



Latent Structure Models for NLP

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deep-spin.github.io/tutorial

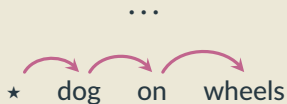
I. Introduction

Structured prediction and NLP

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

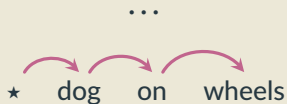
Examples of structure in NLP

Dependency parsing

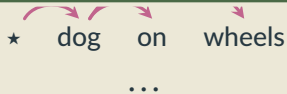


Examples of structure in NLP

Dependency parsing



Exponentially many parse trees!
Cannot enumerate.



Examples of structure in NLP

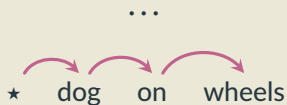
POS tagging

VERB PREP NOUN
dog on wheels

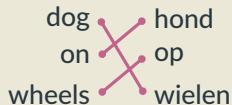
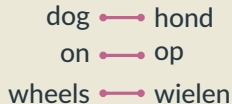
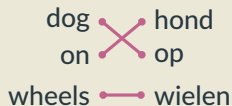
NOUN PREP NOUN
dog on wheels

NOUN DET NOUN
dog on wheels

Dependency parsing



Word alignments



NLP 5 years ago:

Structured prediction and pipelines



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- **Advantages:** fast and simple to train, can rearrange pieces 😊

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NLP 5 years ago:

Structured prediction and pipelines

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

NLP today:

End-to-end training



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End-to-end training

- Forget pipelines—train everything from scratch!
- No more error propagation or linguistic annotations! 🎉

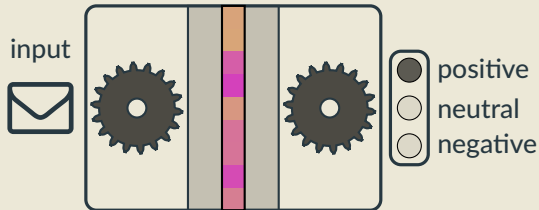
NLP today:

End-to-end training

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

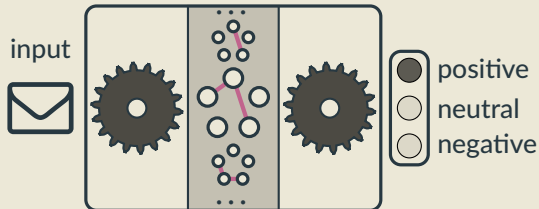
Latent structure models

- Seek *structured* hidden representations instead!



Latent structure models

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Latent structure models aren't so new!

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

Why do we love latent structure models?

- The inferred latent variables can bring us some **interpretability**
- They offer a way of injecting prior knowledge as a **structured bias**
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 - smaller carbon footprint!

What this tutorial is about:

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

This tutorial is *not* about:

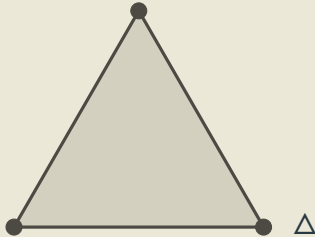
- It's not about continuous latent variables
- It's not about deep generative learning
- We won't cover GANs, VAEs, etc.
- There are (very good) recent tutorials on deep variational models for NLP:
 - “Variational Inference and Deep Generative Models” (Schulz and Aziz, ACL 2018)
 - “Deep Latent-Variable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

Background

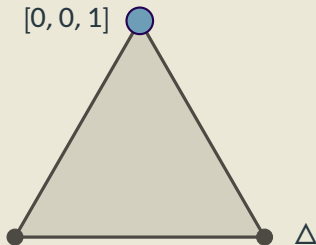
Unstructured vs structured

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

The unstructured case: Probability simplex



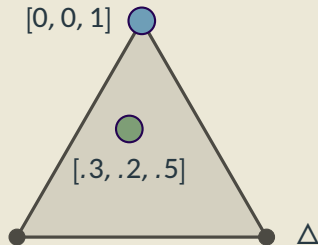
The unstructured case: Probability simplex



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

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

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

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

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

$$\mathbf{p} \geq \mathbf{0}, \quad \sum_c p_c = 1.$$

What's the analogous of Δ for a structure?

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

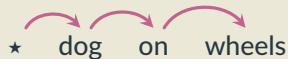
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- A structured object \mathbf{z} can be represented as a *bit vector*.
- Example:
 - a dependency tree can be represented a $O(L^2)$ vector indexed by arcs
 - each entry is 1 iff the arc belongs to the tree
 - **structural constraints:** not all bit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

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



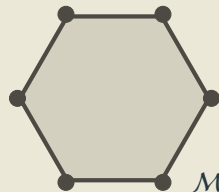
$$\mathbf{z}_2 = [0, 0, 1, 0, 0, 1, 1, 0, 0]$$



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

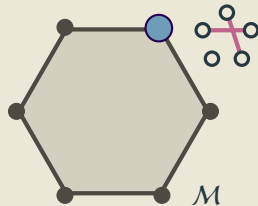


The structured case: Marginal polytope



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



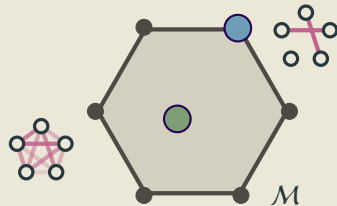
The structured case: Marginal polytope

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

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

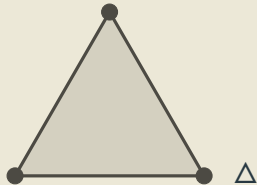
$$\begin{aligned} p_1 &= 0.2, & \mathbf{z}_1 &= [1, 0, 0, 0, 1, 0, 0, 0, 1] \\ p_2 &= 0.7, & \mathbf{z}_2 &= [0, 0, 1, 0, 0, 1, 1, 0, 0] \\ p_3 &= 0.1, & \mathbf{z}_3 &= [1, 0, 0, 0, 1, 0, 0, 1, 0] \end{aligned}$$

$$\Rightarrow \boldsymbol{\mu} = [.3, 0, .7, 0, .3, .7, .7, .1, .2].$$

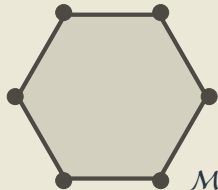


Unstructured vs Structured

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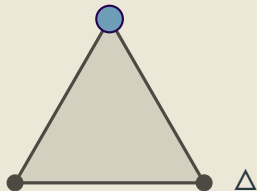


- Structured case: marginal polytope \mathcal{M}

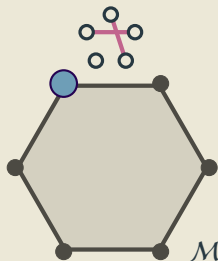


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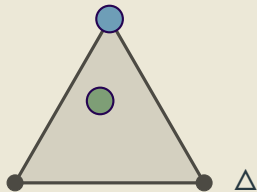


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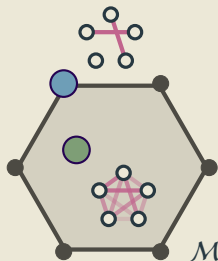


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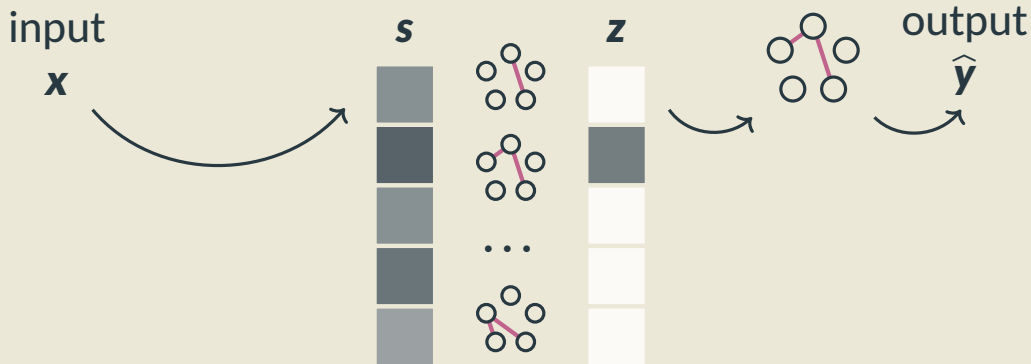


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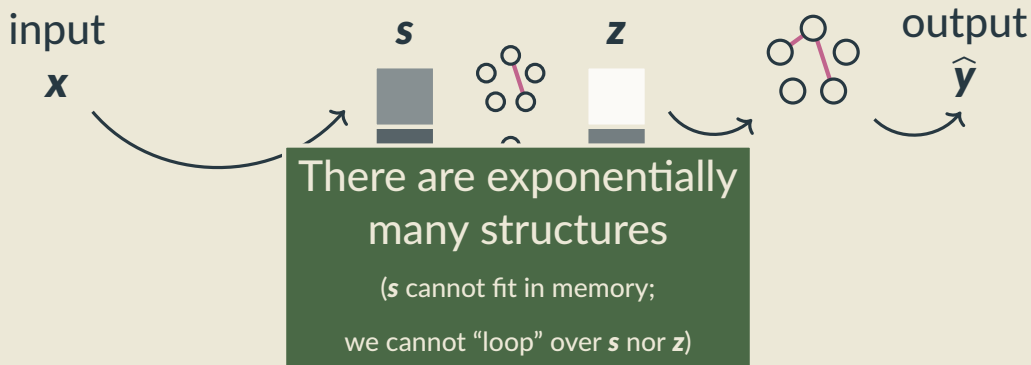
Computing the most likely structure

is a very high-dimensional argmax

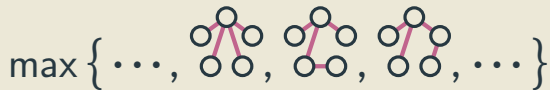
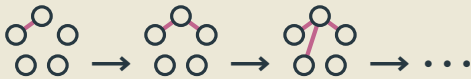


Computing the most likely structure

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Dealing with the combinatorial explosion



1. Incremental structures

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

2. Factorization into parts

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

The challenge of discrete choices.

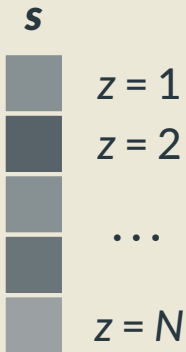
$$z = 1$$

$$z = 2$$

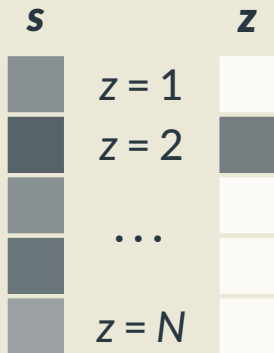
...

$$z = N$$

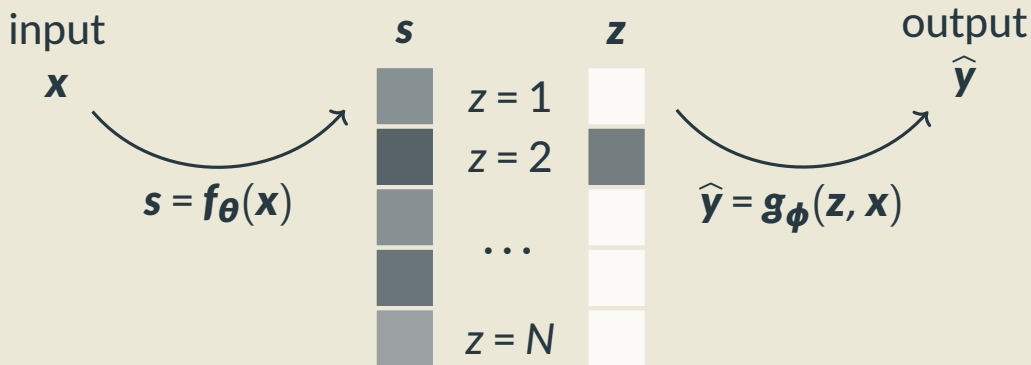
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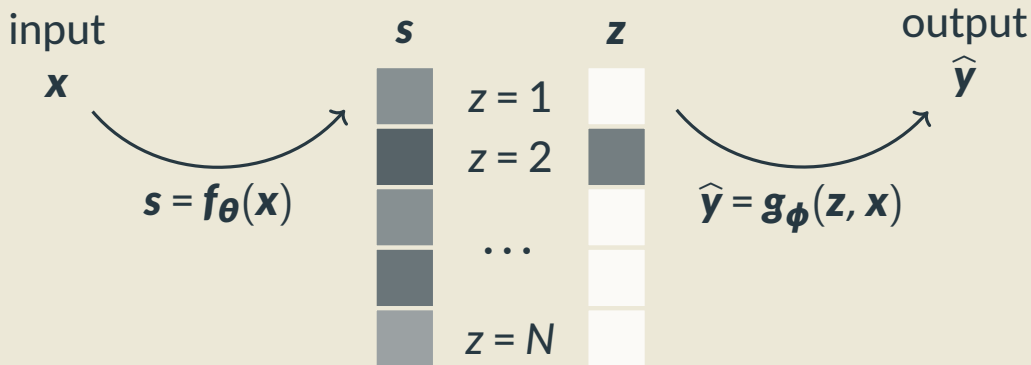
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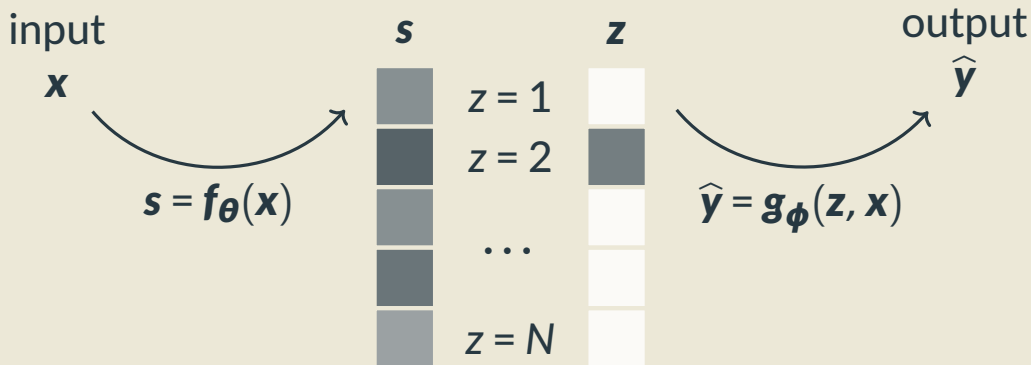


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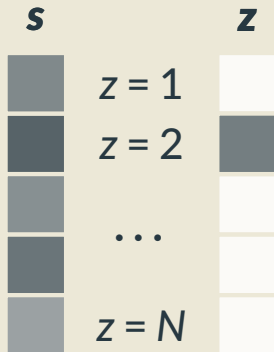
$$\frac{\partial L(\hat{\mathbf{y}}, \mathbf{y})}{\partial \mathbf{w}} = ?$$

The challenge of discrete choices.



