# Learning with Sparse Latent Structure

**Vlad Niculae**

Instituto de Telecomunicações; Lisbon → University of Amsterdam (PhD opening!)

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github.com/deep-spin/lp-sparsemap @vnfrombucharest https://vene.ro

# Rich Underlying Structure

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

author

date

body

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segmentation:
sentences,
words,
and so on

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relationships

*e.g.*, dependency

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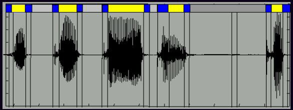
Most of this structure is **hidden**.

# Rich Underlying Structure

## Widely occuring pattern!

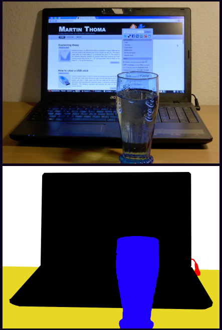
*speech*

(Andre-Obrecht, 1988)



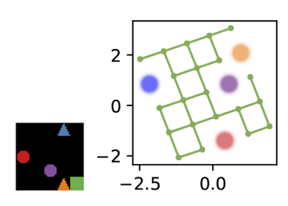
*objects*

(Long et al., 2015)




*transition graphs*

(Kipf, Pol, et al., 2020)



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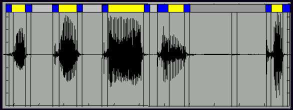

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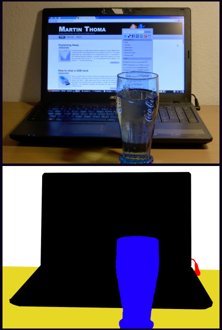


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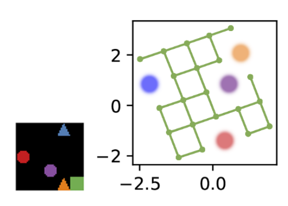
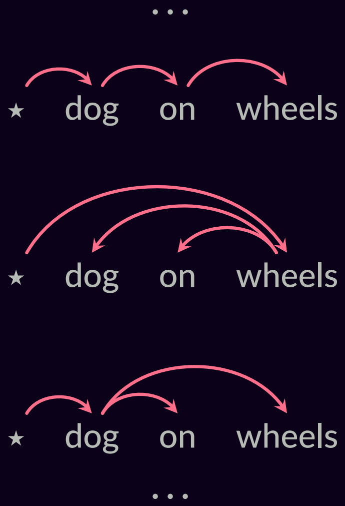



But we'll focus on NLP.

# Structured Prediction



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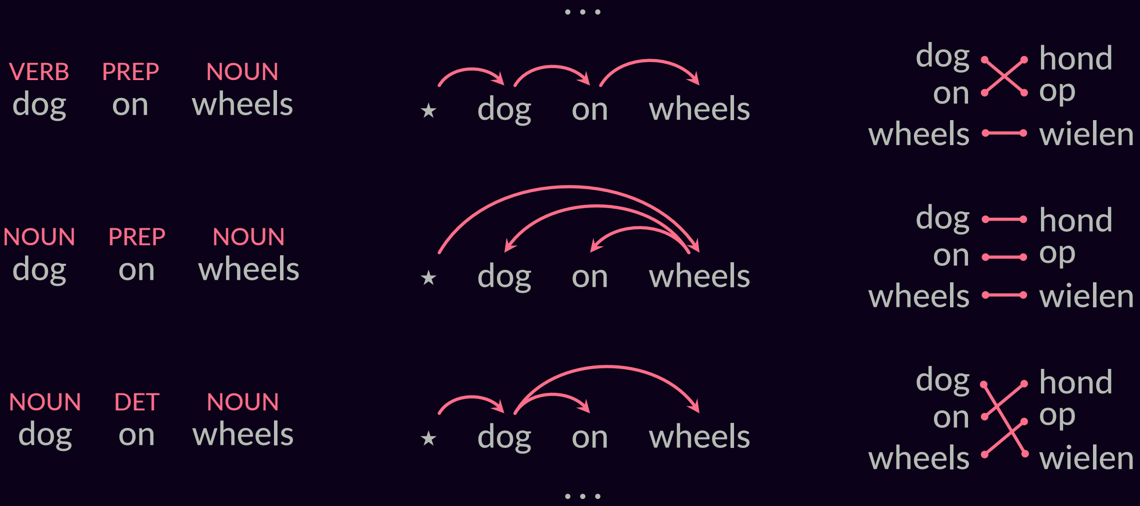

