
[Peng et al., 2018, Martins and Niculae, 2019]

Straight-Through in the structured case

- Structured STE: perceptron update with induced annotation

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

(one step of gradient descent)



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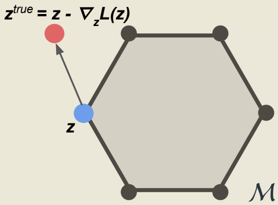

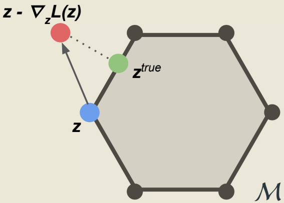

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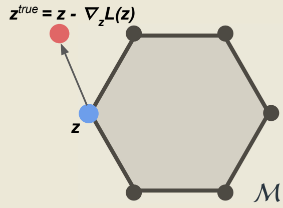
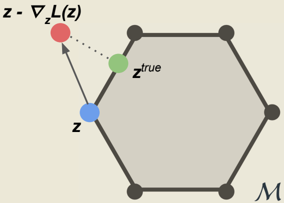
- We discuss a generic way to compute the projection in part 4.





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We saw how to use the *Straight-Through Estimator* to allow learning models with *argmax* in the middle of the computation graph.

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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:

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

Categorical reparameterization

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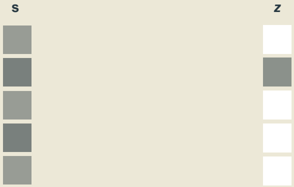
- Sampling from a categorical value in the middle of the computation graph.
  $\boldsymbol{z} \sim \pi_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x) \propto \exp \boldsymbol{s}_{\boldsymbol{\theta}}(\boldsymbol{z} \mid x)$



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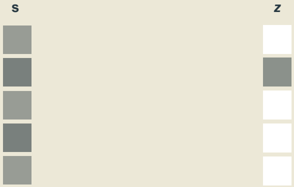

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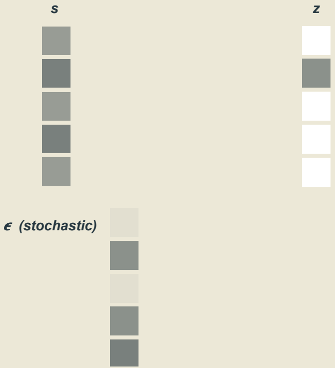

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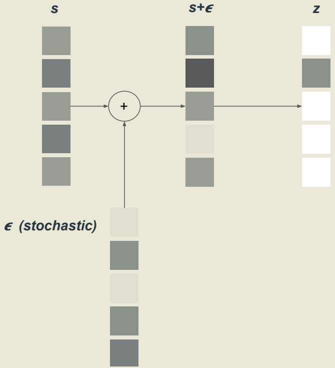

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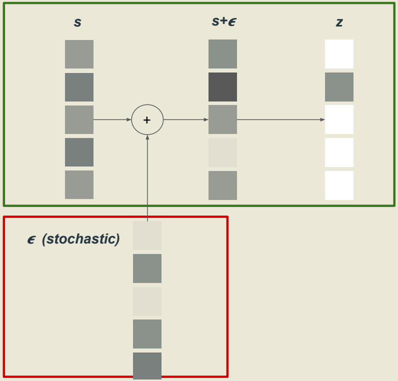

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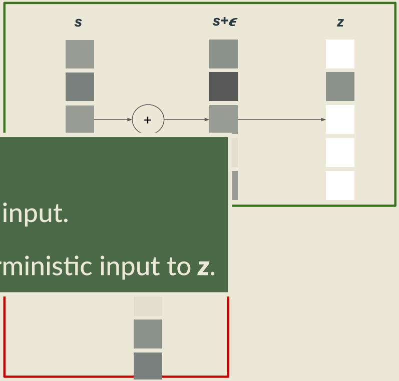

As a result:

Stochasticity is moved as an input.

We can backpropagate through the deterministic input to $\boldsymbol{z}$.

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

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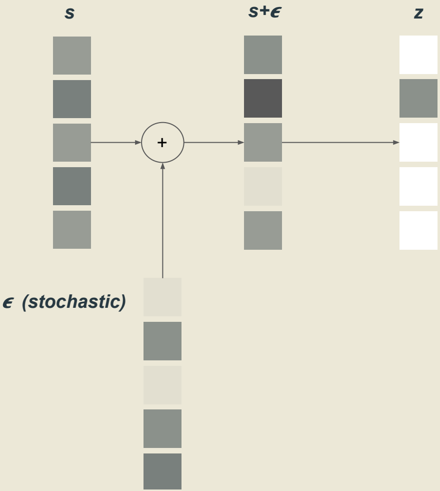

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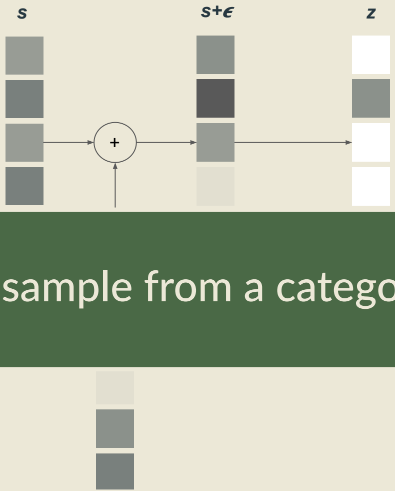

How do we sample from a categorical variable?

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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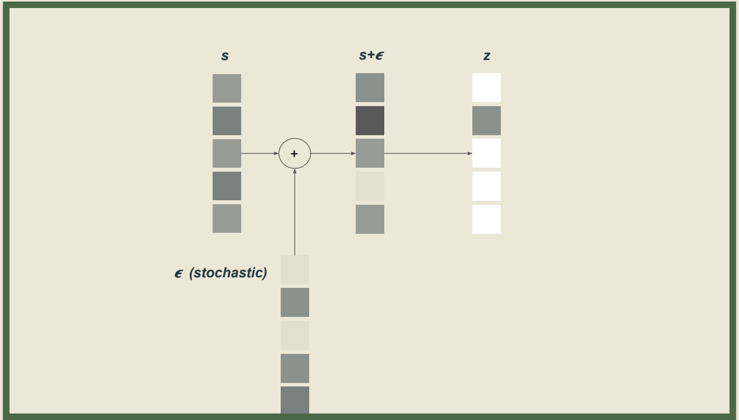

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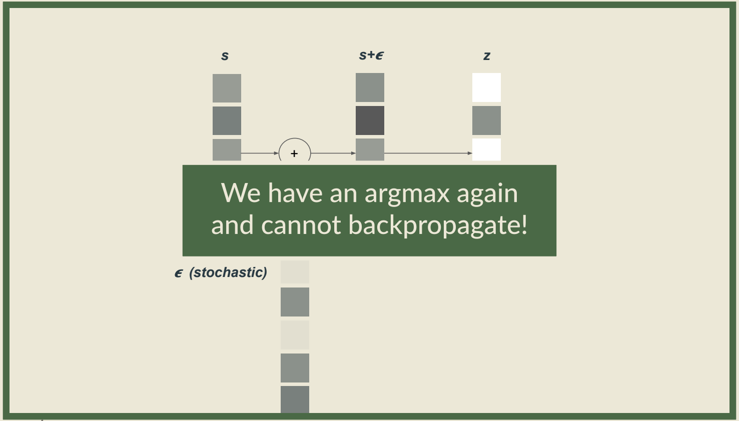

We have an argmax again and cannot backpropagate!

