




Latent Structure Models for NLP

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 deep-spin.github.io/tutorial

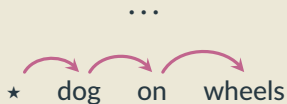
I. Introduction

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

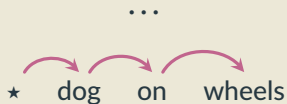
POS tagging

VERB PREP NOUN
dog on wheels

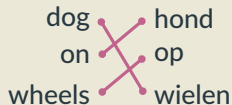
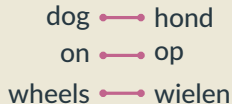
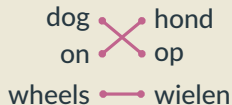
NOUN PREP NOUN
dog on wheels

NOUN DET NOUN
dog on wheels

Dependency parsing

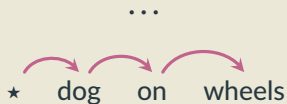


Word alignments



Examples of structure in NLP

Dependency parsing



Exponentially many structures!



...

NLP 5 years ago:

Structured prediction and pipelines



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Structured prediction and pipelines

- Big pipeline systems, connecting different structured predictors, trained separately
- **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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- **Disadvantage:** linguistic annotations required for each component 😓
- **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! 🎉

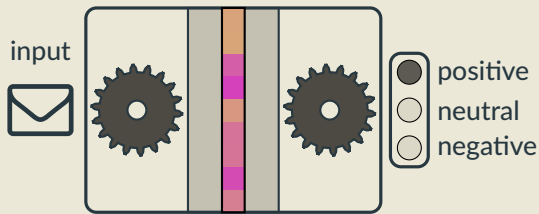
NLP today:

End-to-end training

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

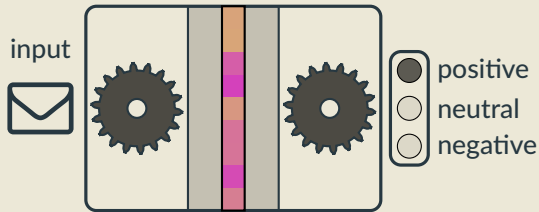
Representation learning

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



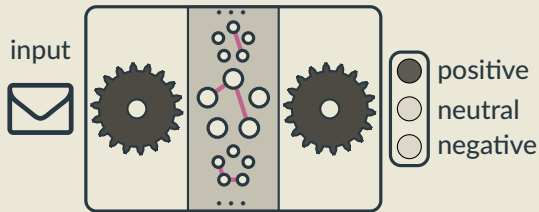
Latent structure models

- Seek *structured* hidden representations instead!



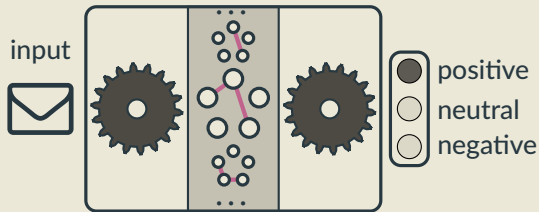
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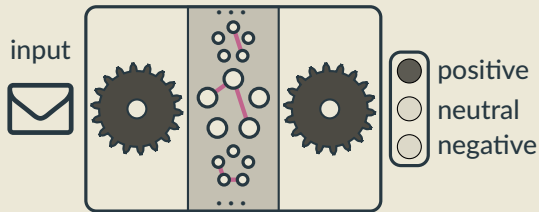
Latent structure models

- Seek *structured* hidden representations instead!
- They can bring us:
 - More interpretability;



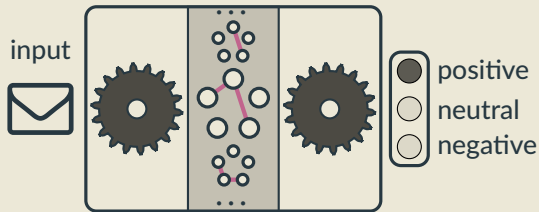
Latent structure models

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Latent structure models

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



Latent structure models aren't so new!

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

What this tutorial is about:

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

This tutorial is *not* about:

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

Background

Unstructured vs structured

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

The challenge of discrete choices

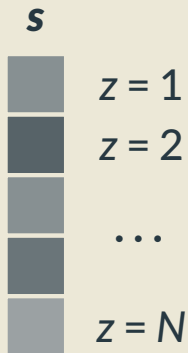
$$z = 1$$

$$z = 2$$

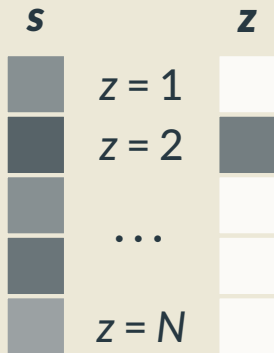
...

$$z = N$$

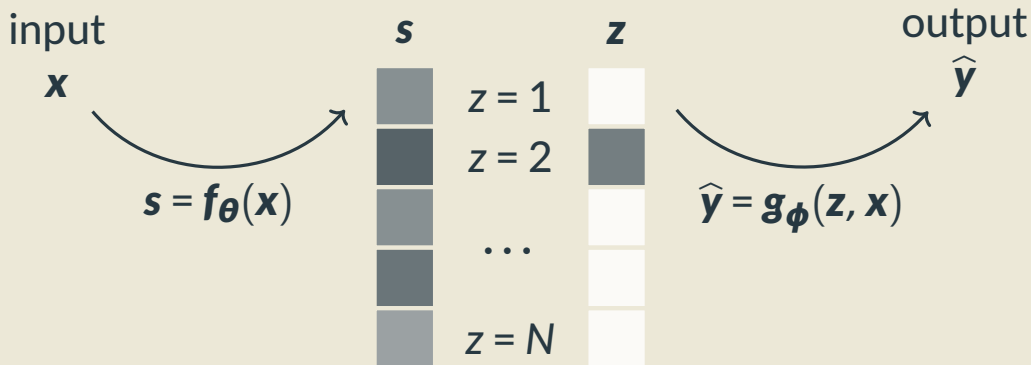
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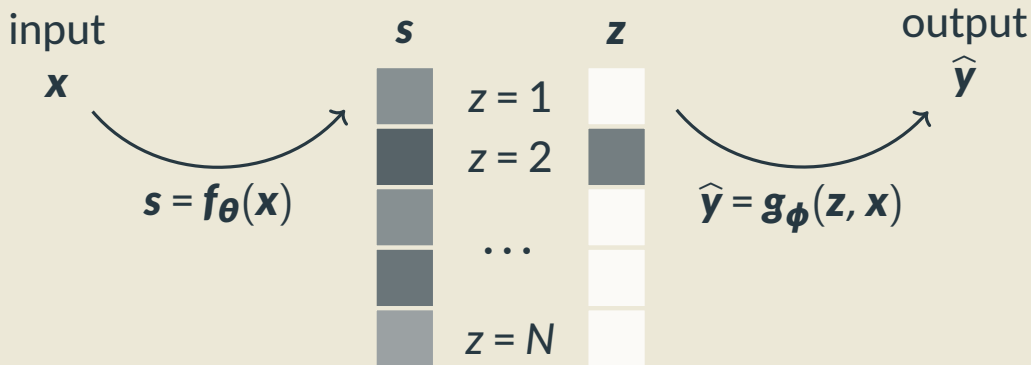
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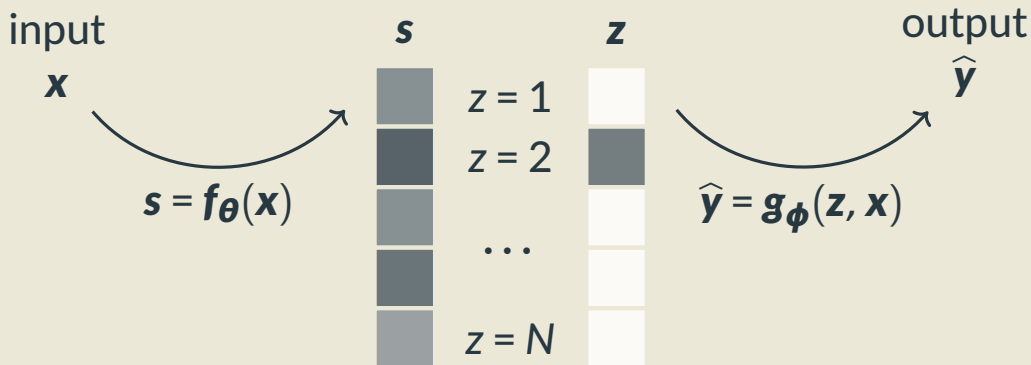


The challenge of discrete choices



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

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or, essentially,

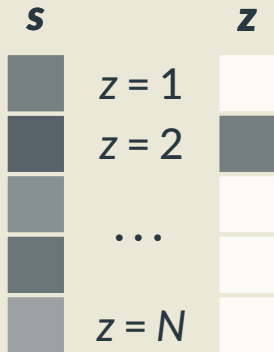
$$\frac{\partial \mathbf{z}}{\partial \mathbf{s}} = ?$$

Discrete mappings are “flat”



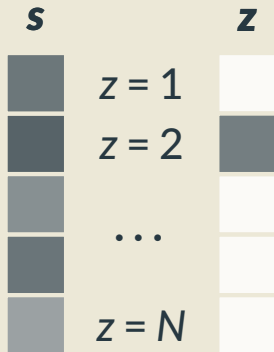
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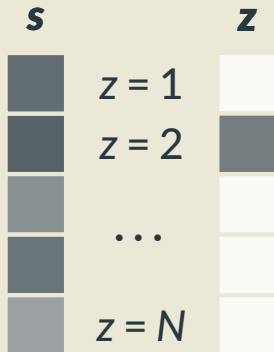
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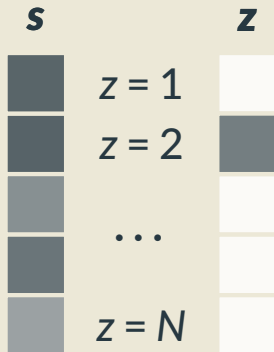
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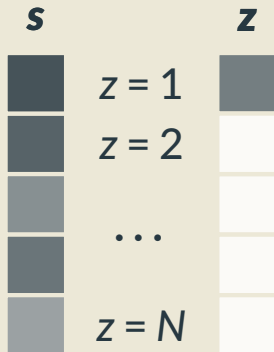
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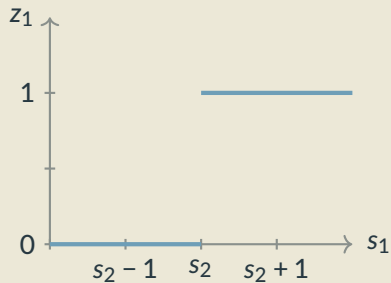


$$\frac{\partial \mathbf{z}}{\partial \mathbf{s}} = ?$$

Argmax

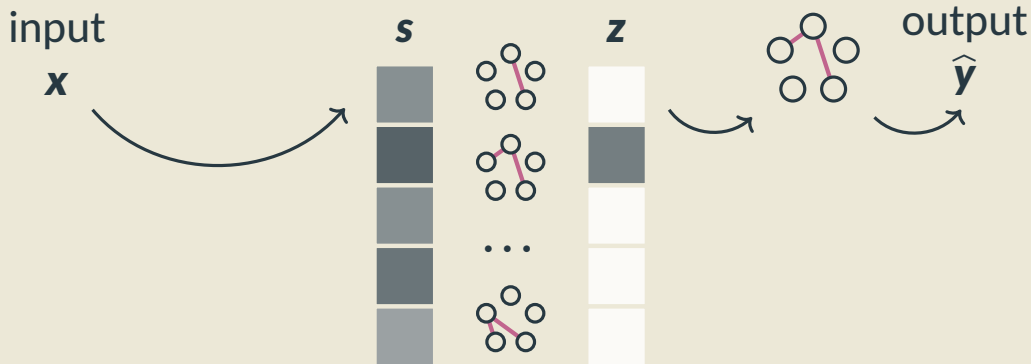


$$\frac{\partial \mathbf{z}}{\partial \mathbf{s}} = \mathbf{0}$$



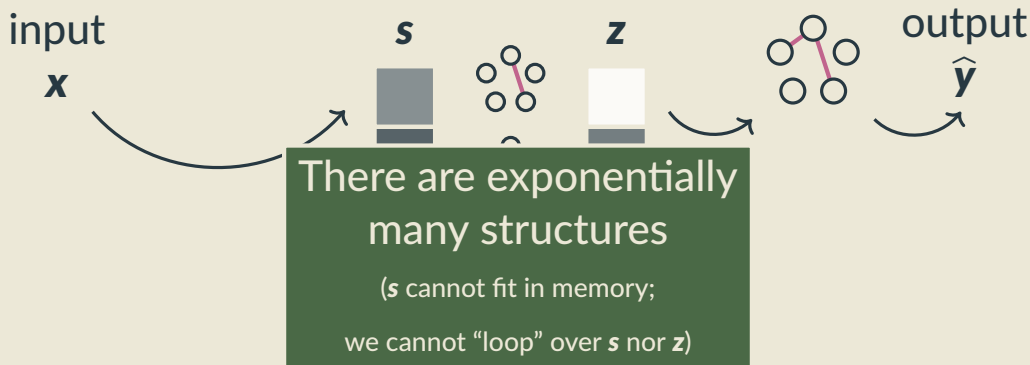
Computing the most likely structure

is a very high-dimensional argmax

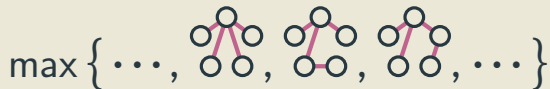
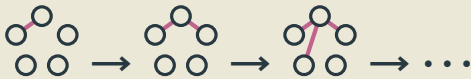


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Dealing with the combinatorial explosion



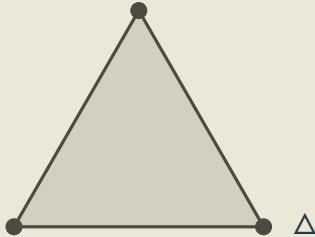
1. Incremental structures

- 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.