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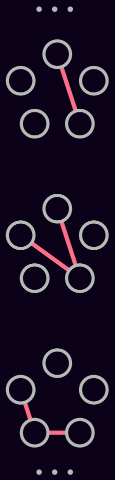

# Traditional Pipeline Approach

input

output

positive

neutral

negative

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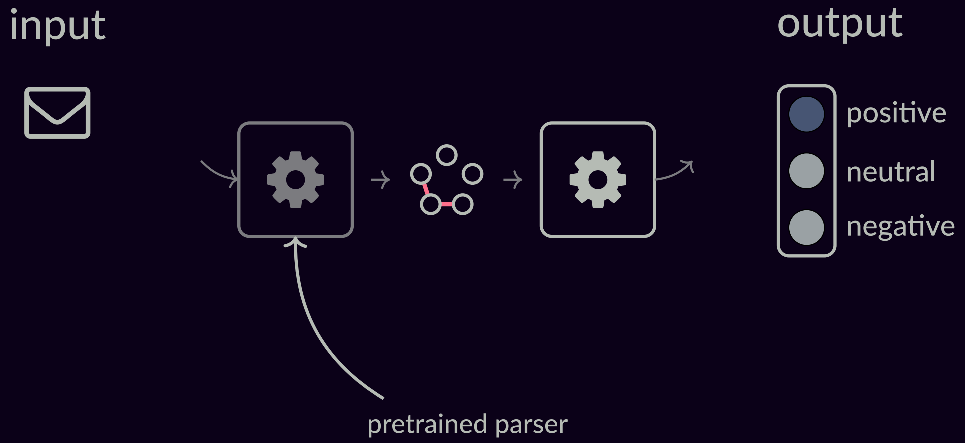
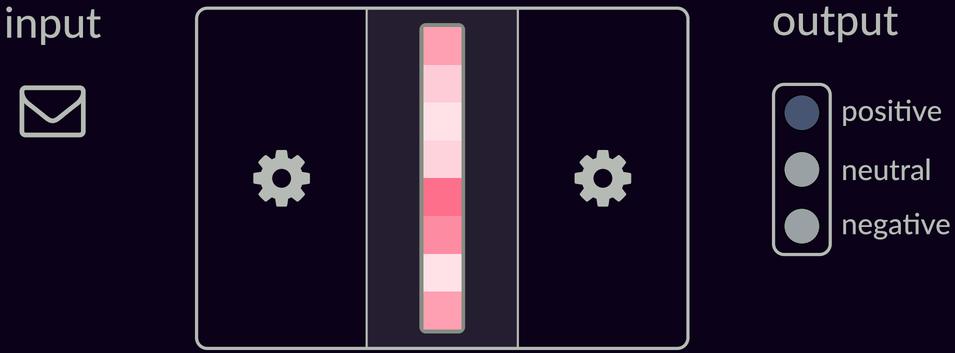