[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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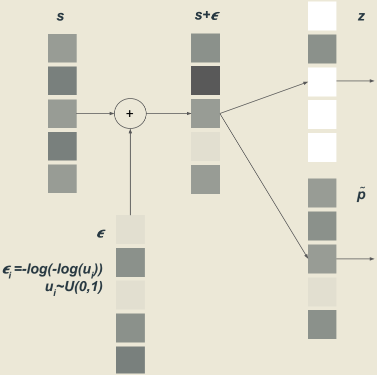

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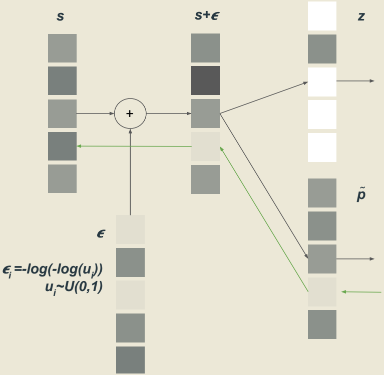

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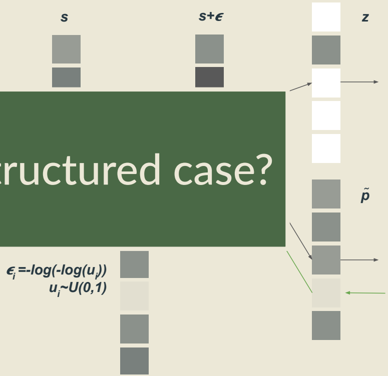
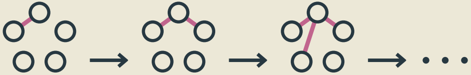
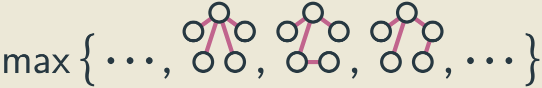


What about the structured case?

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.

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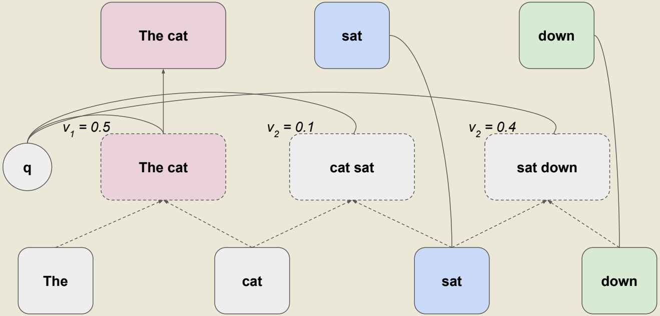
Example: Gumbel Tree-LSTM [Choi et al., 2018].

[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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- Sample from the standard Gumbel distribution.
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Perturb-and-MAP

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

- Sample from the standard Gumbel distribution.
- Perturb the arc scores with the Gumbel noise.
- Compute MAP (task-specific algorithm).

- $\boldsymbol{\epsilon} \sim G(0, 1)$
- $\tilde{\boldsymbol{\eta}} = \boldsymbol{\eta} + \boldsymbol{\epsilon}$
- $\arg\max_{\boldsymbol{z} \in \mathcal{Z}} \tilde{\boldsymbol{\eta}}^\top \boldsymbol{z}$

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Perturb-and-MAP

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

- Sample from the standard Gumbel distribution.
- Perturb the arc scores with the Gumbel noise.
- Compute MAP (task-specific algorithm).
- Backward: we could use Straight-Through with Identity.

- $\boldsymbol{\epsilon} \sim G(0, 1)$
- $\tilde{\boldsymbol{\eta}} = \boldsymbol{\eta} + \boldsymbol{\epsilon}$
- $\arg\max_{\boldsymbol{z} \in \mathcal{Z}} \tilde{\boldsymbol{\eta}}^\top \boldsymbol{z}$

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

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

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

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

- Straight-Through
- SPIGOT

Overview

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

- REINFORCE
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- Structured Attn. Nets
- SparseMAP

And more, in the next section!

IV. End-to-end Differentiable Relaxations

End-to-end differentiable relaxations

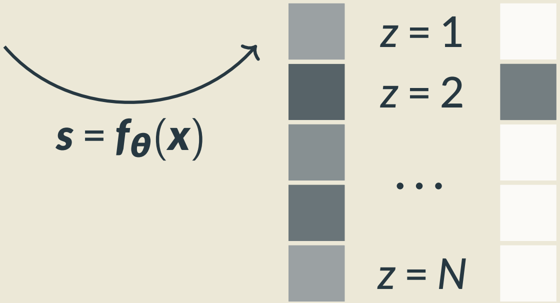
1. Digging into softmax
2. Alternatives to softmax
3. Generalizing to structured prediction
4. Stochasticity and global structures

Recall: Discrete choices & differentiability

input

$\boldsymbol{x}$

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



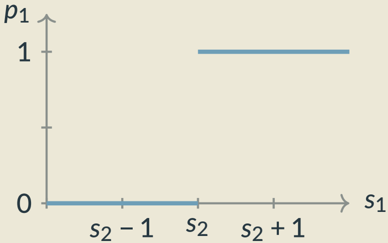
output

$\widehat{\boldsymbol{y}}$

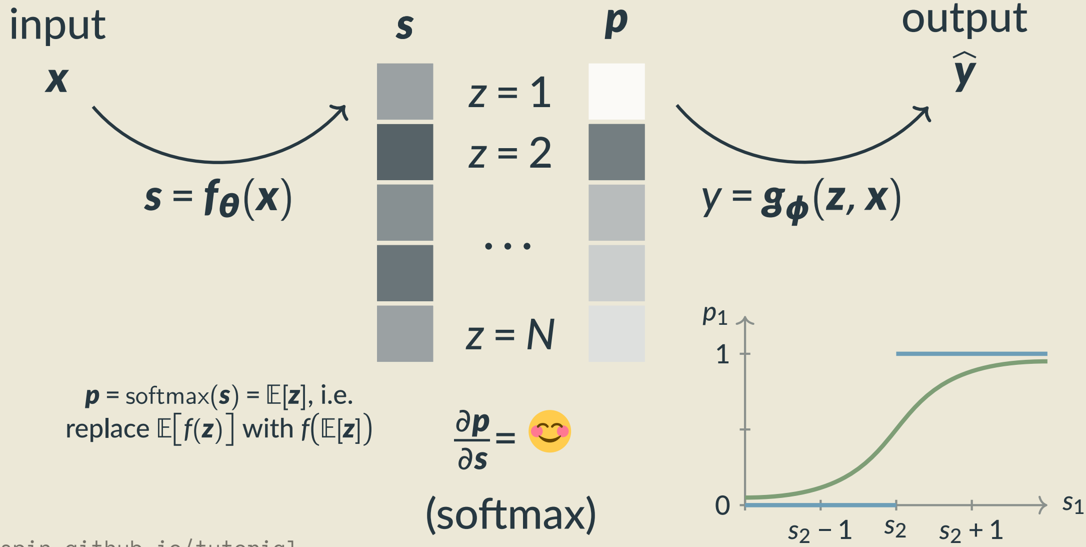
$y = \boldsymbol{g_\phi}(\boldsymbol{z}, \boldsymbol{x})$

