



# Learning with Sparse Latent Structure

**Vlad Niculae** University of Amsterdam (PhD opening!)

Work with: Wilker Aziz, Mathieu Blondel, Claire Cardie, Gonalo M. Correia, Andr  Martins.

# Rich Underlying Structure



## **A disastrous show of pompous and inconsequential gibberish, garish visuals and tedious storytelling**

[themadmoviemane](#) 21 December 2019

I've got nothing against movie musicals, director Tom Hooper, or even anybody who's a part of making this film. But goodness me, *Cats* is an absolute monstrosity. Garish, non-sensical, boring and everything in between, it's a pompous and pointless musical that plays out with barely a redeeming feature, proving one of the most unbearable cinema experiences I've had in a very long time.

While I haven't been a big fan of Hooper's work in the past, particularly *Les Misérables*, *Cats* pales in comparison to anything the director has made before, failing on all levels in its pathetic attempts to provide even a semblance of fun, magical theatre, and instead staggering along through its repetitive and frankly tedious story on its way to a terrible ending that can't come soon enough.

# Rich Underlying Structure



title

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body

# Rich Underlying Structure



segmentation:  
sentences,  
words,  
and so on

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# Rich Underlying Structure



segmentation:  
sentences,  
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and so on

entities

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relationships  
e.g., dependency

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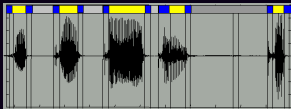
Most of this structure is **hidden**.

# Rich Underlying Structure

## Widely occurring pattern!

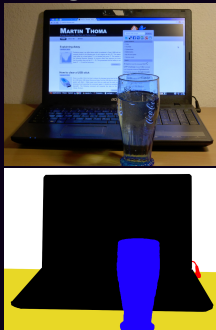
*speech*

(Andre-Obrecht, 1988)



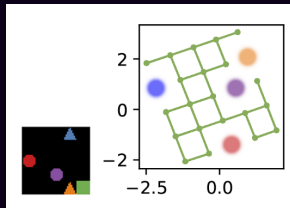
*objects*

(Long et al., 2015)



*transition graphs*

(Kipf, Pol, et al., 2020)



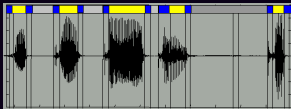


# Rich Underlying Structure

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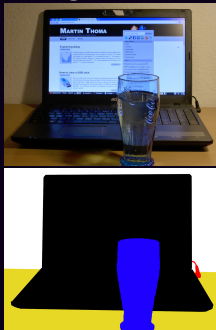
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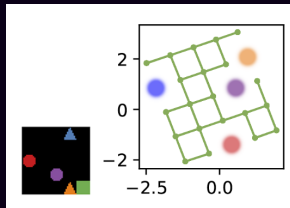
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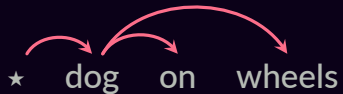
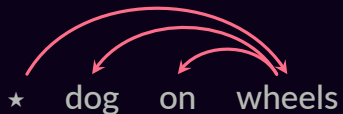
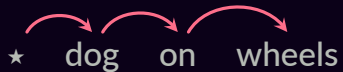
(Kipf, Pol, et al., 2020)



But we'll focus on NLP.

# Structured Prediction

...

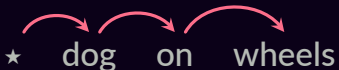


...

# Structured Prediction

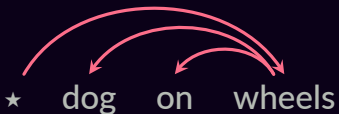
...

VERB    PREP    NOUN  
dog    on    wheels



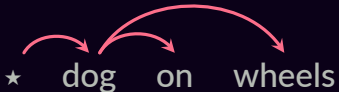
dog    hond  
on    op  
wheels    wielen

NOUN    PREP    NOUN  
dog    on    wheels



dog    hond  
on    op  
wheels    wielen

NOUN    DET    NOUN  
dog    on    wheels



dog    hond  
on    op  
wheels    wielen

...

# Structured Prediction



# Traditional Pipeline Approach

input



output



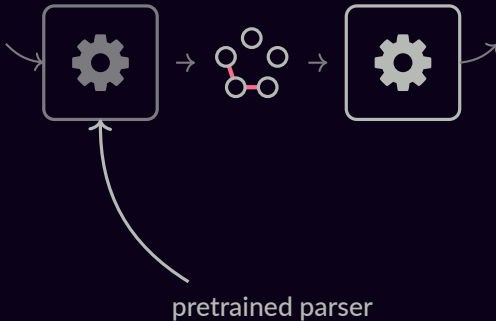
positive

neutral

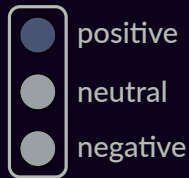
negative

# Traditional Pipeline Approach

input

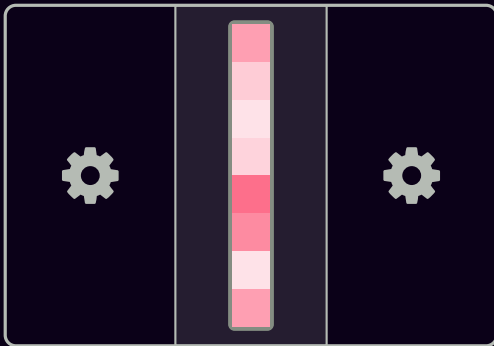


output

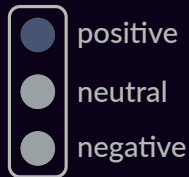


# Deep Learning & Hidden Representations

input

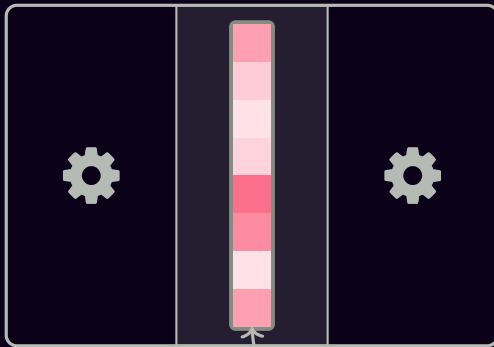


output



# Deep Learning & Hidden Representations

input



output



positive

neutral

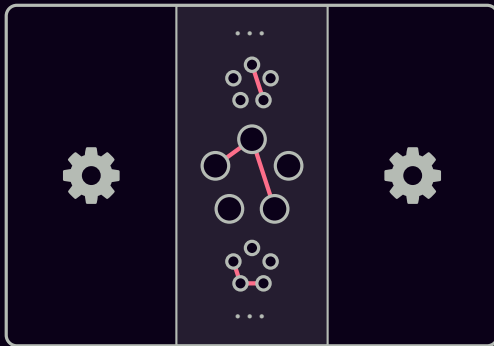
negative

dense vector

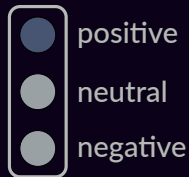


# Latent Structure Models

input



output



\*record scratch\*

\*freeze frame\*

**How to select an item  
from a set?**

# How to select an item from a set?



...



# How to select an item from a set?

$c_1$

$c_2$

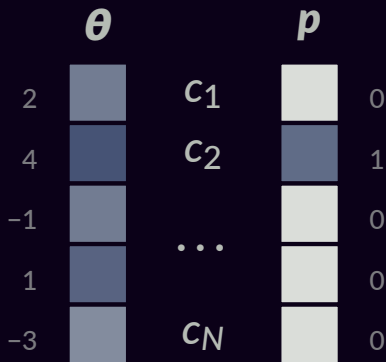
...

$c_N$

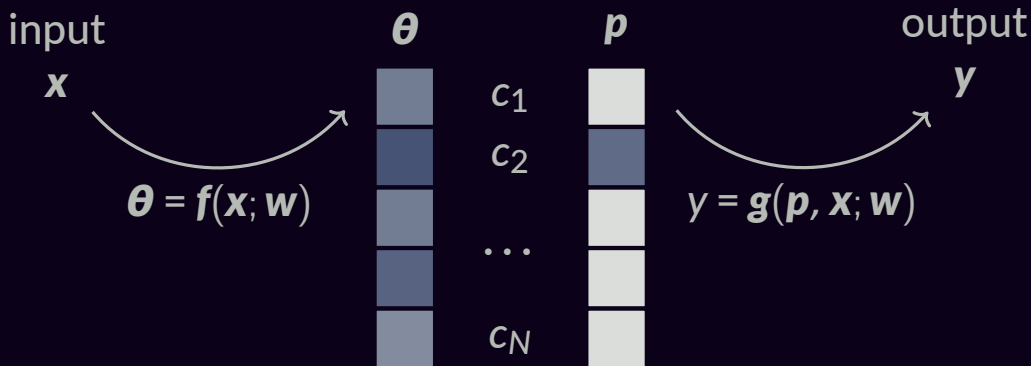
# How to select an item from a set?



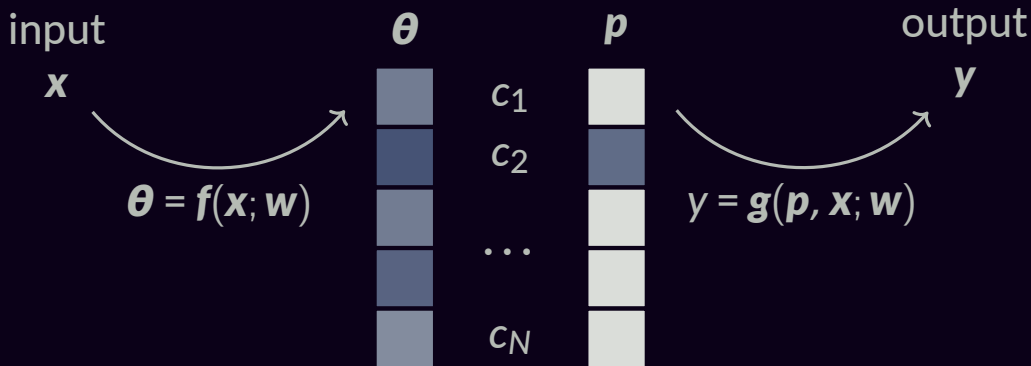
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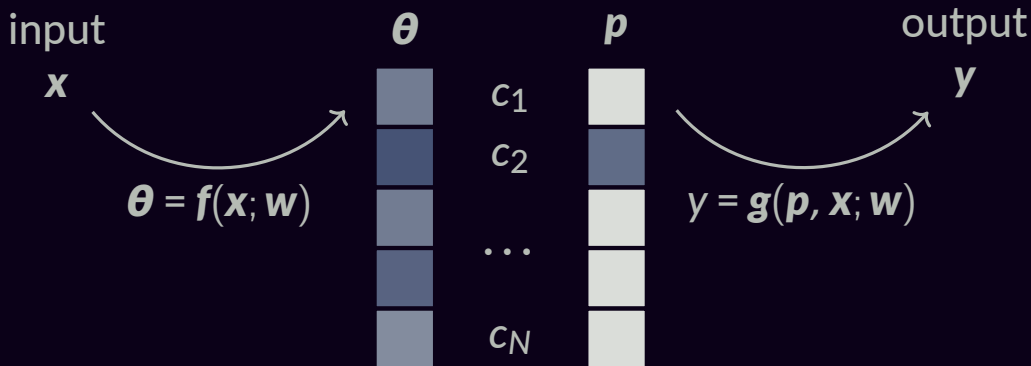
# How to select an item from a set?



$$\frac{\partial y}{\partial w} = ?$$



# How to select an item from a set?

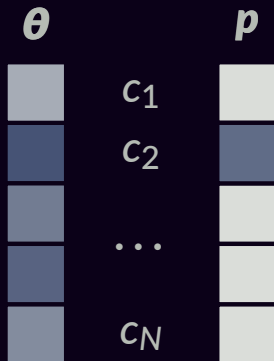


$$\frac{\partial y}{\partial w} = ?$$

or, essentially,









$$\frac{\partial p}{\partial \theta} = ?$$

# Argmax











$$\frac{\partial p}{\partial \theta} = ?$$

# Argmax

$\theta$		$p$
	$c_1$	
	$c_2$	
	$\dots$	
		
	$c_N$	








$$\frac{\partial p}{\partial \theta} = ?$$

# Argmax

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# Argmax



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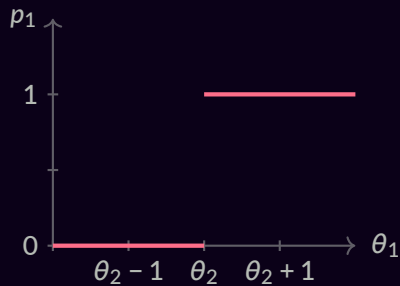
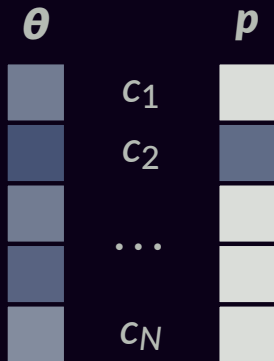
# Argmax



$$\frac{\partial p}{\partial \theta} = ?$$



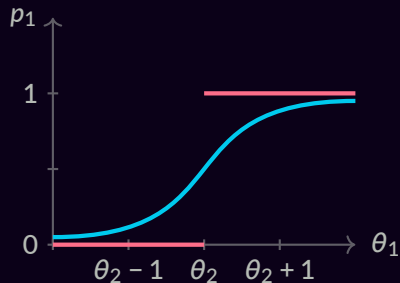
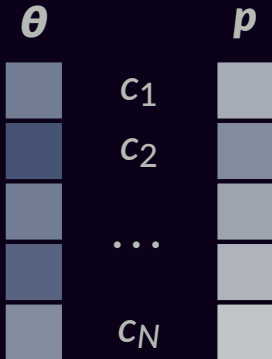
# Argmax



$$\frac{\partial p}{\partial \theta} = \mathbf{0}$$

# Argmax vs. Softmax

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



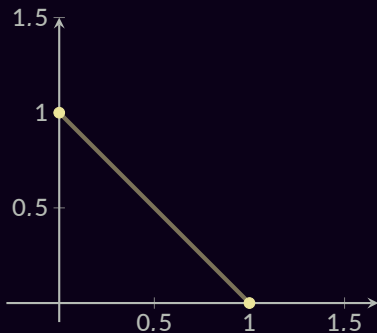
$$\frac{\partial \mathbf{p}}{\partial \boldsymbol{\theta}} = \text{diag}(\mathbf{p}) - \mathbf{p}\mathbf{p}^T$$