# Deep Learning & Hidden Representations



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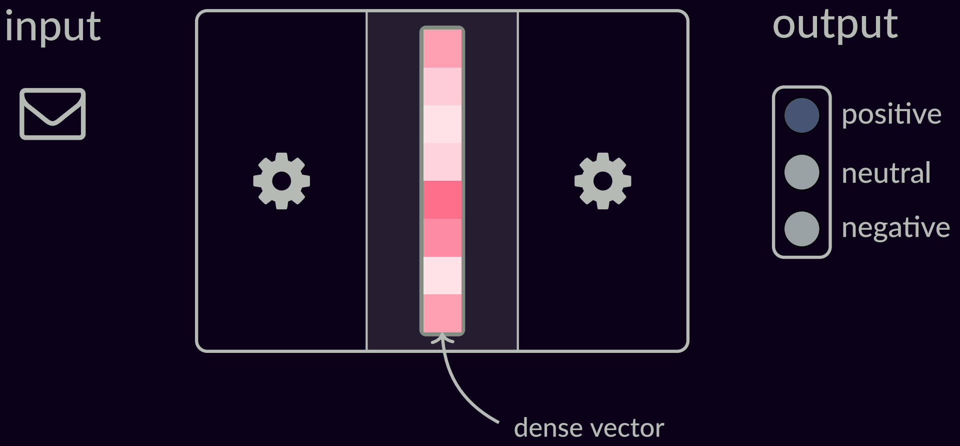
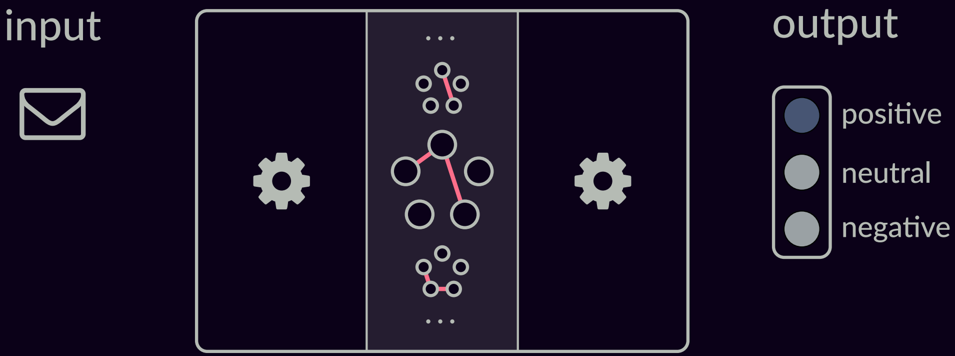


# Latent Structure Models



*record scratch*

*freeze frame*

# How to select an item from a set?

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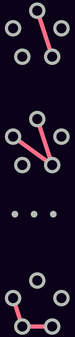

# How to select an item from a set?

$$c_1$$

$$c_2$$

$$\dots$$

$$c_N$$

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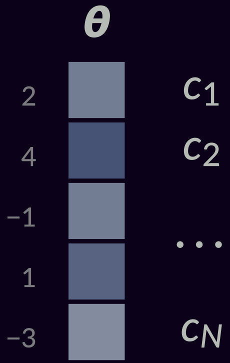

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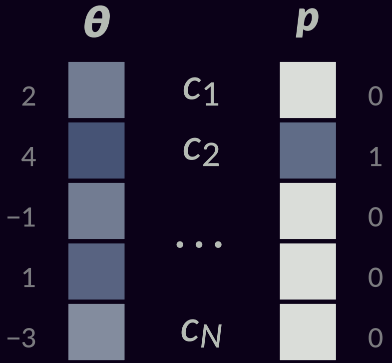

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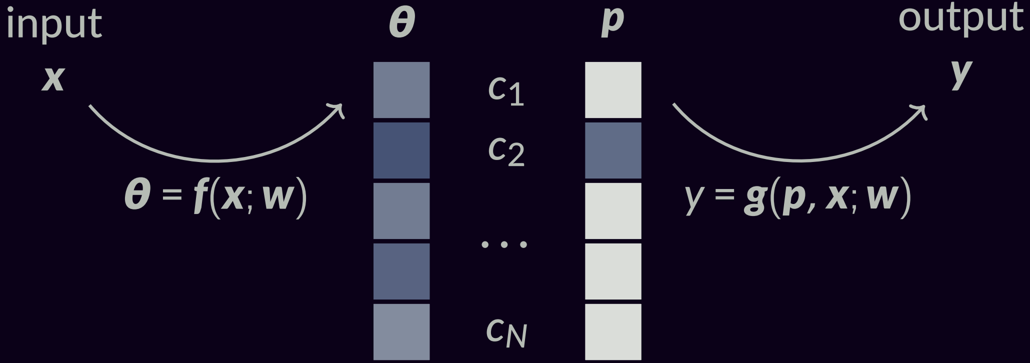