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

(argmax)



One solution: smooth relaxation



input $\boldsymbol{x}$

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

$\boldsymbol{s}$

$z = 1$

$z = 2$

$\dots$

$z = N$

$\boldsymbol{p}$

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

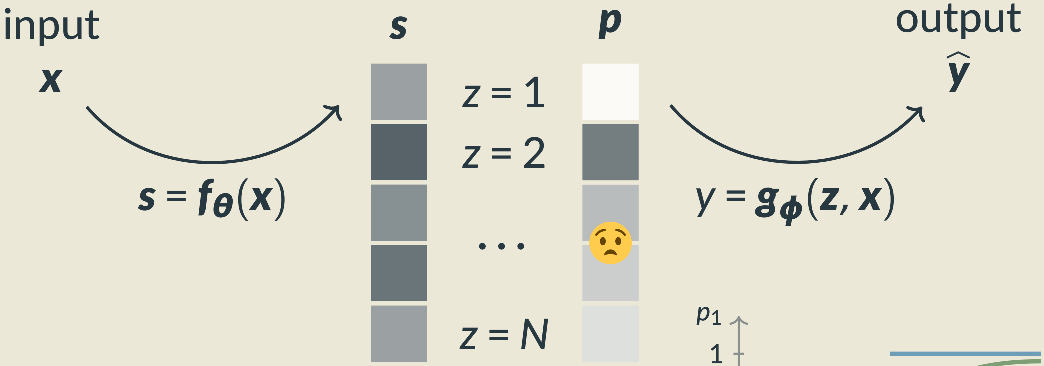
output $\widehat{\boldsymbol{y}}$

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

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

(softmax)

One solution: smooth relaxation



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$z = 1$

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$\cdots$

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$\boldsymbol{p}$

😟

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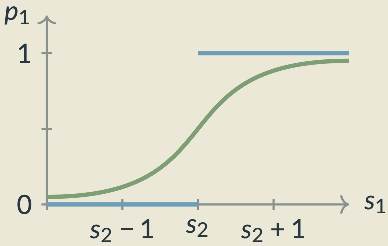

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What is softmax?

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

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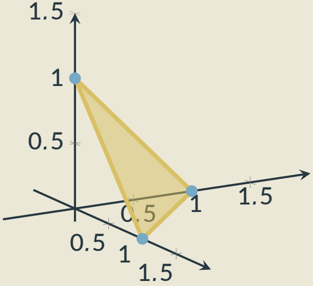
$\boldsymbol{p} \in \triangle$: probability distribution over choices



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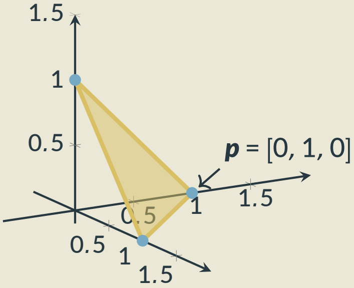

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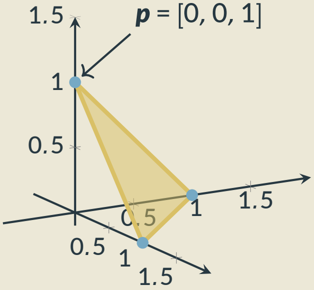

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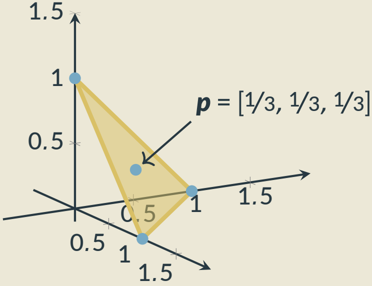

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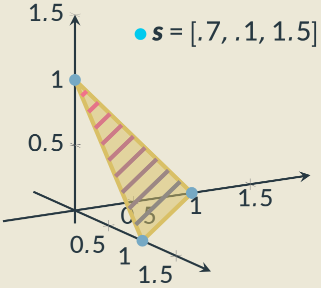

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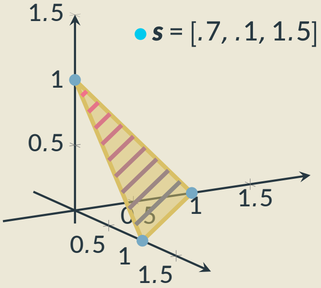
argmax



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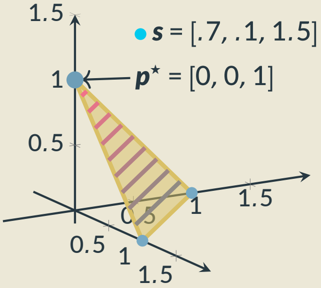
argmax maximizes **expected score**



● $\boldsymbol{s} = [.7, .1, 1.5]$

$\boldsymbol{p}^\star = [0, 0, 1]$

$$\underset{\boldsymbol{p}\in\triangle}{\arg\max}\, \boldsymbol{p}^\top \boldsymbol{s}$$

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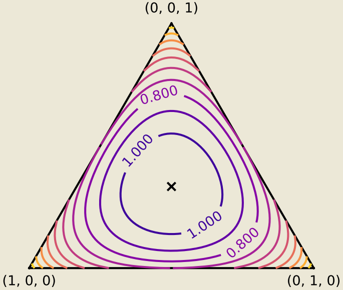
Shannon entropy of $\boldsymbol{p}$: $\mathrm{H}(\boldsymbol{p}) = -\sum_i p_i \log p_i$



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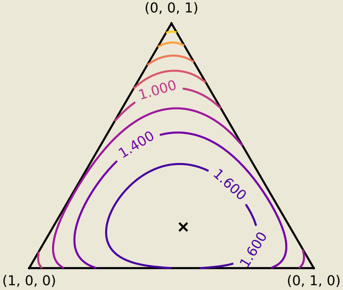
argmax maximizes **expected score**

Shannon entropy of $\boldsymbol{p}$: $\mathrm{H}(\boldsymbol{p}) = -\sum_i p_i \log p_i$

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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Explicit form of the optimization problem:

$$\begin{aligned} \text{maximize} \quad & \textstyle\sum_j p_j s_j - p_j \log p_j \\ \text{subject to} \quad & \boldsymbol{p} \geq 0,\ \boldsymbol{p}^\top \mathbf{1} = 1 \end{aligned}$$

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Lagrangian:

$$\mathcal{L}(\boldsymbol{p}, \boldsymbol{\nu}, \tau) = -\textstyle\sum_j p_j s_j - p_j \log p_j - \boldsymbol{p}^\top \boldsymbol{\nu} + \tau(\boldsymbol{p}^\top \mathbf{1} - 1)$$

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Optimality conditions (KKT):

$$\begin{aligned} 0 = \nabla_{p_i} \mathcal{L}(\boldsymbol{p}, \boldsymbol{\nu}, \tau) &= -s_i + \log p_i + 1 - \nu_i + \tau \\ \boldsymbol{p}^\top \boldsymbol{\nu} &= 0 \\ \boldsymbol{p} &\in \triangle \\ \boldsymbol{\nu} &\geq \mathbf{0} \end{aligned}$$

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if $p_i = 0$, r.h.s. must be $-\infty$,
thus $p_i > 0$, so $\nu_i = 0$.