# A Softmax Origin Story

$$\Delta = \{\mathbf{p} \in \mathbb{R}^N : \mathbf{p} \geq \mathbf{0}, \mathbf{1}^\top \mathbf{p} = 1\}$$

# A Softmax Origin Story

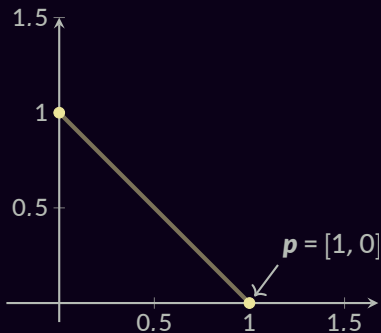
$$\Delta = \{p \in \mathbb{R}^N : p \geq 0, \mathbf{1}^\top p = 1\}$$



$N = 2$

# A Softmax Origin Story

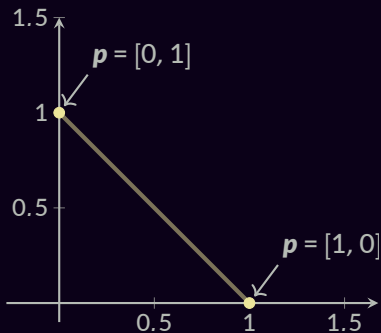
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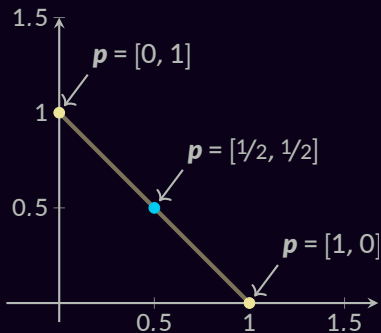
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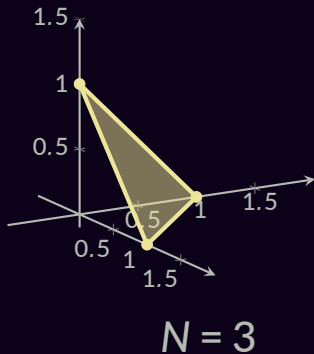
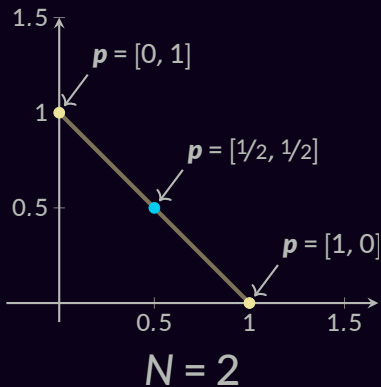
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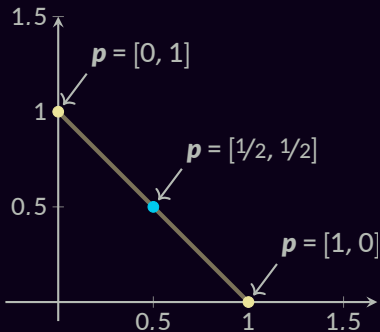
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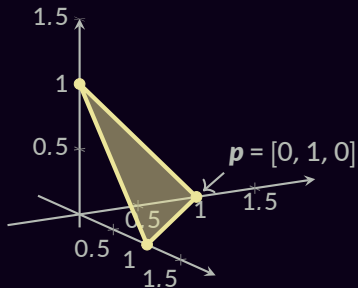


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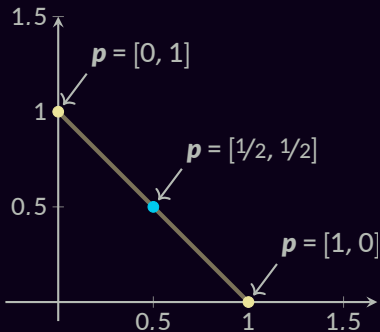
$N = 2$



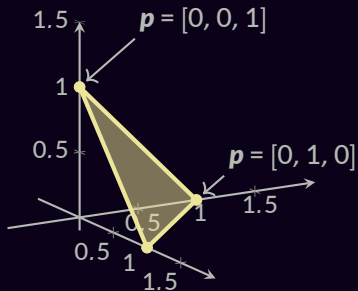
$N = 3$

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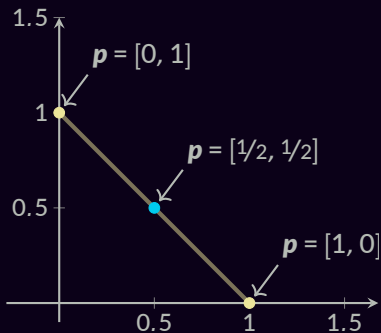
$N = 2$



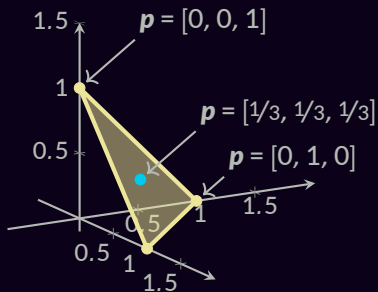
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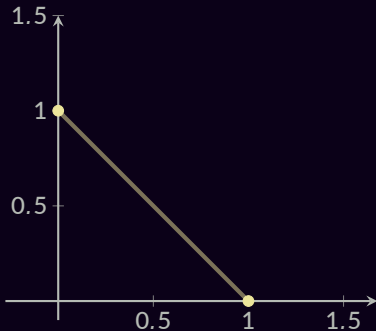


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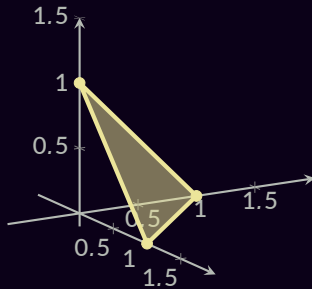
# A Softmax Origin Story

$$\max_j \theta_j = \max_{p \in \Delta} p^T \theta$$

Fundamental Thm. Lin. Prog.  
(Dantzig et al., 1955)



$N = 2$

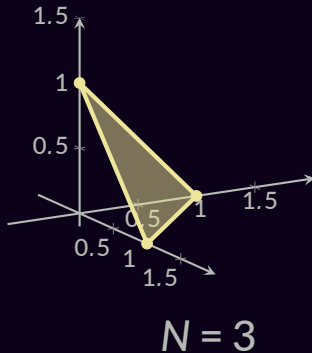
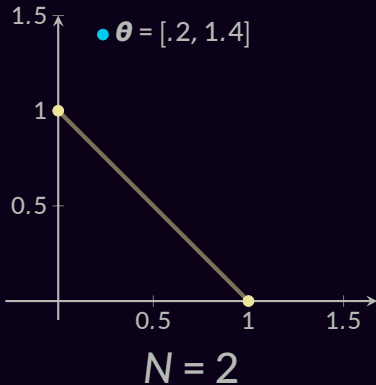


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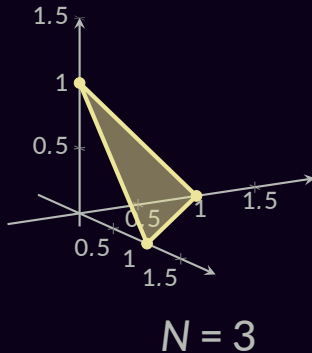
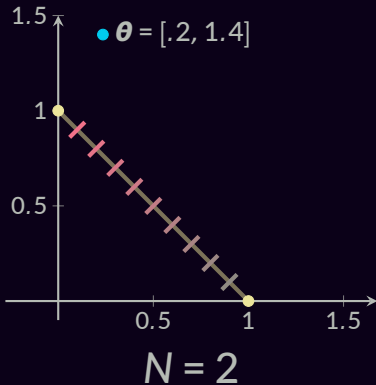
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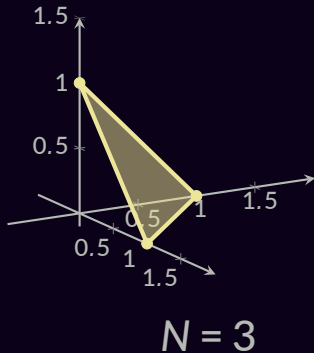
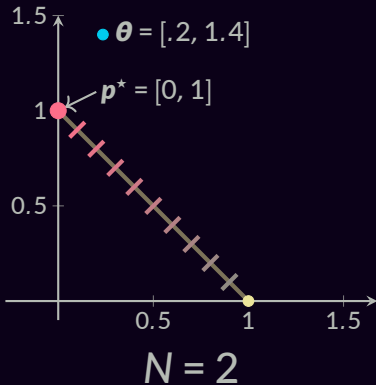
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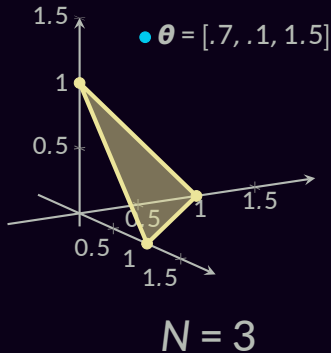
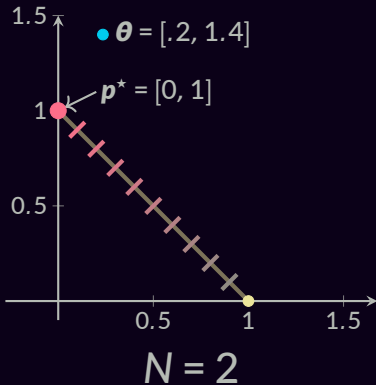
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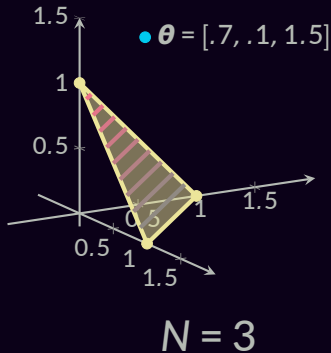
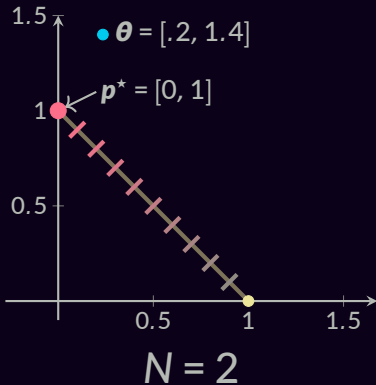




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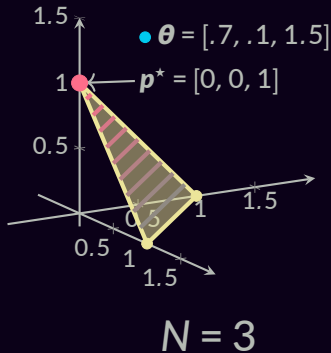
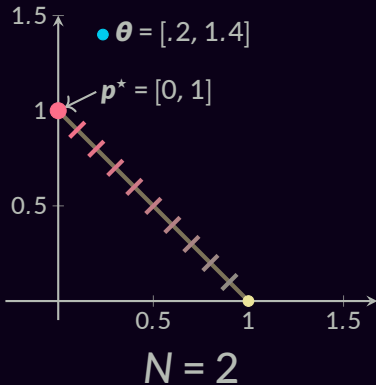
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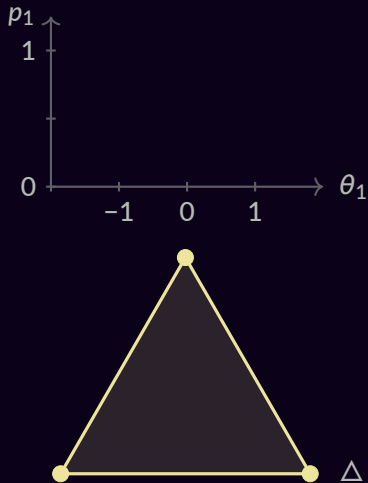
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Fundamental Thm. Lin. Prog.  
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# Smoothed Max Operators

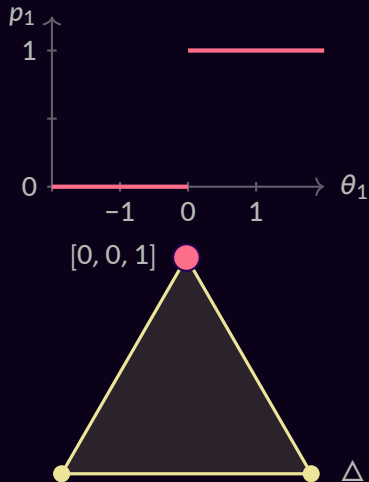
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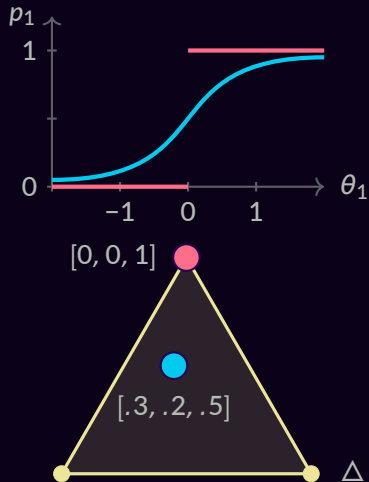
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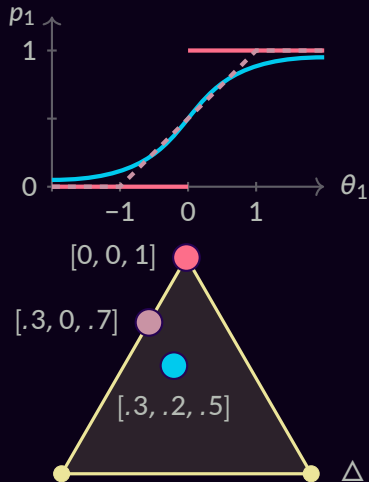
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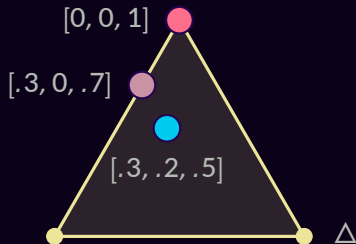
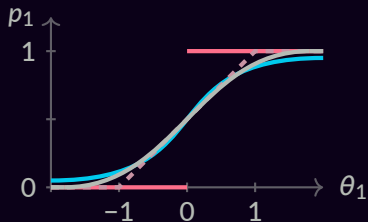
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Tsallis (1988); a generalized entropy (Grünwald and Dawid, 2004)  
 (Blondel, Martins, and Niculae 2019a;  
 Peters, Niculae, and Martins 2019;  
 Correia, Niculae, and Martins 2019)