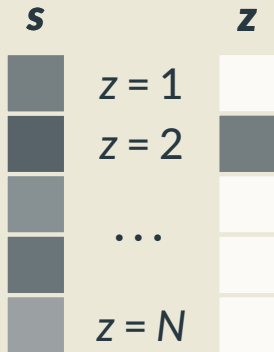
$$\frac{\partial L(\hat{\mathbf{y}}, \mathbf{y})}{\partial \mathbf{w}} = ? \quad \text{or, essentially,} \quad \frac{\partial \mathbf{z}}{\partial \mathbf{s}} = ?$$

Discrete mappings are “flat”



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Discrete mappings are “flat”



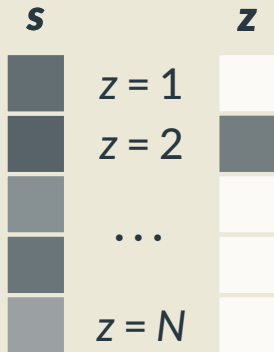
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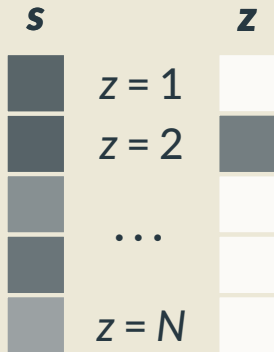
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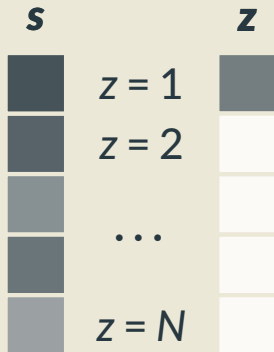
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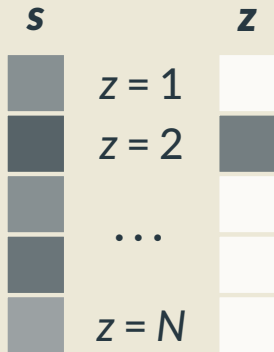
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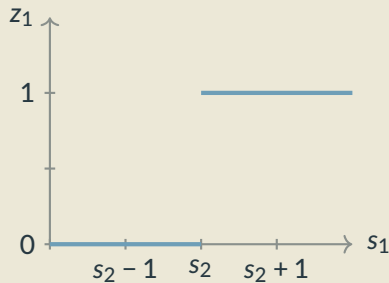


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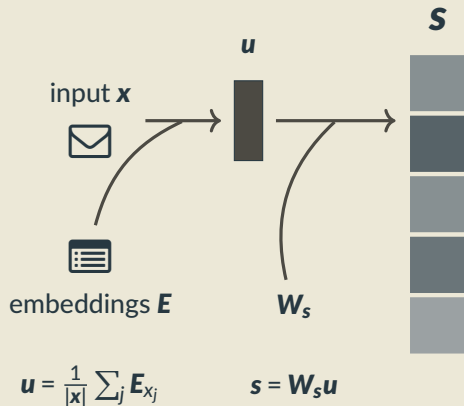
Argmax



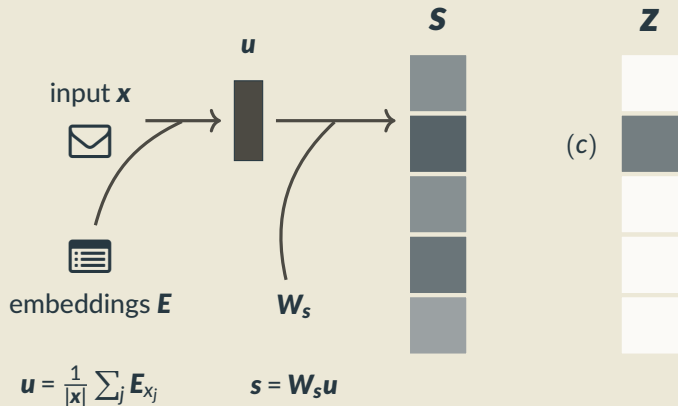
$$\frac{\partial \mathbf{z}}{\partial \mathbf{s}} = \mathbf{0}$$



Example: Regression with latent categorization

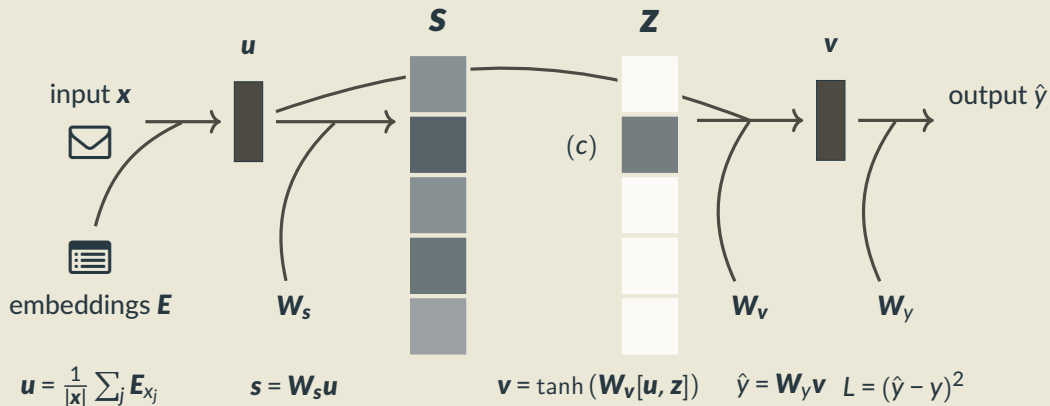


Example: Regression with latent categorization



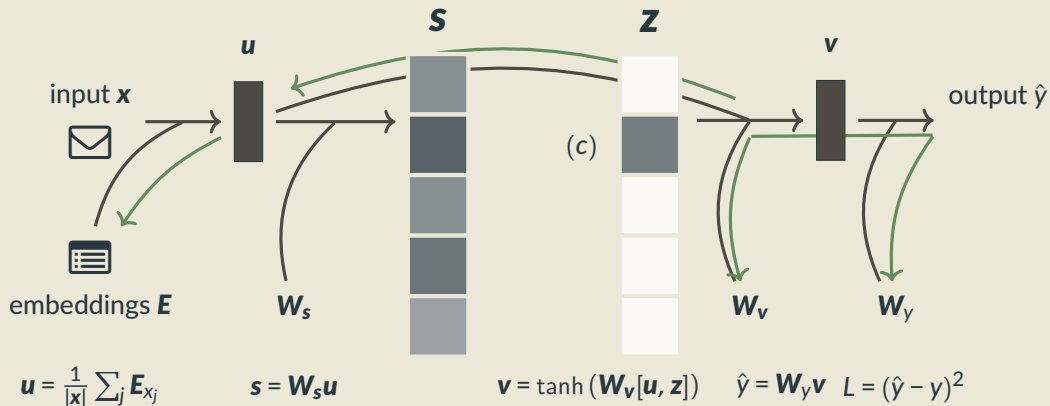
predict topic c ($z = e_c$)

Example: Regression with latent categorization

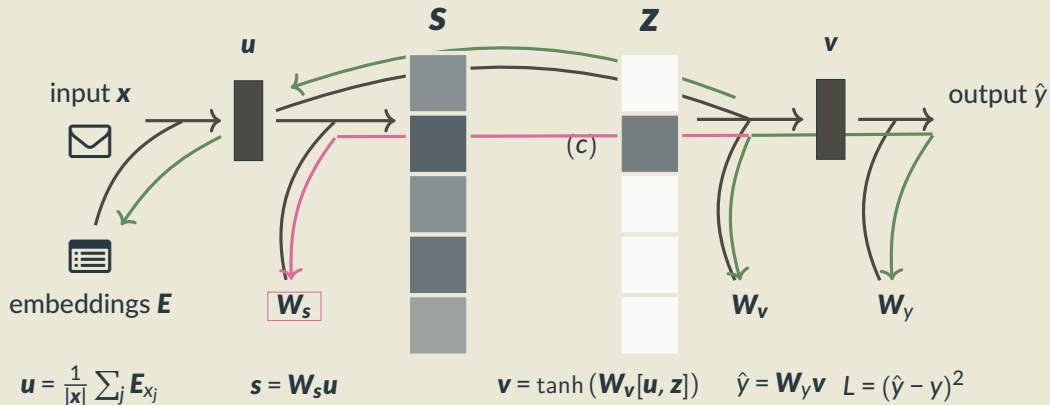


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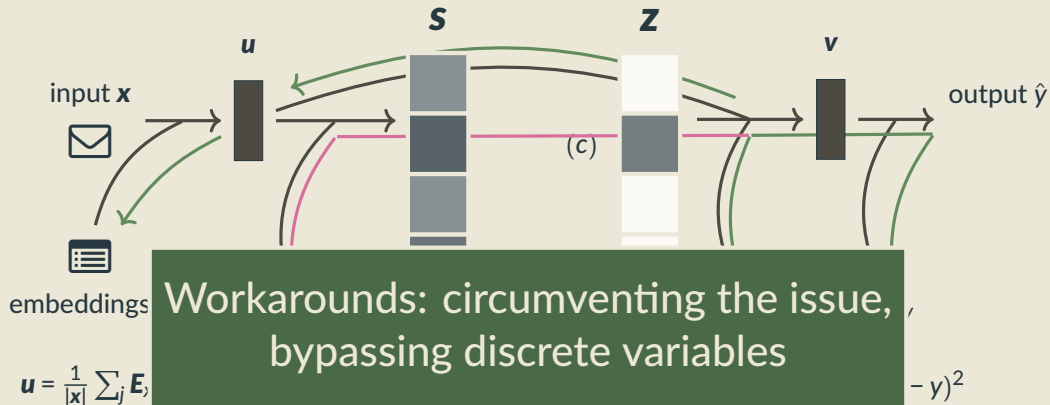


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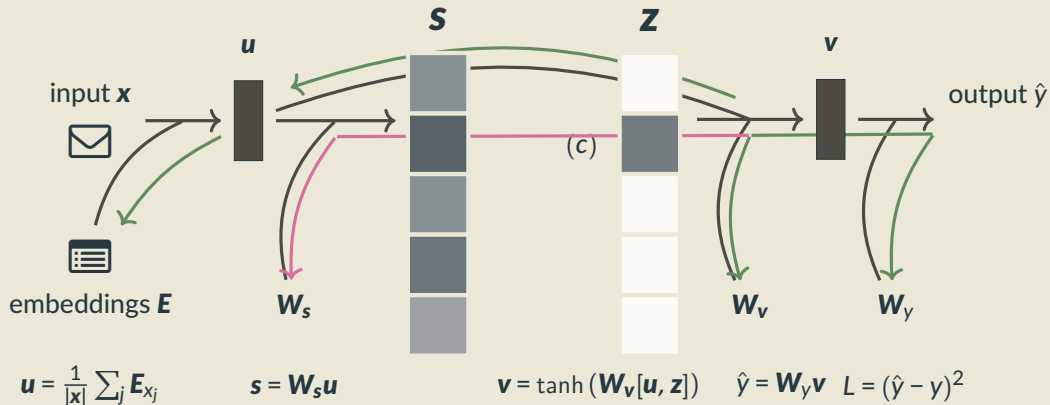


$$\frac{\partial L}{\partial W_s} = \frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial v} \frac{\partial v}{\partial z} \underbrace{\frac{\partial z}{\partial s}}_{\equiv 0} \frac{\partial s}{\partial W_s}$$

Example: Regression with latent categorization

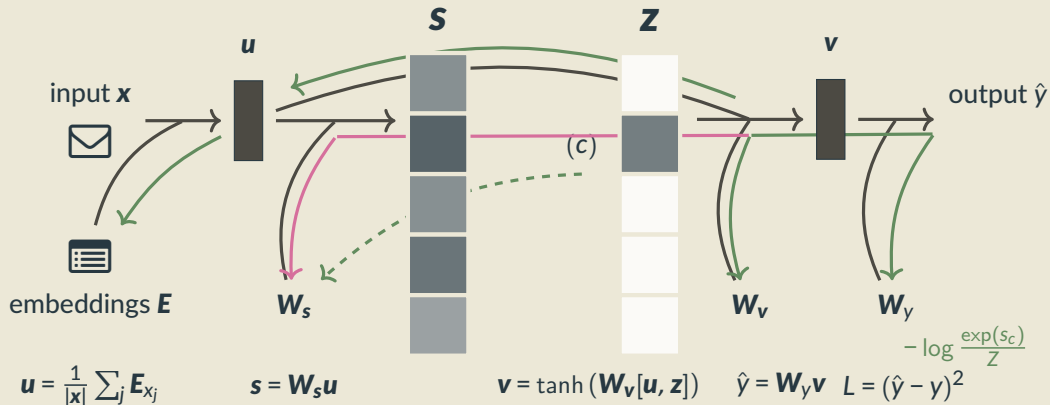


Example: Regression with latent categorization



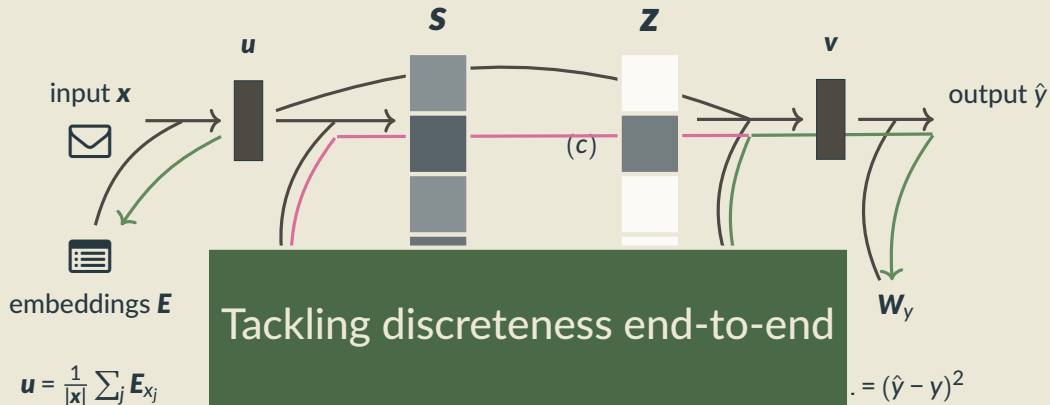
Option 1. Pretrain latent classifier W_s