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if $p_i = 0$, r.h.s. must be $-\infty$,
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$p_i = \exp(s_i)/\exp(\tau+1) = \exp(s_i)/Z$

Must find Z such that $\sum_j p_j = 1$.

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

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Must find Z such that $\sum_j p_j = 1$.
Answer: $Z = \sum_j \exp(s_j)$

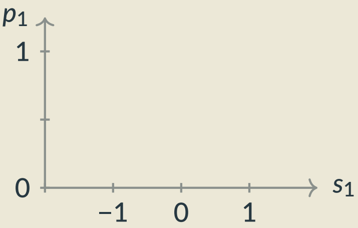
So, $p_i = \dfrac{\exp(s_i)}{\sum_j \exp(s_j)}$.

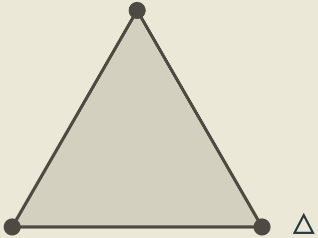
Classic result, e.g., [Boyd and Vandenberghe, 2004, Wainwright and Jordan, 2008]

[Niculae and Blondel, 2017]

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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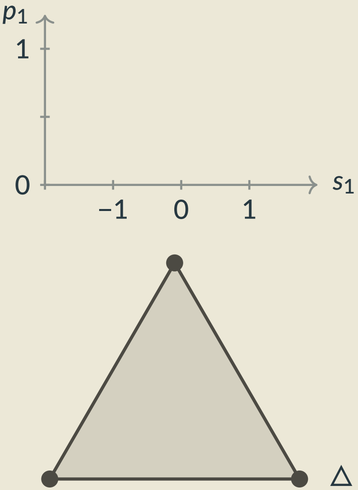

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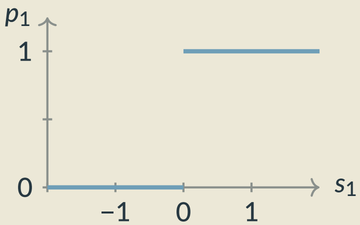
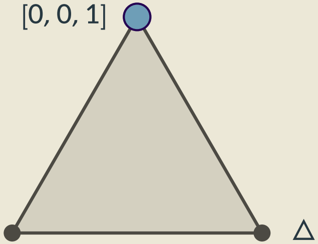
Generalizing softmax: Smoothed argmaxes

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

● argmax: $\Omega(\boldsymbol{p}) = 0$





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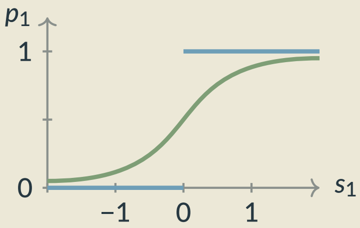
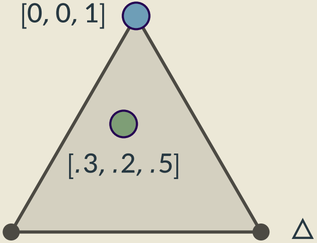
Generalizing softmax: Smoothed argmaxes

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

- ● argmax: $\Omega(\boldsymbol{p}) = 0$
- ● softmax: $\Omega(\boldsymbol{p}) = \sum_j p_j \log p_j$



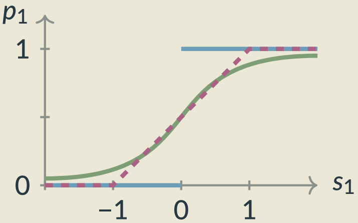


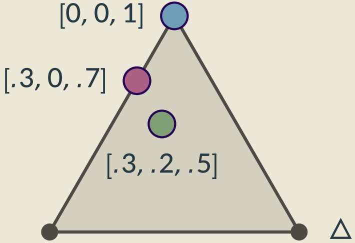
[Niculae and Blondel, 2017, Martins and Astudillo, 2016]

Generalizing softmax: Smoothed argmaxes

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

- ● argmax: $\Omega(\boldsymbol{p}) = 0$
- ● softmax: $\Omega(\boldsymbol{p}) = \sum_j p_j \log p_j$
- ● sparsemax: $\Omega(\boldsymbol{p}) = 1/2\|\boldsymbol{p}\|_2^2$





[Niculae and Blondel, 2017, Blondel et al., 2019]

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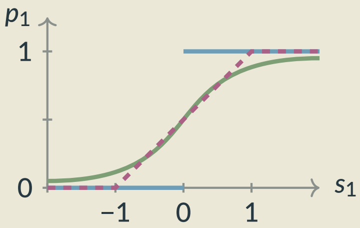
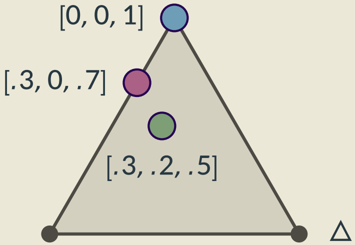
- α-entmax: $\Omega(\boldsymbol{p}) = 1/\alpha(\alpha-1) \sum_j p_j^\alpha$





Generalized entropy interpolates in between [Tsallis, 1988]
Used in Sparse Seq2Seq: [Peters et al., 2019] and Adaptively Sparse Transformers [Correia et al., 2019]

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

Generalizing softmax: Smoothed argmaxes

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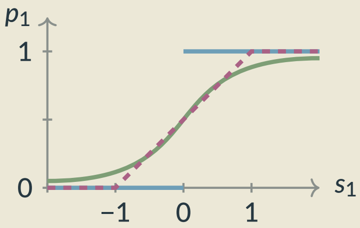
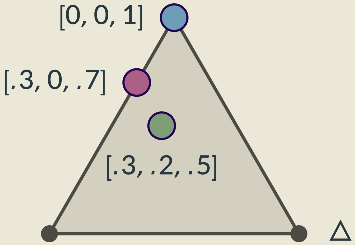
α-entmax: $\Omega(\boldsymbol{p}) = 1/\alpha(\alpha-1) \sum_j p_i^\alpha$

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

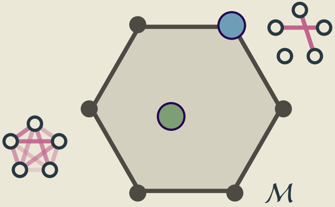




[Wainwright and Jordan, 2008]

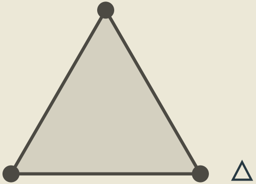
The structured case: Marginal polytope

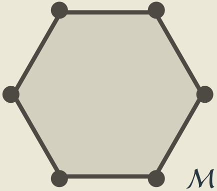
- Each vertex corresponds to one such *bit vector* $\boldsymbol{z}$
- Points inside correspond to *marginal distributions*: convex combinations of structured objects