# Sparsemax

$$\begin{aligned}\text{sparsemax}(\boldsymbol{\theta}) &= \arg \max_{\boldsymbol{p} \in \Delta} \boldsymbol{p}^\top \boldsymbol{\theta} - 1/2 \|\boldsymbol{p}\|_2^2 \\ &= \arg \min_{\boldsymbol{p} \in \Delta} \|\boldsymbol{p} - \boldsymbol{\theta}\|_2^2\end{aligned}$$



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**Computation:**

$$\mathbf{p}^\star = [\boldsymbol{\theta} - \tau \mathbf{1}]_+$$

$$\theta_i > \theta_j \Rightarrow p_i \geq p_j$$

$O(d)$  via partial sort

(Held et al., 1974; Brucker, 1984; Condat, 2016)

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**Backward pass:**

$$\mathbf{J}_{\text{sparsemax}} = \text{diag}(\mathbf{s}) - \frac{1}{|\mathcal{S}|} \mathbf{s} \mathbf{s}^\top$$

$$\text{where } \mathcal{S} = \{j : p_j^\star > 0\},$$

$$s_j = \mathbb{I}[j \in \mathcal{S}]$$

(Martins and Astudillo, 2016)

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**Computation:**

$\mathbf{p}^* = [\theta_i - \theta_j]$   
 $\theta_i > \theta_j$   
 $O(d)$  via

**argmin differentiation**

(Gould et al., 2016; Amos and Kolter, 2017)

**Backward pass:**

$g(\mathbf{s}) - \frac{1}{|S|} \mathbf{s} \mathbf{s}^\top$   
 $: p_j^* > 0\}$ ,  
 $\in S]$

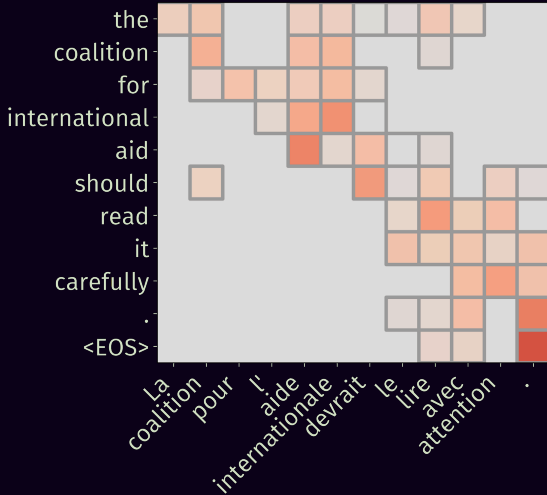
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(Martins and Astudillo, 2016)

## First applications:

## sparse attention

(Martins and Astudillo, 2016; Correia, Niculae, and Martins, 2019)



sparse losses (& seq2seq)

(Blondel et al., 2019a; Peters et al., 2019)

d → r → a → w → e → d → </s>  
 66.4%  
 32.2%  
 1.4%

# Latent variable models!

$$\begin{aligned} p(y \mid x) &= \sum_{h \in \mathcal{H}} p_{\boldsymbol{\phi}}(y \mid h, x) p_{\boldsymbol{\pi}}(h \mid x) \\ &= \mathbb{E}_{h \sim p_{\boldsymbol{\pi}}(h|x)} p_{\boldsymbol{\phi}}(y \mid h, x) \end{aligned}$$

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receiver

sender

- Emergent communication:  $h$  is a word from a big vocabulary.  $p_{\phi}(y | h)$  is expensive.

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sum over  
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- **Idea: parametrize  $p_{\pi}(h | x)$  using sparsemax!** Sum only over  $|\bar{\mathcal{H}}| \ll |\mathcal{H}|$ .  
No bias AND no variance by **changing the question**

# Emergent Communication



... but make it harder:  $|\mathcal{H}| = 256$



Method	success (%)	Dec. calls
<i>Monte Carlo</i>		
SFE	33.05 $\pm 2.84$	1
NVIL	37.04 $\pm 1.61$	1
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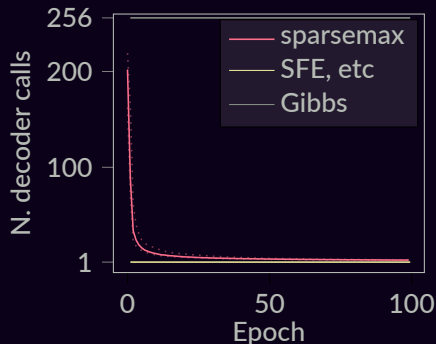
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# Limitations

- Mostly (and eventually) very sparse.  
But  $\text{sparsemax}(\mathbf{0}) = 1/d \mathbf{1}$ : fully dense worst case.
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One solution: **top-k sparsemax**

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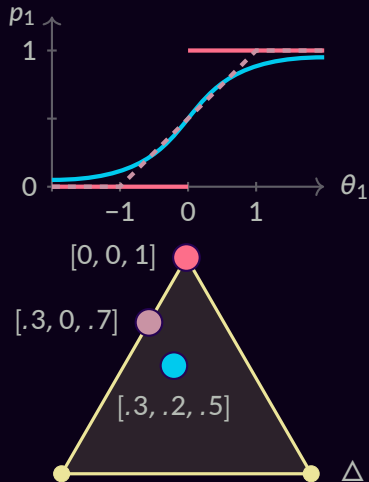
- Non-convex but easy: sparsemax over the  $k$  highest scores (Kyrillidis et al., 2013).
- Top-k oracle available for some structured problems.
- Certificate: if at least one of the top-k  $h$  gets  $p(h) = 0$ , **k-sparsemax = sparsemax!**  
thus, for latent variables: biased early on, but it goes away.



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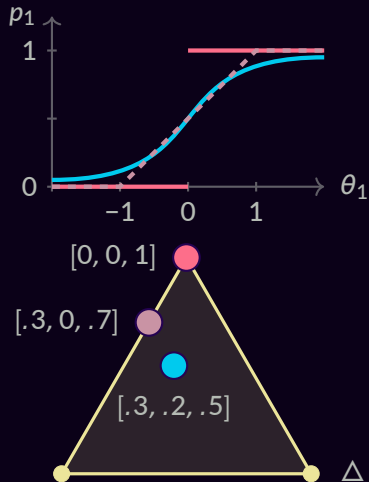
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- fusedmax:  $\Omega(\mathbf{p}) = 1/2 \|\mathbf{p}\|_2^2 + \sum_j |p_j - p_{j-1}|$

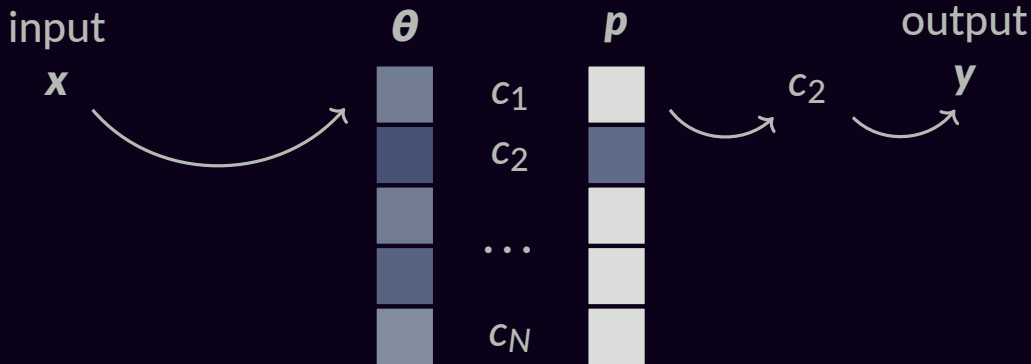


# Structured Prediction

finally

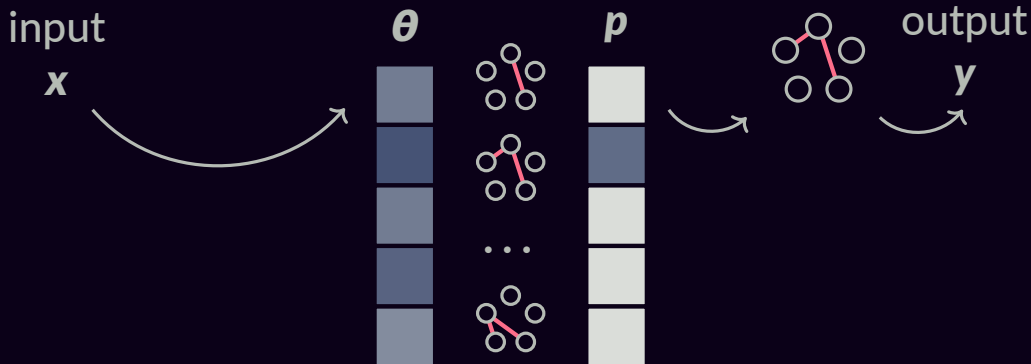
# Structured Prediction

is essentially a (very high-dimensional) argmax



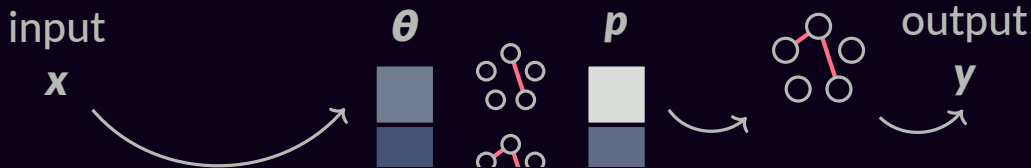
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There are exponentially  
many structures

( $\theta$  cannot fit in memory!)

# Factorization Into Parts



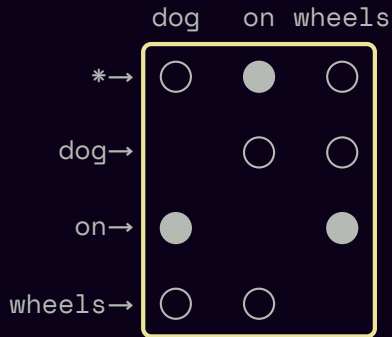
# Factorization Into Parts



	dog	on	wheels
*→	<input type="radio"/>	<input checked="" type="radio"/>	<input type="radio"/>
dog→		<input type="radio"/>	<input type="radio"/>
on→	<input checked="" type="radio"/>		<input checked="" type="radio"/>
wheels→	<input type="radio"/>	<input type="radio"/>	

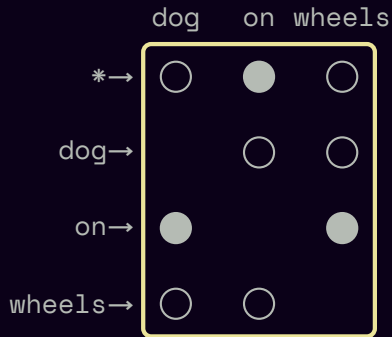


# Factorization Into Parts



TREE

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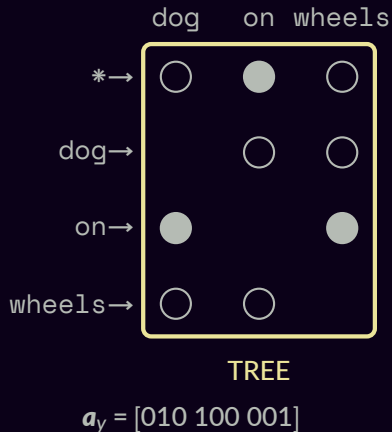
TREE

$$\mathbf{a}_y = [010 \ 100 \ 001]$$

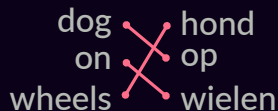
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$$\mathbf{A} = \begin{array}{l} \text{star} \rightarrow \text{dog} \\ \text{on} \rightarrow \text{dog} \\ \text{wheels} \rightarrow \text{dog} \\ \text{star} \rightarrow \text{on} \\ \text{dog} \rightarrow \text{on} \\ \text{wheels} \rightarrow \text{on} \\ \text{star} \rightarrow \text{wheels} \\ \text{dog} \rightarrow \text{wheels} \\ \text{on} \rightarrow \text{wheels} \end{array} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ \hline 0 & 1 & 1 \\ 1 & \dots & 0 & 0 & \dots \\ 0 & 0 & 0 \\ \hline 0 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \quad \boldsymbol{\eta} = \begin{bmatrix} .1 \\ .2 \\ -.1 \\ \hline .3 \\ .8 \\ .1 \\ \hline -.3 \\ .2 \\ -.1 \end{bmatrix}$$

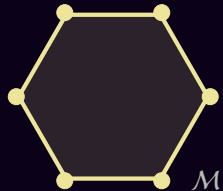
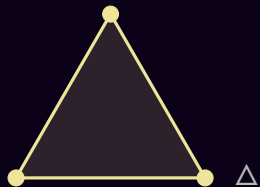


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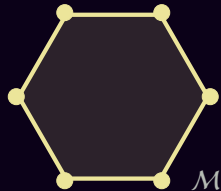
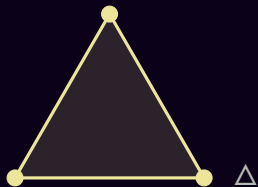


$$\mathbf{A} = \begin{bmatrix} \star \rightarrow \text{dog} & 1 & 0 & 0 \\ \text{on} \rightarrow \text{dog} & 0 & 1 & 1 \\ \text{wheels} \rightarrow \text{dog} & 0 & 0 & 0 \\ \hline \star \rightarrow \text{on} & 0 & 1 & 1 \\ \text{dog} \rightarrow \text{on} & 1 & \dots & 0 & 0 & \dots \\ \text{wheels} \rightarrow \text{on} & 0 & 0 & 0 \\ \hline \star \rightarrow \text{wheels} & 0 & 0 & 0 \\ \text{dog} \rightarrow \text{wheels} & 0 & 1 & 0 \\ \text{on} \rightarrow \text{wheels} & 1 & 0 & 1 \end{bmatrix} \quad \boldsymbol{\eta} = \begin{bmatrix} .1 \\ .2 \\ -.1 \\ \hline .3 \\ .8 \\ .1 \\ \hline -.3 \\ .2 \\ -.1 \end{bmatrix}$$