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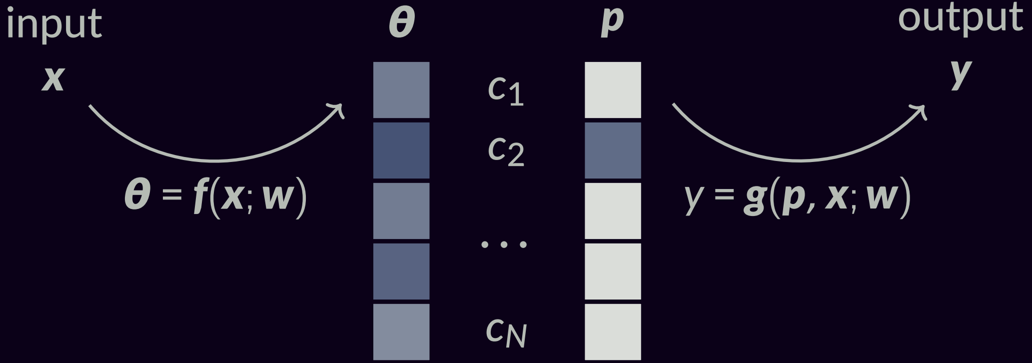
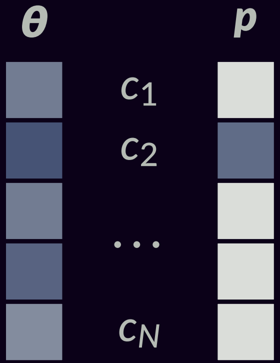



$$\frac{\partial y}{\partial \boldsymbol{w}} = ?$$

# How to select an item from a set?

input $\boldsymbol{x}$

$\boldsymbol{\theta} = \boldsymbol{f}(\boldsymbol{x}; \boldsymbol{w})$

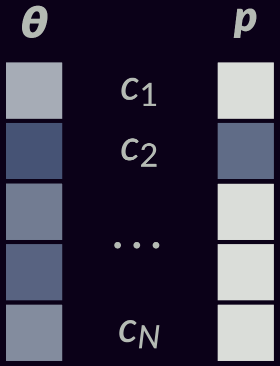



output $\boldsymbol{y}$

$y = \boldsymbol{g}(\boldsymbol{p}, \boldsymbol{x}; \boldsymbol{w})$

$\frac{\partial y}{\partial \boldsymbol{w}} = ?$ or, essentially, $\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{\theta}} = ?$

# Argmax

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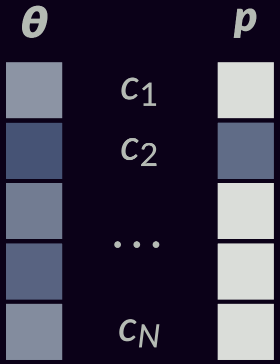


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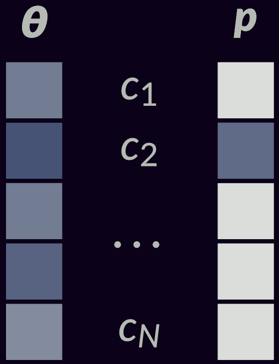


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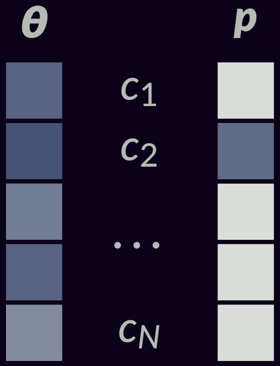