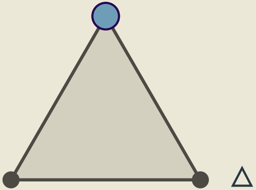
$$\boldsymbol{\mu} = \underbrace{p_1\boldsymbol{z}_1 + \ldots + p_N\boldsymbol{z}_N}_{\text{exponentially many terms}}, \ \boldsymbol{p} \in \Delta.$$

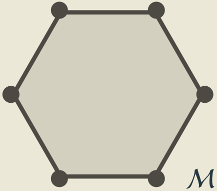
$$\begin{aligned} p_1 &= 0.2, \quad \boldsymbol{z}_1 = [1, 0, 0, 0, 1, 0, 0, 0, 1] \\ p_2 &= 0.7, \quad \boldsymbol{z}_2 = [0, 0, 1, 0, 0, 1, 1, 0, 0] \\ p_3 &= 0.1, \quad \boldsymbol{z}_3 = [1, 0, 0, 0, 1, 0, 0, 1, 0] \end{aligned} \quad \Rightarrow \quad \boldsymbol{\mu} = [.3, 0, .7, 0, .3, .7, .7,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


$\triangle$


$\mathcal{M}$

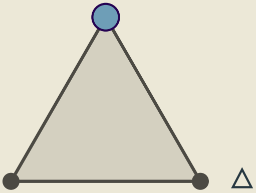
● **argmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s}$

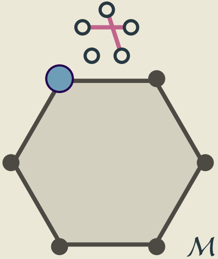




argmax $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s}$

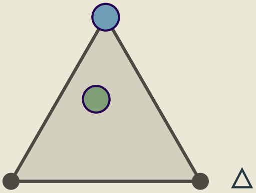
MAP $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta}$

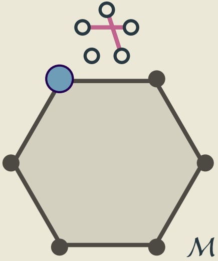




- ● **argmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s}$
- ● **softmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s} + \mathrm{H}(\boldsymbol{p})$

MAP $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta}$ ●





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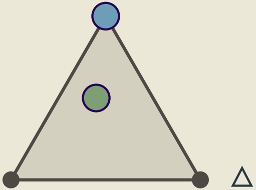
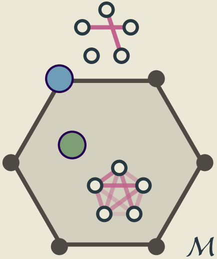
MAP $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta}$ ●

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





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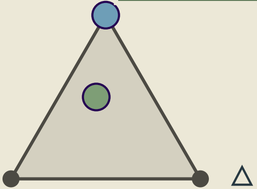
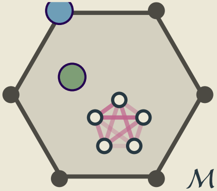
Just like softmax relaxes argmax, marginals relax MAP **differentiably**!





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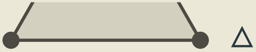
Just like softmax relaxes argmax, marginals relax MAP **differentiably**!

Unlike argmax/softmax, computation is not obvious!



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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Derivatives of marginals 1: DP

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 $k$
for $i \in n-1, \ldots, 1$ do                                     # backward log-probabilities
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$Z = \sum_k \exp \alpha_{n,k}$                                      # partition function
return $\boldsymbol{\mu} = \exp\left(\boldsymbol{\alpha} + \boldsymbol{\beta} - \log Z\right)$                          # marginals
```

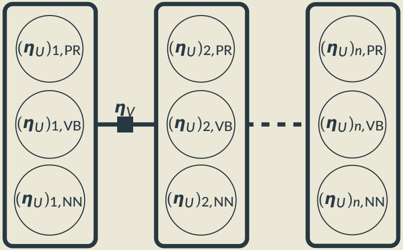
$(\boldsymbol{\eta}_U)_{1,\mathrm{PR}}$
$(\boldsymbol{\eta}_U)_{1,\mathrm{VB}}$
$(\boldsymbol{\eta}_U)_{1,\mathrm{NN}}$
$\boldsymbol{\eta}_V$
$(\boldsymbol{\eta}_U)_{2,\mathrm{PR}}$
$(\boldsymbol{\eta}_U)_{2,\mathrm{VB}}$
$(\boldsymbol{\eta}_U)_{2,\mathrm{NN}}$
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$Z = \sum_k \exp \alpha_{n,k}$                                       # partition function
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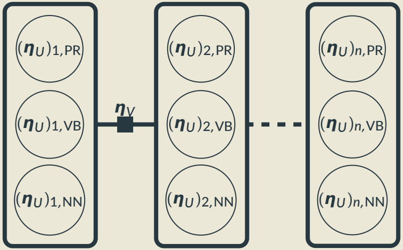
```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for $i \in 2, \ldots, n$ do                                                  # forward log-probabilities
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for $i \in n-1, \ldots, 1$ do                                              # backward log-probabilities
    $\beta_{i,k} = \log \sum_{k'} \exp\left(\beta_{i+1,k'} + (\boldsymbol{\eta}_U)_{i+1,k'} + (\boldsymbol{\eta}_V)_{k,k'}\right)$   for all $k$
$Z = \sum_k \exp \alpha_{n,k}$                                                      # partition function
return $\boldsymbol{\mu} = \exp\left(\boldsymbol{\alpha} + \boldsymbol{\beta} - \log Z\right)$                                   # marginals
```

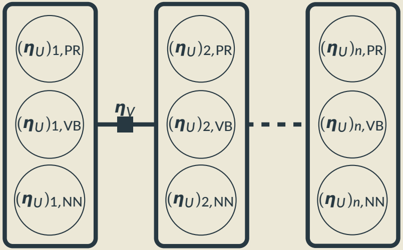
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- Alg. consists of differentiable ops: PyTorch autograd can handle it! (v. bad idea)
- Better book-keeping: Li and Eisner [2009], Mensch and Blondel [2018]
- With circular dependencies, this breaks! Can get an approximation [Stoyanov et al., 2011]

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```
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$Z = \sum_k \exp \alpha_{n,k}$                                                  # partition function
return $\boldsymbol{\mu} = \exp\left(\boldsymbol{\alpha} + \boldsymbol{\beta} - \log Z\right)$                                  # marginals
```

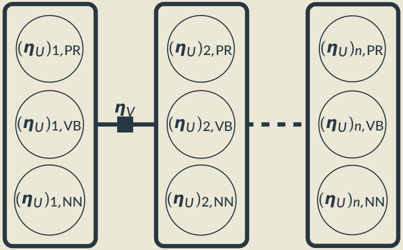
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$(\boldsymbol{\eta}_U)_{n,\mathrm{PR}}$
$(\boldsymbol{\eta}_U)_{n,\mathrm{VB}}$
$(\boldsymbol{\eta}_U)_{n,\mathrm{NN}}$