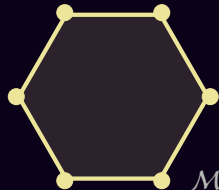
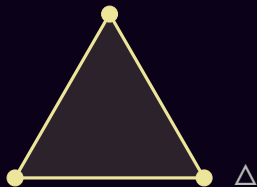
$$\mathbf{A} = \begin{bmatrix} \text{dog} - \text{hond} & 1 & 0 & 0 \\ \text{dog} - \text{op} & 0 & 1 & 1 \\ \text{dog} - \text{wielen} & 0 & 0 & 0 \\ \hline \text{on} - \text{hond} & 0 & 0 & 0 \\ \text{on} - \text{op} & 1 & \dots & 0 & 0 & \dots \\ \text{on} - \text{wielen} & 0 & 1 & 1 \\ \hline \text{wheels} - \text{hond} & 0 & 1 & 0 \\ \text{wheels} - \text{op} & 0 & 0 & 0 \\ \text{wheels} - \text{wielen} & 1 & 0 & 1 \end{bmatrix} \quad \boldsymbol{\eta} = \begin{bmatrix} .1 \\ .2 \\ -.1 \\ \hline .3 \\ .8 \\ .1 \\ \hline -.3 \\ .2 \\ -.1 \end{bmatrix}$$



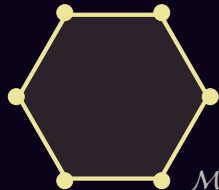
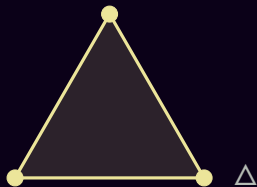
$$\mathcal{M} := \text{conv} \{ \mathbf{a}_h : h \in \mathcal{H} \}$$



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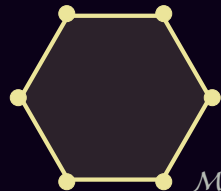
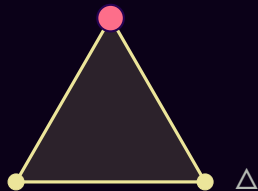


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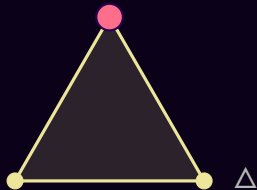




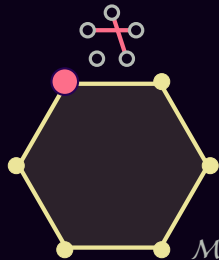
●  $\mathbf{argmax} \arg \max_{p \in \Delta} p^T \theta$



• **argmax**  $\arg \max_{p \in \Delta} p^\top \theta$



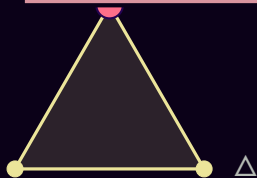
• **MAP**  $\arg \max_{\mu \in \mathcal{M}} \mu^\top \eta$



●  $\mathbf{argmax}_{p \in \Delta} p^T \theta$

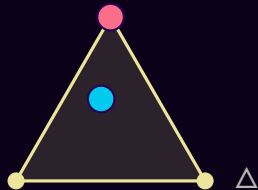
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e.g. dependency parsing → **Chu-Liu/Edmonds**  
matching → **Kuhn-Munkres**

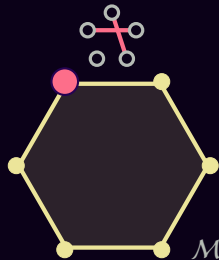


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- **softmax**  $\arg \max_{p \in \Delta} p^\top \theta + H(p)$

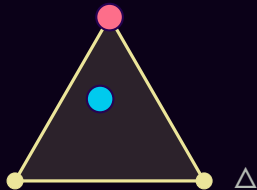


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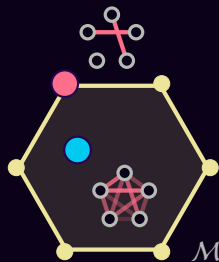
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● **marginals**  $\arg \max_{\mu \in \mathcal{M}} \mu^\top \eta + \tilde{H}(\mu)$



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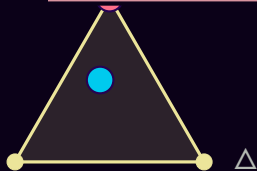
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● **marginals**  $\arg \max_{\mu \in \mathcal{M}} \mu^\top \eta + \tilde{H}(\mu)$

e.g. sequence labeling  $\rightarrow$  forward-backward

(Rabiner, 1989)

As attention: (Kim et al., 2017)



- **argmax**  $\arg \max_{p \in \Delta} p^\top \theta$

- **softmax**  $\arg \max_{p \in \Delta} p^\top \theta + H(p)$

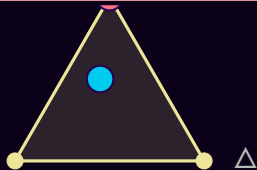
- **MAP**  $\arg \max_{\mu \in \mathcal{M}} \mu^\top \eta$

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e.g. dependency parsing → **the Matrix-Tree theorem**

(Koo et al., 2007; D. A. Smith and N. A. Smith, 2007; McDonald and Satta, 2007)

As attention: (Liu and Lapata, 2018)



● **argmax**  $\arg \max_{p \in \Delta} p^\top \theta$

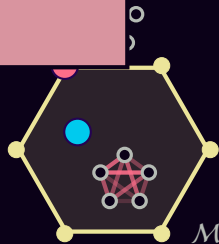
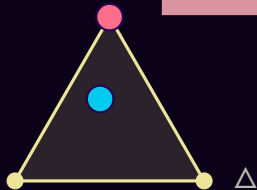
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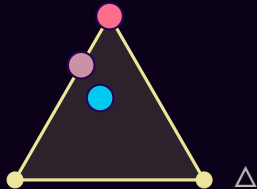
e.g. matchings  $\rightarrow$  **#P-complete!**

(Taskar, 2004; Valiant, 1979)



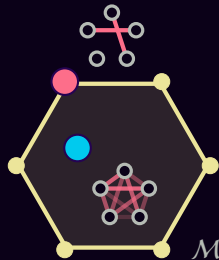


- **argmax**  $\arg \max_{p \in \Delta} p^\top \theta$
- **softmax**  $\arg \max_{p \in \Delta} p^\top \theta + H(p)$
- **sparsemax**  $\arg \max_{p \in \Delta} p^\top \theta - 1/2 \|p\|^2$



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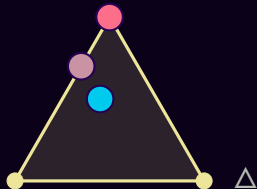
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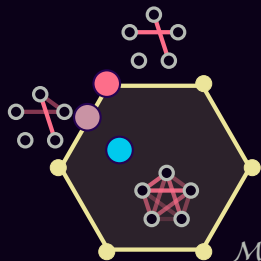
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● **MAP**  $\arg \max_{\mu \in \mathcal{M}} \mu^\top \eta$

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

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



# Algorithms for SparseMAP

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

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linear constraints  
(*alas, exponentially many!*)

quadratic objective

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(Frank and Wolfe, 1956; Lacoste-Julien and Jaggi, 2015)

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

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(Frank and Wolfe, 1956; Lacoste-Julien and Jaggi, 2015)

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quadratic objective

## Conditional Gradient

(Frank and Wolfe, 1956; Lacoste-Julien and Jaggi, 2015)

- select a new corner
- update the (sparse) **Active Set achieves finite & linear convergence!**

- Update rules: van
- Quadratic objective: **Active Set**

(Nocedal and Wright, 1999, Ch. 16.4 & 16.5)

(Wolfe, 1976; Vinyes and Obozinski, 2017)

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

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

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linear constraints  
(*alas, exponentially many!*)

quadratic objective

**Condition** Completely modular: just add MAP pass

(Frank and Wolfe, 1956)

- select a new corner of  $\mathcal{M}$
- update the (sparse) coefficients of  $\mathbf{p}$ 
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takes  $O(\dim(\boldsymbol{\mu}) \text{nnz}(\mathbf{p}^*))$

# SparseMAP Applications

- **Sparse alignment attention**  
(Nicolae, Martins, Blondel, and Cardie, 2018)
- **Latent TreeLSTM**  
(Nicolae, Martins, and Cardie, 2018)
- **As loss: supervised dependency parsing**  
(Nicolae, Martins, Blondel, and Cardie 2018;  
Blondel, Martins, and Nicolae 2019b)

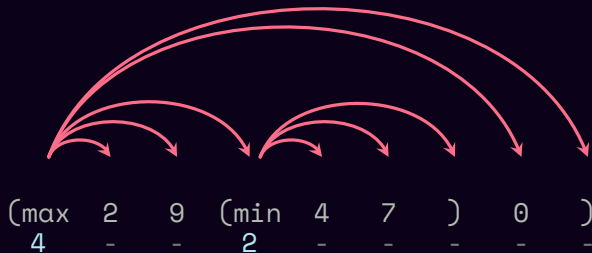
# Latent Dependency Trees

Arity tagging with latent GCN (Corro and Titov, 2019; Kipf and Welling, 2017)

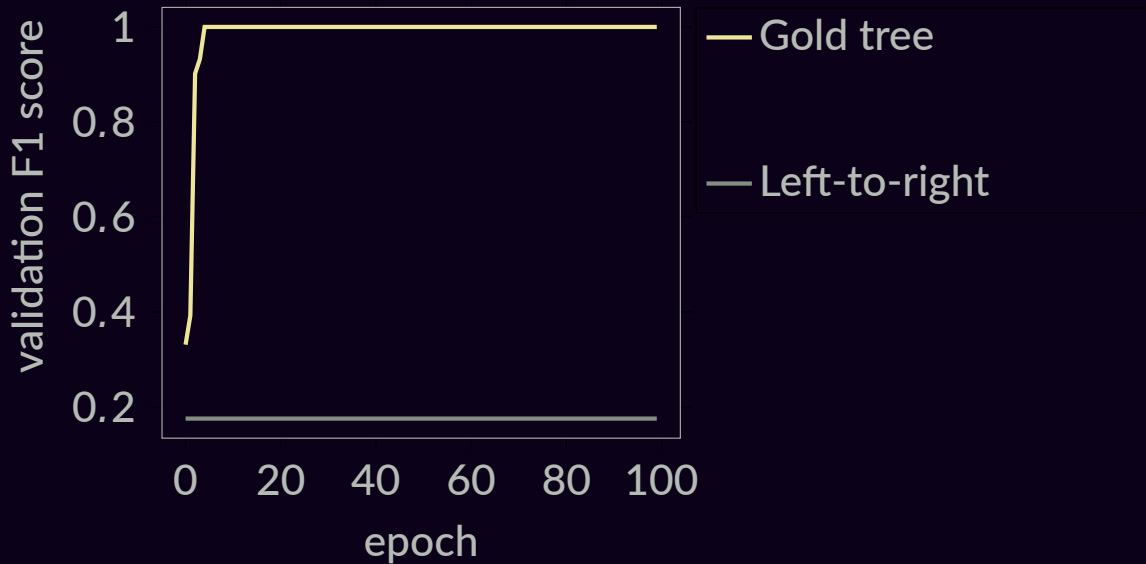
(max 2 9 (min 4 7 ) 0 )

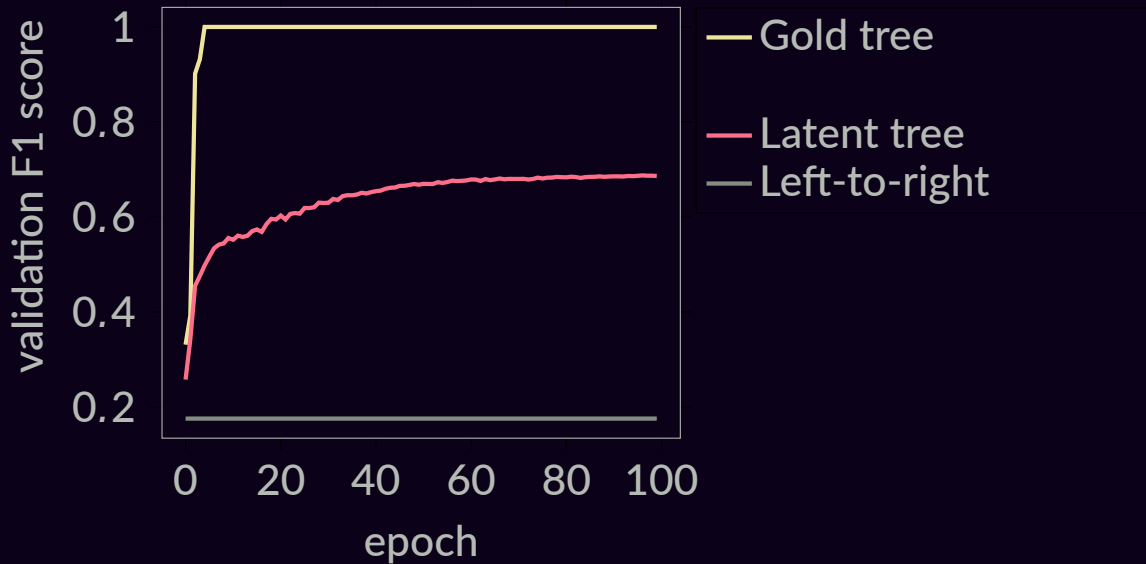
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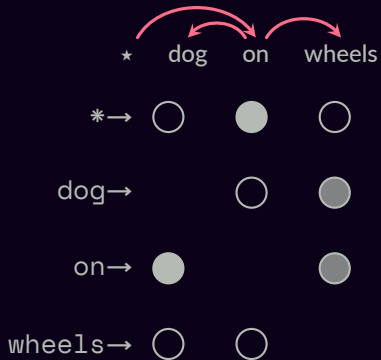