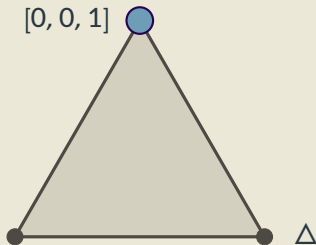
2. Factorization into parts

- 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 unstructured case: Probability simplex



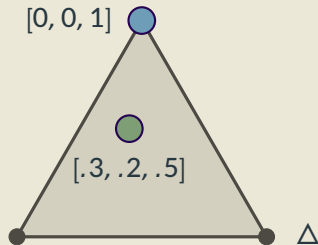
The unstructured case: Probability simplex



- 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*.

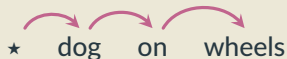
What's the analogous of Δ for a structure?

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

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



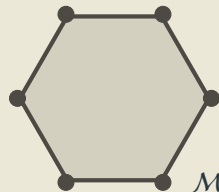
$$\mathbf{z}_2 = [0, 0, 1, 0, 0, 1, 1, 0, 0]$$



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

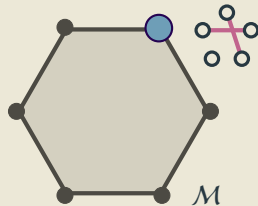


The structured case: Marginal polytope



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



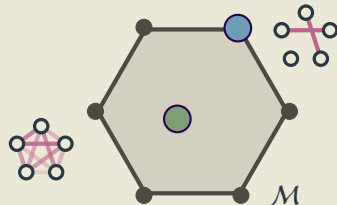
The structured case: Marginal polytope

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

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

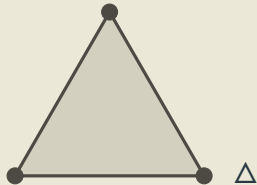
$$\begin{aligned} p_1 &= 0.2, & \mathbf{z}_1 &= [1, 0, 0, 0, 1, 0, 0, 0, 1] \\ p_2 &= 0.7, & \mathbf{z}_2 &= [0, 0, 1, 0, 0, 1, 1, 0, 0] \\ p_3 &= 0.1, & \mathbf{z}_3 &= [1, 0, 0, 0, 1, 0, 0, 1, 0] \end{aligned}$$

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

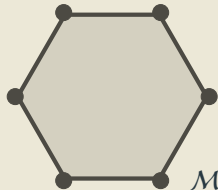


Unstructured vs Structured

- Unstructured case: simplex Δ

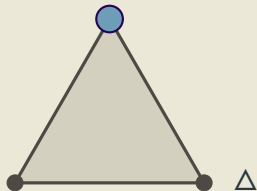


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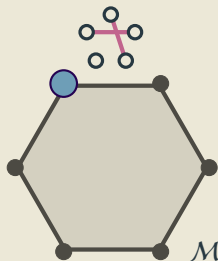


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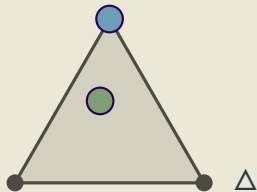


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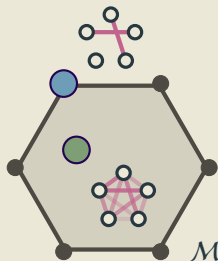


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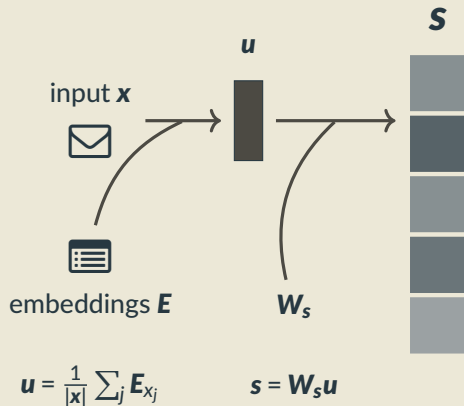
- Unstructured case: simplex Δ



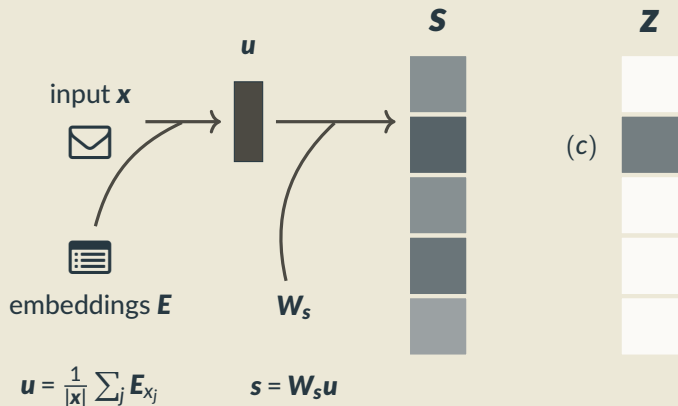
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Example: Regression with latent categorization

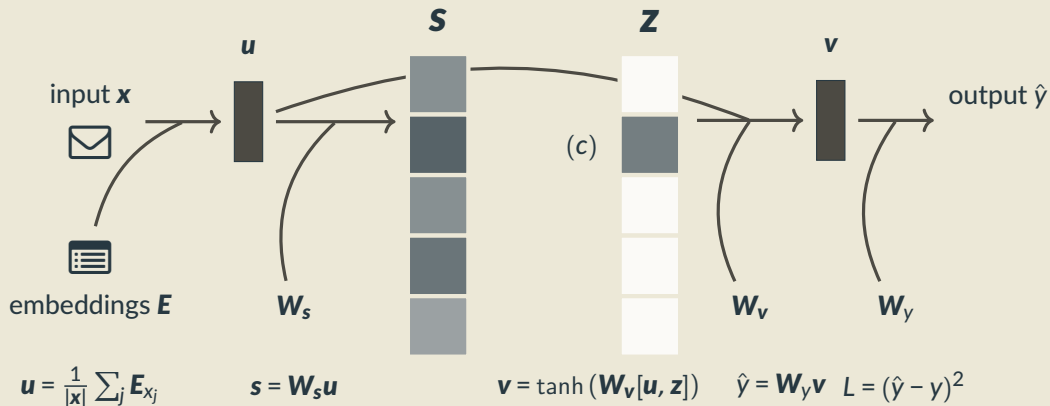


Example: Regression with latent categorization



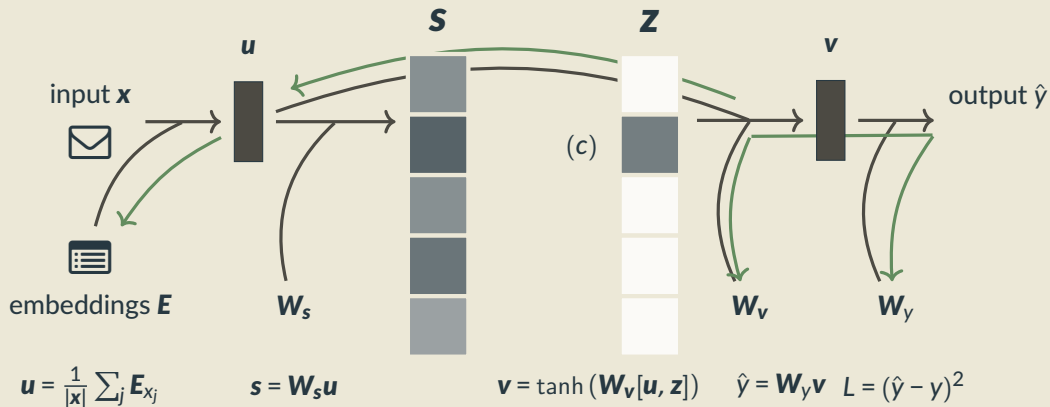
predict topic c ($z = e_c$)

Example: Regression with latent categorization

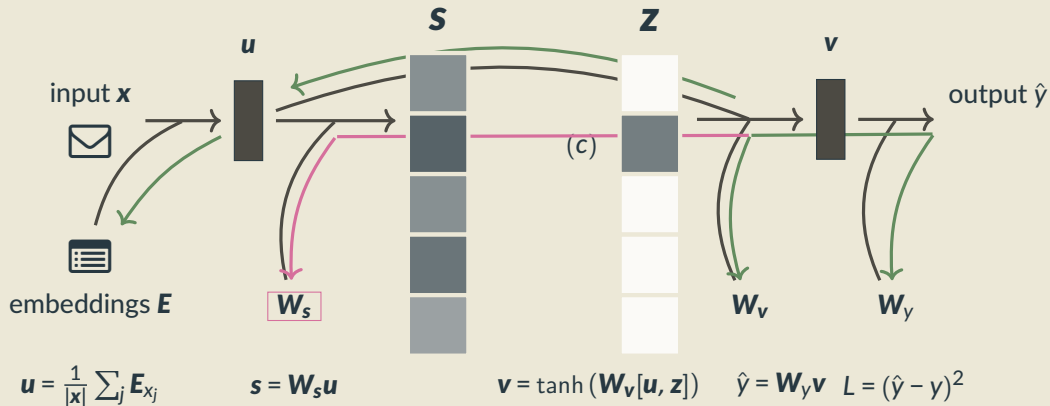


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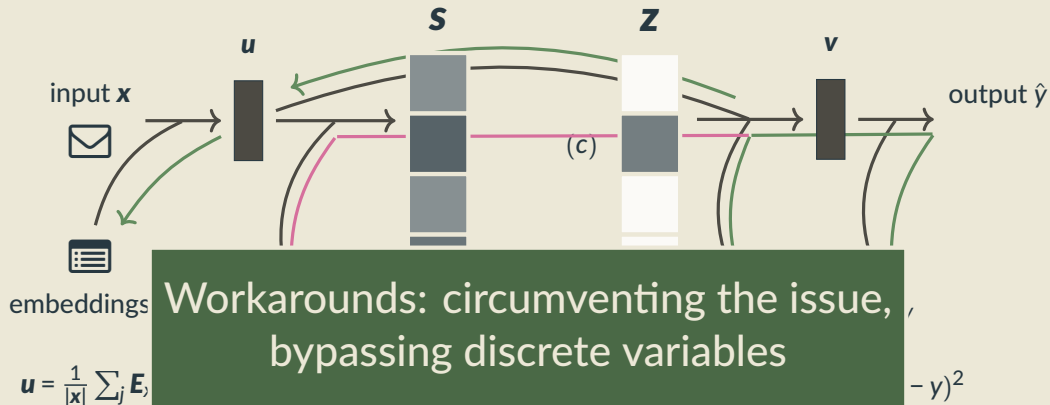


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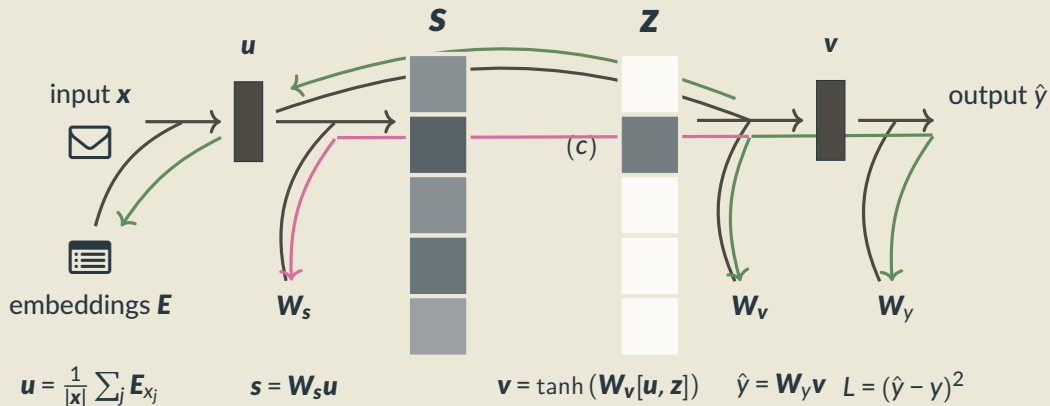


$$\frac{\partial L}{\partial W_s} = \frac{\partial L}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial v} \frac{\partial v}{\partial z} \underbrace{\frac{\partial z}{\partial s}}_{\equiv 0} \frac{\partial s}{\partial W_s}$$

Example: Regression with latent categorization

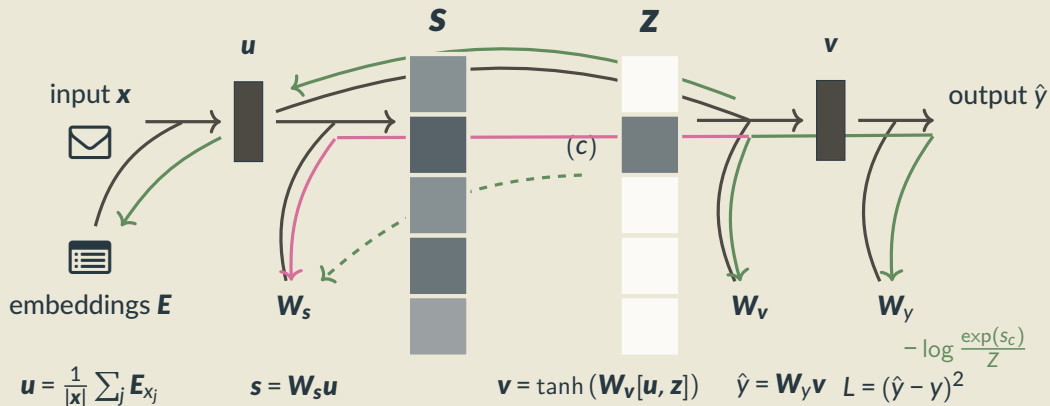


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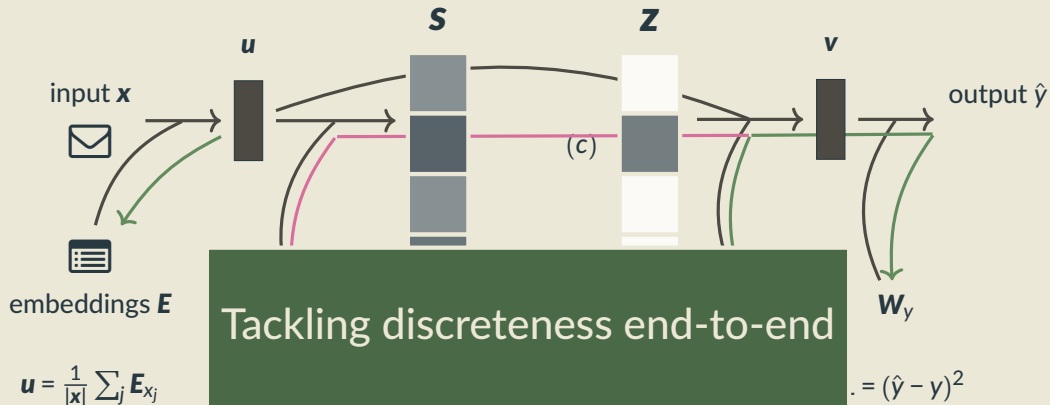
Option 1. Pretrain latent classifier W_s