Example: Regression with latent categorization

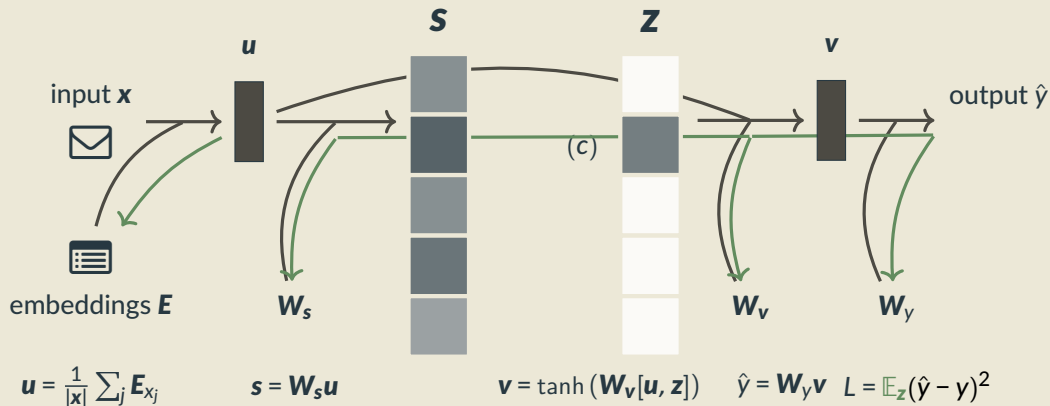


Option 2. Multi-task learning

Example: Regression with latent categorization

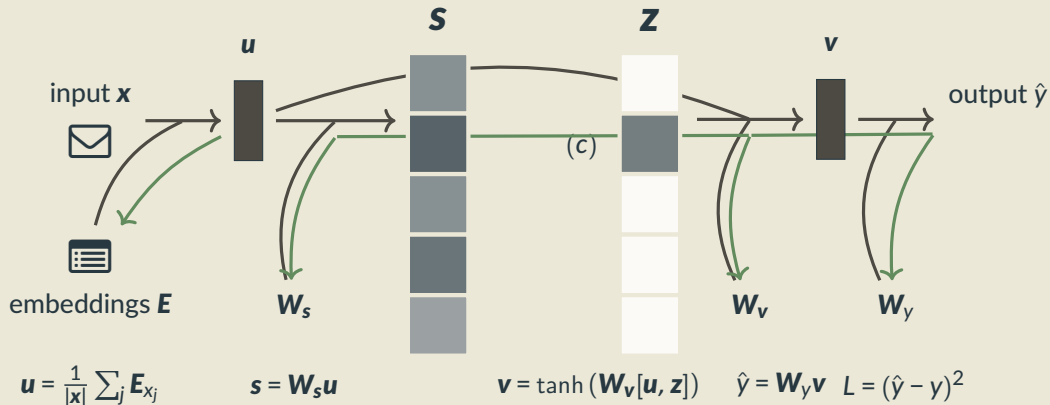


Example: Regression with latent categorization



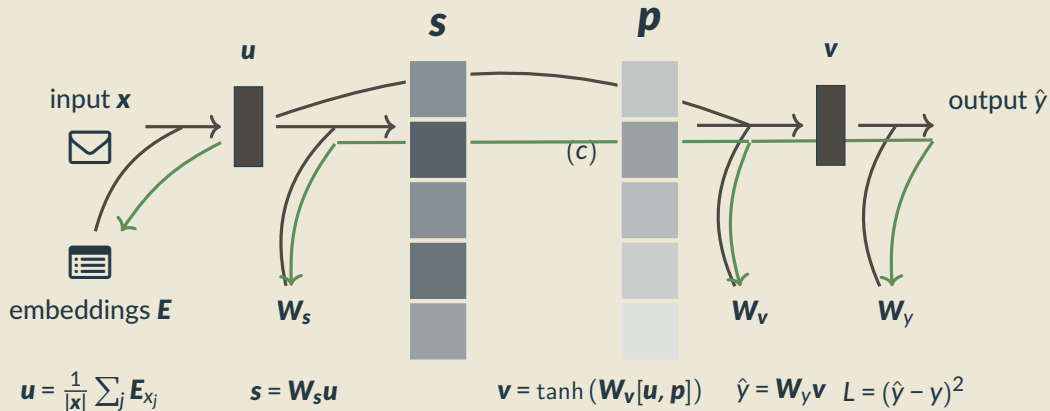
Option 3. Stochasticity! $\frac{\partial \mathbb{E}_z(\hat{y}(z) - y)^2}{\partial W_s} \neq 0$

Example: Regression with latent categorization



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

Example: Regression with latent categorization



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

Dealing with discrete latent variables

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

Dealing with discrete latent variables

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

Roadmap of the tutorial

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

Coffee Break

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

II. Reinforcement Learning Methods

Latent structure via marginalization

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

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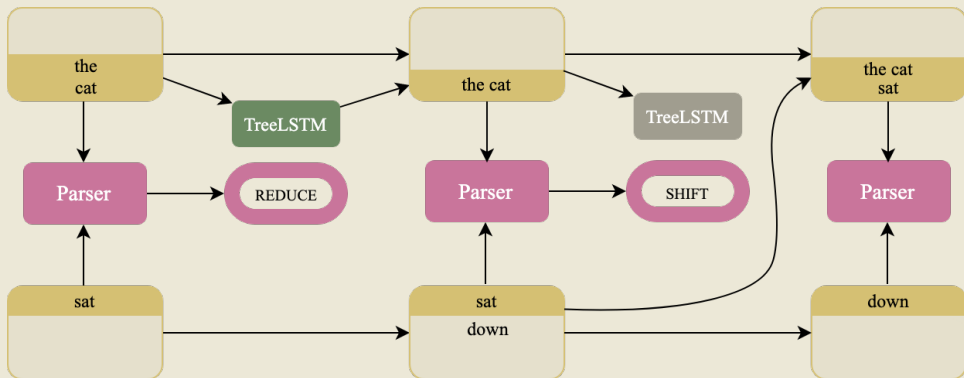
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- But we don't know \mathbf{z} !
- In this section:
we jointly learn a structured prediction model $\pi_{\theta}(\mathbf{z} \mid x)$
by optimizing the **expected loss**,

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

**But first, supervised
SPINN**

Stack-augmented Parser-Interpreter Neural-Network



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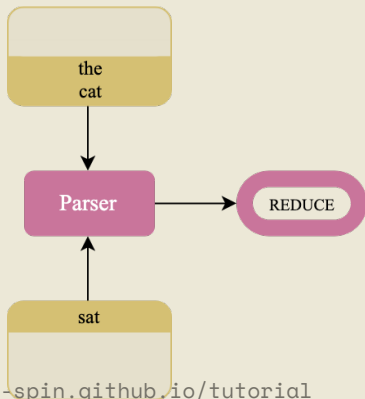
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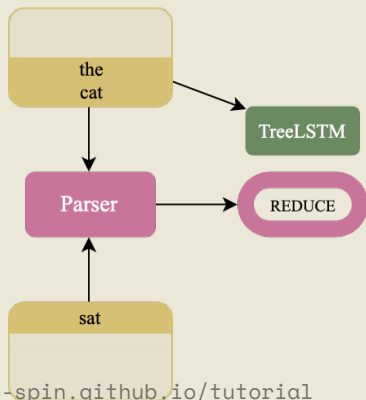
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- **TreeLSTM** combines top two elements of the stack when the parser chooses the REDUCE action.

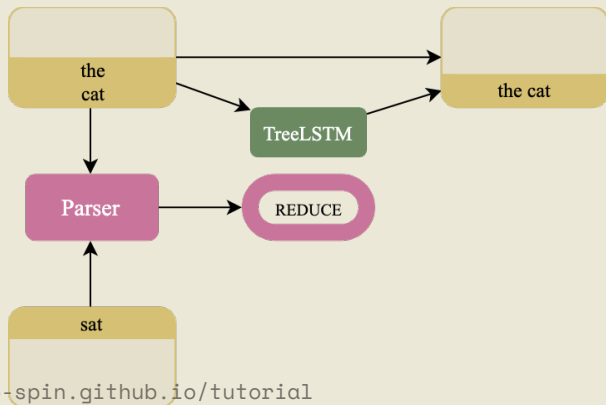
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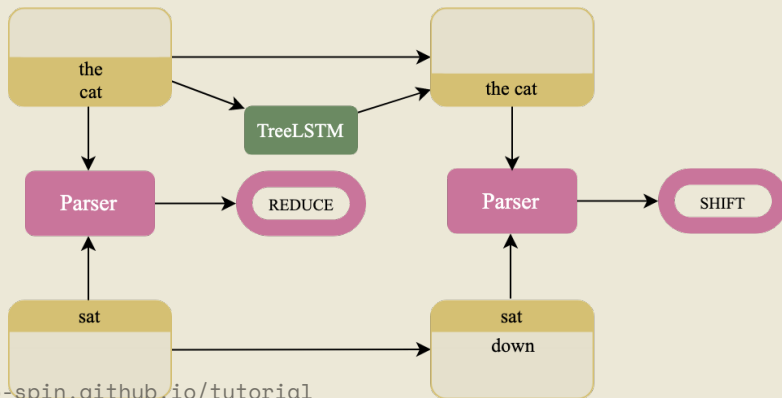
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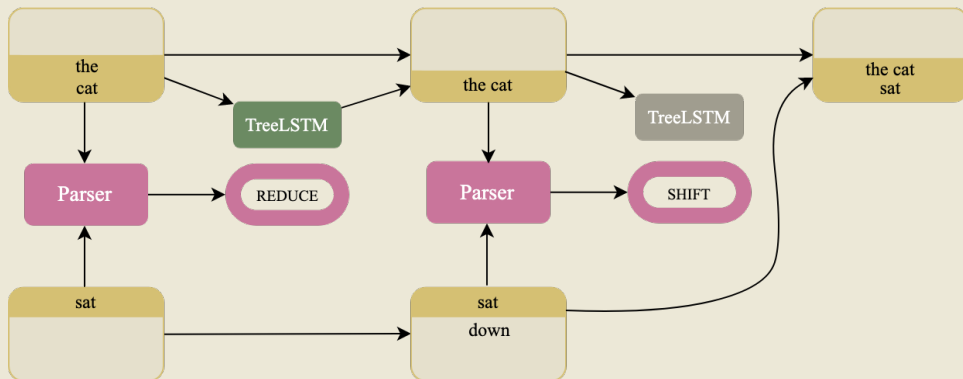
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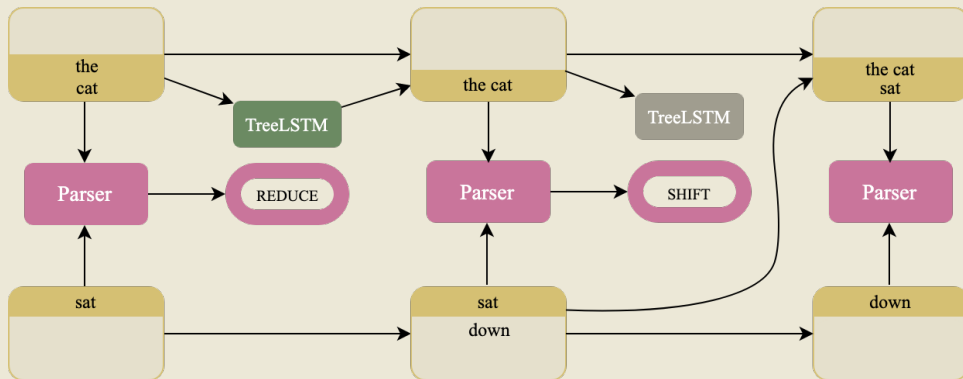
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Shift-Reduce parsing

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

$$\mathbf{z} = \{z_1, \dots, z_{2L-1}\}$$

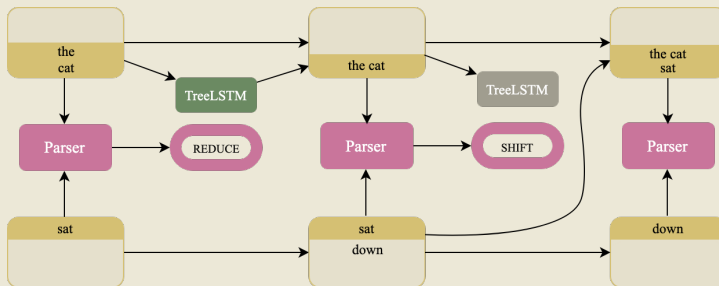
where, $z_j \in \{0, 1\} \ \forall j \in [1, 2L - 1]$

Shift-Reduce parsing

A sequence of Bernoulli trials but with conditional dependence,

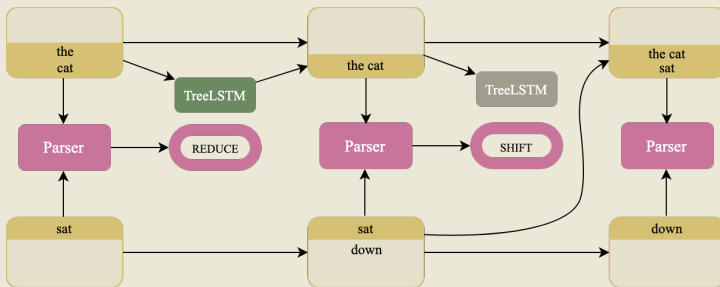
$$p(z_1, z_2, \dots, z_{2L-1}) = \prod_{j=1}^{2L-1} p(z_j \mid z_{<j})$$

Latent structure learning with SPINN



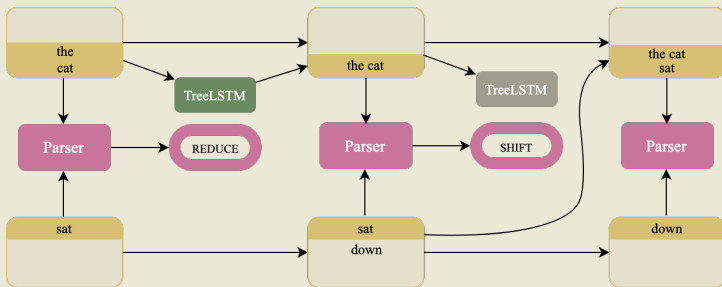
Latent structure learning with SPINN

- But now, remove syntactic supervision from SPINN.



Latent structure learning with SPINN

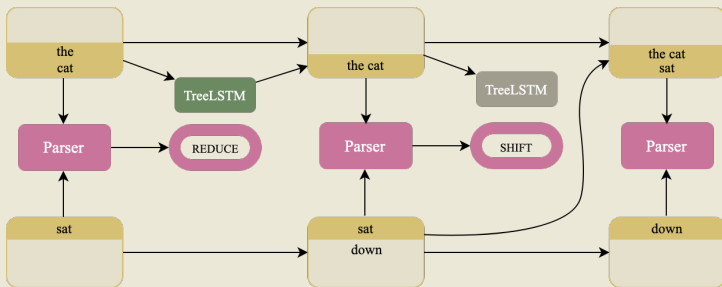
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- We model the parse, \mathbf{z} , as a latent variable with our parser as the score function estimator, $f_{\theta}(\mathbf{x})$.

Latent structure learning with SPINN

- But now, remove syntactic supervision from SPINN.



- We model the parse, \mathbf{z} , as a latent variable with our parser as the score function estimator, $f_{\theta}(\mathbf{x})$.
- 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.