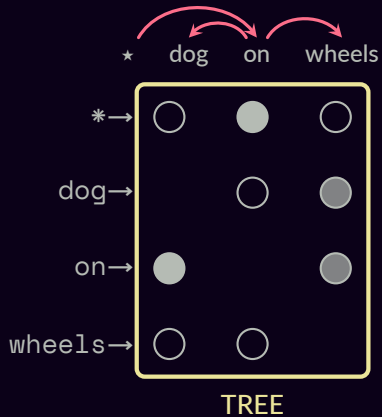


**What if MAP is not  
available?**

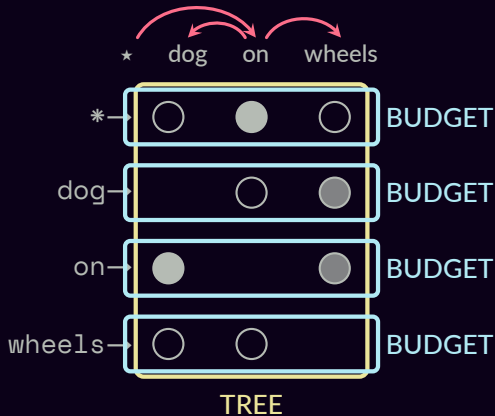
# Multiple, Overlapping Factors



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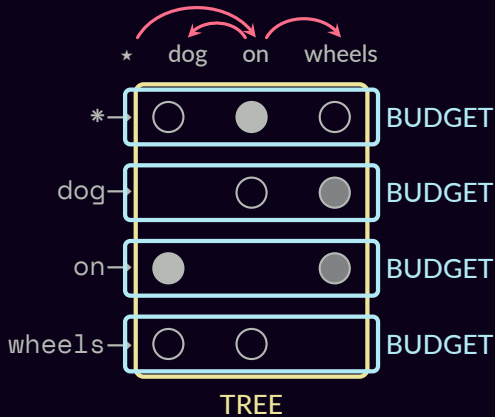


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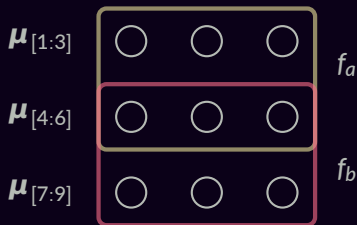


# Multiple, Overlapping Factors

Maximization in factor graphs: NP-hard, even when each factor is tractable.

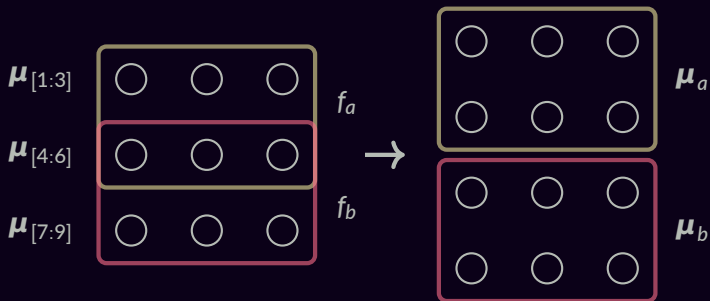


# Optimization as Consensus-Seeking

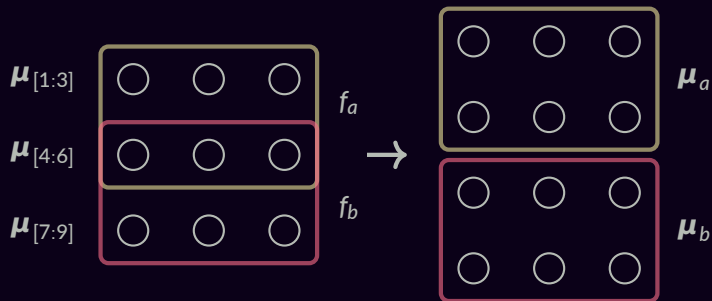




# Optimization as Consensus-Seeking



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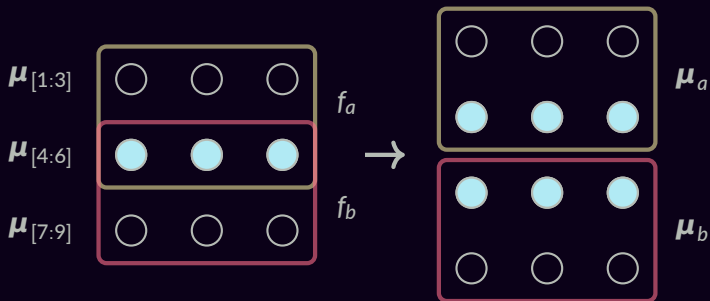


$$\max_{\mu_f} \sum_{f \in \mathcal{F}} \eta_f^\top \mu_f$$

s.t.

$$\mu_f \in \mathcal{M}_f \text{ for } f \in \mathcal{F}$$

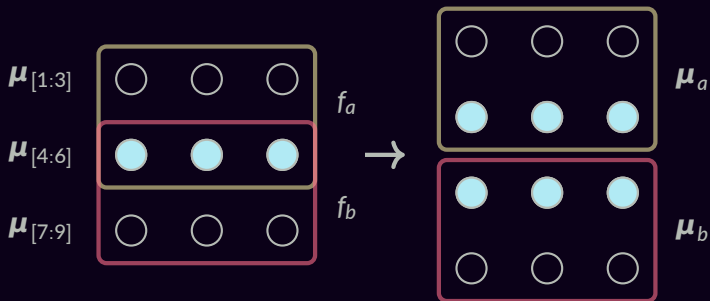
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Agreement on overlap:  $\boldsymbol{\mu}_{a,[4:6]} = \boldsymbol{\mu}_{b,[4:6]} = \boldsymbol{\mu}_{[4:6]}$

$$\max_{\boldsymbol{\mu}_f} \sum_{f \in \mathcal{F}} \boldsymbol{\eta}_f^\top \boldsymbol{\mu}_f \quad \text{s.t.} \quad \boldsymbol{\mu}_f \in \mathcal{M}_f \text{ for } f \in \mathcal{F}$$

# Optimization as Consensus-Seeking



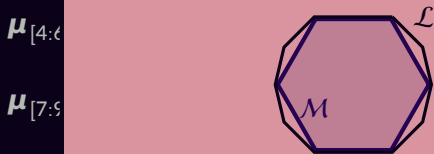
Agreement on overlap:  $\boldsymbol{\mu}_{a,[4:6]} = \boldsymbol{\mu}_{b,[4:6]} = \boldsymbol{\mu}_{[4:6]}$

$$\max_{\boldsymbol{\mu}, \boldsymbol{\mu}_f} \sum_{f \in \mathcal{F}} \boldsymbol{\eta}_f^\top \boldsymbol{\mu}_f$$

$$\text{s.t. } \mathbf{C}_f \boldsymbol{\mu} = \boldsymbol{\mu}_f, \boldsymbol{\mu}_f \in \mathcal{M}_f \text{ for } f \in \mathcal{F}$$

the local polytope:

$$\mathcal{L} := \{\boldsymbol{\mu} : \mathbf{C}_f \boldsymbol{\mu} \in \mathcal{M}_f, f \in \mathcal{F}\} \supseteq \mathcal{M}$$

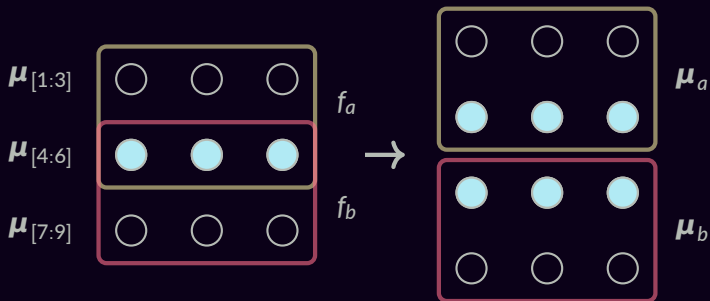


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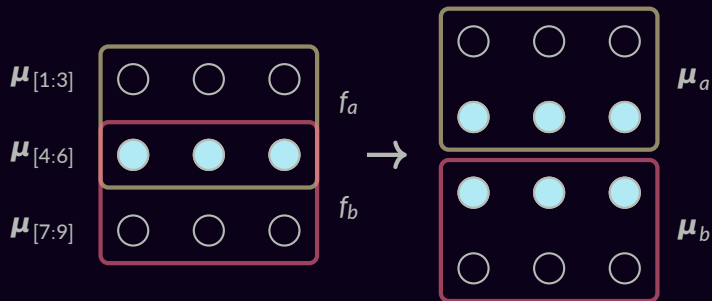


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# Algorithms for LP-SparseMAP

## Forward pass

$$\begin{aligned} & \arg \max_{\mathbf{C}_f \boldsymbol{\mu} = \boldsymbol{\mu}_f} \left( \sum_{f \in \mathcal{F}} \boldsymbol{\eta}_f^\top \boldsymbol{\mu}_f \right) - 1/2 \|\boldsymbol{\mu}\|^2 \\ &= \arg \max_{\mathbf{C}_f \boldsymbol{\mu} = \boldsymbol{\mu}_f} \sum_{f \in \mathcal{F}} \left( \boldsymbol{\eta}_f^\top \boldsymbol{\mu}_f - 1/2 \|\mathbf{D}_f \boldsymbol{\mu}_f\|^2 \right) \end{aligned}$$

- Separable objective,  
agreement constraints  
ADMM in consensus form
- SparseMAP subproblem for each  $f$



# Algorithms for LP-SparseMAP

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- Separable objective, agreement constraints  
ADMM in consensus form
- SparseMAP subproblem for each  $f$

## Backward pass

- Jacobian fixed-point characterization

$$\mathbf{J} = \begin{bmatrix} \mathbf{C}_{f_a} \\ \mathbf{C}_{f_b} \\ \vdots \end{bmatrix}^\top \begin{bmatrix} \mathbf{J}_{f_a} & \cdots & 0 \\ \vdots & \mathbf{J}_{f_b} & \vdots \\ 0 & \cdots & \ddots \end{bmatrix} \begin{bmatrix} \mathbf{C}_{f_a} \\ \mathbf{C}_{f_b} \\ \vdots \end{bmatrix} \mathbf{J}$$

- Efficient iteration for vjp
- Combines the SparseMAP Jacobians of each factor

(use specialized impl. when available: many commonly used factors derived in paper.)

# Differentiable Sparse Structured Prediction



```
fg = FactorGraph()
var = [fg.variable() for i in range(n)] # handwave

fg.add(Tree(var))

for i in range(n):
    fg.add(Budget(var[i, :], budget=5))

mu = fg.lp_sparsemap(eta)
```

Factor graphs as a hidden-layer DSL!

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If  $|\mathcal{F}| = 1$ , recovers SparseMAP.

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Factor graphs as a hidden-layer DSL!

If  $|\mathcal{F}| = 1$ , recovers SparseMAP.

Modular library.

Built-in specialized factors:

- OR, XOR, AND
- OR-with-output
- Budget, Knapsack
- Pairwise

```
class Factor:
    def map( $\eta_f$ ): # abstract, private
        raise NotImplemented

    def sparsemap( $\eta_f$ ):
        # active set algo, uses self.map

    def backward( $d\mu_f$ ):
        # analytic, uses active set result
```

```
class Budget(Factor):
    def sparsemap( $\eta_f$ ):
        # specialized

    def backward( $d\mu_f$ ):
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```

# Differentiable Sparse Structured Prediction



Factor graphs as a hidden-layer DSL!

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New factors only require MAP.

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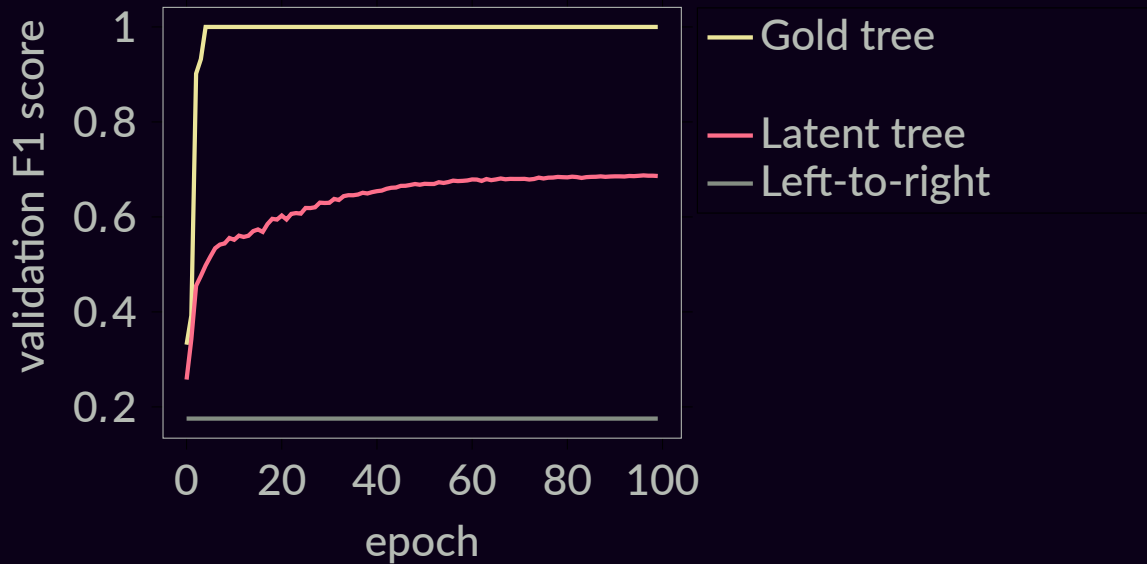
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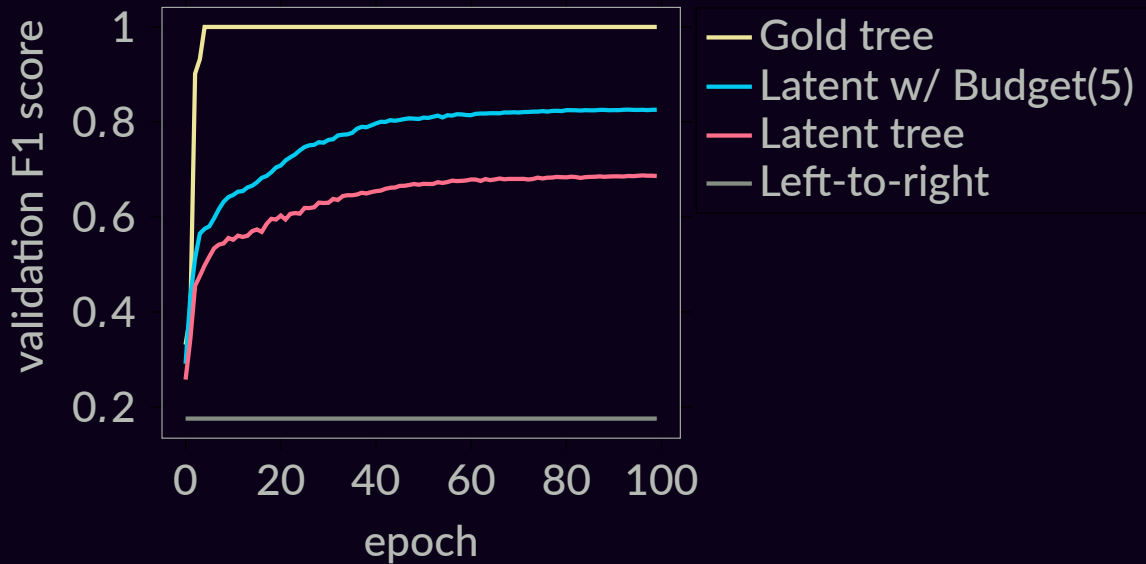
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```