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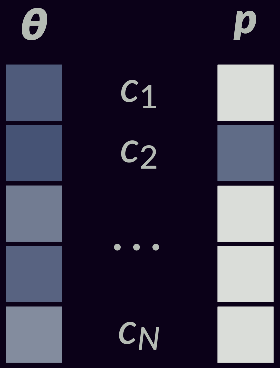


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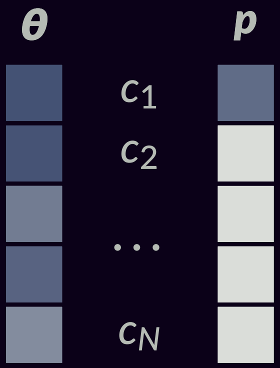


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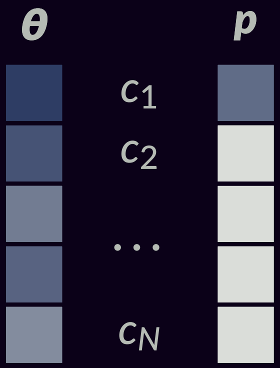


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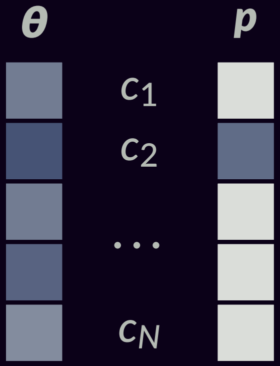
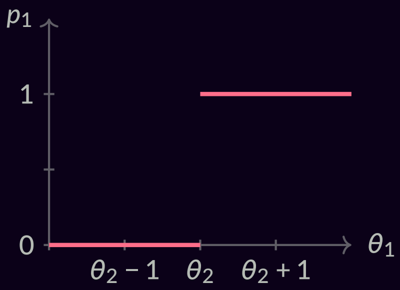
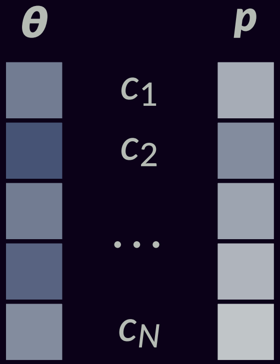


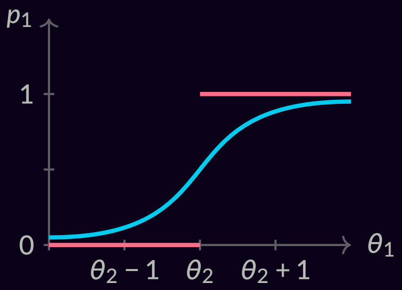




$$\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{\theta}} = \mathbf{0}$$

# Argmax vs. Softmax

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




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

# A Softmax Origin Story 🦸🏽‍♀️

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

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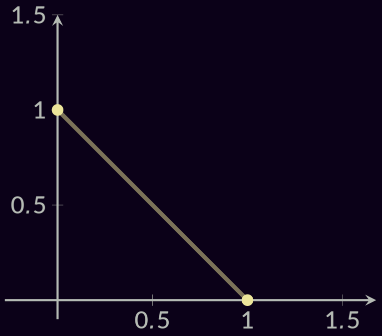


$N = 2$

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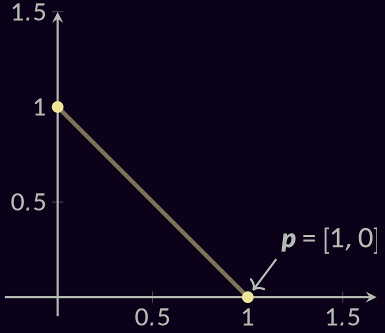