SPINN with REINFORCE

Some basic terminology,

- The action space is $z_j \in \{\text{SHIFT}, \text{REDUCE}\}$, and \mathbf{z} is a sequence of actions.

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- Maximize the reward, where \mathcal{R} is performance on the downstream task like sentence classification.

SPINN with REINFORCE

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 - The state \mathbf{h} is the top two elements of the stack and the top element of the buffer
 - Learn
 - Maximize
- NOTE: Only a single reward at the end of parsing.**
- like sentence classification.

Through the looking glass of REINFORCE

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

Through the looking glass of REINFORCE

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

(By definition of expectation. How to evaluate?)

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SPINN with REINFORCE, aka RL-SPINN

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This model fails to solve a simple toy problem.

Toy problem: ListOps



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

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

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3 tokens \Rightarrow 5 trees

5 tokens \Rightarrow 42 trees

10 tokens \Rightarrow 16796 trees

High variance

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

High variance

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

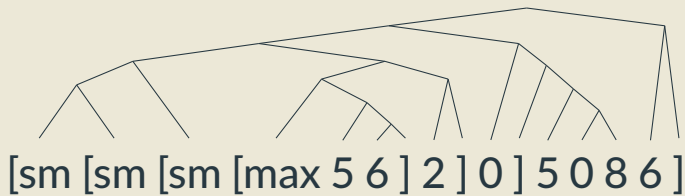


Figure: Truth: 7; Pred: 7

High variance

Sometimes it doesn't:



Figure: Truth: 6; Pred: 5

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

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Possible solutions,

1. Gradient normalization
2. Control variates, aka baselines

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Which we can do because,

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

Issues with SPINN with REINFORCE

This system faces two big problems,

1. High variance of gradients
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Coadaptation problem

Learning composition function parameters ϕ with backpropagation,
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Difference in variance of two gradient estimates.

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ma

Dif

Possible solution:

Proximal Policy Optimization (Schulman et al., 2017)

Making REINFORCE+SPINN work

Havrylov et al. [2019] use,

1. Input dependent control variate
2. Gradient normalization
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- Has not yet been very effective at learning English syntax.

III. Gradient Surrogates

So far:

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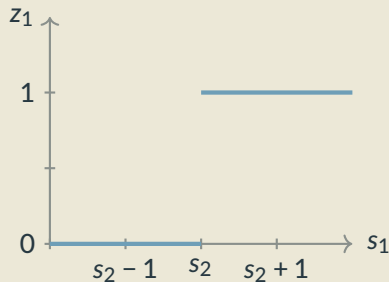
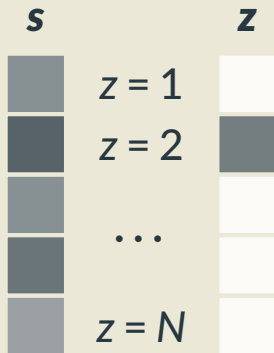
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- 3A: try to optimize the deterministic loss directly
- 3B: use this strategy to reduce variance in the stochastic model.

Recap: The argmax problem

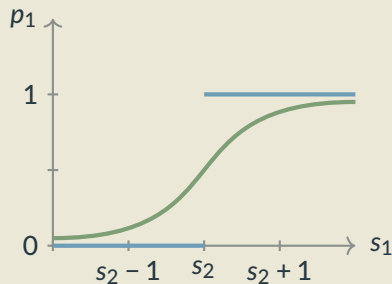
$$\mathbf{z} = \arg \max(\mathbf{s})$$



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

Softmax

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



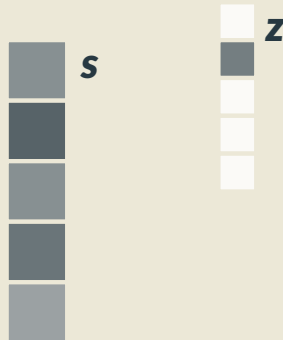
$$\frac{\partial \mathbf{p}}{\partial \mathbf{s}} = \text{diag}(\mathbf{p}) - \mathbf{p}\mathbf{p}^\top$$

Straight-Through Estimator



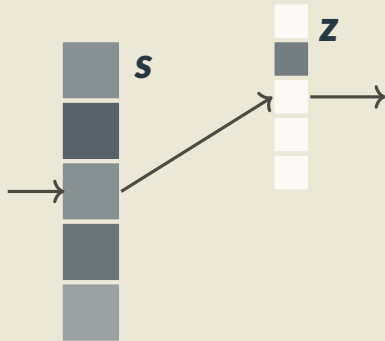
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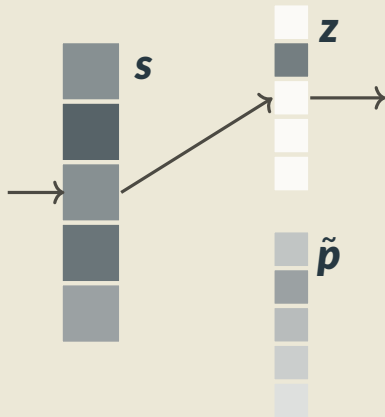
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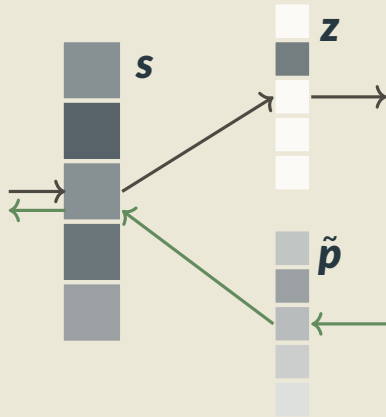
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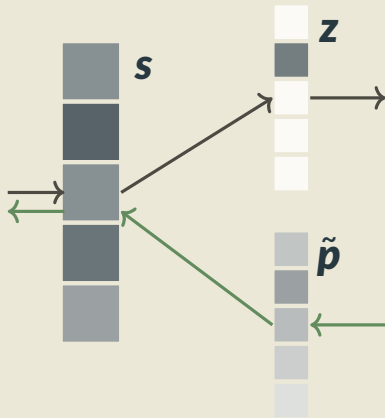
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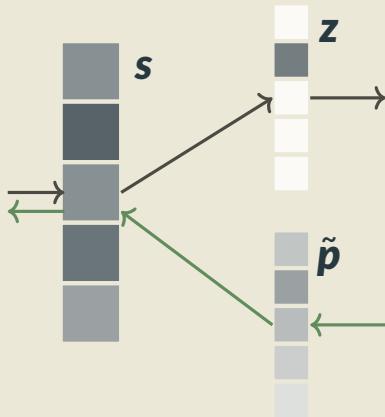
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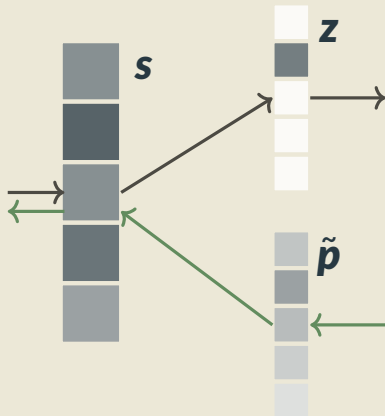
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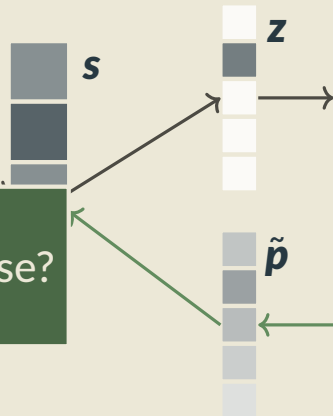
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- More explanation in a while



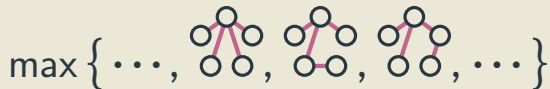
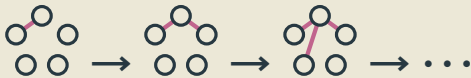
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- More explanation

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.

STE for incremental structures

STE for incremental structures

- Build a structure as a sequence of discrete choices (e.g., shift-reduce)

STE for incremental structures

- Build a structure as a sequence of discrete choices (e.g., shift-reduce)
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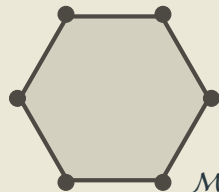
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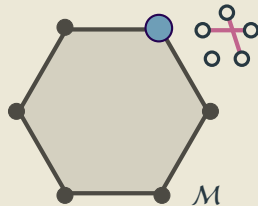
Example: Latent Tree Learning with Differentiable Parsers: Shift-Reduce Parsing and Chart Parsing [Maillard and Clark, 2018] (STE through beam search).

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



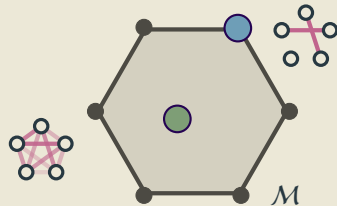
The structured case: Marginal polytope

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

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

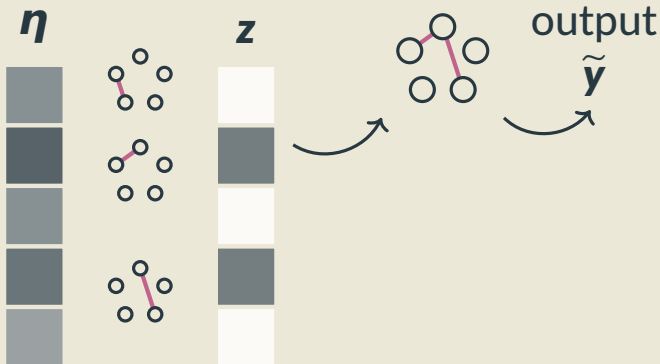
$$\begin{aligned} p_1 &= 0.2, & \mathbf{z}_1 &= [1, 0, 0, 0, 1, 0, 0, 0, 1] \\ p_2 &= 0.7, & \mathbf{z}_2 &= [0, 0, 1, 0, 0, 1, 1, 0, 0] \\ p_3 &= 0.1, & \mathbf{z}_3 &= [1, 0, 0, 0, 1, 0, 0, 1, 0] \end{aligned}$$

$$\Rightarrow \boldsymbol{\mu} = [.3, 0, .7, 0, .3, .7, .7, .1, .2].$$



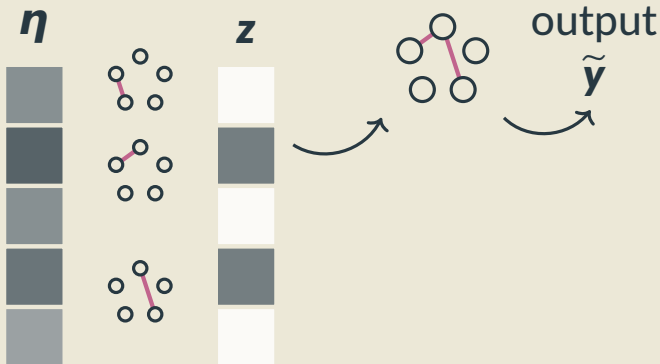
STE for factorization into parts

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



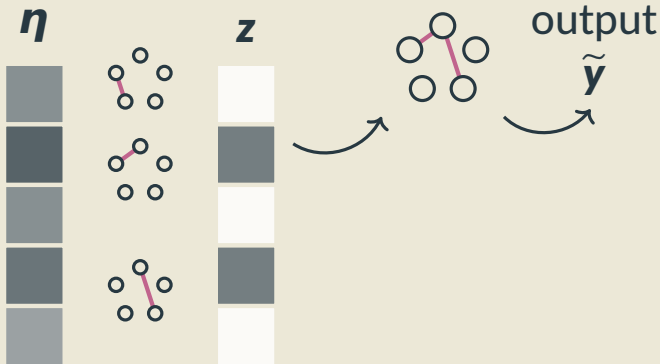
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- Backward: identity $\frac{\partial \tilde{\mu}}{\partial \eta} = I$



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]

Straight-Through Estimator

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- Structured STE: perceptron update with fake annotation

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

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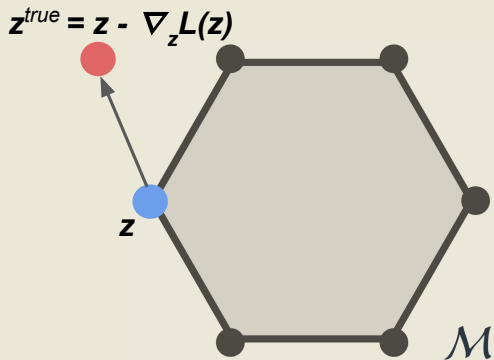
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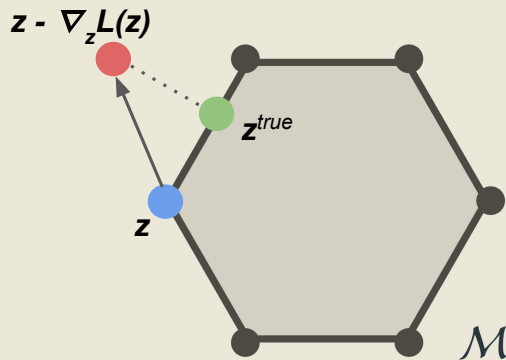
- We discuss a generic way to compute the projection in part 3.

SPIGOT vs STE

STE



SPIGOT



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Now we will see how to apply STE for stochastic graphs, as an alternative approach of the score-function estimators.

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- An alternative is using the *reparameterization trick* [Kingma and Welling, 2014].

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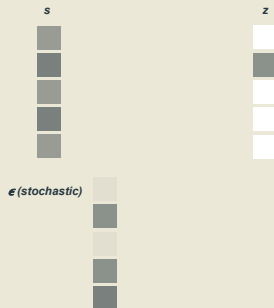


z



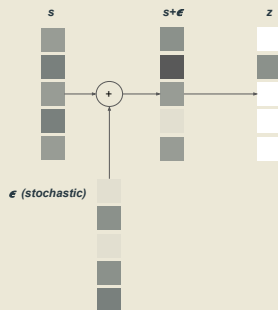
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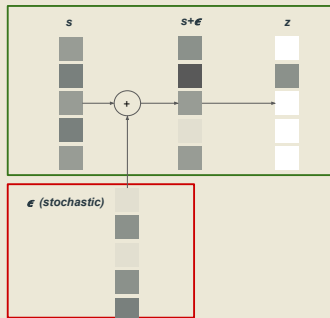
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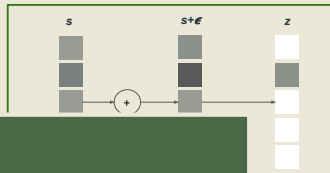


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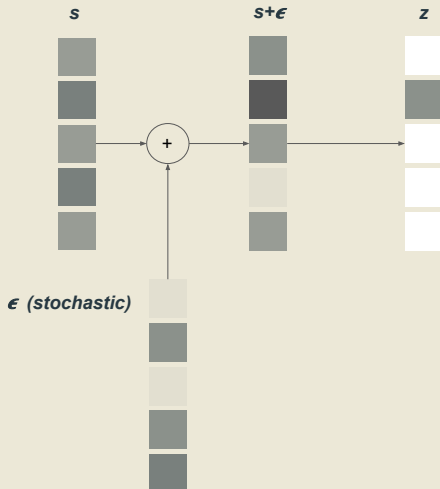
As a result:

Stochasticity is moved as an input.