Derivatives of marginals 2: Matrix-Tree

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

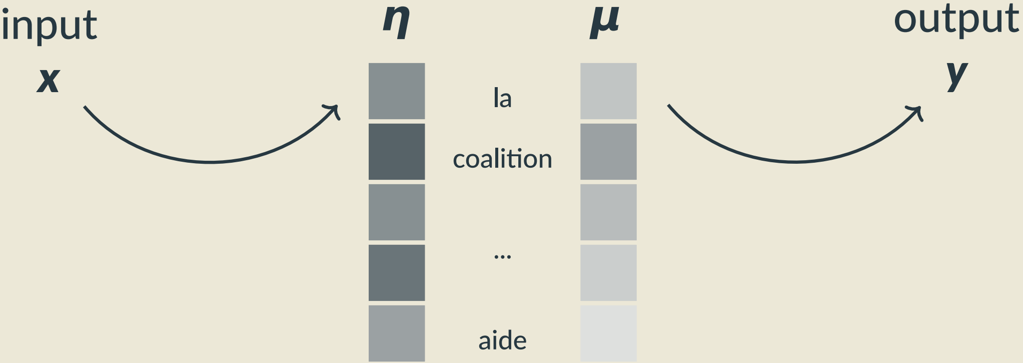
$$Z = \det \boldsymbol{L}(\boldsymbol{s})$$

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

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

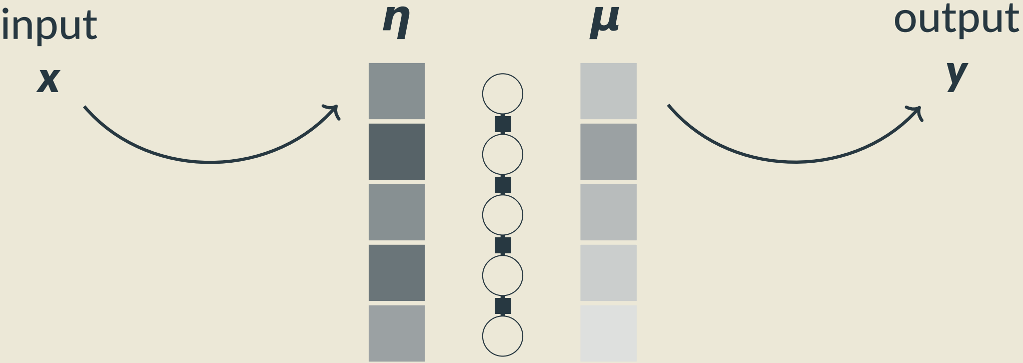
[Kim et al., 2017]

Structured Attention Networks



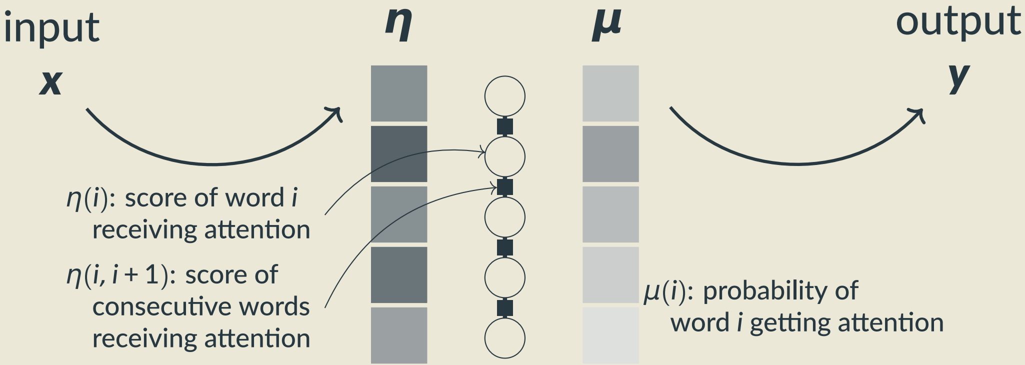
[Kim et al., 2017]

Structured Attention Networks



[Kim et al., 2017]

Structured Attention Networks



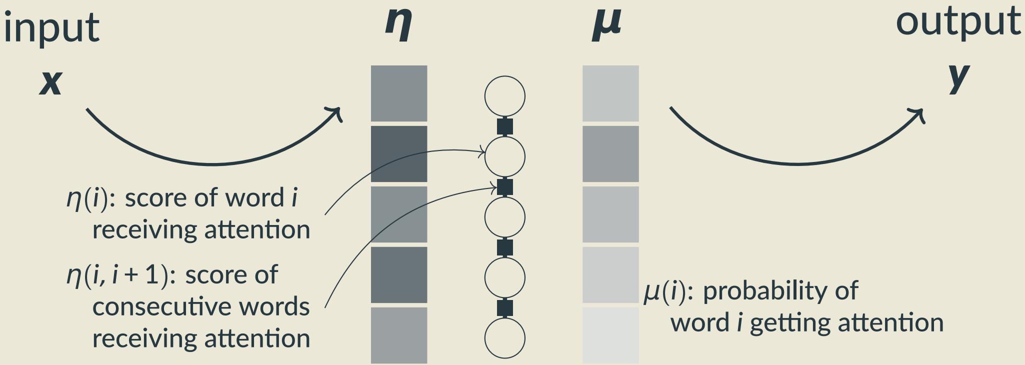
$\eta(i)$: score of word i receiving attention

$\eta(i, i+1)$: score of consecutive words receiving attention

$\mu(i)$: probability of word i getting attention

[Kim et al., 2017]

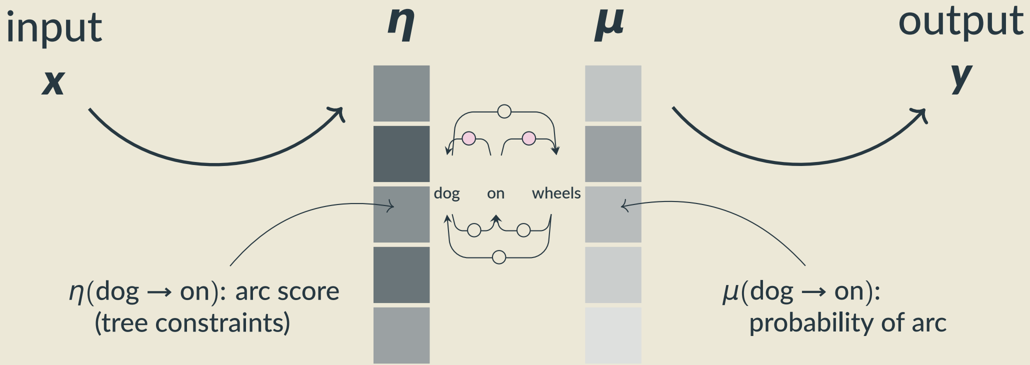
Structured Attention Networks


input
$\boldsymbol{x}$
$\boldsymbol{\eta}$
$\boldsymbol{\mu}$
output
$\boldsymbol{y}$
$\eta(i)$: score of word i receiving attention
$\eta(i, i+1)$: score of consecutive words receiving attention
$\mu(i)$: probability of word i getting attention

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

[Kim et al., 2017]