Example: Regression with latent categorization

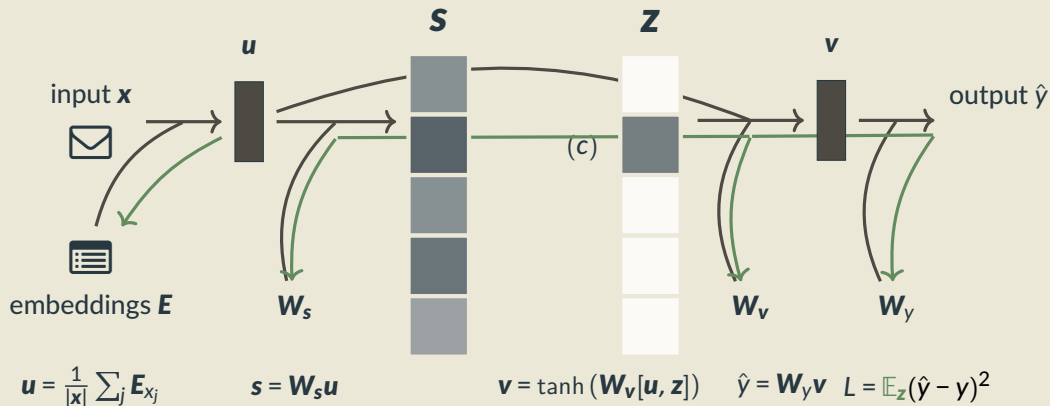


Option 2. Multi-task learning

Example: Regression with latent categorization

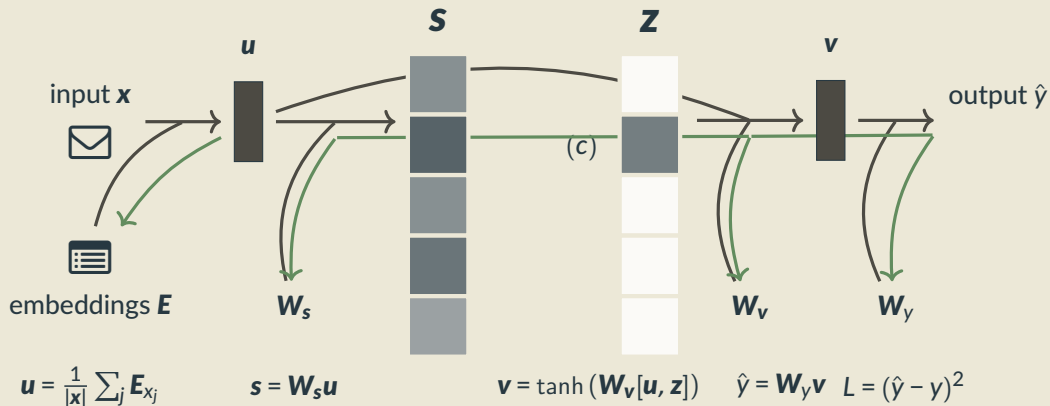


Example: Regression with latent categorization



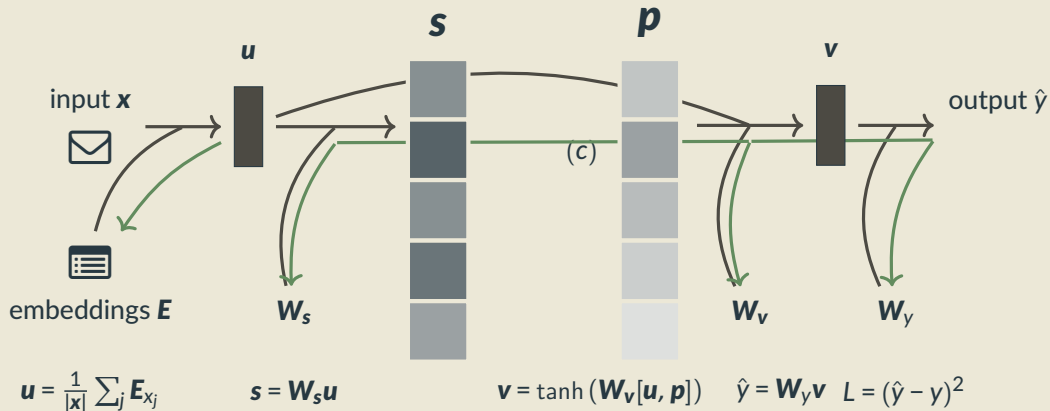
Option 3. Stochasticity! $\frac{\partial \mathbb{E}_z(\hat{y}(z) - y)^2}{\partial W_s} \neq 0$

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

Coffee Break

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

Coffee Break

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

II. Reinforcement Learning Methods

Latent structure via marginalization

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

Latent structure via marginalization

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$$L(\hat{y}(\mathbf{z}; x), y)$$

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- But we don't know \mathbf{z} !

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

Latent structure via marginalization

- Given a sentence-label pair (x, y) and its **known** parse tree \mathbf{z} , we can make a prediction $\hat{y}(\mathbf{z}; x)$ and incur a loss,

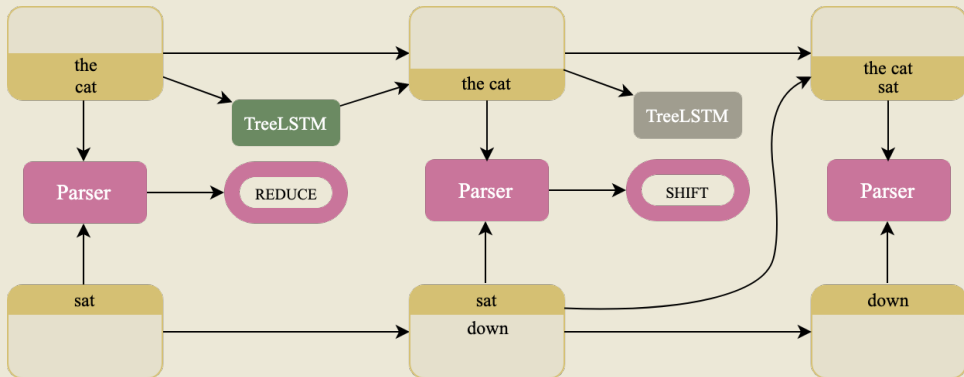
$$L(\hat{y}(\mathbf{z}; x), y) \text{ or simply } L(\mathbf{z})$$

- 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**,

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

**But first, supervised
SPINN**

Stack-augmented Parser-Interpreter Neural-Network



Stack-augmented Parser-Interpreter Neural-Network

- Joint learning: Combines a constituency parser and a sentence representation model.

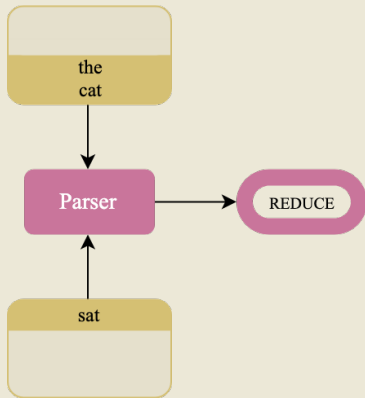
Stack-augmented Parser-Interpreter Neural-Network

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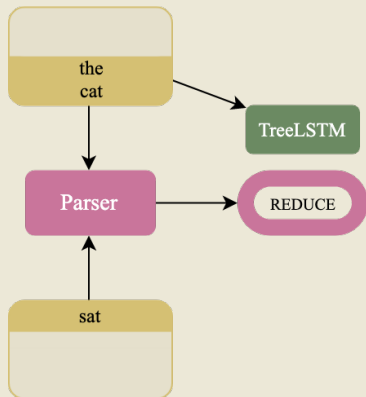
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- Joint learning: Combines a constituency parser and a sentence representation model.
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- **TreeLSTM** combines top two elements of the stack when the parser chooses the REDUCE action.

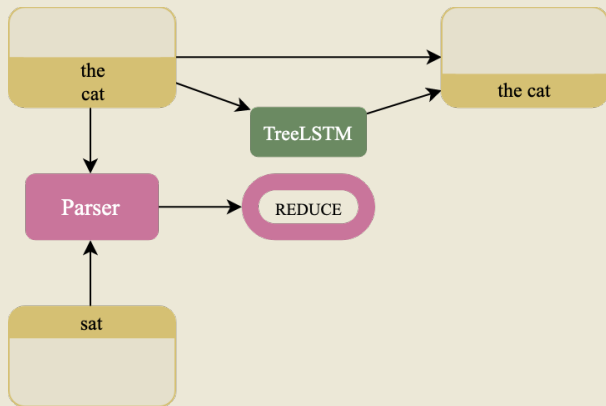
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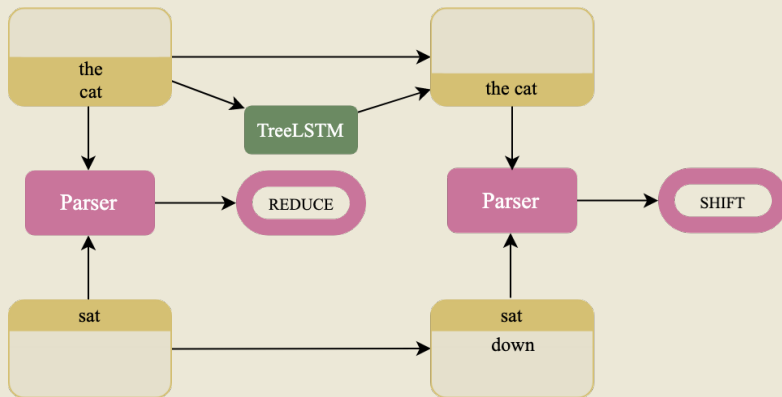
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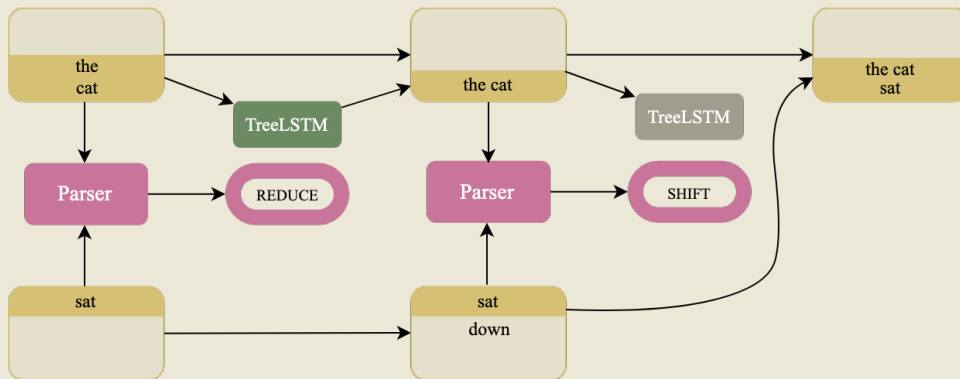
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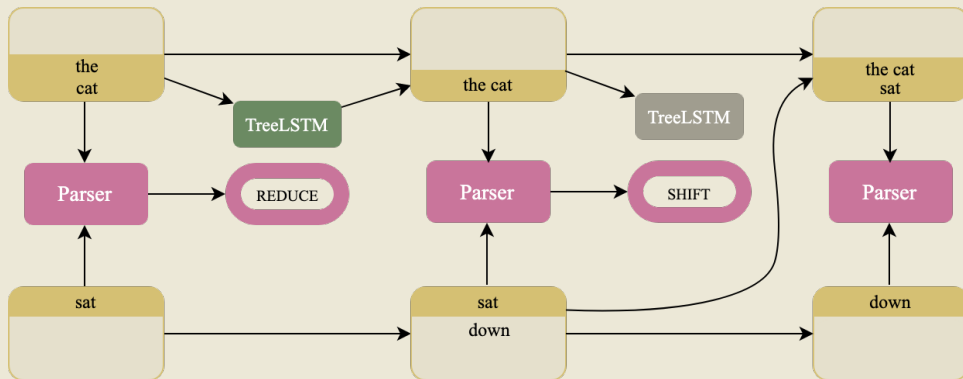
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Shift-Reduce parsing

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

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

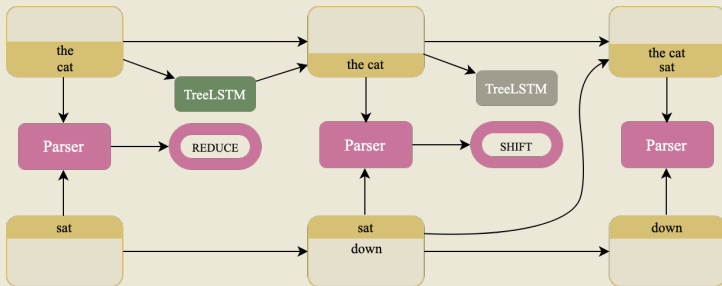
where, $z_j \in \{0, 1\} \ \forall j \in [1, 2L - 1]$

Shift-Reduce parsing

A sequence of Bernoulli trials but with conditional dependence,

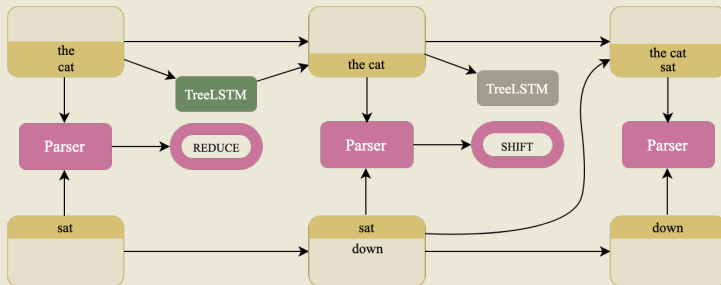
$$p(z_1, z_2, \dots, z_{2L-1}) = \prod_{j=1}^{2L-1} p(z_j \mid z_{<j})$$

Latent structure learning with SPINN



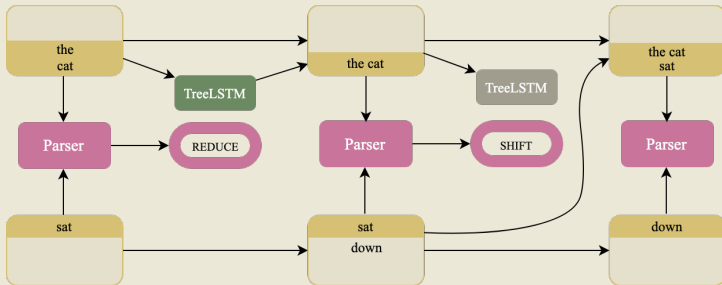
Latent structure learning with SPINN

- But now, remove syntactic supervision from SPINN.