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



Categorical reparameterization



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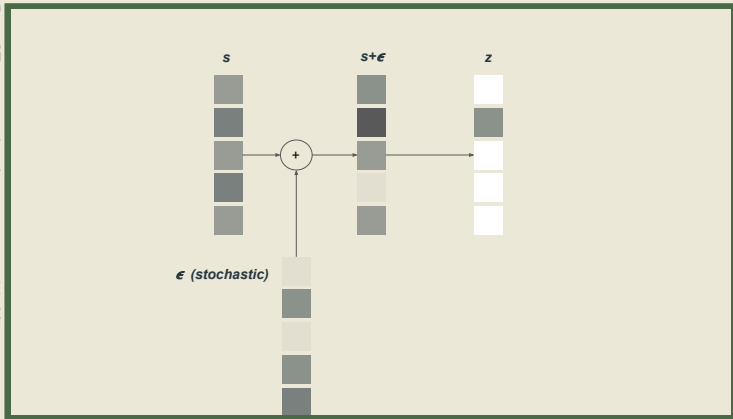
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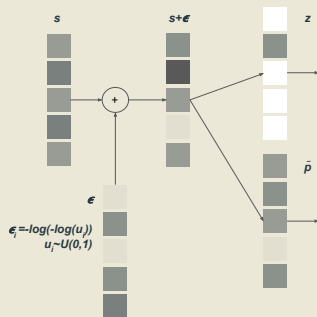


Straight-Through Gumbel Estimator

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

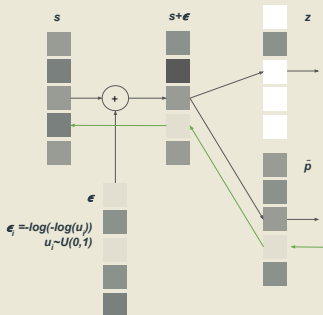
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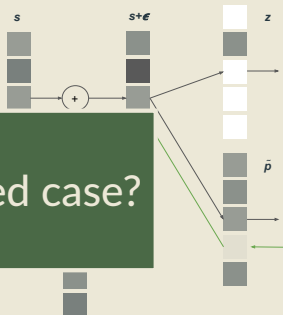
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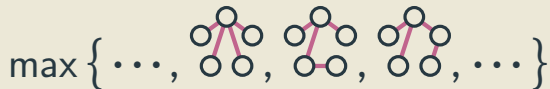
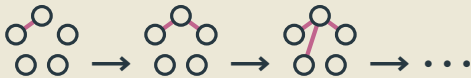
- Backward: precompute

$$\tilde{\mathbf{p}} = \text{softmax}(\mathbf{s} + \epsilon)$$

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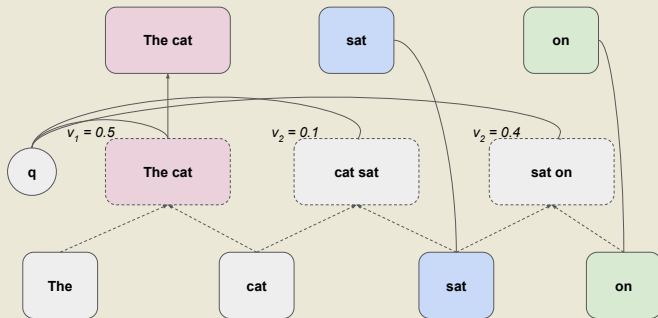
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Example: Gumbel Tree-LSTM [Choi et al., 2018].

Example: Gumbel Tree-LSTM

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



Sampling from factorized models

Perturb-and-MAP

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

- Sample from the normal Gumbel distribution.
- Perturb the arc scores with the Gumbel noise.
- Compute MAP (task-specific algorithm).
- $\epsilon \sim G(0, 1)$
- $\tilde{\eta} = \eta + \epsilon$
- $\arg \max_{\mathbf{z} \in \mathcal{Z}} \tilde{\eta}^T \mathbf{z}$

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

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

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

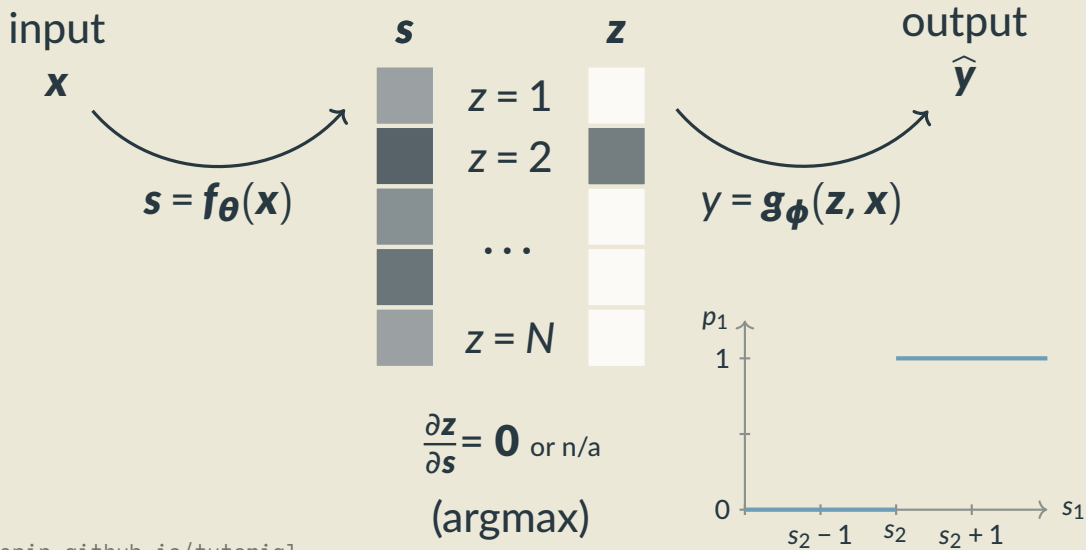
- REINFORCE
- Straight Through-Gumbel (Perturb & MAP)
- Straight Through
- SPIGOT

IV. End-to-end differentiable methods

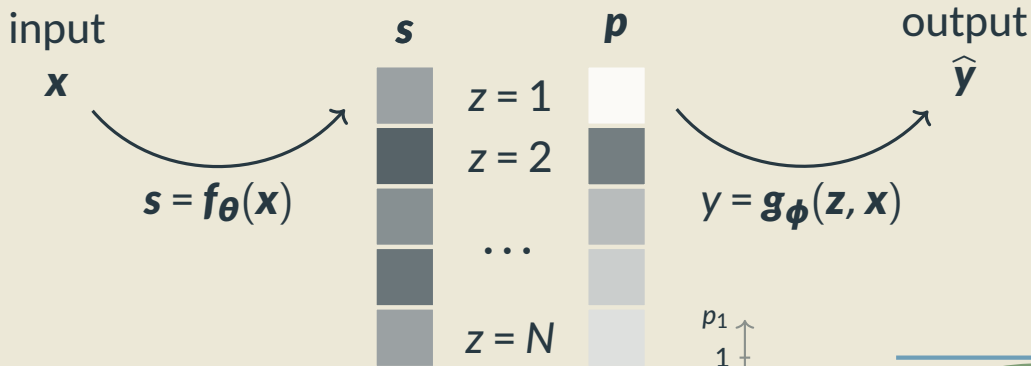
End-to-end differentiable methods

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

Recall: Discrete choices & differentiability



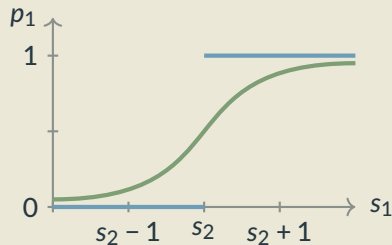
One solution: smooth relaxation



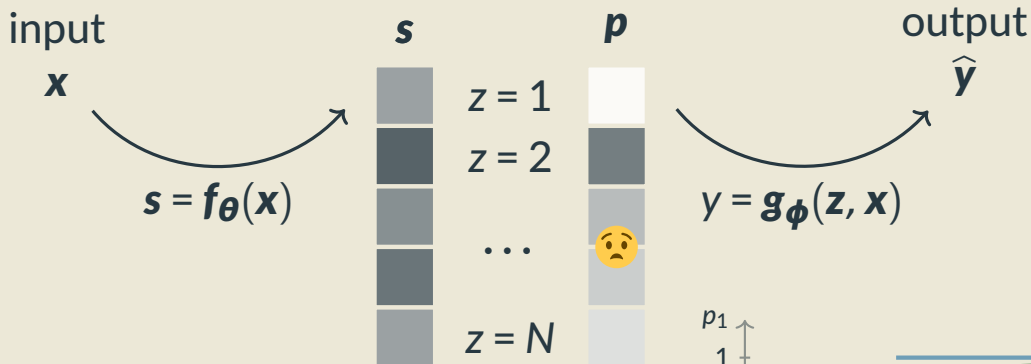
$\mathbf{p} = \text{softmax}(\mathbf{s}) = \mathbb{E}[\mathbf{z}]$, i.e.
replace $\mathbb{E}[f(\mathbf{z})]$ with $f(\mathbb{E}[\mathbf{z}])$

$$\frac{\partial \mathbf{p}}{\partial \mathbf{s}} = \text{😊}$$

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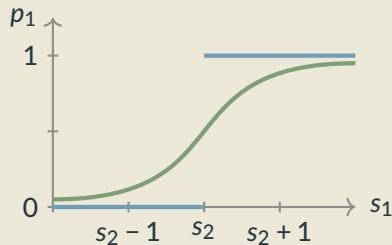


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Overview

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

- REINFORCE
 - Straight Through–Gumbel (Perturb & MAP)
 - SparseMAP
-
- $\text{dom } L$ may be only \mathcal{Z} ,
 - $\nabla_{\mathbf{z}} L$ need not exist!

$$L(\arg \max_{\mathbf{z}} \pi_{\theta}(\mathbf{z} | x))$$

- Straight Through
- SPIGOT

Model restrictions:

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

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

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

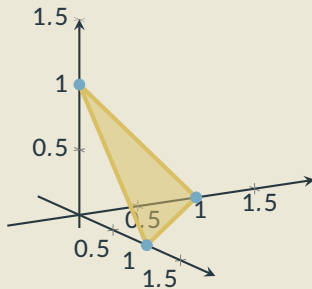
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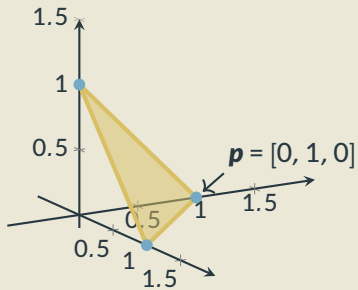
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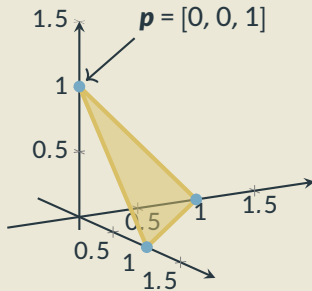
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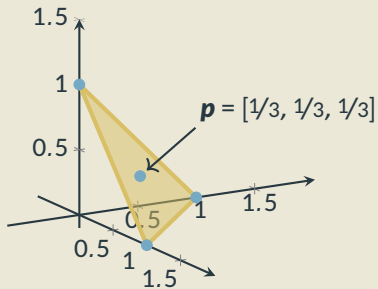
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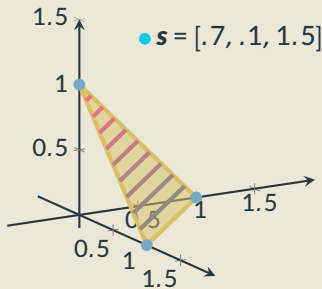


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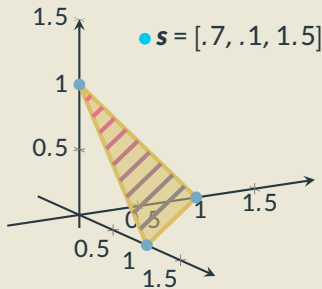
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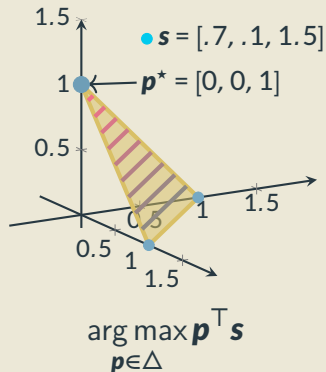
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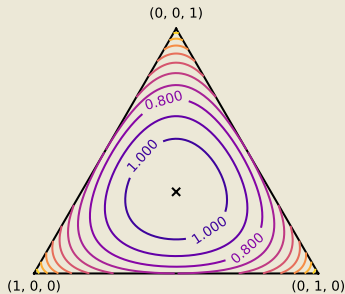
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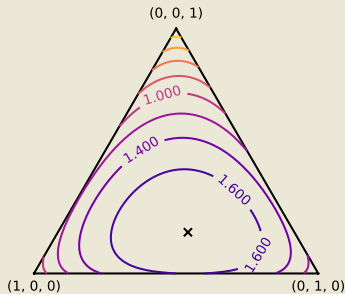
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softmax maximizes **expected score + entropy**:



$$\arg \max_{\mathbf{p} \in \Delta} \mathbf{p}^\top \mathbf{s} + H(\mathbf{p})$$

Variational form of softmax

Proposition. The unique solution to $\arg \max_{\mathbf{p} \in \Delta} \mathbf{p}^\top \mathbf{s} + H(\mathbf{p})$ is given by $p_j = \frac{\exp s_j}{\sum_i \exp s_i}$.