```
class Budget(Factor):
    def sparsemap( $\eta_f$ ):
        # specialized

    def backward( $d\mu_f$ ):
        # specialized
```

```
class Tree(Factor):
    def map( $\eta$ ):
        # Chu-Liu/Edmonds algo
```





# Structured Attention for Alignments

NLI

premise: A gentleman overlooking a neighborhood situation.  
hypothesis: A police officer watches a situation closely.

input

(P, H)

⚙	A	A	⚙
	gentleman	police	
	overlooking	officer	
	...	...	
	situation	closely	

output



entails

contradicts

neutral

(Model: decomposable attention (Parikh et al., 2016))



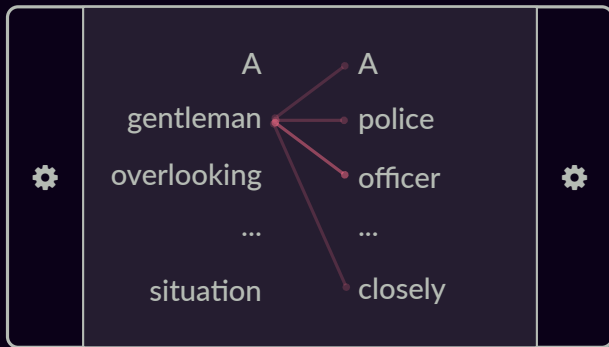
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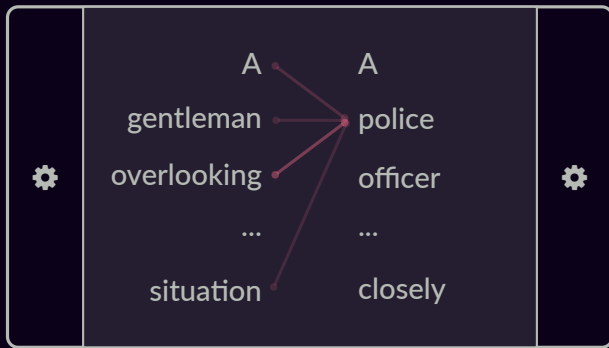
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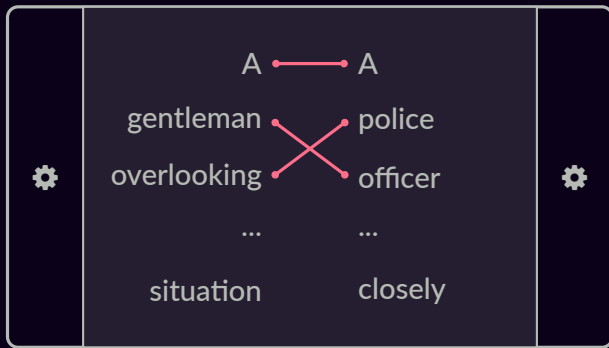
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NLI

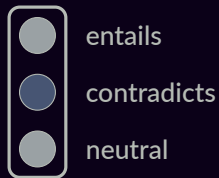
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(P, H)



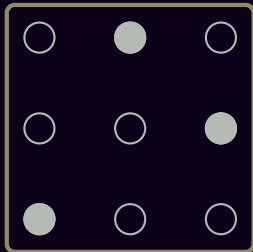
output



(Proposed model: global structured alignment.)

# Structured Alignment Models

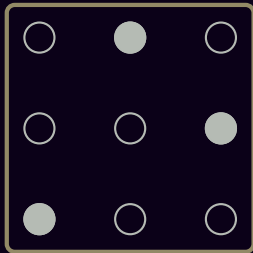
*matching*



SparseMAP w/ Kuhn-Munkres  
(Kuhn, 1955)

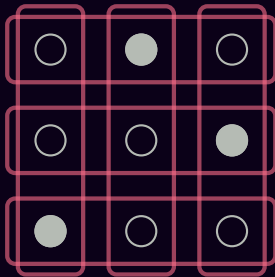
# Structured Alignment Models

*matching*



SparseMAP w/ Kuhn-Munkres  
(Kuhn, 1955)

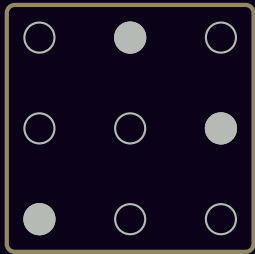
*LP-matching*



LP-SparseMAP w/ XORs  
(equivalent; different solver)

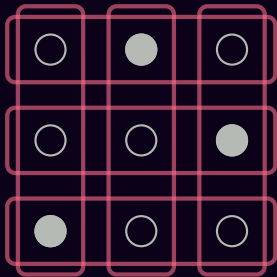
# Structured Alignment Models

*matching*



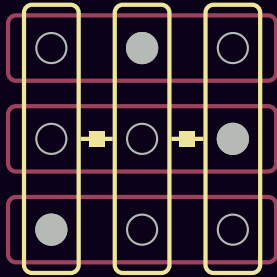
SparseMAP w/ Kuhn-Munkres  
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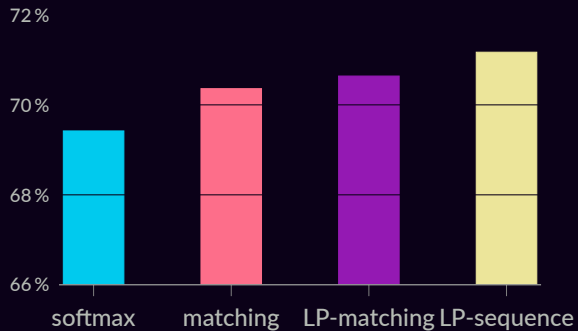
LP-SparseMAP w/ XORs  
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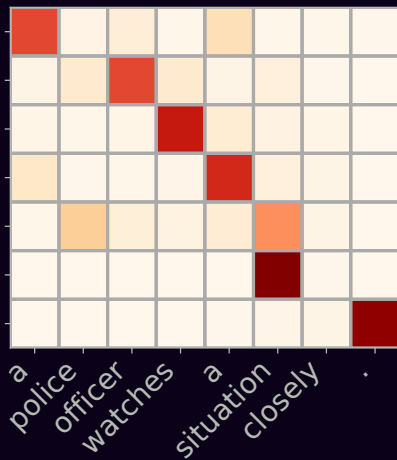
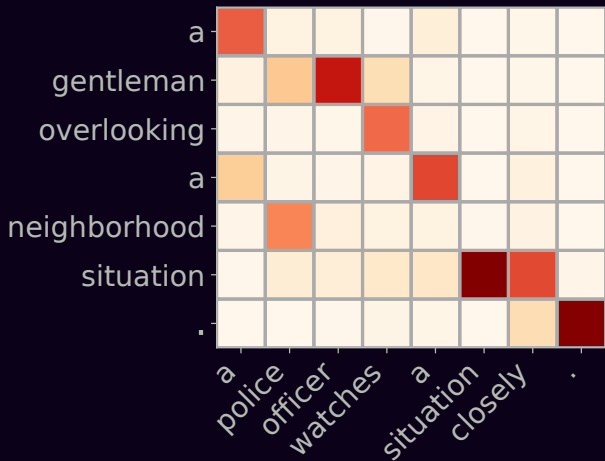
*LP-sequence*



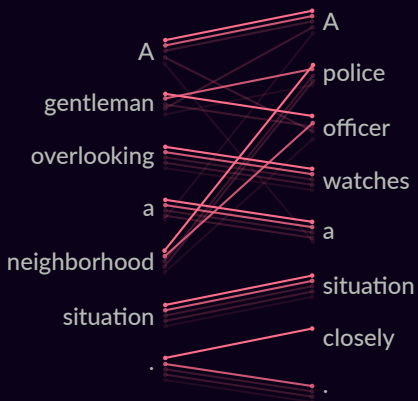
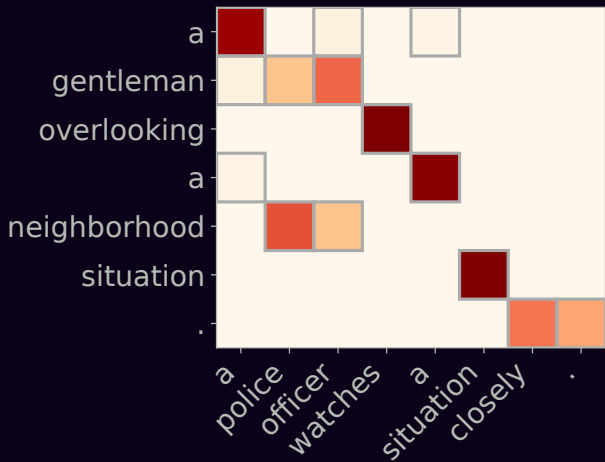
additional score  
for *contiguous alignments*  
 $(i, j) - (i + 1, j \pm 1)$

## MultiNLI (Williams et al., 2017)







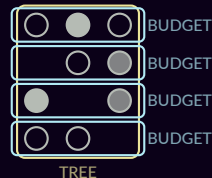
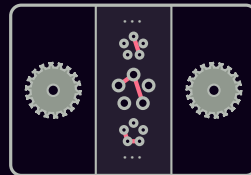


# Conclusions

Differentiable & sparse  
structured inference

Generic, extensible, efficient algorithms

Interpretable **structured attention**



# Conclusions

Differentiable & sparse  
structured inference

Generic, extensible, efficient algorithms

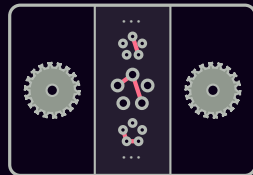
Interpretable **structured attention**

# Future work

Structure beyond NLP

Weak & semi-supervision

Generative latent structure models



**Extra slides**

# Acknowledgements



This work was supported by the European Research Council (ERC StG DeepSPIN 758969) and by the Fundação para a Ciência e Tecnologia through contract UID/EEA/50008/2013.

Some icons by Dave Gandy and Freepik via flaticon.com.

# Fusedmax

$$\begin{aligned}\text{fusedmax}(\boldsymbol{\theta}) &= \arg \max_{\mathbf{p} \in \Delta} \mathbf{p}^T \boldsymbol{\theta} - 1/2 \|\mathbf{p}\|_2^2 - \sum_{2 \leq j \leq d} |p_j - p_{j-1}| \\ &= \arg \min_{\mathbf{p} \in \Delta} \|\mathbf{p} - \boldsymbol{\theta}\|_2^2 + \sum_{2 \leq j \leq d} |p_j - p_{j-1}| \\ \text{prox}_{\text{fused}}(\boldsymbol{\theta}) &= \arg \min_{\mathbf{p} \in \mathbb{R}^d} \|\mathbf{p} - \boldsymbol{\theta}\|_2^2 + \sum_{2 \leq j \leq d} |p_j - p_{j-1}|\end{aligned}$$

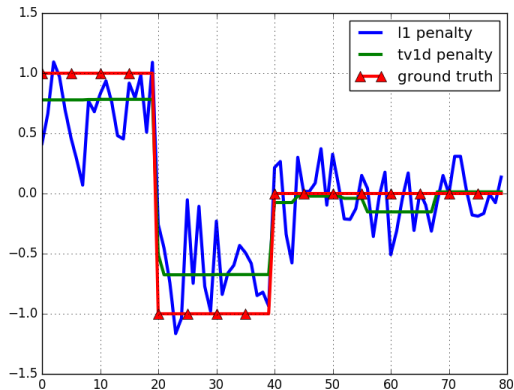
**Proposition:**  $\text{fusedmax}(\boldsymbol{\theta}) = \text{sparsemax}(\text{prox}_{\text{fused}}(\boldsymbol{\theta}))$

(Niculae and Blondel, 2017)

fusedmax(

prox<sub>fused</sub>(

Proposi



“Fused Lasso” a.k.a. 1-d Total Variation

(Tibshirani et al., 2005)

(Niculae and Blondel, 2017)

$|p_j - p_{j-1}|$

$|p_{j-1}|$

$|p_{j-1}|$

fused( $\theta$ )

# Danskin's Theorem

Let  $\phi : \mathbb{R}^d \times \mathcal{Z} \rightarrow \mathbb{R}$ ,  $\mathcal{Z} \subset \mathbb{R}^d$  compact.