Latent structure learning with SPINN

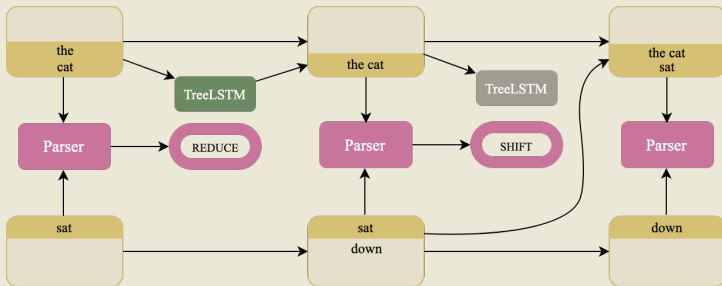
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- We model the parse, \mathbf{z} , as a latent variable scored by $f_{\theta}(\mathbf{x})$.

Latent structure learning with SPINN

- But now, remove syntactic supervision from SPINN.



- We model the parse, \mathbf{z} , as a latent variable scored by $f_{\theta}(\mathbf{x})$.
- 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.

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 - The state \mathbf{h} is the top two elements of the stack and the top element of the buffer
 - Learning
 - Maximizing
- 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

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

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

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

Through the looking glass of REINFORCE

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$$\begin{aligned} &= \sum_{\mathbf{z}} L(\mathbf{z}) \nabla_{\boldsymbol{\theta}} \pi_{\boldsymbol{\theta}}(\mathbf{z} | x) \\ &= \sum_{\mathbf{z}} L(\mathbf{z}) \pi_{\boldsymbol{\theta}}(\mathbf{z} | x) \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(\mathbf{z} | x) \\ &= \mathbb{E}_{\mathbf{z} \sim \pi_{\boldsymbol{\theta}}(\mathbf{z} | x)} [L(\mathbf{z}) \nabla_{\boldsymbol{\theta}} \log \pi_{\boldsymbol{\theta}}(\mathbf{z} | x)] \end{aligned}$$

SPINN with REINFORCE, aka RL-SPINN

Yogatama et al. [2017] uses REINFORCE to train 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
Random Trees	24.0	24.0	24.2	5.2

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But why?

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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”:

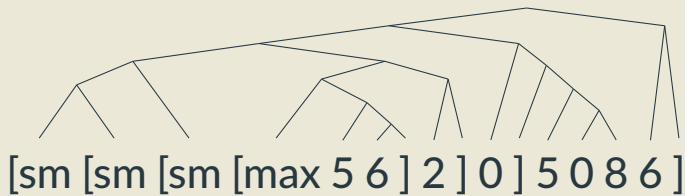


Figure: Truth: 7; Pred: 7

High variance

Sometimes it doesn't:

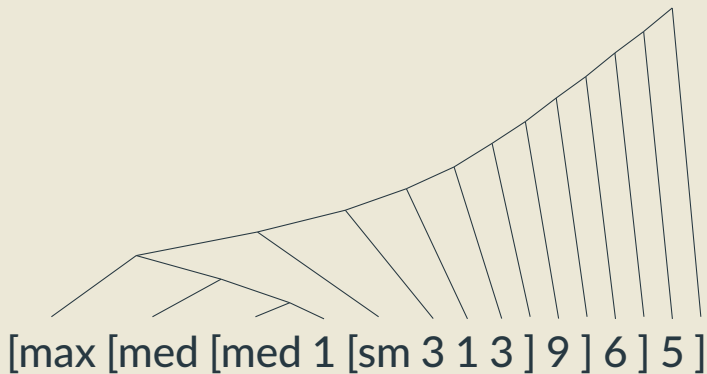


Figure: Truth: 6; Pred: 5

High variance

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

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Possible solutions,

1. Gradient normalization
2. Control variates, aka baselines

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So,

$$\nabla \mathbb{E}_{\mathbf{z} \sim \pi(\mathbf{z})} = \mathbb{E}_{\mathbf{z} \sim \pi(\mathbf{z})} [(\textcolor{blue}{L}(\mathbf{z}) - \textcolor{red}{b}(\mathbf{x})) \nabla \pi(\mathbf{z})]$$

Which we can do because,

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

Issues with SPINN with REINFORCE

This system faces two big problems,

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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

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1. Input dependent control variate
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However, does not learn English grammars.

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Roadmap of the tutorial

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

Coffee Break

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

Coffee Break

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

III. Gradient Surrogates

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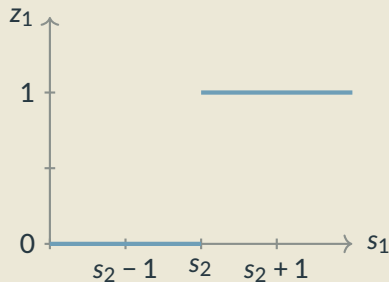
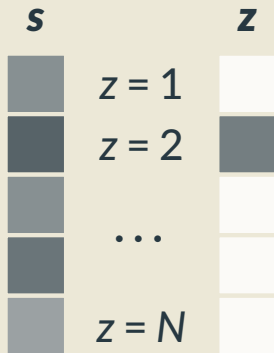
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incur loss $L(\hat{\mathbf{z}}(x))$
- 3A: try to optimize the deterministic loss directly
- 3B: use this strategy to reduce variance in the stochastic model.

Recap: The argmax problem

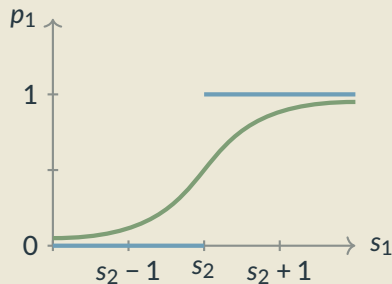
$$\mathbf{z} = \arg \max(\mathbf{s})$$



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

Softmax

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



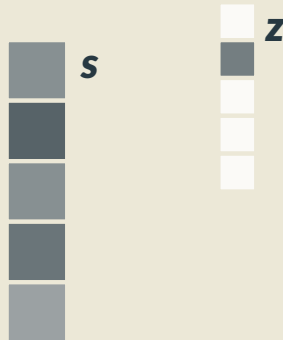
$$\frac{\partial \mathbf{p}}{\partial \mathbf{s}} = \text{diag}(\mathbf{p}) - \mathbf{p}\mathbf{p}^\top$$

Straight-Through Estimator



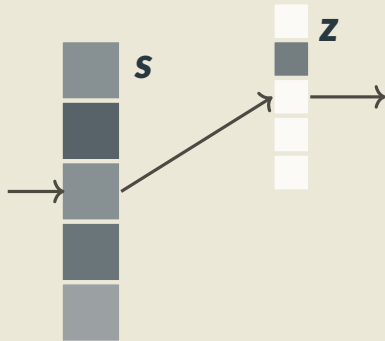
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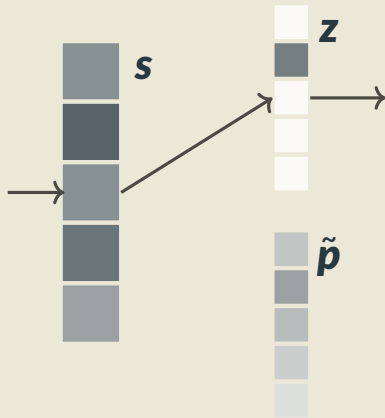
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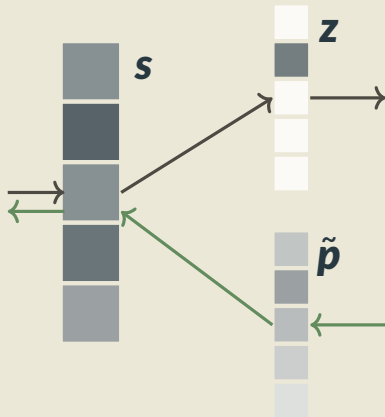
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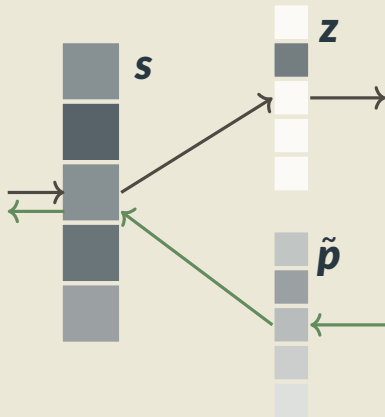
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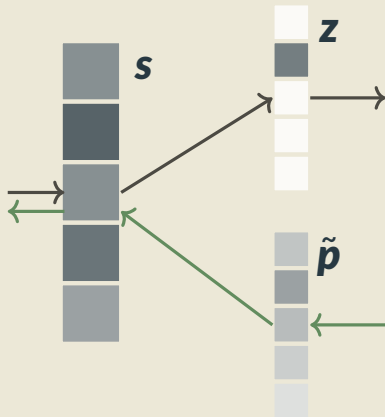
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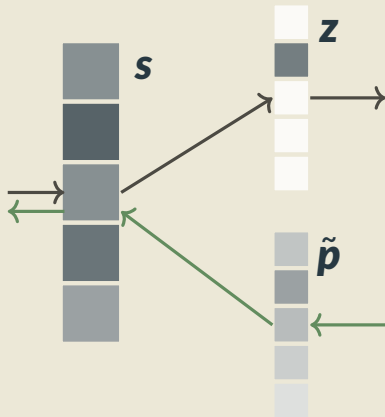
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 - others, e.g. softmax $\tilde{\mathbf{p}}(\mathbf{s}) = \text{softmax}(\mathbf{s})$, $\frac{\partial \tilde{\mathbf{p}}}{\partial \mathbf{s}} = \text{diag}(\tilde{\mathbf{p}}) - \tilde{\mathbf{p}}\tilde{\mathbf{p}}^T$



Straight-Through Estimator

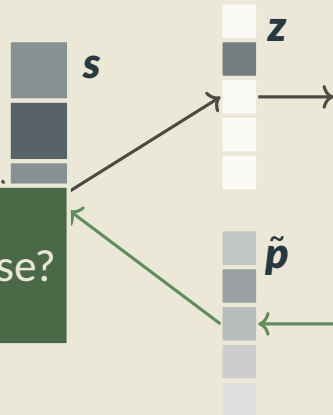
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 - others, e.g. softmax $\tilde{\mathbf{p}}(\mathbf{s}) = \text{softmax}(\mathbf{s})$, $\frac{\partial \tilde{\mathbf{p}}}{\partial \mathbf{s}} = \text{diag}(\tilde{\mathbf{p}}) - \tilde{\mathbf{p}}\tilde{\mathbf{p}}^T$
- More explanation in a while



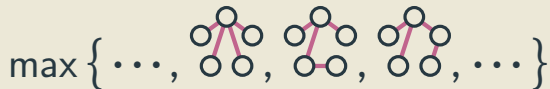
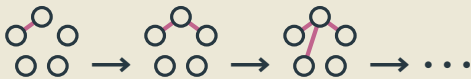
Straight-Through Estimator

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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.

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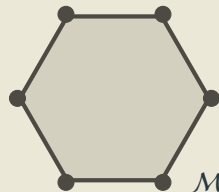
Example: Latent Tree Learning with Differentiable Parsers: Shift-Reduce Parsing and Chart Parsing [Maillard and Clark, 2018] (STE through beam search).

STE for the factorized approach

Requires a bit more work:

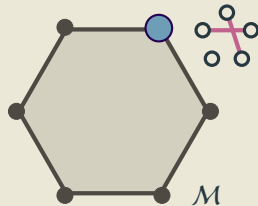
- Recap: marginal polytope
- Predicting structures globally: Maximum A Posteriori (MAP)
- Deriving Straight-Through and SPIGOT

The structured case: Marginal polytope



The structured case: Marginal polytope

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



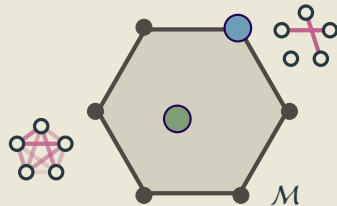
The structured case: Marginal polytope

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

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

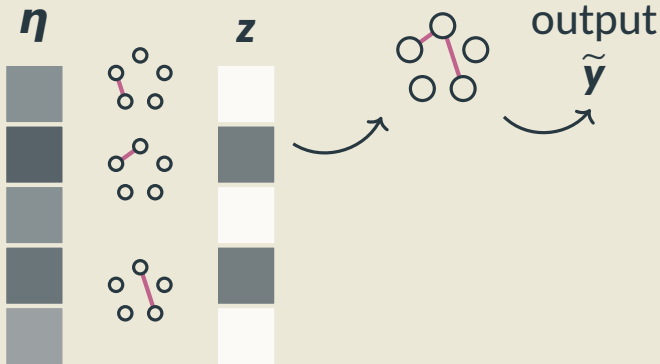
$$\begin{aligned} p_1 &= 0.2, & \mathbf{z}_1 &= [1, 0, 0, 0, 1, 0, 0, 0, 1] \\ p_2 &= 0.7, & \mathbf{z}_2 &= [0, 0, 1, 0, 0, 1, 1, 0, 0] \\ p_3 &= 0.1, & \mathbf{z}_3 &= [1, 0, 0, 0, 1, 0, 0, 1, 0] \end{aligned}$$

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



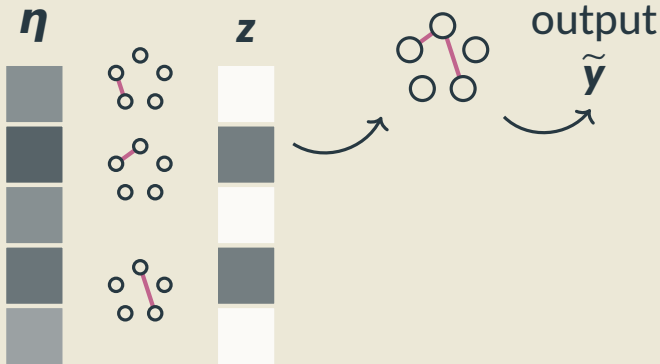
Predicting structures from scores of parts

- $\eta(i \rightarrow j)$: score of arc $i \rightarrow j$
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Predicting structures from scores of parts

- $\eta(i \rightarrow j)$: score of arc $i \rightarrow j$
- $z(i \rightarrow j)$: is arc $i \rightarrow j$ selected?
- Task-specific algorithm for the highest-scoring structure.