Structured Attention Networks

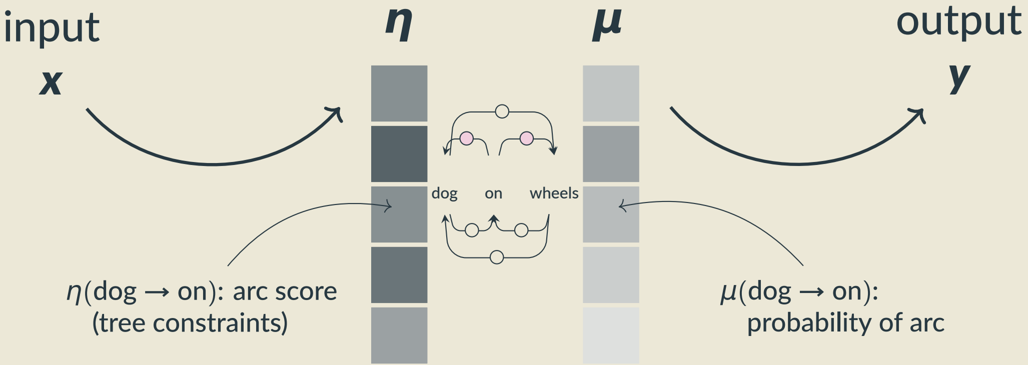


CRF marginals (from *forward–backward*) give attention weights ∈ (0, 1)

Similar idea for projective dependency trees with *inside–outside*

[Kim et al., 2017]

Structured Attention Networks



input $\boldsymbol{x}$

$\boldsymbol{\eta}$

$\boldsymbol{\mu}$

output $\boldsymbol{y}$

dog on wheels

$\eta(\text{dog} \rightarrow \text{on})$: arc score (tree constraints)

$\mu(\text{dog} \rightarrow \text{on})$: probability of arc

CRF marginals (from *forward–backward*) give attention weights ∈ (0, 1)

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)

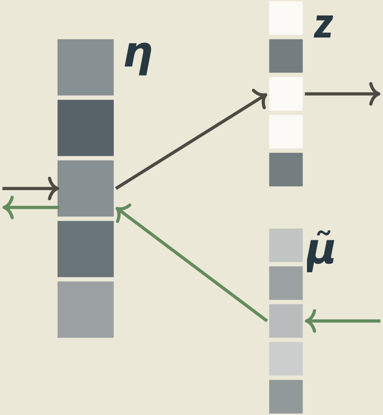
  $$\boldsymbol{z} = \underset{\boldsymbol{z}\in\mathcal{Z}}{\arg\max}(\boldsymbol{\eta}+\boldsymbol{\epsilon})^{\top}\boldsymbol{z}$$

- Backward pass:

  pretend we did marginal inference

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

  (or some similar relaxation)



Back-propagating through marginals

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- Familiar algorithms for NLPers,