$$\partial \max_{\mathbf{z} \in \mathcal{Z}} \phi(\mathbf{x}, \mathbf{z}) = \text{conv} \{ \nabla_{\mathbf{x}} \phi(\mathbf{x}, \mathbf{z}^*) \mid \mathbf{z}^* \in \arg \max_{\mathbf{z} \in \mathcal{Z}} \phi(\mathbf{x}, \mathbf{z}) \}.$$

**Example: maximum of a vector**



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**Example: maximum of a vector**

$$\begin{aligned} \partial \max_{j \in [d]} \theta_j &= \partial \max_{\mathbf{p} \in \Delta} \mathbf{p}^\top \boldsymbol{\theta} \\ &= \partial \max_{\mathbf{p} \in \Delta} \phi(\mathbf{p}, \boldsymbol{\theta}) \\ &= \text{conv} \{ \nabla_{\boldsymbol{\theta}} \phi(\mathbf{p}^*, \boldsymbol{\theta}) \} \\ &= \text{conv} \{ \mathbf{p}^* \} \end{aligned}$$

# Danskin's Theorem

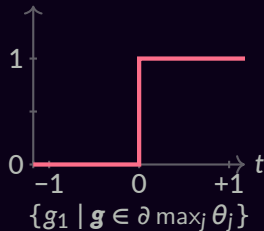
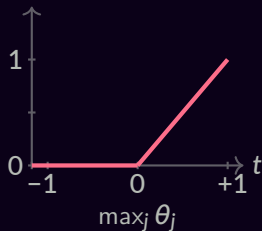
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$$\boldsymbol{\theta} = [t, 0]$$



**Dynamically inferring  
the computation graph**

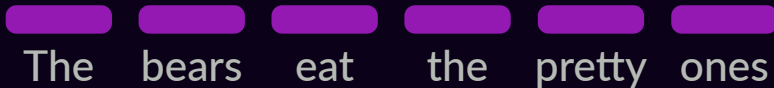
So far: a structured hidden layer

$$\mathbb{E}_H[\mathbf{a}_H]$$

Network must handle “soft” combinations of structures.  
Fine for attention, but can be limiting.

# Dependency TreeLSTM

(Tai et al., 2015)

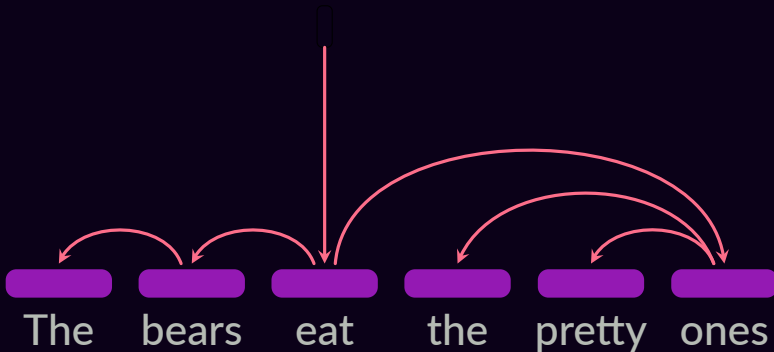


The diagram illustrates word embeddings for the sentence "The bears eat the pretty ones". Each word is represented by a blue rounded rectangle. The words are arranged in a horizontal line, with "The" and "bears" on the left, "eat" in the center, and "the", "pretty", and "ones" on the right. The rectangles are connected by thin lines, suggesting a sequence or relationship between the words.

The bears eat the pretty ones

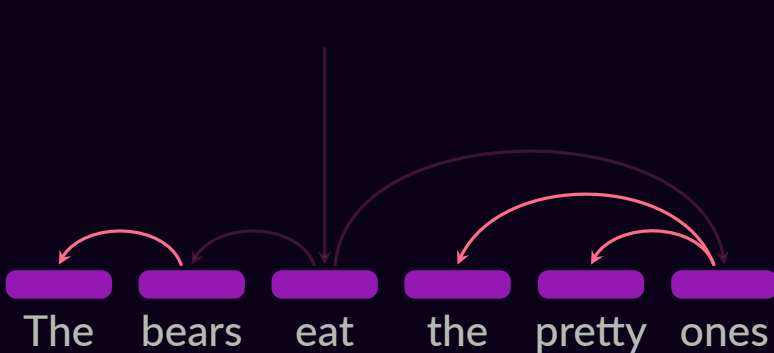
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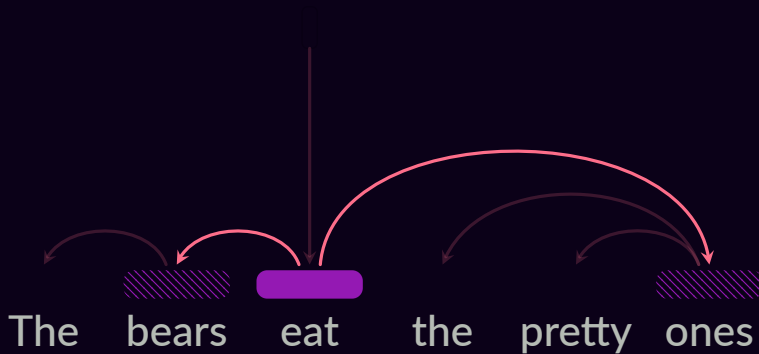
(Tai et al., 2015)





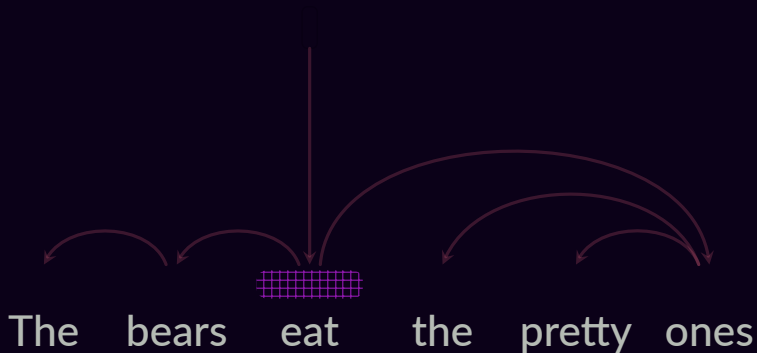
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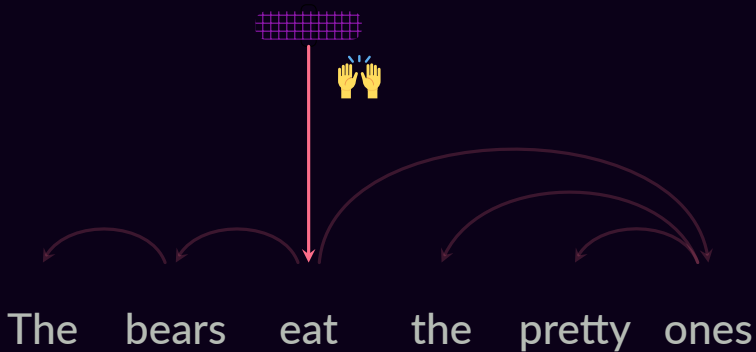
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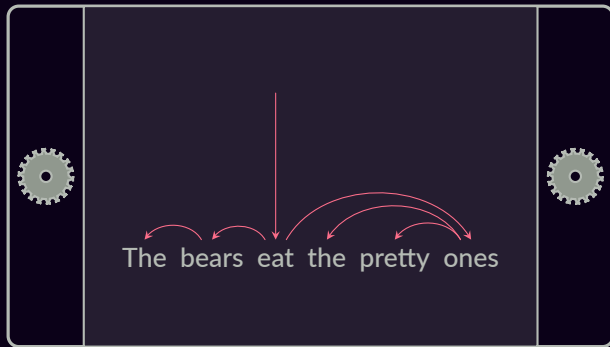


# Latent Dependency TreeLSTM

(Niculae, Martins, and Cardie, 2018)

input

$x$



output

$y$

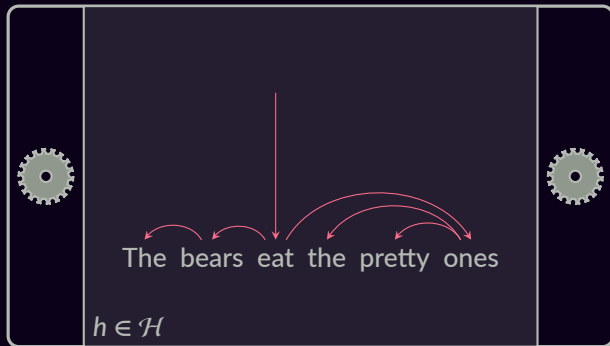
# Latent Dependency TreeLSTM

(Niculae, Martins, and Cardie, 2018)

$$p(y|x) = \sum_{h \in \mathcal{H}} p(y | h, x) p(h | x)$$

input

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output

$y$

# Structured Latent Variable Models

$$p(y | x) = \sum_{h \in \mathcal{H}} p(y | h, x) p(h | x)$$


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e.g., a TreeLSTM defined by  $h$





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$$p(y | x) = \sum_{h \in \mathcal{H}} p_{\phi}(y | h, x) p_{\pi}(h | x)$$

e.g., a TreeLSTM defined by  $h$

latent classifier

The diagram illustrates the components of the equation. A curved arrow points from the text 'e.g., a TreeLSTM defined by  $h$ ' to the parameter  $\phi$  in the term  $p_{\phi}(y | h, x)$ . Another curved arrow points from the text 'latent classifier' to the parameter  $\pi$  in the term  $p_{\pi}(h | x)$ .

# Structured Latent Variable Models

sum over  
all possible trees

e.g., a TreeLSTM defined by  $h$

$$p(y | x) = \sum_{h \in \mathcal{H}} p_{\phi}(y | h, x) p_{\pi}(h | x)$$

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Exponentially large sum!

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How to define  $p_{\pi}$ ?

idea 1

idea 2

idea 3

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argmax

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softmax

idea 3

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SparseMAP



# SparseMAP

 $= .7$

 $+ .3$



# SparseMAP

$$\begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} = .7$$

$$\begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} + .3$$

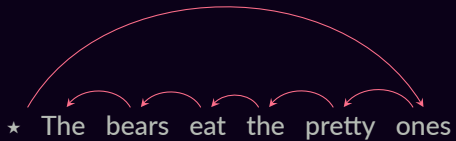
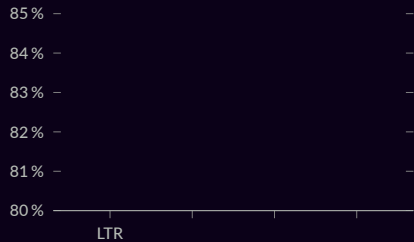
$$\begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} + 0 \begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} + \dots$$

# SparseMAP

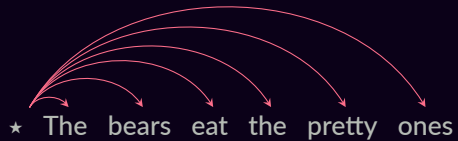
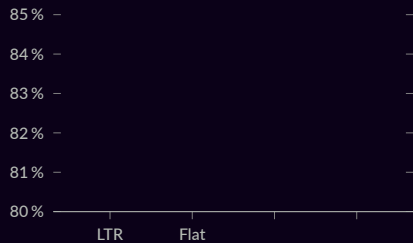