Algorithms for specific structures

Best structure (MAP)

Sequence tagging

Viterbi
[Rabiner, 1989]

Constituent trees

CKY
[Kasami, 1966, Younger, 1967]
[Cocke and Schwartz, 1970]

Temporal alignments

DTW
[Sakoe and Chiba, 1978]

Dependency trees

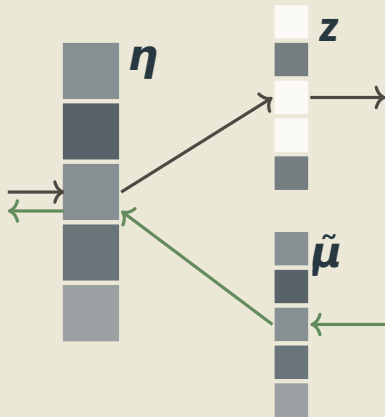
Max. Spanning Arborescence
[Chu and Liu, 1965, Edmonds, 1967]

Assignments

Kuhn-Munkres
[Kuhn, 1955, Jonker and Volgenant, 1987]

Structured Straight-Through

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



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Revisited

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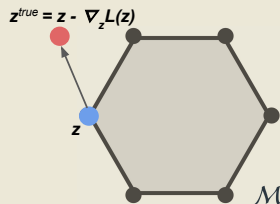
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Straight-Through in the structured case

- Structured STE: perceptron update with induced annotation

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

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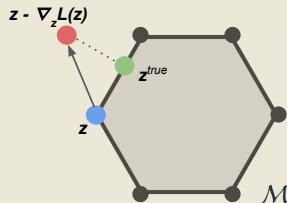
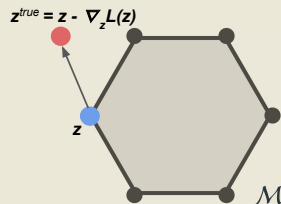
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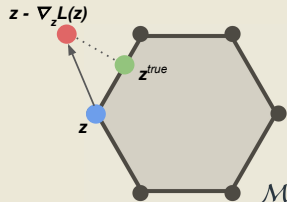
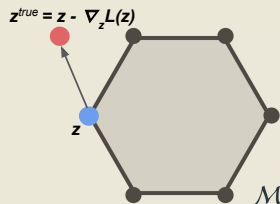
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- We discuss a generic way to compute the projection in part 4.



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

Stochastic node in the computation graph

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Recall the stochastic objective:

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

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

Categorical reparameterization

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- Sampling from a categorical value in the middle of the computation graph.

$$\mathbf{z} \sim \pi_{\boldsymbol{\theta}}(\mathbf{z} \mid \mathbf{x}) \propto \exp \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{z} \mid \mathbf{x})$$

s



z



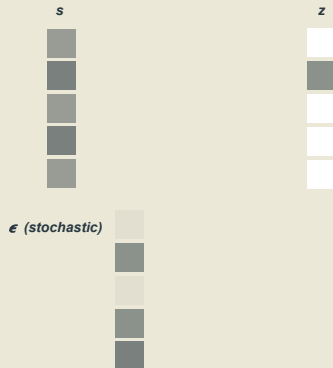
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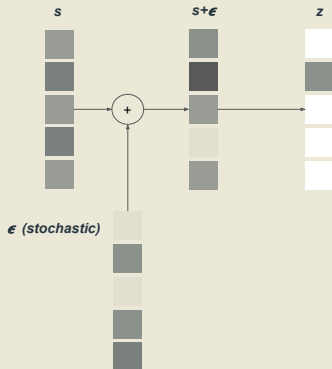
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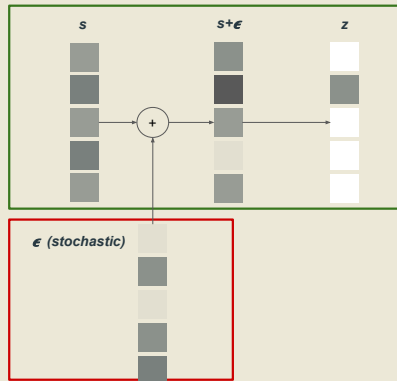
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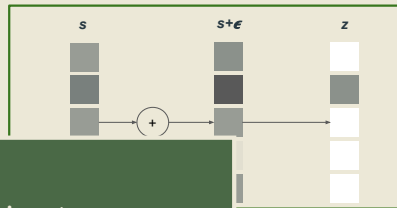
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- Reparameterizing stochasticity

- Makes \mathbf{z} deterministic



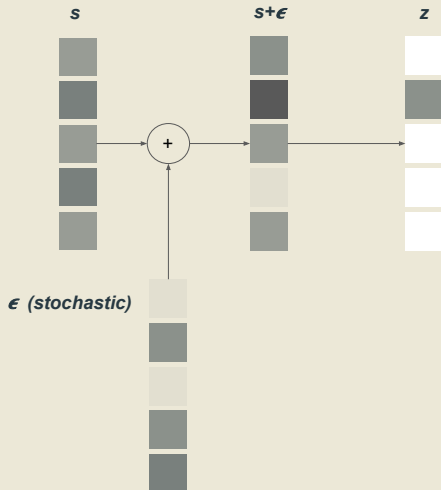
As a result:

Stochasticity is moved as an input.

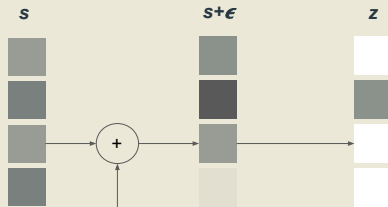
We can backpropagate through the deterministic input to \mathbf{z} .



Categorical reparameterization



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How do we sample from a categorical variable?



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The two methods are equivalent. *(Not obvious, but we will not prove it now.)*

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- return $\mathbf{z} = \mathbf{e}_t$ s.t. $c_t \leq u < c_{t+1}$

2. The Gumbel-Max trick:

- $u_i \sim \text{Uniform}(0, 1)$
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- $\mathbf{z} = \arg \max(\mathbf{s} + \boldsymbol{\epsilon})$

The two methods are equivalent. *(Not obvious, but we will not prove it now.)*
Requires sampling from the Standard Gumbel Distribution $G(0,1)$.

Sampling from a categorical variable

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

1. Inverse transform sampling:

- $\mathbf{p} = \text{softmax}(\mathbf{s})$
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Derivation & more info: [Adams, 2013, Vieira, 2014]

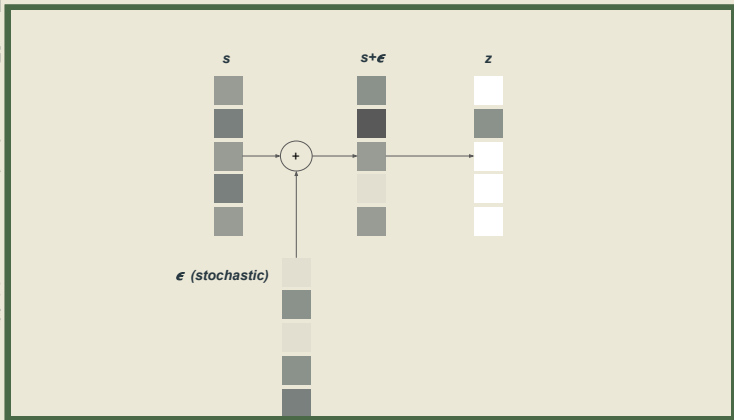
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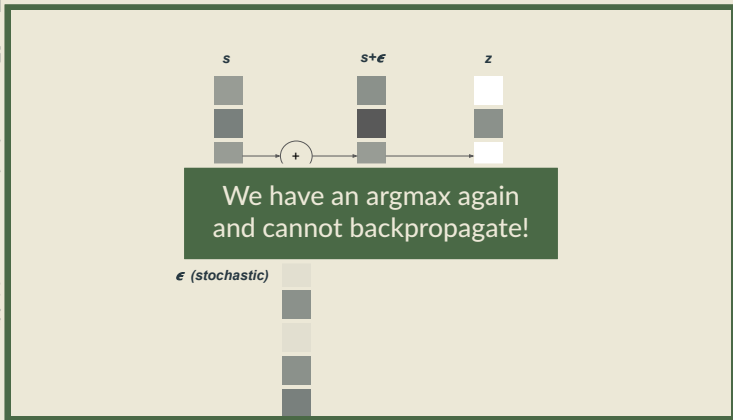
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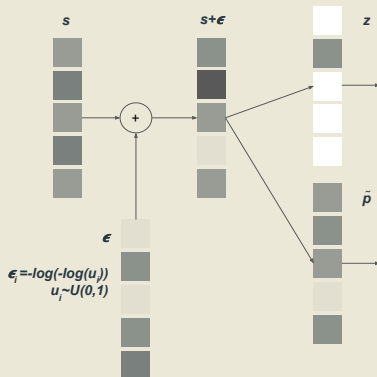
Straight-Through Gumbel Estimator

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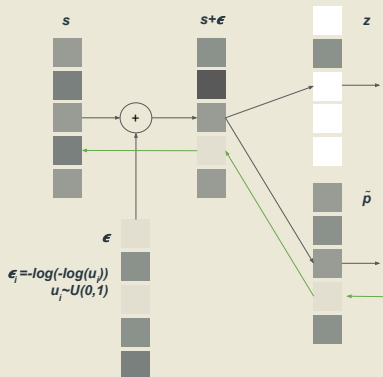
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 $\tilde{\mathbf{p}} = \text{softmax}(\mathbf{s} + \boldsymbol{\epsilon})$



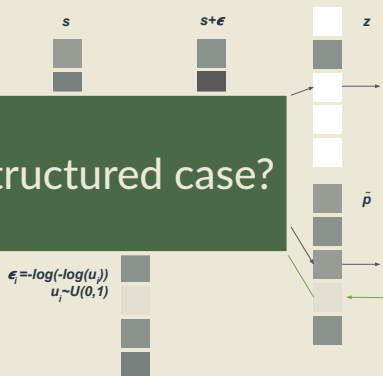
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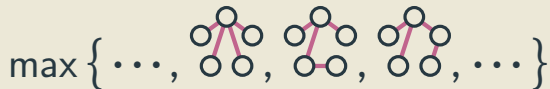
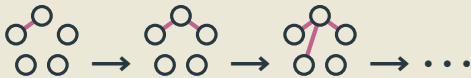
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What about the structured case?



Dealing with the combinatorial explosion



1. Incremental structures

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

2. Factorization into parts

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

Sampling from incremental structures

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- Backward: pretend we had used a **differentiable surrogate function**

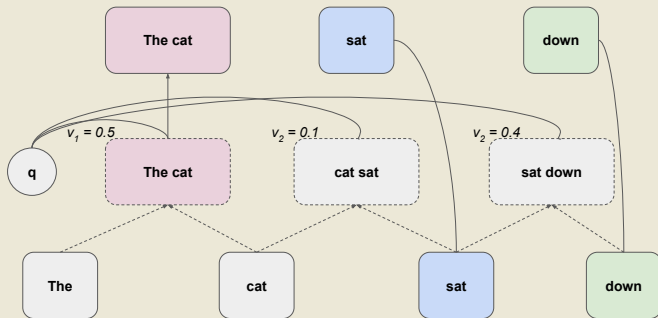
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Example: Gumbel Tree-LSTM [Choi et al., 2018].

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!)

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- $\tilde{\eta} = \eta + \epsilon$

Sampling from factorized models

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- Sample from the normal Gumbel distribution.
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- Compute MAP (task-specific algorithm).
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- $\arg \max_{\mathbf{z} \in \mathcal{Z}} \tilde{\eta}^T \mathbf{z}$

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).
- Backward: we could use Straight-Through with Identity.
- $\epsilon \sim G(0, 1)$
- $\tilde{\eta} = \eta + \epsilon$
- $\arg \max_{\mathbf{z} \in \mathcal{Z}} \tilde{\eta}^T \mathbf{z}$

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
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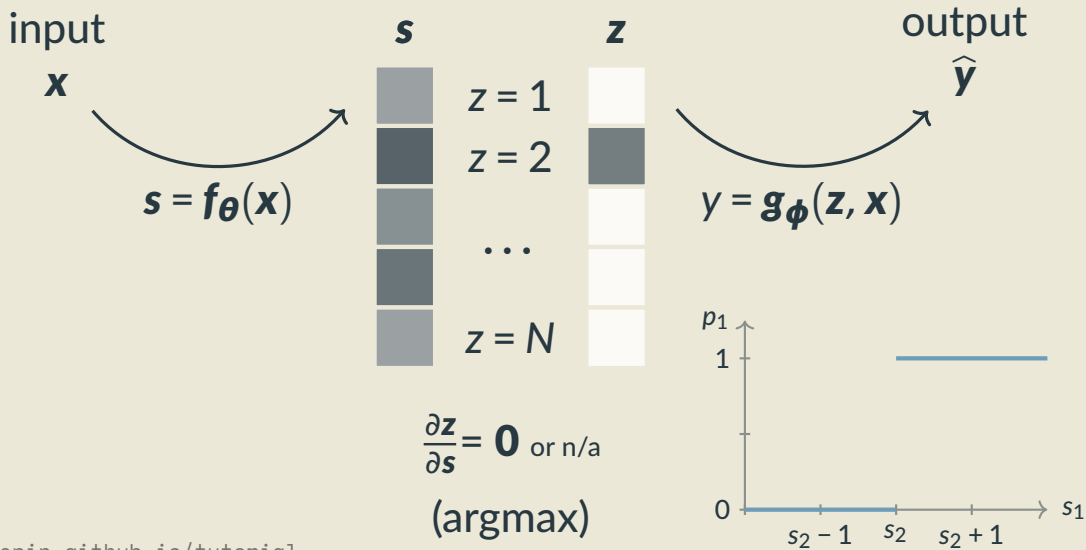
And more, in the next section!