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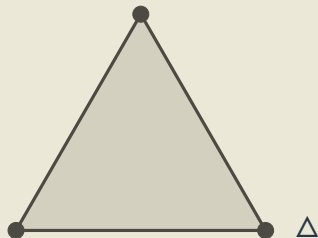
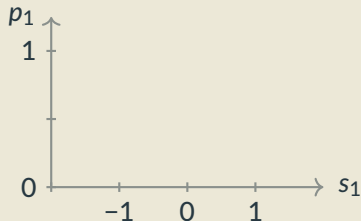
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$$\text{So, } p_i = \frac{\exp(s_i)}{\sum_j \exp(s_j)}.$$

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

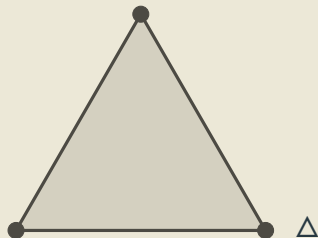
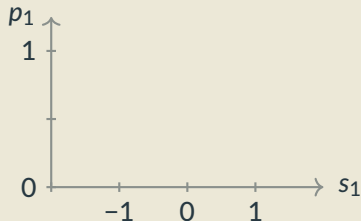
Generalizing softmax: Smoothed argmaxes

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



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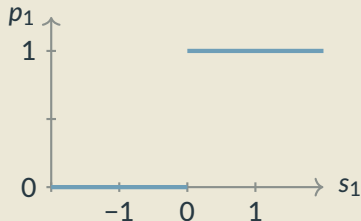
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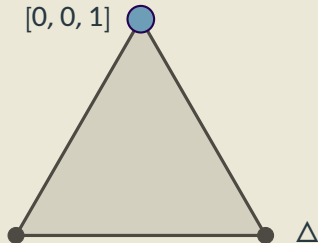
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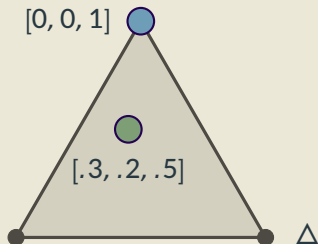
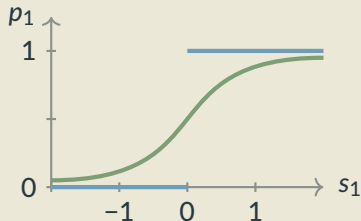
$[0, 0, 1]$



Generalizing softmax: Smoothed argmaxes

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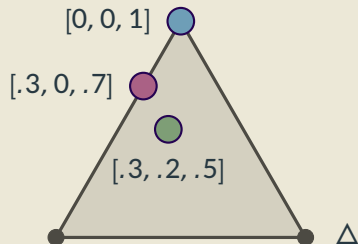
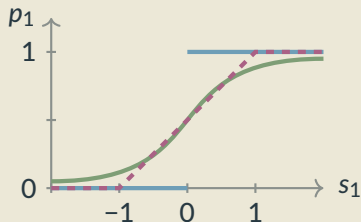
- argmax: $\Omega(\mathbf{p}) = 0$
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Generalizing softmax: Smoothed argmaxes

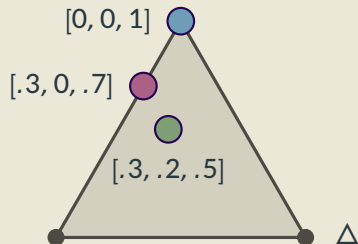
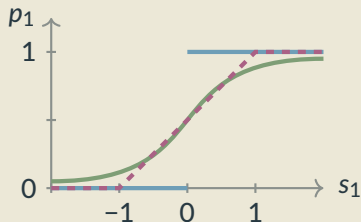
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- α -entmax: $\Omega(\mathbf{p}) = 1/\alpha(\alpha-1) \sum_j p_j^{\alpha}$

Generalized entropy interpolates in between [Tsallis, 1988]

Used in Sparse Seq2Seq: [Peters et al., 2019]

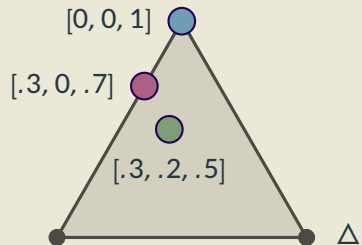
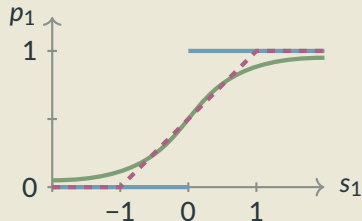
(Mon 13:50, poster session 2D)



Generalizing softmax: Smoothed argmaxes

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- fusedmax: $\Omega(\mathbf{p}) = 1/2 \|\mathbf{p}\|_2^2 + \sum_j |p_j - p_{j-1}|$
- csparsesmax: $\Omega(\mathbf{p}) = 1/2 \|\mathbf{p}\|_2^2 + \iota(\mathbf{a} \leq \mathbf{p} \leq \mathbf{b})$
- csoftmax: $\Omega(\mathbf{p}) = \sum_j p_j \log p_j + \iota(\mathbf{a} \leq \mathbf{p} \leq \mathbf{b})$



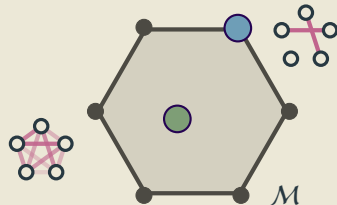
The structured case: Marginal polytope

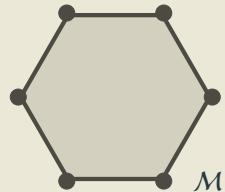
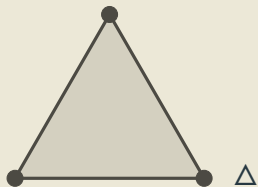
- Each vertex corresponds to one such *bit* vector \mathbf{z}
- Points inside correspond to *marginal distributions*: convex combinations of structured objects

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

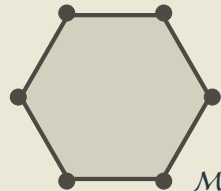
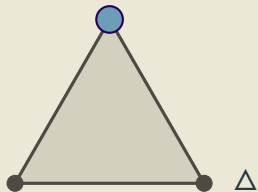
$$\begin{aligned} p_1 &= 0.2, & \mathbf{z}_1 &= [1, 0, 0, 0, 1, 0, 0, 0, 1] \\ p_2 &= 0.7, & \mathbf{z}_2 &= [0, 0, 1, 0, 0, 1, 1, 0, 0] \\ p_3 &= 0.1, & \mathbf{z}_3 &= [1, 0, 0, 0, 1, 0, 0, 1, 0] \end{aligned}$$

$$\Rightarrow \boldsymbol{\mu} = [.3, 0, .7, 0, .3, .7, .7, .1, .2].$$

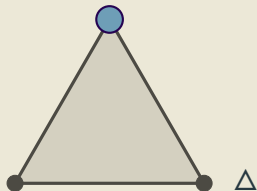




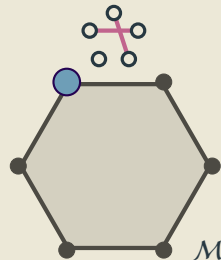
- $\operatorname{argmax}_{\mathbf{p} \in \Delta} \operatorname{argmax} \mathbf{p}^T \mathbf{s}$



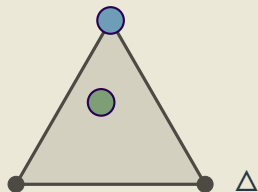
• **argmax** $\arg \max_{\mathbf{p} \in \Delta} \mathbf{p}^T \mathbf{s}$



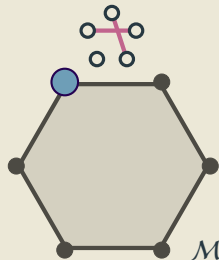
• **MAP** $\arg \max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^T \boldsymbol{\eta}$



- **argmax** $\arg \max_{\mathbf{p} \in \Delta} \mathbf{p}^T \mathbf{s}$
- **softmax** $\arg \max_{\mathbf{p} \in \Delta} \mathbf{p}^T \mathbf{s} + H(\mathbf{p})$

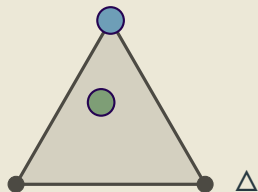


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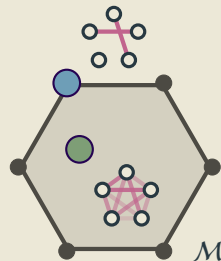
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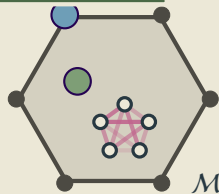
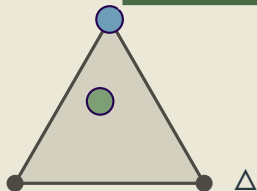
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Just like softmax relaxes argmax,
marginals relax MAP **differentiably!**



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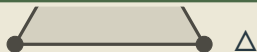
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Unlike argmax/softmax, computation is not obvious!



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

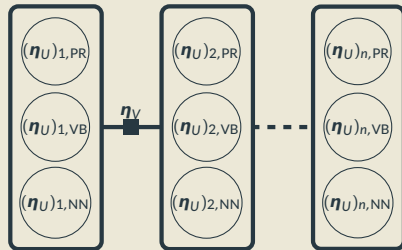
Dynamic programming: marginals by **Forward-Backward, Inside-Outside**, etc.

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Marginals in a sequence tagging model.

```
1 input:  $d$  tags,  $n$  tokens,  $\boldsymbol{\eta}_U \in \mathbb{R}^{n \times d}$ ,  $\boldsymbol{\eta}_V \in \mathbb{R}^{d \times d}$ 
2 initialize  $\boldsymbol{\alpha}_1 = \mathbf{0}$ ,  $\boldsymbol{\beta}_n = \mathbf{0}$ 
3 for  $i \in 2, \dots, n$  do                                # forward log-probabilities
4    $\alpha_{i,k} = \log \sum_{k'} \exp(\alpha_{i-1,k'} + (\boldsymbol{\eta}_U)_{i,k} + (\boldsymbol{\eta}_V)_{k',k})$  for all  $k$ 
5 for  $i \in n-1, \dots, 1$  do                                # backward log-probabilities
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7  $Z = \sum_k \exp \alpha_{n,k}$                                     # partition function
8 return  $\boldsymbol{\mu} = \exp(\boldsymbol{\alpha} + \boldsymbol{\beta} - \log Z)$                 # marginals
```



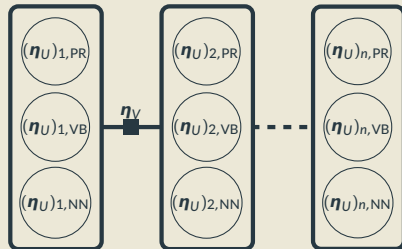
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- Alg. consists of differentiable ops: PyTorch autograd can handle it! (v. bad idea)

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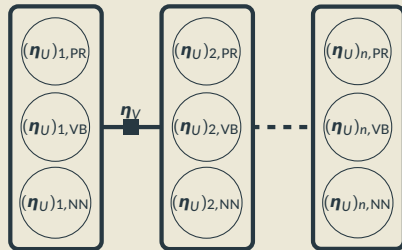
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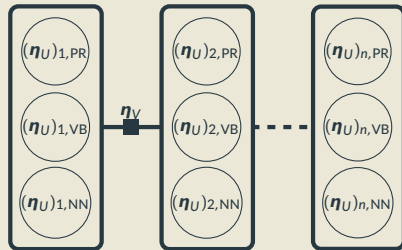
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- With circular dependencies, this breaks! Can get an approximation Stoyanov et al. [2011]

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Derivatives of marginals 2: Matrix-Tree

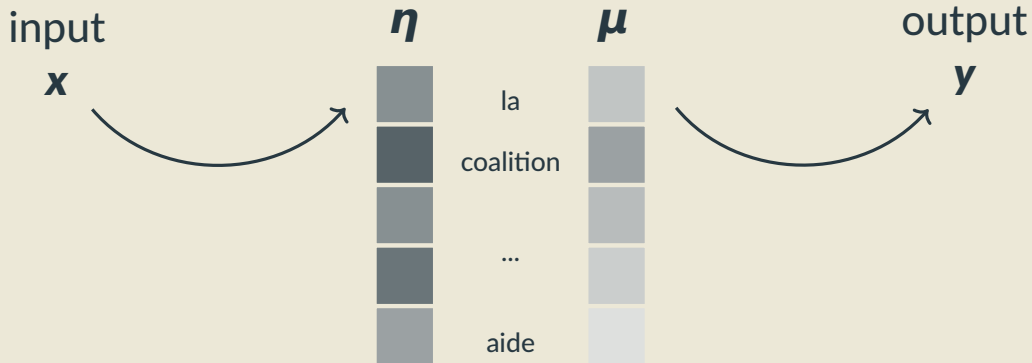
$\mathbf{L}(\mathbf{s})$: Laplacian of the edge score graph

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

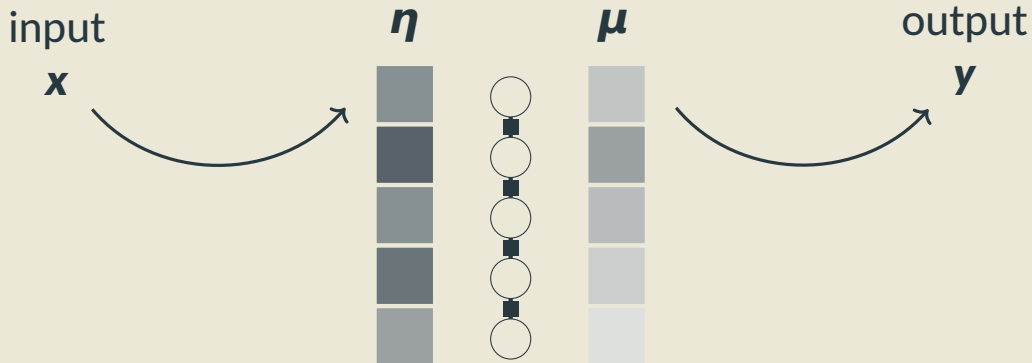
$$\boldsymbol{\mu} = \mathbf{L}(\mathbf{s})^{-1}$$