$$\begin{aligned}
 & \text{Diagram 1} = .7 \quad \text{Diagram 2} + .3 \quad \text{Diagram 3} + 0 \text{Diagram 4} + \dots \\
 p(y | x) = & .7 p_{\phi}(y | \text{Diagram 1}) + .3 p_{\phi}(y | \text{Diagram 2})
 \end{aligned}$$



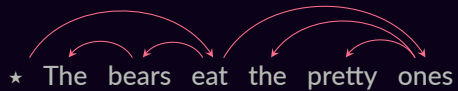
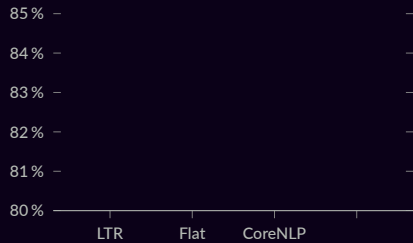




Left-to-right: regular LSTM



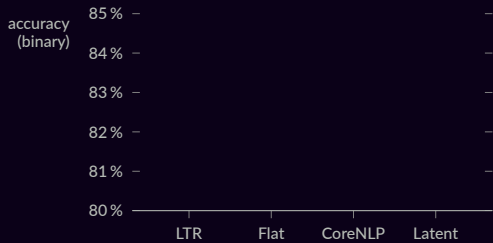
Flat: bag-of-words-like



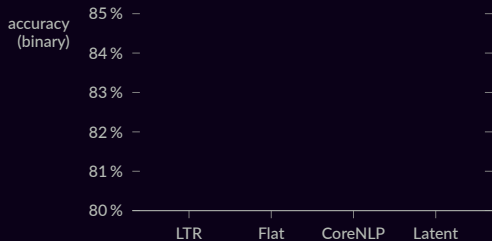
CoreNLP: off-line parser



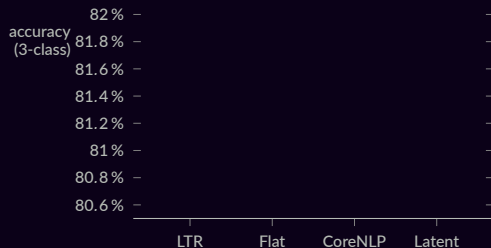
## Sentiment classification (SST)



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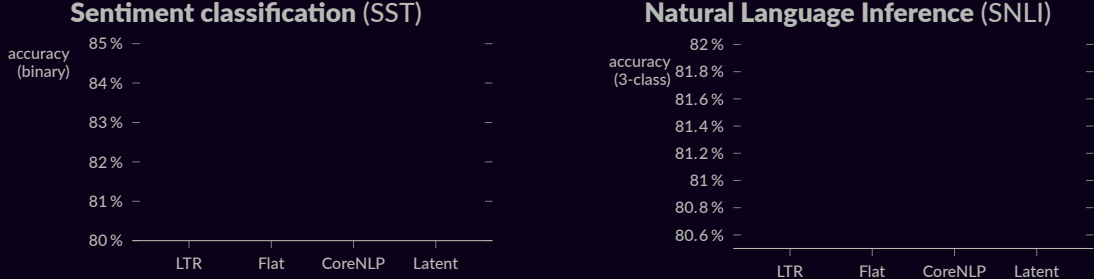


## Natural Language Inference (SNLI)



## Sentence pair classification ( $P, H$ )

$$p(y \mid P, H) = \sum_{h_P \in \mathcal{H}(P)} \sum_{h_H \in \mathcal{H}(H)} p_{\phi}(y \mid h_P, h_H) p_{\pi}(h_P \mid P) p_{\pi}(h_H \mid H)$$

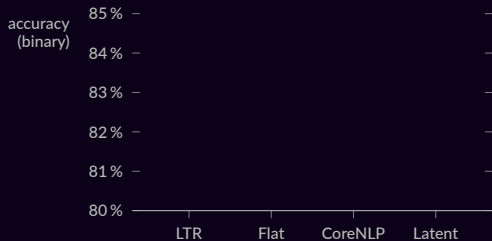


## Reverse dictionary lookup

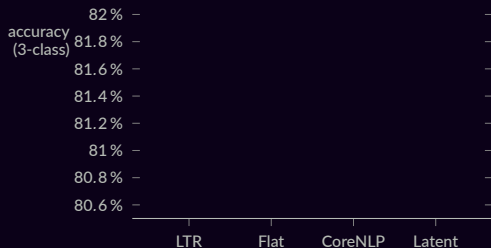
given word description, predict word embedding (Hill et al., 2016)

instead of  $p(y | x)$ , we model  $\mathbb{E}_{p_{\pi}} \mathbf{g}(x) = \sum_{h \in \mathcal{H}} \mathbf{g}(x; h) p_{\pi}(h | x)$

## Sentiment classification (SST)

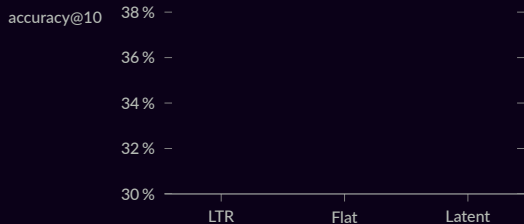


## Natural Language Inference (SNLI)

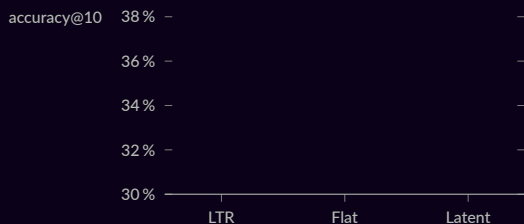


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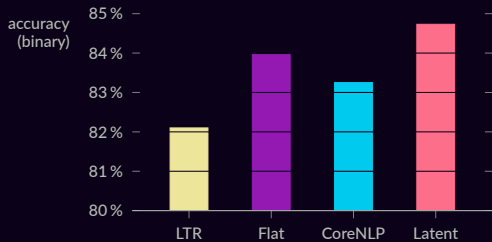
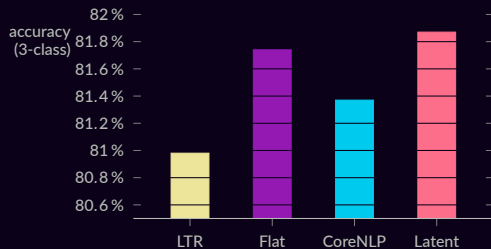
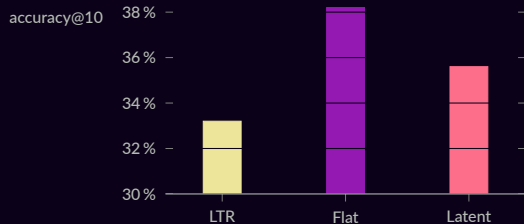
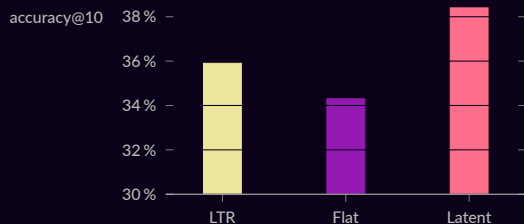
(definitions)



(concepts)

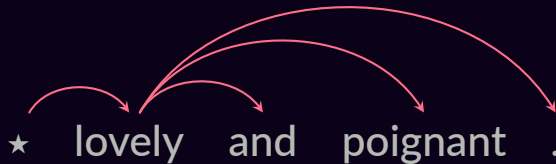




**Sentiment classification (SST)****Natural Language Inference (SNLI)****Reverse dictionary lookup****(definitions)****(concepts)**

# Syntax vs. Composition Order

CoreNLP parse,  $p = 21.4\%$

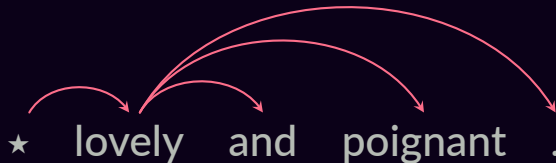


# Syntax vs. Composition Order

$p = 22.6\%$

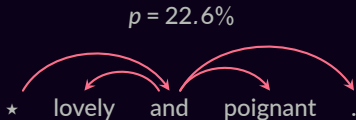


CoreNLP parse,  $p = 21.4\%$

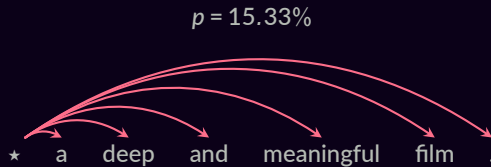


...

# Syntax vs. Composition Order



CoreNLP parse,  $p = 21.4\%$



$p = 15.27\%$



CoreNLP parse,  $p = 0\%$



# Structured Output Prediction

SparseMAP

$$L_A(\boldsymbol{\eta}, \bar{\boldsymbol{\mu}}) = \max_{\boldsymbol{\mu} \in \mathcal{M}} \left\{ \boldsymbol{\eta}^\top \boldsymbol{\mu} - 1/2 \|\boldsymbol{\mu}\|^2 \right\} \\ - \boldsymbol{\eta}^\top \bar{\boldsymbol{\mu}} + 1/2 \|\bar{\boldsymbol{\mu}}\|^2$$

Instance of a structured Fenchel-Young loss, like CRF, SVM, etc. (Blondel, Martins, and Niculae, 2019b)

# Structured Output Prediction

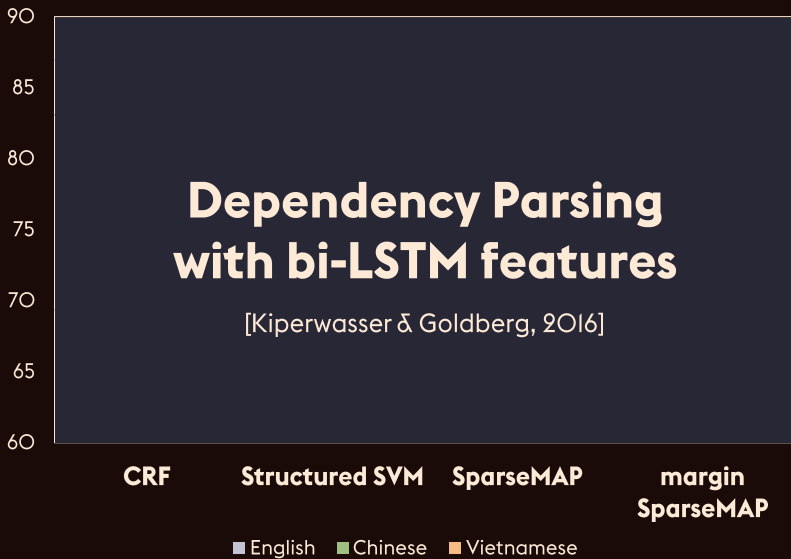
SparseMAP

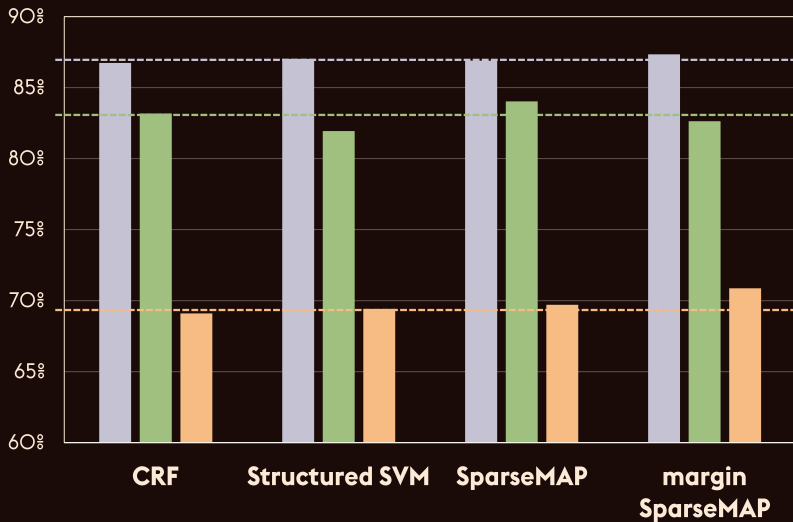
$$L_A(\boldsymbol{\eta}, \bar{\boldsymbol{\mu}}) = \max_{\boldsymbol{\mu} \in \mathcal{M}} \left\{ \boldsymbol{\eta}^\top \boldsymbol{\mu} - 1/2 \|\boldsymbol{\mu}\|^2 \right. \\ \left. - \boldsymbol{\eta}^\top \bar{\boldsymbol{\mu}} + 1/2 \|\bar{\boldsymbol{\mu}}\|^2 \right\}$$

cost-SparseMAP

$$L_A^\rho(\boldsymbol{\eta}, \bar{\boldsymbol{\mu}}) = \max_{\boldsymbol{\mu} \in \mathcal{M}} \left\{ \boldsymbol{\eta}^\top \boldsymbol{\mu} - 1/2 \|\boldsymbol{\mu}\|^2 + \rho(\boldsymbol{\mu}, \bar{\boldsymbol{\mu}}) \right\} \\ - \boldsymbol{\eta}^\top \bar{\boldsymbol{\mu}} + 1/2 \|\bar{\boldsymbol{\mu}}\|^2$$

Instance of a structured Fenchel-Young loss, like CRF, SVM, etc. (Blondel, Martins, and Niculae, 2019b)





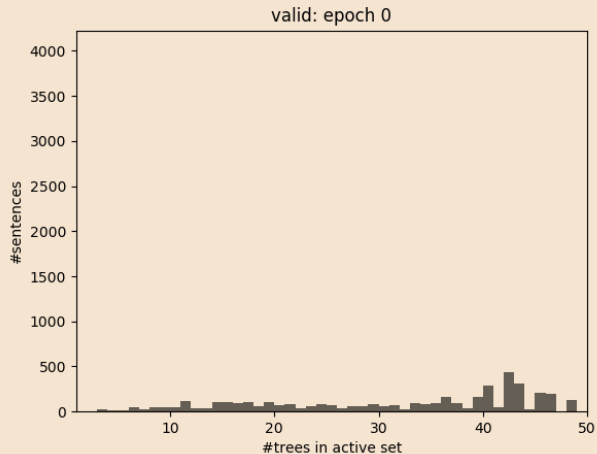
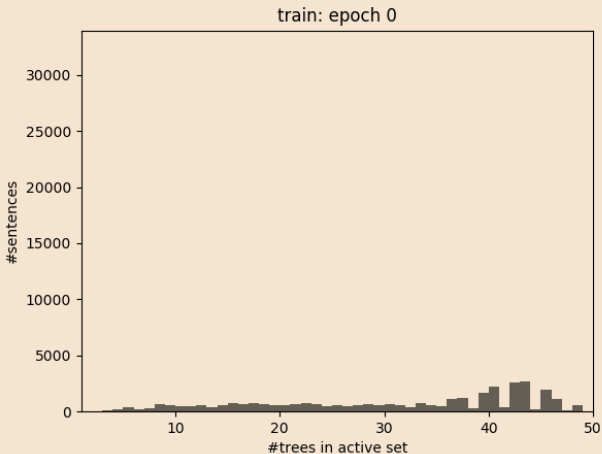
Unlabeled Accuracy (UAS)  
Universal Dependencies dataset

■ English ■ Chinese ■ Vietnamese



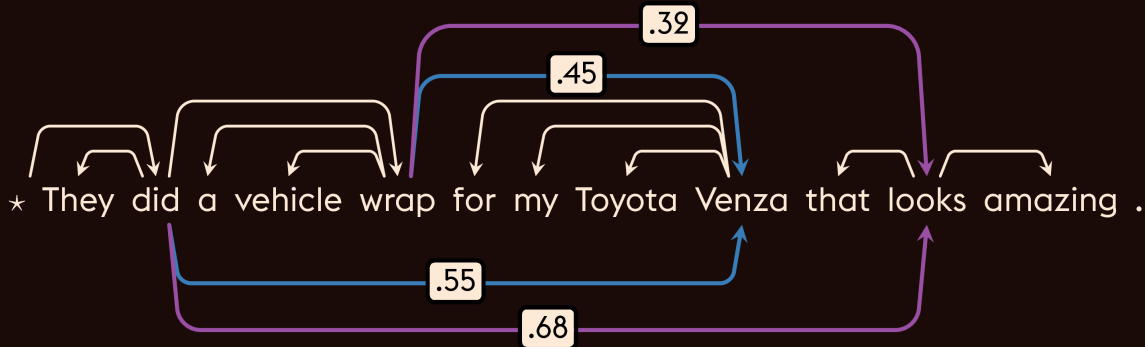
# Sparse Structured Output Prediction

As models train, inference gets sparser!



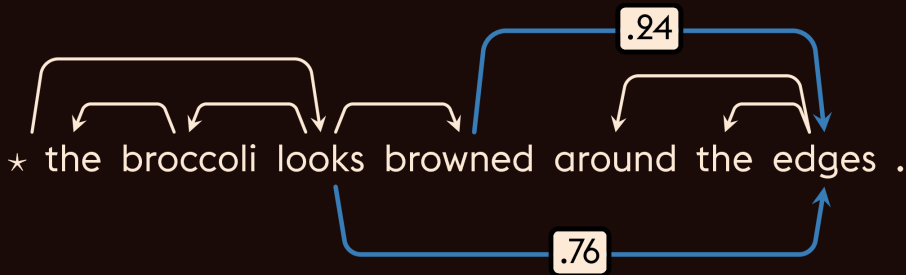
# Sparse Structured Output Prediction

**Inference captures linguistic ambiguity!**



# Sparse Structured Output Prediction

**Inference captures linguistic ambiguity!**



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