IV. End-to-end Differentiable Relaxations

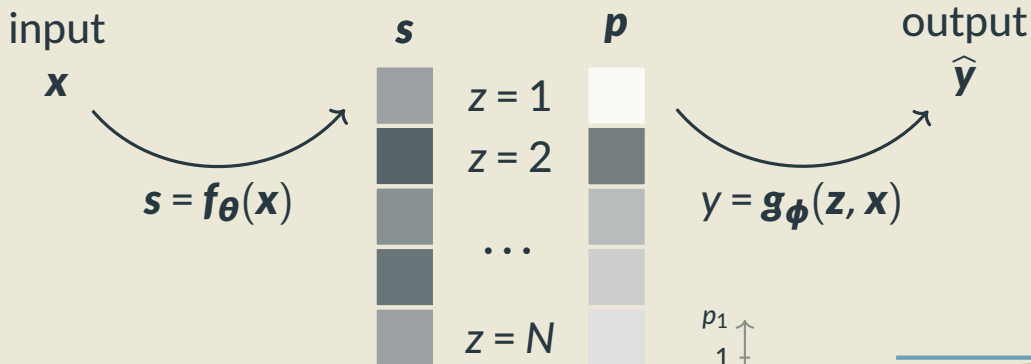
End-to-end differentiable relaxations

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

Recall: Discrete choices & differentiability



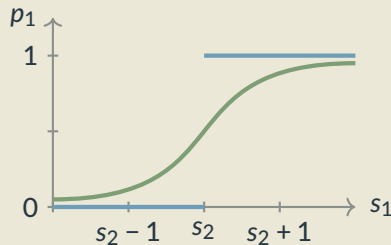
One solution: smooth relaxation



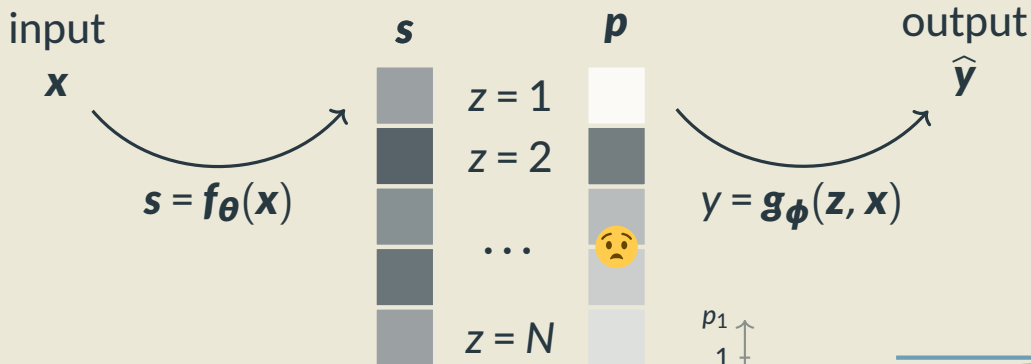
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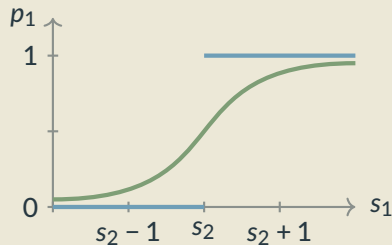


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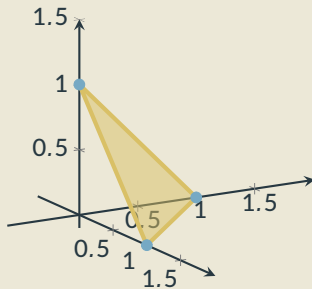
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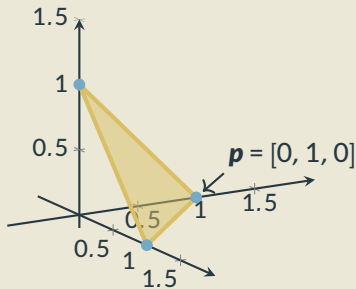
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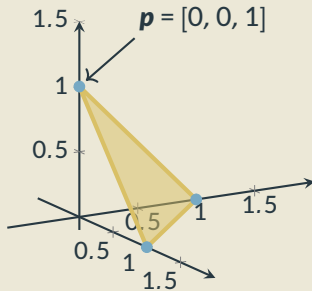
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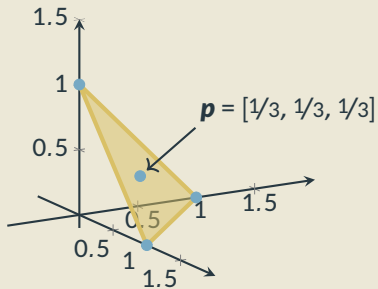
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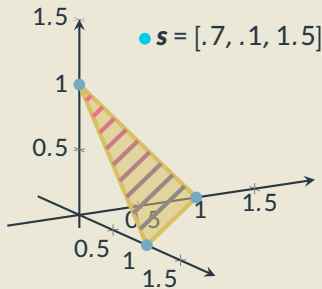


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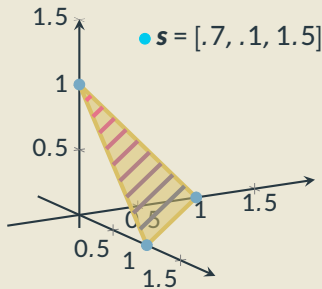
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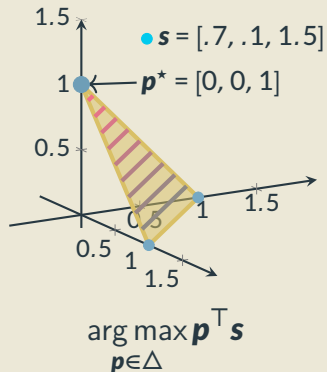
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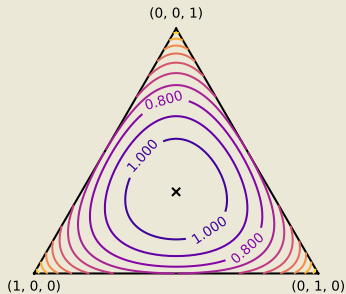
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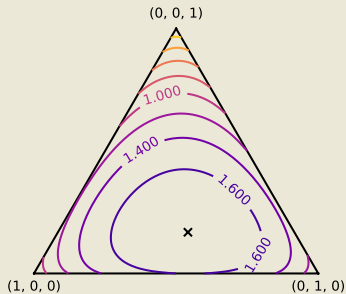
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softmax maximizes **expected score + entropy**:



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

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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$$p_i = \exp(s_i) / \exp(\tau + 1) = \exp(s_i) / Z$$

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$$p_i = \exp(s_i) / \exp(\tau + 1) = \exp(s_i) / Z$$

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

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 $p_j = \frac{\exp s_j}{\sum_i \exp s_i}$.

Explicit form of the optimization problem:

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

Lagrangian:

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

Optimality conditions (KKT):

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

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

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$$\mathbf{p}^\top \boldsymbol{\nu} = 0$$

$$\mathbf{p} \in \Delta$$

$$\boldsymbol{\nu} \geq 0$$

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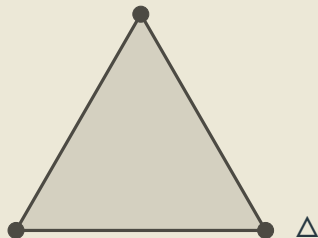
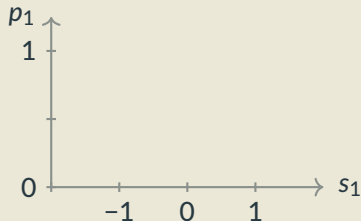
Answer: $Z = \sum_j \exp(s_j)$

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

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

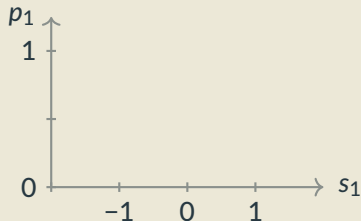
Generalizing softmax: Smoothed argmaxes

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



Generalizing softmax: Smoothed argmaxes

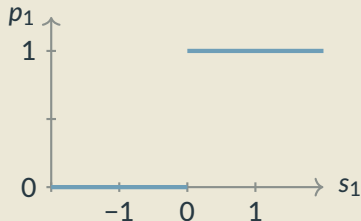
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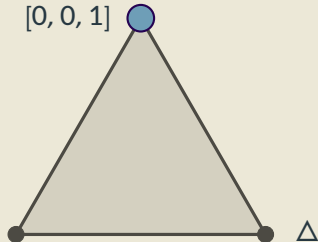
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- argmax: $\Omega(\mathbf{p}) = 0$



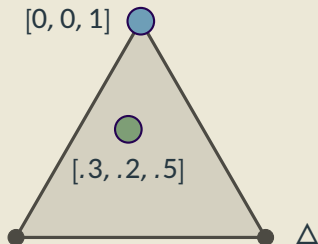
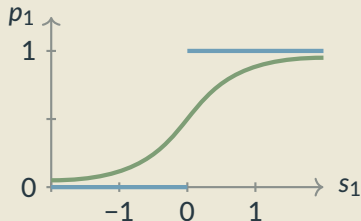
$[0, 0, 1]$



Generalizing softmax: Smoothed argmaxes

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

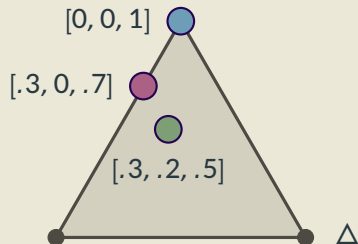
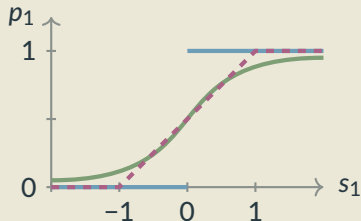
- argmax: $\Omega(\mathbf{p}) = 0$
- softmax: $\Omega(\mathbf{p}) = \sum_j p_j \log p_j$



Generalizing softmax: Smoothed argmaxes

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

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

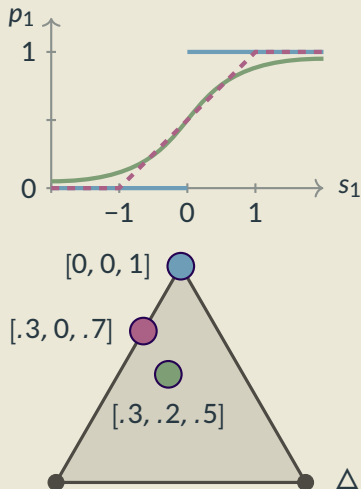


Generalizing softmax: Smoothed argmaxes

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

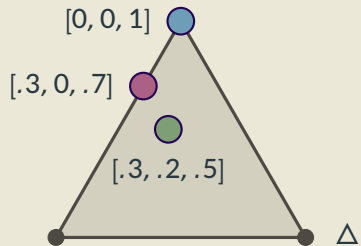
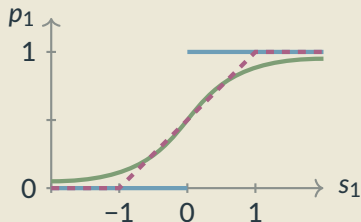
Generalized entropy interpolates in between [Tsallis, 1988]
 Used in Sparse Seq2Seq: [Peters et al., 2019] and Adaptively
 Sparse Transformers [Correia et al., 2019]



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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- α -entmax: $\Omega(\mathbf{p}) = 1/\alpha(\alpha-1) \sum_j p_j^{\alpha}$
- 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: $\Omega(\mathbf{p}) = \sum_j p_j \log p_j + \iota(\mathbf{a} \leq \mathbf{p} \leq \mathbf{b})$



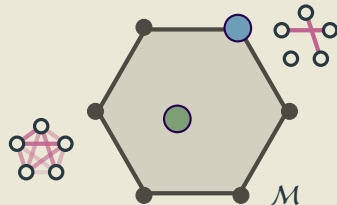
The structured case: Marginal polytope

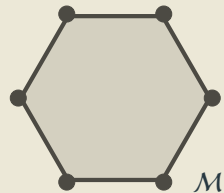
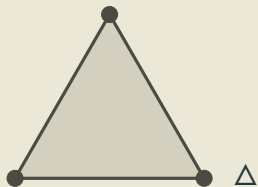
- Each vertex corresponds to one such *bit vector* \mathbf{z}
- Points inside correspond to *marginal distributions*: convex combinations of structured objects

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

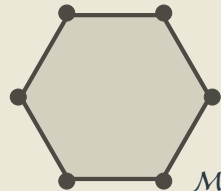
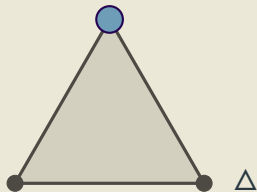
$$\begin{aligned} p_1 &= 0.2, & \mathbf{z}_1 &= [1, 0, 0, 0, 1, 0, 0, 0, 1] \\ p_2 &= 0.7, & \mathbf{z}_2 &= [0, 0, 1, 0, 0, 1, 1, 0, 0] \\ p_3 &= 0.1, & \mathbf{z}_3 &= [1, 0, 0, 0, 1, 0, 0, 1, 0] \end{aligned}$$

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

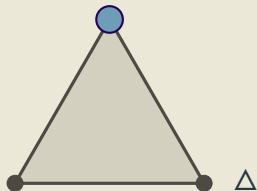




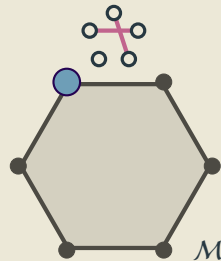
- $\operatorname{argmax}_{\mathbf{p} \in \Delta} \arg \max \mathbf{p}^T \mathbf{s}$



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

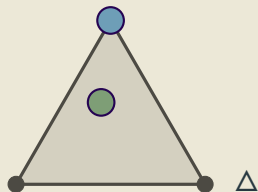


• **MAP** $\arg \max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^T \boldsymbol{\eta}$

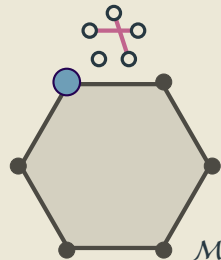


- **argmax** $\arg \max_{\mathbf{p} \in \Delta} \mathbf{p}^T \mathbf{s}$

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

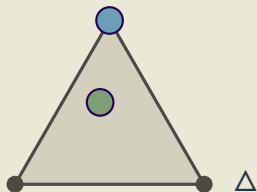


- **MAP** $\arg \max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^T \boldsymbol{\eta}$



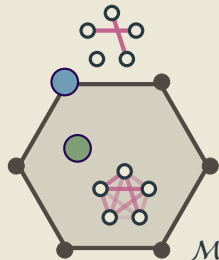
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- **MAP** $\arg \max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^T \boldsymbol{\eta}$

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



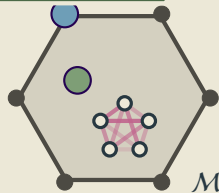
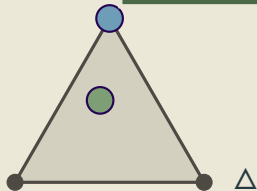
- **argmax** $\arg \max_{\mathbf{p} \in \Delta} \mathbf{p}^T \mathbf{s}$

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



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

Unlike argmax/softmax, computation is not obvious!