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

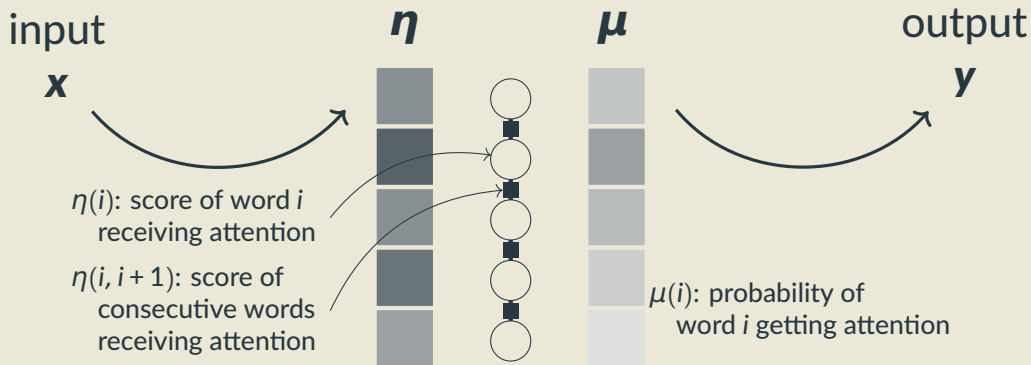
Structured Attention Networks



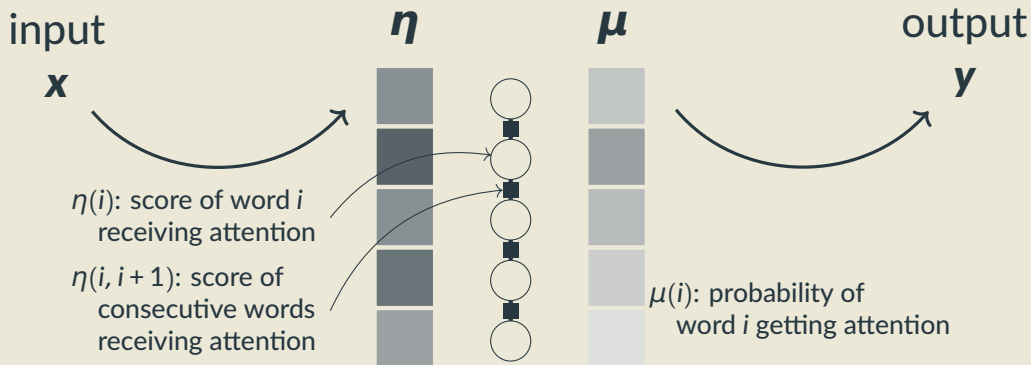
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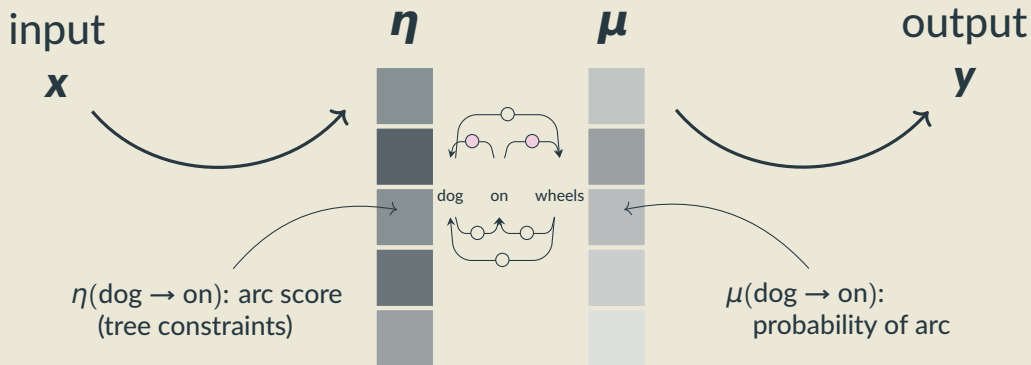


Structured Attention Networks



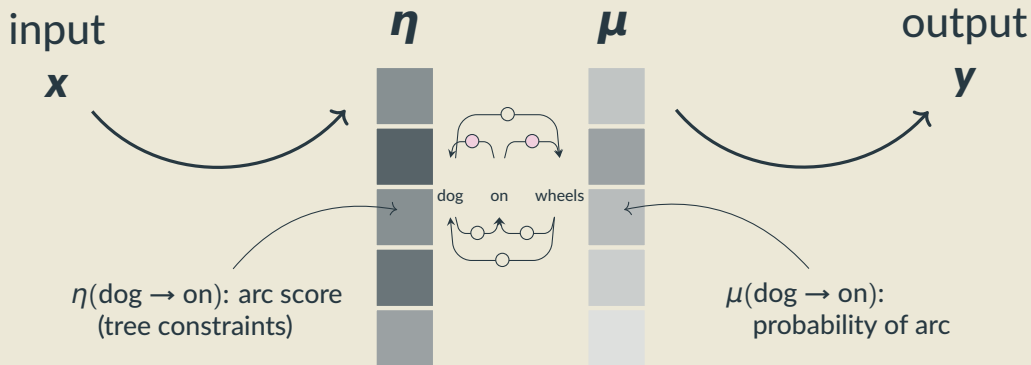
CRF marginals (from *forward-backward*) give attention weights $\in (0, 1)$

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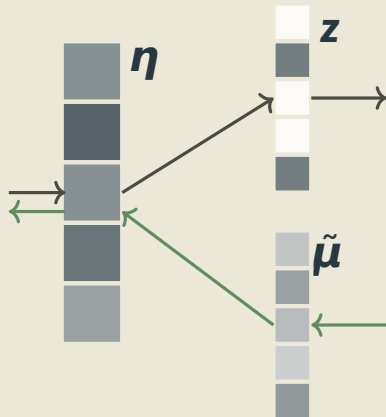
CRF marginals (from *forward-backward*) give attention weights $\in (0, 1)$
 Similar idea for projective dependency trees with *inside-outside*
 and non-projective with the Matrix-Tree theorem [Liu and Lapata, 2018].

Differentiable Perturb & Parse

Extending Gumbel-Softmax to structured stochastic models

- Forward pass:
sample structure \mathbf{z} (approximately)
$$\mathbf{z} = \arg \max_{\mathbf{z} \in \mathcal{Z}} (\boldsymbol{\eta} + \boldsymbol{\epsilon})^\top \mathbf{z}$$
- Backward pass:
pretend we did marginal inference
$$\tilde{\boldsymbol{\mu}} = \arg \max_{\boldsymbol{\mu} \in \mathcal{M}} (\boldsymbol{\eta} + \boldsymbol{\epsilon})^\top \mathbf{z} + \tilde{H}(\boldsymbol{\mu})$$

(or some similar relaxation)



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- (Structured Attention Net

Cons:

- (Structured Attention Net (fixed by Perturb & MA
- Efficient & numerically stable (somewhat alleviated b
- Not applicable when mar
- Case-by-case algorithms

```

procedure BACKPROPINSIDEOUTSIDE( $\theta, p, \nabla_p^T$ )
  for  $s, t = 1, \dots, n, s \neq t$  do  $\triangleright$  Backpropagation uses the identity  $\nabla_p^T = (p \odot \nabla_p^T) / \nabla_p^{T+P}$ 
     $d[s, t] \leftarrow \log p[s, t] \odot \log \nabla_p^T[s, t]$   $\triangleright d = \log(p \odot \nabla_p^T)$ 
     $\nabla_p^T, \nabla_p^T \leftarrow \log \nabla_p^T \leftarrow -\infty$   $\triangleright$  Initialize inside ( $\nabla_p^T$ ), outside ( $\nabla_p^T$ ) gradients, and log of  $\nabla_p^T$ 
    for  $s = 1, \dots, n - 1$  do  $\triangleright$  Backpropagate  $d$  to  $\nabla_p^T$  and  $\nabla_p^T$ 
      for  $t = s + 1, \dots, n$  do
         $\nabla_p^T[s, t, R, 0], \nabla_p^T[s, t, R, 1] \leftarrow d[s, t]$ 
         $\nabla_p^T[1, n, R, 1] \leftarrow -d[s, t]$ 
        if  $s > 1$  then
           $\nabla_p^T[s, t, L, 0], \nabla_p^T[s, t, L, 1] \leftarrow -d[s, t]$ 
           $\nabla_p^T[1, n, R, 1] \leftarrow -d[s, t]$ 
        for  $k = 1, \dots, n$  do  $\triangleright$  Backpropagate through outside vsp
          for  $s = 1, \dots, n - k$  do
             $t \leftarrow s + k$ 
             $v \leftarrow \nabla_p^T[s, t, R, 0] \odot \beta[s, t, R, 0]$   $\triangleright v, \gamma$  are temporary values
            for  $u = 1, \dots, n$  do
               $\nabla_p^T[s, u, R, 1], \nabla_p^T[s, u, R, 1] \leftarrow v \odot \beta[s, u, R, 1] \odot \alpha[t, u, R, 1]$ 
            if  $s > 1$  then
               $v \leftarrow \nabla_p^T[s, t, L, 0] \odot \beta[s, t, L, 0]$ 
              for  $u = 1, \dots, s$  do
                 $\nabla_p^T[s, t, L, 1], \nabla_p^T[s, s, L, 1] \leftarrow v \odot \beta[s, t, L, 1] \odot \alpha[u, s, L, 1]$ 
               $v \leftarrow \nabla_p^T[s, t, L, 1] \odot \beta[s, t, L, 1]$ 
              for  $u = 1, \dots, n$  do
                 $\nabla_p^T[s, u, L, 1], \nabla_p^T[u, L, 0] \leftarrow v \odot \beta[s, u, L, 1] \odot \alpha[u, s, L, 1]$ 
            for  $u = 1, \dots, s - 1$  do
               $\gamma \leftarrow \beta[s, t, R, 0] \odot \alpha[u, s - 1, R, 1] \odot \theta_{s,t}$ 
               $\nabla_p^T[s, t, R, 0], \nabla_p^T[u, s - 1, R, 1], \log \nabla_p^T[u, t] \leftarrow v \odot \gamma$ 
               $\gamma \leftarrow \beta[s, t, L, 0] \odot \alpha[u, s - 1, L, 1] \odot \theta_{s,t}$ 
               $\nabla_p^T[s, t, L, 0], \nabla_p^T[u, s - 1, L, 1], \log \nabla_p^T[u, t] \leftarrow v \odot \gamma$ 
             $v \leftarrow \nabla_p^T[s, t, R, 1] \odot \beta[s, t, R, 1]$ 
            for  $u = 1, \dots, s$  do
               $\nabla_p^T[s, t, R, 1], \nabla_p^T[s, u, R, 0] \leftarrow v \odot \beta[s, t, R, 1] \odot \alpha[u, s, R, 0]$ 
            for  $u = t + 1, \dots, n$  do
               $\gamma \leftarrow \beta[s, u, R, 0] \odot \alpha[t + 1, u, L, 1] \odot \theta_{s,t}$ 
               $\nabla_p^T[s, u, R, 0], \nabla_p^T[t + 1, u, L, 1], \log \nabla_p^T[s, u] \leftarrow v \odot \gamma$ 
               $\gamma \leftarrow \beta[s, u, L, 0] \odot \alpha[t + 1, u, L, 1] \odot \theta_{s,t}$ 
               $\nabla_p^T[s, u, L, 0], \nabla_p^T[t + 1, u, L, 1], \log \nabla_p^T[s, u] \leftarrow v \odot \gamma$ 
          for  $k = n, \dots, 1$  do  $\triangleright$  Backpropagate through inside vsp
            for  $s = 1, \dots, n - k$  do
               $t \leftarrow s + k$ 
               $v \leftarrow \nabla_p^T[s, t, R, 1] \odot \alpha[s, t, R, 1]$ 
              for  $u = s + 1, \dots, t$  do
                 $\nabla_p^T[s, t, R, 0], \nabla_p^T[s, t, R, 1] \leftarrow v \odot \alpha[s, u, R, 0] \odot \alpha[s, t, R, 1]$ 
              if  $s > 1$  then
                 $v \leftarrow \nabla_p^T[s, t, L, 1] \odot \alpha[s, t, L, 1]$ 
                for  $u = s, \dots, t - 1$  do
                   $\nabla_p^T[s, u, L, 1], \nabla_p^T[s, t, L, 0] \leftarrow v \odot \alpha[s, u, L, 1] \odot \alpha[s, t, L, 0]$ 
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                for  $u = s, \dots, t - 1$  do
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                   $\nabla_p^T[s, u, R, 1], \nabla_p^T[s + 1, t, L, 1], \log \nabla_p^T[s, t] \leftarrow v \odot \gamma$ 
              return sign exp log  $\nabla_p^T$   $\triangleright$  Exponentiate log gradient, multiply by sign, and return  $\nabla_p^T$ 

```

Figure 7: Backpropagation through the inside-outside algorithm to calculate the gradient with respect to the input potentials. ∇_p^T denotes the Jacobian of α with respect to θ (∇_p^T is the gradient with respect to θ). $\alpha, \beta \leftarrow \infty$ means $\alpha = \alpha \odot \infty$ and $\beta = \beta \odot \infty$.

xact.

inals are dense;
nation)

ugh DPs is tricky;

Back-propagating through marginals

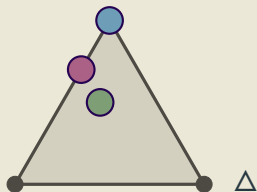
Pros:

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

Cons:

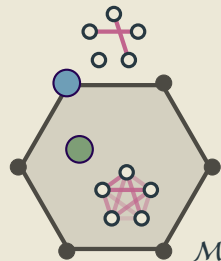
- (Structured Attention Networks:) forward pass marginals are dense;
(fixed by Perturb & MAP, at cost of rough approximation)
- Efficient & numerically stable back-propagation through DPs is tricky;
(somewhat alleviated by [Mensch and Blondel, 2018])
- Not applicable when marginals are unavailable.
-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

- **argmax** $\arg \max_{\mathbf{p} \in \Delta} \mathbf{p}^T \mathbf{s}$
- **softmax** $\arg \max_{\mathbf{p} \in \Delta} \mathbf{p}^T \mathbf{s} + H(\mathbf{p})$
- **sparsemax** $\arg \max_{\mathbf{p} \in \Delta} \mathbf{p}^T \mathbf{s} - 1/2 \|\mathbf{p}\|^2$

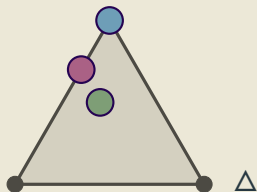


● **MAP** $\arg \max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^T \boldsymbol{\eta}$

● **marginals** $\arg \max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^T \boldsymbol{\eta} + \tilde{H}(\boldsymbol{\mu})$



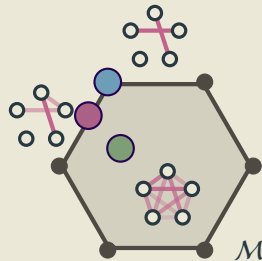
- **argmax** $\arg \max_{\mathbf{p} \in \Delta} \mathbf{p}^T \mathbf{s}$
- **softmax** $\arg \max_{\mathbf{p} \in \Delta} \mathbf{p}^T \mathbf{s} + H(\mathbf{p})$
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- **MAP** $\arg \max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^T \boldsymbol{\eta}$

- **marginals** $\arg \max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^T \boldsymbol{\eta} + \tilde{H}(\boldsymbol{\mu})$

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



SparseMAP solution

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

$$= \begin{array}{c} \circ \quad \circ \\ \diagup \quad \diagdown \\ \circ \quad \circ \end{array} = .6 \begin{array}{c} \circ \quad \circ \\ \diagup \quad \diagdown \\ \circ \quad \circ \end{array} + .4 \begin{array}{c} \circ \quad \circ \\ \diagup \quad \diagdown \\ \circ \quad \circ \end{array}$$

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

Algorithms for SparseMAP

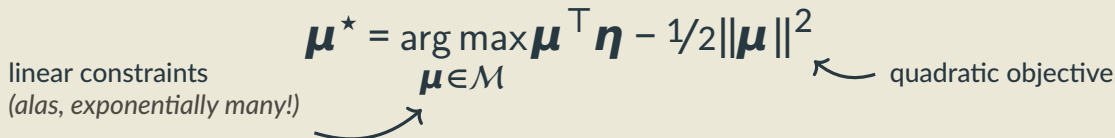
$$\boldsymbol{\mu}^{\star} = \arg \max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^{\top} \boldsymbol{\eta} - 1/2 \|\boldsymbol{\mu}\|^2$$