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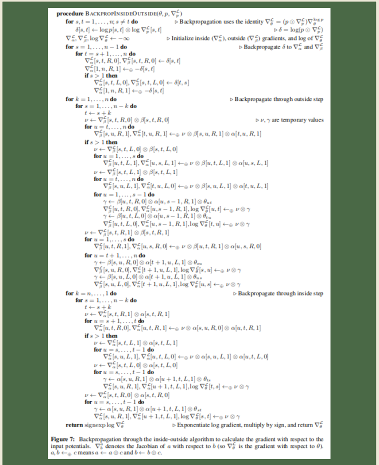

```
procedure BACKPROPINSIDEOUTSIDE($\theta, p, \nabla_p^{\mathcal{L}}$)
    for $s, t = 1, \ldots, n; s \neq t$ do        ▷ Backpropagation uses the identity $\nabla_\theta^{\mathcal{L}} = (p \odot \nabla_p^{\mathcal{L}})\nabla_\theta^{\log p}$
        $\delta[s,t] \leftarrow \log p[s,t] \otimes \log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

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

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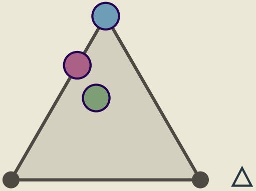
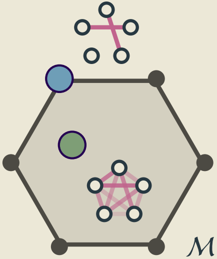
[Niculae et al., 2018a]

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





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● **sparsemax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{s} - 1/2\|\boldsymbol{p}\|^2$

MAP $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta}$ ●

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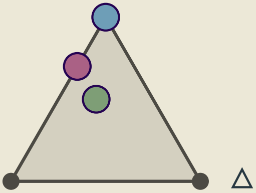
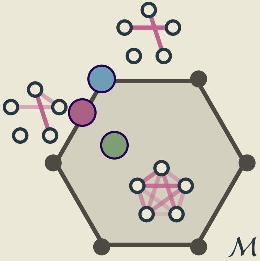
SparseMAP $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta} - 1/2\|\boldsymbol{\mu}\|^2$ ●

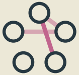
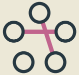
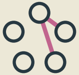




[Niculae et al., 2018a]

SparseMAP solution

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

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

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

Algorithms for SparseMAP

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

This is also $\text{proj}_{\mathcal{M}}$ required by SPIGOT!

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

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Conditional Gradient

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

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

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[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

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

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

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

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

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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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Completely modular: just add MAP

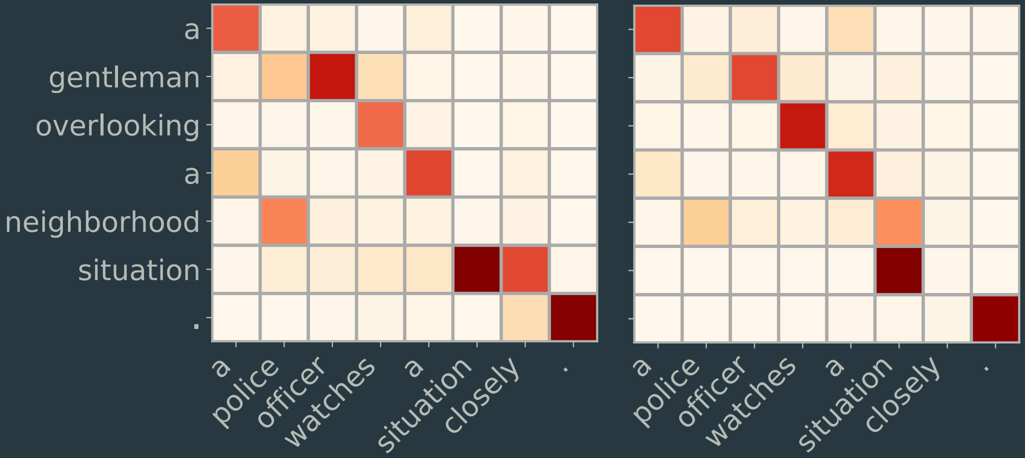
pass

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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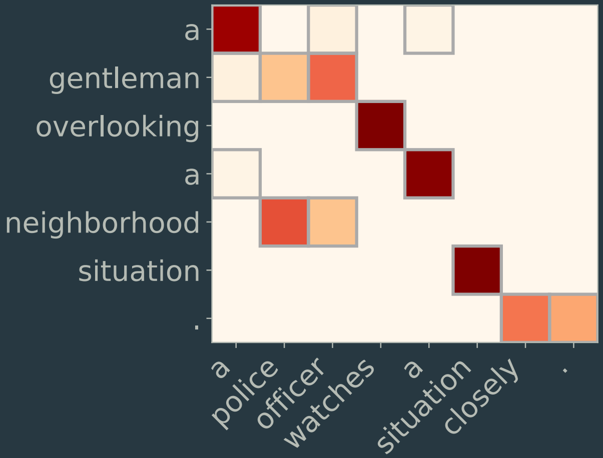

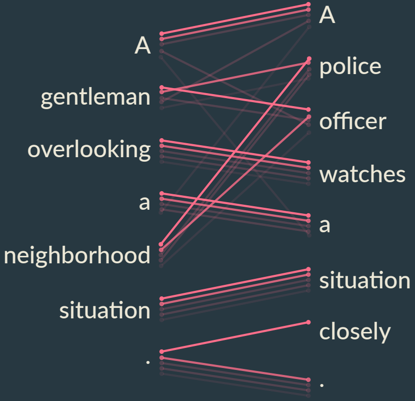

Overview

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

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

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

- Straight-Through
- SPIGOT

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

- Structured Attn. Nets
- SparseMAP

Structured latent variables without sampling

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

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 $\boldsymbol{z}$

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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 $\boldsymbol{z}$

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

parsing model,
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Exponentially large sum!

Structured latent variables without sampling

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parsing model,
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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 $\boldsymbol{z}$

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

parsing model,
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$$\sum_{h\in\mathcal{H}}$$

idea 1

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Structured latent variables without sampling

sum over
all possible trees

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

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

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

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

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

idea 1

idea 2

idea 3

Structured latent variables without sampling

sum over
all possible trees

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

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

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

idea 2

idea 3

Structured latent variables without sampling

sum over
all possible trees

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parsing model,
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Structured latent variables without sampling

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parsing model,
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How to define $\pi_{\boldsymbol{\theta}}$?

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

idea 2

idea 3

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

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idea 2	$\pi_{\boldsymbol{\theta}}(\boldsymbol{z}) = 1$ if $\boldsymbol{z} = \mathrm{MAP}(f_{\boldsymbol{\theta}}(\cdot))$ else 0	argmax		
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Structured latent variables without sampling

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

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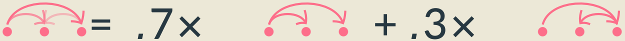
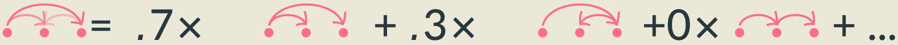
idea 3		SparseMAP	😊	😊

Structured latent variables without sampling



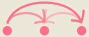
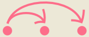
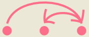
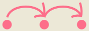
= .7× + .3×

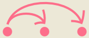
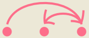
Structured latent variables without sampling



= .7× + .3× +0× + ...

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

V. Conclusions

[Corro and Titov, 2019b, Havrylov et al., 2019]

Stanford Natural Language Inference (Accuracy)

[Kim et al., 2017]	
Simple Attention	86.2
Structured Attention	86.8
[Liu and Lapata, 2018]	
100D Structured Attention	86.8
[Yogatama et al., 2017]	
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
[Havrylov et al., 2019]	
100D TreeLSTM + tricks	84.3

Stanford Sentiment (Accuracy)

[Socher et al., 2013]	
Bigram Naive Bayes	83.1
[Niculae et al., 2018b]	
DepTreeLSTM w/ CoreNLP	83.2
DepTreeLSTM w/ SparseMAP	84.7
[Corro and Titov, 2019b]	
GCN w/ CoreNLP	83.8
GCN w/ Perturb-and-MAP	84.6
[Choi et al., 2018]	
ST Gumbel-Tree	90.7
[Havrylov et al., 2019]	
TreeLSTM + tricks	90.2

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]

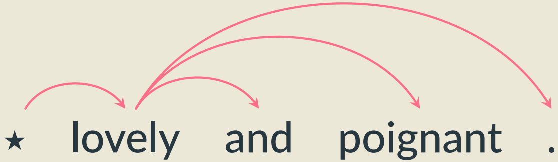
  (future work: more inductive biases and constraints?)
- Common to compare latent structures with parser outputs.

  But is this always a meaningful comparison?

[Niculae et al., 2018b]

Syntax vs. Composition Order

CoreNLP parse, $p = 21.4\%$

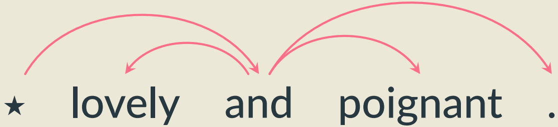


⋆ lovely and poignant .

[Niculae et al., 2018b]

Syntax vs. Composition Order

$p = 22.6\%$



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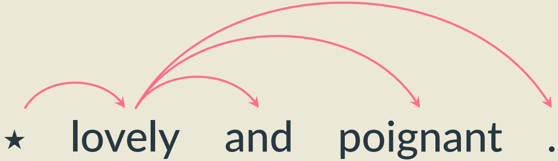

★ lovely and poignant .

. . .

[Niculae et al., 2018b]

Syntax vs. Composition Order

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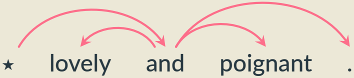
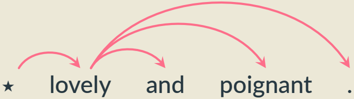
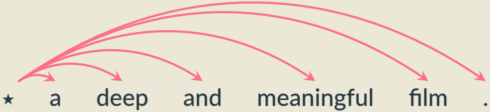

★ lovely and poignant .

CoreNLP parse, $p = 21.4\%$

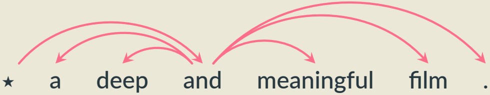

★ lovely and poignant .

...

$p = 15.33\%$

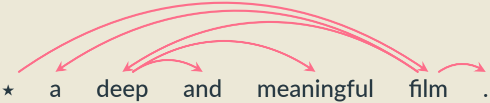

★ a deep and meaningful film .

$p = 15.27\%$


★ a deep and meaningful film .

...

CoreNLP parse, $p = 0\%$


★ a deep and meaningful film .

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]

Overview

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

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

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

- Straight-Through
- SPIGOT

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

- Structured Attn. Nets
- SparseMAP

Overview

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

- REINFORCE$^{\text{SPL}}$
- Straight-Through Gumbel (Perturb & MAP)$^{\text{SPL},\text{MRG}}$
- SparseMAP$^{\text{MAP+}}$

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

- Straight-Through$^{\text{MAP},\text{MRG}}$
- SPIGOT$^{\text{MAP+}}$

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

- Structured Attn. Nets$^{\text{MRG}}$
- SparseMAP$^{\text{MAP+}}$

Computation:

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

MAP: Finding the highest-scoring structure.

MRG: Marginal inference.

Overview

Thank you!

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

- REINFORCE$^{\text{SPL}}$
- Straight-Through Gumbel (Perturb & MAP)$^{\text{SPL,MRG}}$
- SparseMAP$^{\text{MAP+}}$

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

- Straight-Through$^{\text{MAP,MRG}}$
- SPIGOT$^{\text{MAP+}}$

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

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Computation:

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