Algorithms for specific structures

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

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Derivatives of marginals 1: DP

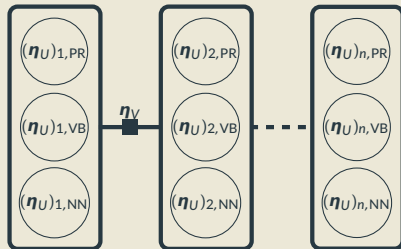
Dynamic programming: marginals by **Forward-Backward**, **Inside-Outside**, etc.

Derivatives of marginals 1: DP

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

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
6    $\beta_{i,k} = \log \sum_{k'} \exp(\beta_{i+1,k'} + (\boldsymbol{\eta}_U)_{i+1,k'} + (\boldsymbol{\eta}_V)_{k,k'})$  for all  $k$ 
7  $Z = \sum_k \exp \alpha_{n,k}$                                     # partition function
8 return  $\boldsymbol{\mu} = \exp(\boldsymbol{\alpha} + \boldsymbol{\beta} - \log Z)$                 # marginals
```



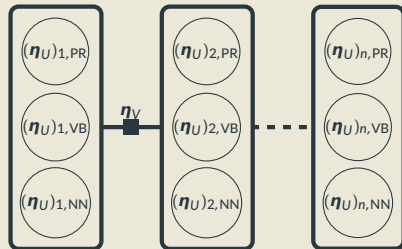
Derivatives of marginals 1: DP

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

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

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```



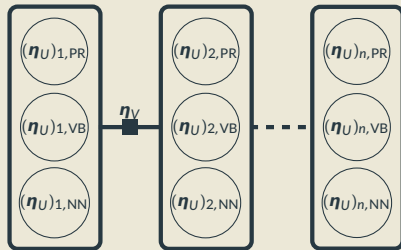
Derivatives of marginals 1: DP

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- Better book-keeping: Li and Eisner [2009], Mensch and Blondel [2018]

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```



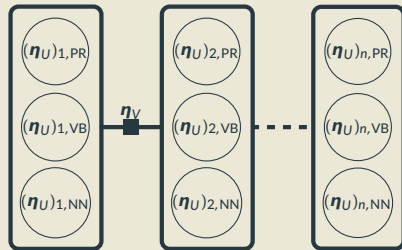
Derivatives of marginals 1: DP

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

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

Marginals in a sequence tagging model.

```
1 input:  $d$  tags,  $n$  tokens,  $\boldsymbol{\eta}_U \in \mathbb{R}^{n \times d}$ ,  $\boldsymbol{\eta}_V \in \mathbb{R}^{d \times d}$ 
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```



Derivatives of marginals 2: Matrix-Tree

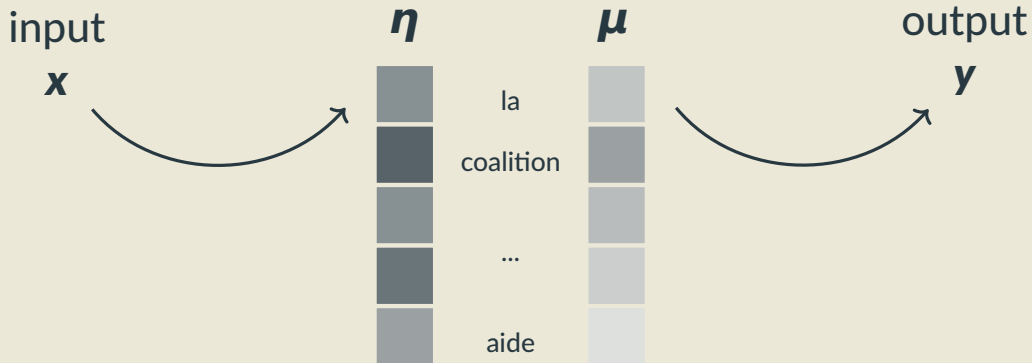
$\mathbf{L}(\mathbf{s})$: Laplacian of the edge score graph

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

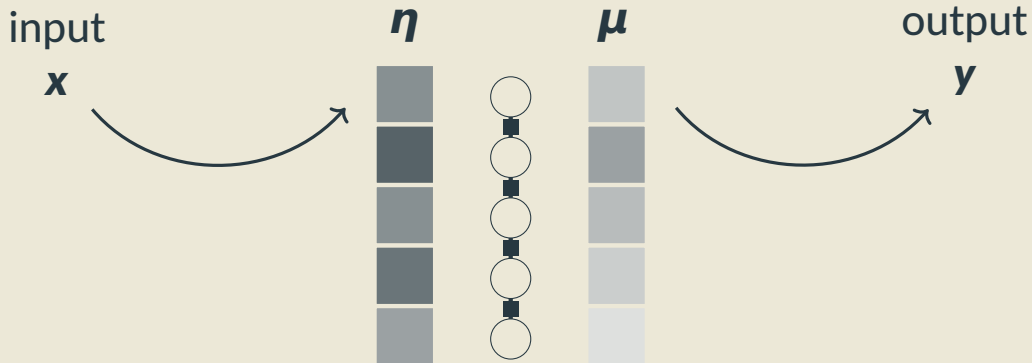
$$\boldsymbol{\mu} = \mathbf{L}(\mathbf{s})^{-1}$$

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

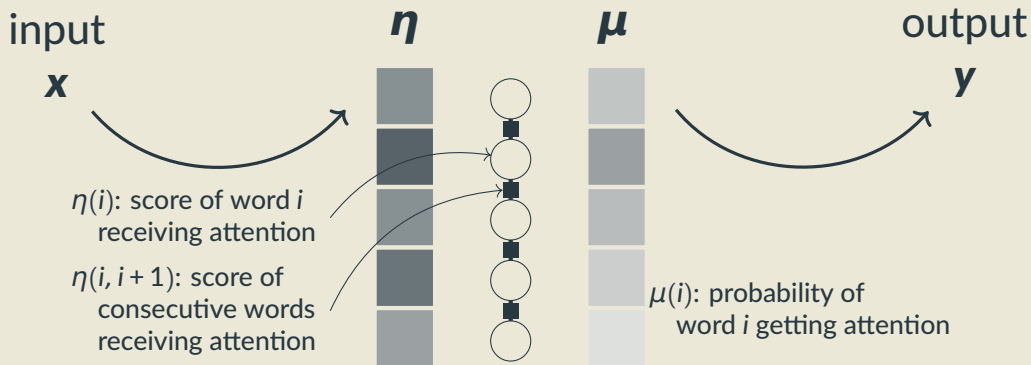
Structured Attention Networks



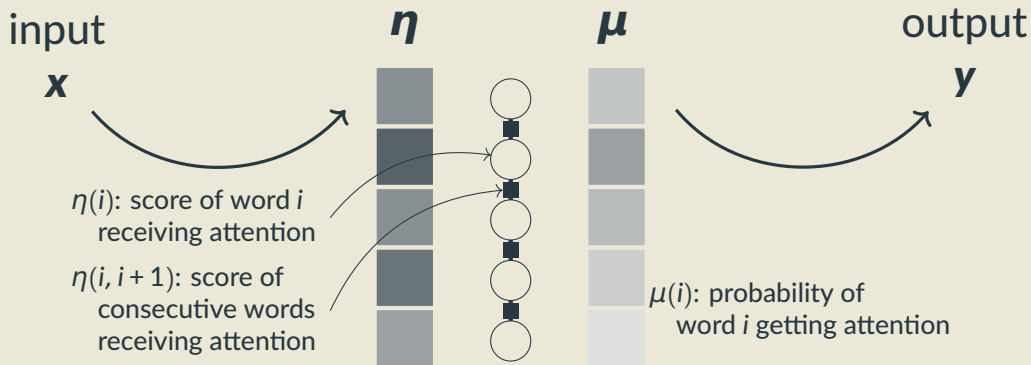
Structured Attention Networks



Structured Attention Networks

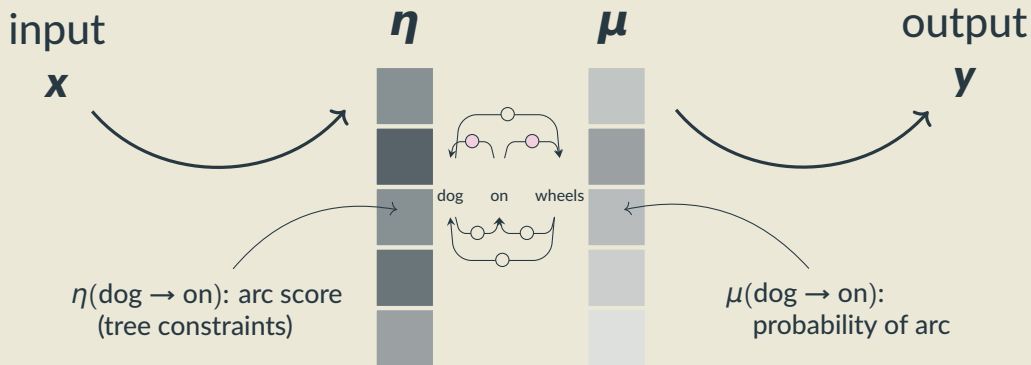


Structured Attention Networks



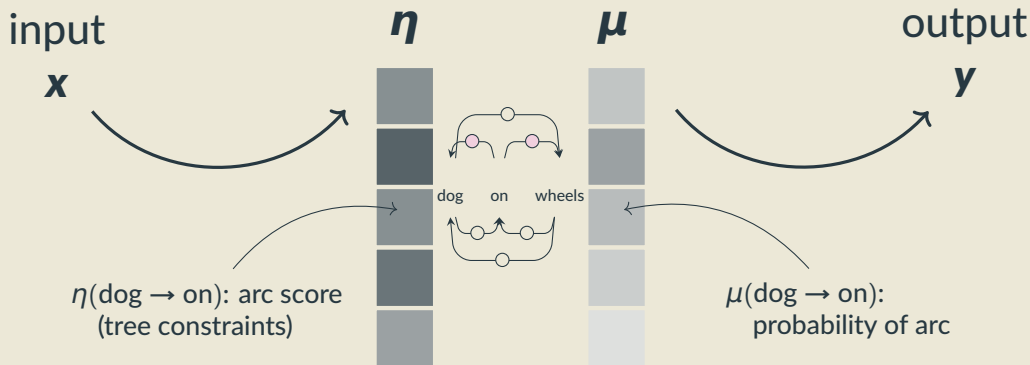
CRF marginals (from *forward-backward*) give attention weights $\in (0, 1)$

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

Structured Attention Networks



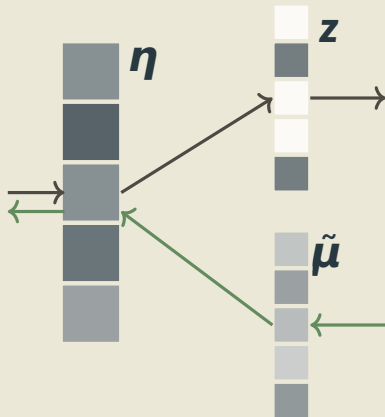
CRF marginals (from *forward-backward*) give attention weights $\in (0, 1)$
 Similar idea for projective dependency trees with *inside-outside*
 and non-projective with the Matrix-Tree theorem [Liu and Lapata, 2018].