Algorithms for SparseMAP

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

linear constraints
(*alas, exponentially many!*)

quadratic objective

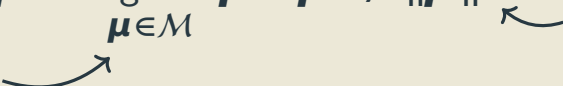


Algorithms for SparseMAP

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

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quadratic objective



Conditional Gradient

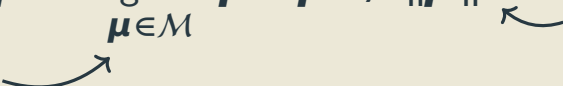
[Frank and Wolfe, 1956, Lacoste-Julien and Jaggi, 2015]

Algorithms for SparseMAP

linear constraints
(*alas, exponentially many!*)

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

quadratic objective



Conditional Gradient

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

- select a new corner of \mathcal{M}

Algorithms for SparseMAP

linear constraints
(*alas, exponentially many!*)

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

quadratic objective

Conditional Gradient

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

- select a new corner of \mathcal{M}

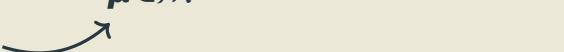
$$\arg \max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \underbrace{(\boldsymbol{\eta} - \boldsymbol{\mu}^{(t-1)})}_{\tilde{\boldsymbol{\eta}}}$$

Algorithms for SparseMAP

linear constraints
(*alas, exponentially many!*)

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

quadratic objective



Conditional Gradient

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

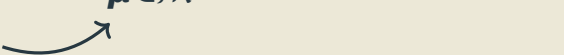
- select a new corner of \mathcal{M}
- update the (sparse) coefficients of \boldsymbol{p}
 - Update rules: vanilla, away-step, pairwise

Algorithms for SparseMAP

linear constraints
(*alas, exponentially many!*)

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

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Conditional Gradient

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

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

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

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

Vinyes and Obozinski, 2017]

Algorithms for SparseMAP

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

linear constraints
(*alas, exponentially many!*)

quadratic objective

Conditional Gradient

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

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

Active Set achieves
finite & linear convergence!

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

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

Vinyes and Obozinski, 2017]

Algorithms for SparseMAP

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

linear constraints
(*alas, exponentially many!*)

quadratic objective

Conditional Gradient

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

- select a new corner of \mathcal{M}
- update the (sparse) coefficients of p
 - Update rules: vanilla, away-step, pairwise
 - Quadratic objective: **Active Set**
a.k.a. Min-Norm Point, [Wolfe, 1976]

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

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Backward pass

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

Algorithms for SparseMAP

linear constraints
(*alas, exponentially many!*)

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

quadratic objective

Conditional Gradient

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

- select a new corner of \mathcal{M}
- update the (sparse) coefficients of \mathbf{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,

Vinyes and Obozinski, 2017]

Backward pass

$\frac{\partial \boldsymbol{\mu}}{\partial \boldsymbol{\eta}}$ is sparse
computing $\left(\frac{\partial \boldsymbol{\mu}}{\partial \boldsymbol{\eta}}\right)^\top d\mathbf{y}$
takes $\mathcal{O}(\dim(\boldsymbol{\mu}) \text{nnz}(\mathbf{p}^*))$

Algorithms for SparseMAP

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

linear constraints
(*alas, exponentially many!*)

quadratic objective

Condition

pass

Completely modular: just add MAP

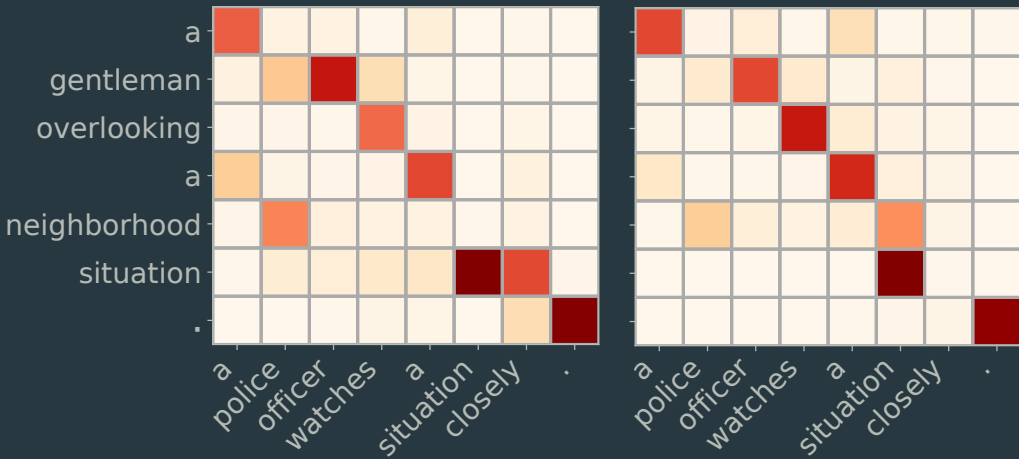
[Frank and Wolfe, 1956]

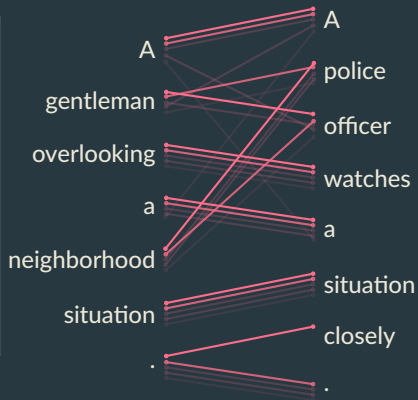
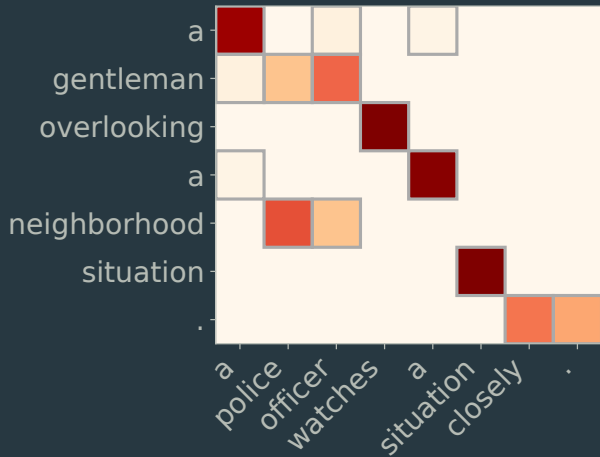
- select a new candidate \mathbf{c}
- update the (sparse) coefficients or \mathbf{p}
 - Update rules: vanilla, away-step, pairwise
 - Quadratic objective: **Active Set**
a.k.a. Min-Norm Point, [Wolfe, 1976]

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

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computing $\left(\frac{\partial \boldsymbol{\mu}}{\partial \boldsymbol{\eta}}\right)^\top d\boldsymbol{\eta}$
takes $\mathcal{O}(\dim(\boldsymbol{\mu}) \text{nnz}(\mathbf{p}^*))$





Overview

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

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

$$L(\arg \max_{\mathbf{z}} \pi_{\theta}(\mathbf{z} | x))$$

- Straight Through
- SPIGOT

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

- Structured Attn. Nets
- SparseMAP

Overview

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

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Model restrictions:

- $\text{dom } L$ may be only \mathcal{Z} ,
- $\nabla_{\mathbf{z}} L$ need not exist!
- $L(\mathbf{z})$ with $\mathbf{z} \in \mathcal{Z}$ in forward
- needs (relaxed) $\nabla_{\mathbf{z}} L$ in backward.
- $L(\mathbf{z})$ must be relaxed and differentiable.
- (sparsity gets us closer to \mathcal{Z}).

Structured latent variables without sampling

$$\mathbb{E}_{\mathbf{z}}[L(\mathbf{z})] = \sum_{\mathbf{z} \in \mathcal{Z}} L(\hat{\mathbf{y}}(\mathbf{z})) \pi(\mathbf{z} | \mathbf{x})$$

Structured latent variables without sampling

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

Structured latent variables without sampling

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

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

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

Structured latent variables without sampling

sum over
all possible trees

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

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

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

Exponentially large sum!

Structured latent variables without sampling

sum over
all possible trees

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

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

How to define π_{θ} ?

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

idea 1

idea 2

idea 3

Structured latent variables without sampling

sum over
all possible trees

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

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

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

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

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

idea 1

idea 2

idea 3

Structured latent variables without sampling

sum over
all possible trees

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

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

How to define π_{θ} ?

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

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

idea 1

idea 2

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Structured latent variables without sampling

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

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

How to define π_{θ} ?

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

idea 1 $\pi_{\theta}(\mathbf{z}) \propto \exp(f_{\theta}(\mathbf{z}))$

softmax

idea 2

idea 3

Structured latent variables without sampling

sum over
all possible trees


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

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

How to define π_{θ} ?

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Structured latent variables without sampling

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

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

How to define π_{θ} ?

parsing model,
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idea 2

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softmax



Structured latent variables without sampling

sum over
all possible trees

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

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

How to define π_{θ} ?

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

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

idea 2

idea 3

Structured latent variables without sampling

sum over
all possible trees



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

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

How to define π_{θ} ?

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

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

idea 1 $\pi_{\theta}(\mathbf{z}) \propto \exp(f_{\theta}(\mathbf{z}))$

softmax

idea 2 $\pi_{\theta}(\mathbf{z}) = 1$ if $\mathbf{z} = \text{MAP}(f_{\theta}(\cdot))$ else 0

argmax

idea 3

Structured latent variables without sampling

sum over
all possible trees

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

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

How to define π_{θ} ?

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

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

idea 1 $\pi_{\theta}(\mathbf{z}) \propto \exp(f_{\theta}(\mathbf{z}))$

softmax



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

$$\frac{\partial \mathbb{E}[L(\mathbf{z})]}{\partial \theta}$$

idea 1 $\pi_{\theta}(\cdot)$

idea 2 $\pi_{\theta}(\mathbf{z}) = 1$ if $\mathbf{z} = \text{MAP}(f_{\theta}(\cdot))$ else 0

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idea 3

softmax

argmax

SparseMAP



Structured latent variables without sampling


$$= .7x \quad + .3x$$

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

Structured latent variables without sampling

$$\begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} = .7 \times \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} + .3 \times \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} + 0 \times \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} + \dots$$

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

Structured latent variables without sampling

$$\begin{aligned} \text{Diagram} &= .7 \times \text{Diagram} + .3 \times \text{Diagram} + 0 \times \text{Diagram} + \dots \\ \mathbb{E}[L(\mathbf{z})] &= .7 \times L(\text{Diagram}) + .3 \times L(\text{Diagram}) \end{aligned}$$

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

Stanford Natural Language Inference (Accuracy)

[Kim et al., 2017]

Simple Attention 86.2

Structured Attention 86.8

[Liu and Lapata, 2018]

100D SAN - 86.8

Yogatama et al

100D RL-SPINN 80.5

[Choi et al., 2018]

100D ST Gumbel-Tree 82.6

300D - 85.6

600D - 86.0

[Corro and Titov, 2019b]

Latent Tree + 1 GCN - 85.2

Latent Tree + 2 GCN - 86.2

Stanford Sentiment (Accuracy)

Socher et al

Bigram Naive Bayes 83.1

[Nicolae et al., 2018b]

TreeLSTM w/ CoreNLP 83.2

TreeLSTM w/ SparseMAP 84.7

[Corro and Titov, 2019b]

GCN w/ CoreNLP 83.8

GCN w/ Perturb-and-MAP 84.6

V. Conclusions

Is it syntax?!

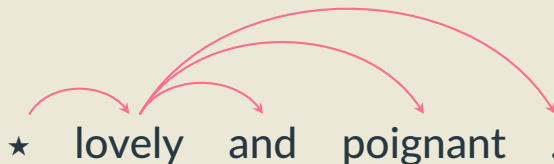
- Unlike e.g. unsupervised parsing, the structures we learn are guided by a **downstream objective** (typically discriminative).
- They don't typically resemble grammatical structure (yet) [Williams et al., 2018]
(future work: more inductive biases and constraints?)

Is it syntax?!

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

Syntax vs. Composition Order

CoreNLP parse, $p = 21.4\%$

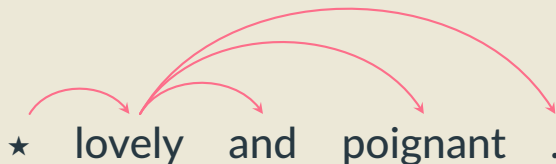


Syntax vs. Composition Order

$p = 22.6\%$

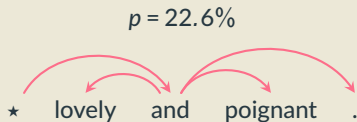


CoreNLP parse, $p = 21.4\%$

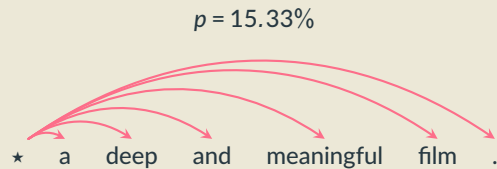


...

Syntax vs. Composition Order



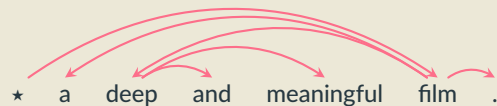
CoreNLP parse, $p = 21.4\%$



$p = 15.27\%$



...
CoreNLP parse, $p = 0\%$



Overview

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

- REINFORCE
 - Straight Through–Gumbel (Perturb & MAP)
 - SparseMAP
-
- $\text{dom } L$ may be only \mathcal{Z} ,
 - $\nabla_{\mathbf{z}} L$ need not exist!

$$L(\arg \max_{\mathbf{z}} \pi_{\theta}(\mathbf{z} | x))$$

- Straight Through
- SPIGOT

Model restrictions:

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

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

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

Overview

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

$$L(\arg \max_{\mathbf{z}} \pi_{\theta}(\mathbf{z} | x))$$

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

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

- Straight Through^{MAP,MRG}
- SPIGOT^{MAP+}

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

Computation:

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

^{MAP}: Finding the highest-scoring structure.

^{MRG}: Marginal inference.

Conclusions

- Latent structure models are desirable for interpretability, structural bias, and higher predictive power with fewer parameters.
- Stochastic latent variables can be dealt with RL or straight-through gradients.
- Deterministic argmax requires surrogate gradients (e.g. SPIGOT).
- Continuous relaxations of argmax include SANs and SparseMAP.
- Intuitively, some of these different methods are trying to do similar things or require the same building blocks (e.g. SPIGOT and SparseMAP).

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