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)



Back-propagating through marginals

Pros:

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- Familiar algorithms for NLPers,

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```

procedure BACKPROPINSIDEOUTSIDE( $\theta, p, \nabla_p^T$ )
  for  $s, t = 1, \dots, n, s \neq t$  do  $\triangleright$  Backpropagation uses the identity  $\nabla_p^T = (p \odot \nabla_p^T) / \nabla_p^{T+P}$ 
     $d[s, t] \leftarrow \log p[s, t] \odot \log \nabla_p^T[s, t]$   $\triangleright d \leftarrow \log(p \odot \nabla_p^T)$ 
     $\nabla_p^T[s, t] \leftarrow \log \nabla_p^T[s, t] \leftarrow -\infty$   $\triangleright$  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
       $t \leftarrow s + k$ 
       $\nu \leftarrow \nabla_p^T[s, t, R, 0] \odot \beta[s, t, R, 0]$   $\triangleright \nu, \gamma$  are temporary values
      for  $u = t, \dots, n$  do
         $\nabla_p^T[s, u, R, 0], \nabla_p^T[s, u, R, 1] \leftarrow \nu \odot \beta[s, u, R, 1] \odot \alpha[t, u, R, 1]$ 
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        for  $u = t, \dots, n$  do
           $\nabla_p^T[s, u, L, 1], \nabla_p^T[s, u, L, 0] \leftarrow \nu \odot \beta[s, u, L, 1] \odot \alpha[t, u, L, 1]$ 
      for  $u = 1, \dots, s - 1$  do
         $\gamma \leftarrow \beta[s, t, R, 0] \odot \alpha[u, s - 1, R, 1] \odot \theta_{s,t}$ 
         $\nabla_p^T[s, t, R, 0], \nabla_p^T[s, t, R, 1] \leftarrow \gamma \odot \log \nabla_p^T[s, t] \leftarrow \nu \odot \gamma$ 
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      for  $u = 1, \dots, s$  do
         $\nabla_p^T[s, u, R, 1], \nabla_p^T[s, u, R, 0] \leftarrow \nu \odot \beta[s, u, R, 1] \odot \alpha[u, s, R, 0]$ 
      for  $u = t + 1, \dots, n$  do
         $\nu \leftarrow \beta[s, u, R, 0] \odot \alpha[t + 1, u, L, 1] \odot \theta_{s,t}$ 
         $\nabla_p^T[s, u, R, 0], \nabla_p^T[s, u, L, 1], \log \nabla_p^T[s, u] \leftarrow \nu \odot \gamma$ 
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         $\nabla_p^T[s, u, L, 0], \nabla_p^T[s, u, L, 1], \log \nabla_p^T[s, u] \leftarrow \nu \odot \gamma$ 
  for  $k = n, \dots, 1$  do  $\triangleright$  Backpropagate through inside vsp
    for  $s = 1, \dots, n - k$  do
       $t \leftarrow s + k$ 
       $\nu \leftarrow \nabla_p^T[s, t, R, 1] \odot \alpha[s, t, R, 1]$ 
      for  $u = s + 1, \dots, t$  do
         $\nabla_p^T[s, u, R, 0], \nabla_p^T[s, u, R, 1] \leftarrow \nu \odot \alpha[s, u, R, 0] \odot \alpha[s, t, R, 1]$ 
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        for  $u = s, \dots, t - 1$  do
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           $\nabla_p^T[s, u, R, 1], \nabla_p^T[s, u + 1, t, L, 1], \log \nabla_p^T[s, u] \leftarrow \nu \odot \gamma$ 
      return signexp 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), $\alpha, \beta \leftarrow \text{emission} \leftarrow \alpha, \beta \leftarrow \text{emission} \leftarrow \alpha, \beta \leftarrow \text{emission}$.

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8])

Back-propagating through marginals

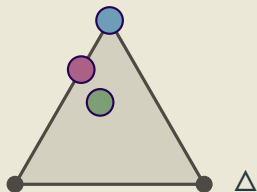
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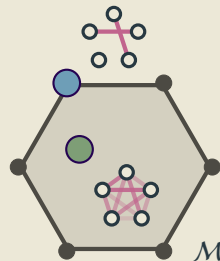
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- **argmax** $\arg \max_{\mathbf{p} \in \Delta} \mathbf{p}^T \mathbf{s}$
- **softmax** $\arg \max_{\mathbf{p} \in \Delta} \mathbf{p}^T \mathbf{s} + H(\mathbf{p})$
- **sparsemax** $\arg \max_{\mathbf{p} \in \Delta} \mathbf{p}^T \mathbf{s} - 1/2 \|\mathbf{p}\|^2$

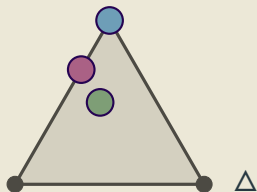


● **MAP** $\arg \max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^T \boldsymbol{\eta}$

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



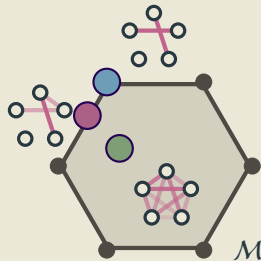
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- **SparseMAP** $\arg \max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^T \boldsymbol{\eta} - 1/2 \|\boldsymbol{\mu}\|^2$



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

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

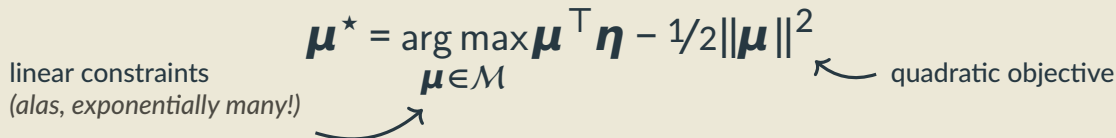
This is also $\text{proj}_{\mathcal{M}}$ required by SPIGOT!

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

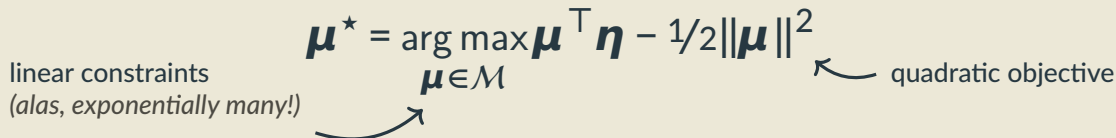


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Conditional Gradient

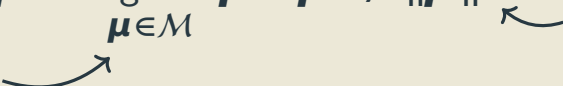
[Frank and Wolfe, 1956, Lacoste-Julien and Jaggi, 2015]

Algorithms for SparseMAP

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Conditional Gradient

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

- select a new corner of \mathcal{M}

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quadratic objective

Conditional Gradient

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

- select a new corner of \mathcal{M}

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

Algorithms for SparseMAP

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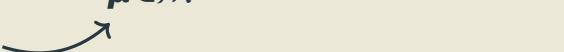
- select a new corner of \mathcal{M}
- update the (sparse) coefficients of \boldsymbol{p}
 - Update rules: vanilla, away-step, pairwise

Algorithms for SparseMAP

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(*alas, exponentially many!*)

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quadratic objective



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

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

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linear constraints
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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]

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Algorithms for SparseMAP

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

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(*alas, exponentially many!*)

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Backward pass

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

Algorithms for SparseMAP

linear constraints
(*alas, exponentially many!*)

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quadratic objective

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

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Backward pass

$\frac{\partial \boldsymbol{\mu}}{\partial \boldsymbol{\eta}}$ is sparse
computing $\left(\frac{\partial \boldsymbol{\mu}}{\partial \boldsymbol{\eta}}\right)^\top d\mathbf{y}$
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

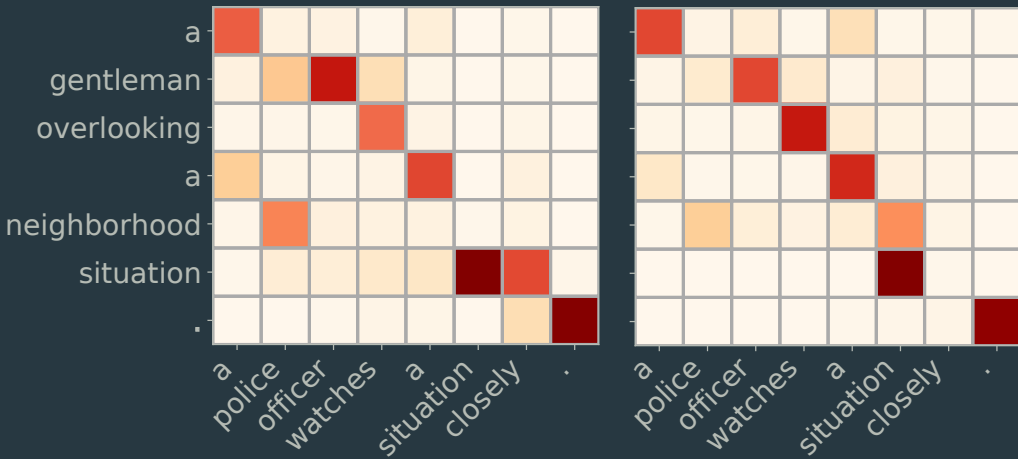
Completely modular: just add MAP

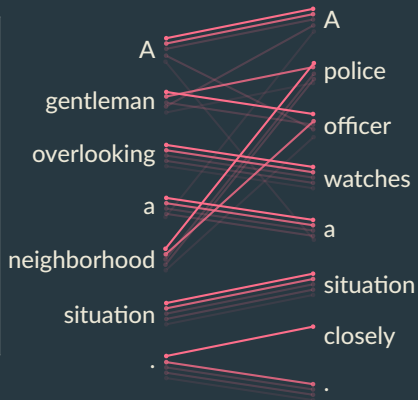
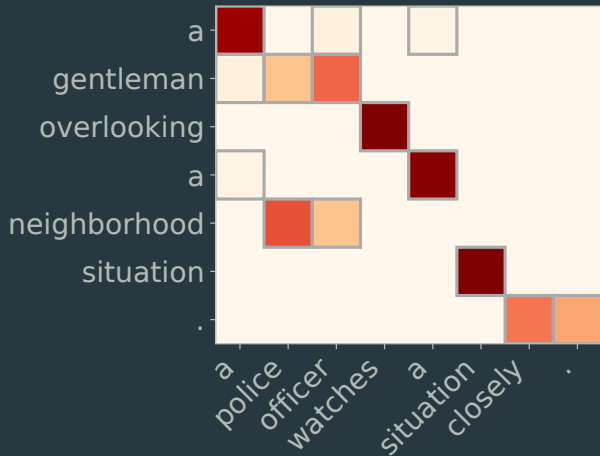
[Frank and Wolfe, 1956]

- select a new candidate \mathbf{c}
- update the (sparse) coefficients or \mathbf{p}
 - Update rules: vanilla, away-step, pairwise
 - Quadratic objective: **Active Set**
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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

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}

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parsing model,
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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}

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

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

idea 2

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Structured latent variables without sampling

sum over
all possible trees

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

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

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

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 $f_{\theta}(\mathbf{z}; x)$

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

softmax 

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

idea 2

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

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SparseMAP



Structured latent variables without sampling

$$\begin{array}{c} \text{•} \quad \text{•} \quad \text{•} \\ \text{↖} \quad \text{↗} \\ \text{•} \end{array} = .7x \quad \begin{array}{c} \text{•} \quad \text{•} \quad \text{•} \\ \text{↖} \quad \text{↗} \\ \text{•} \end{array} + .3x \quad \begin{array}{c} \text{•} \quad \text{•} \quad \text{•} \\ \text{↖} \quad \text{↗} \\ \text{•} \end{array}$$

Structured latent variables without sampling

$$\begin{matrix} \text{•} & \text{•} & \text{•} \\ \text{↖} & \text{↗} & \text{↘} \\ \text{•} & \text{•} & \text{•} \end{matrix} = .7x \quad \begin{matrix} \text{•} & \text{•} & \text{•} \\ \text{↖} & \text{↗} & \text{↘} \\ \text{•} & \text{•} & \text{•} \end{matrix} + .3x \quad \begin{matrix} \text{•} & \text{•} & \text{•} \\ \text{↖} & \text{↗} & \text{↘} \\ \text{•} & \text{•} & \text{•} \end{matrix} + 0x \quad \begin{matrix} \text{•} & \text{•} & \text{•} \\ \text{↖} & \text{↗} & \text{↘} \\ \text{•} & \text{•} & \text{•} \end{matrix} + \dots$$

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

V. Conclusions

Stanford Natural Language Inference (Accuracy)

[Kim et al., 2017]

Simple Attention 86.2

Structured Attention 86.8

[Liu and Lapata, 2018]

100D Structured Attention 86.8

[Yogatama et al., 2017]

100D RL-SPINN 80.5

[Choi et al., 2018]

100D ST Gumbel-Tree 82.6

300D - 85.6

600D - 86.0

[Corro and Titov, 2019b]

Latent Tree + 1 GCN - 85.2

Latent Tree + 2 GCN - 86.2

[Havrylov et al., 2019]

100D TreeLSTM + tricks 84.3

Stanford Sentiment (Accuracy)

[Socher et al., 2013]

Bigram Naive Bayes 83.1

[Niculae et al., 2018b]

DepTreeLSTM w/ CoreNLP 83.2

DepTreeLSTM w/ SparseMAP 84.7

[Corro and Titov, 2019b]

GCN w/ CoreNLP 83.8

GCN w/ Perturb-and-MAP 84.6

[Choi et al., 2018]

ST Gumbel-Tree 90.7

[Havrylov et al., 2019]

TreeLSTM + tricks 90.2

Is it syntax?!

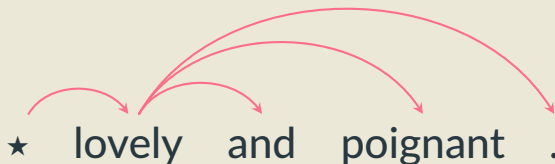
- Unlike e.g. unsupervised parsing, the structures we learn are guided by a **downstream objective** (typically discriminative).
- They don't typically resemble grammatical structure (yet) [Williams et al., 2018]
(future work: more inductive biases and constraints?)

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- 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, $p = 21.4\%$

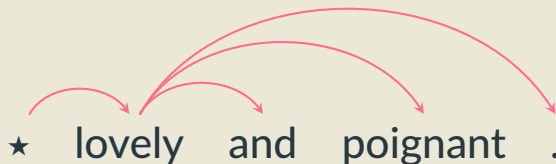


Syntax vs. Composition Order

$p = 22.6\%$

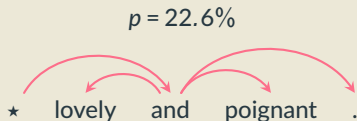


CoreNLP parse, $p = 21.4\%$

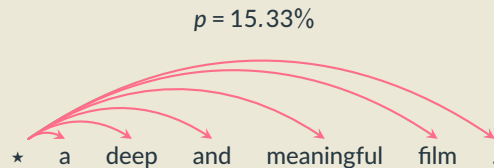
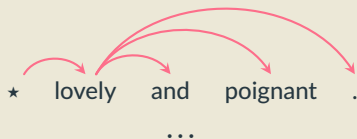


...

Syntax vs. Composition Order



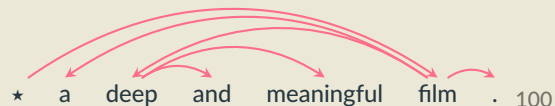
CoreNLP parse, $p = 21.4\%$



$p = 15.27\%$



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



Conclusions

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

Overview

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

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

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

- Straight-Through
- SPIGOT

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

- Structured Attn. Nets
- SparseMAP

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- REINFORCE^{SPL}
- Straight-Through Gumbel
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- SPIGOT^{MAP+}

- Structured Attn. Nets^{MRG}
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Computation:

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

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

^{MRG}: Marginal inference.

Overview

Thank you!

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