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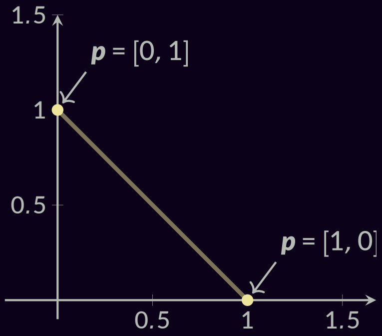


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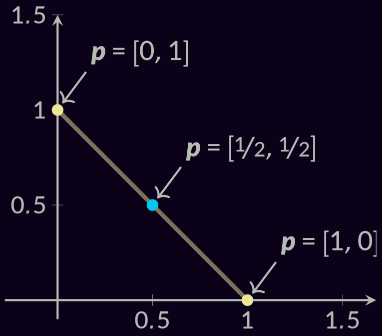


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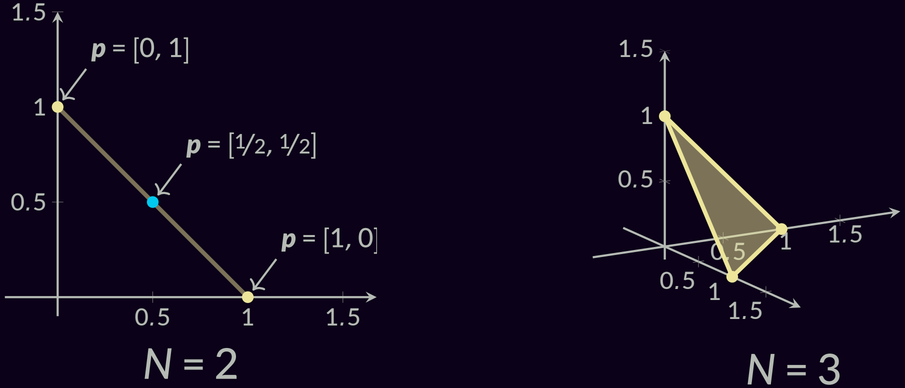

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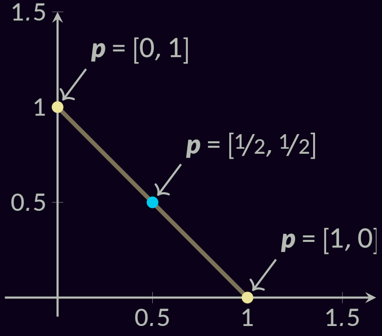


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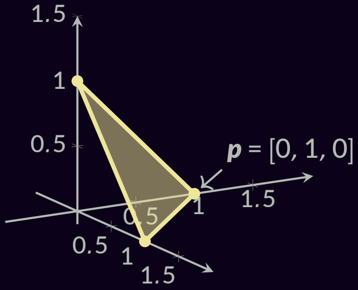


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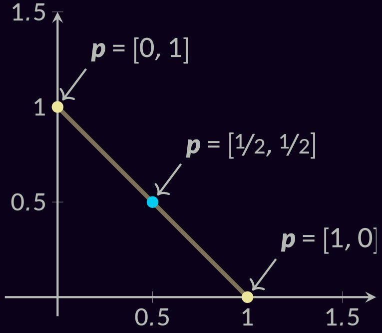


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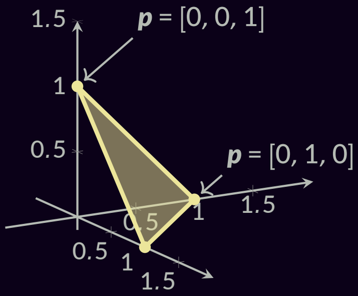


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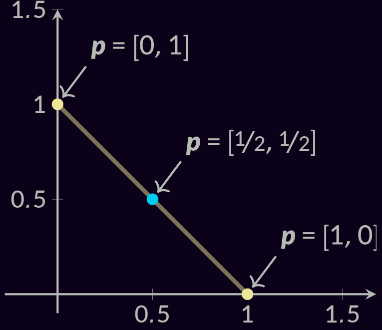


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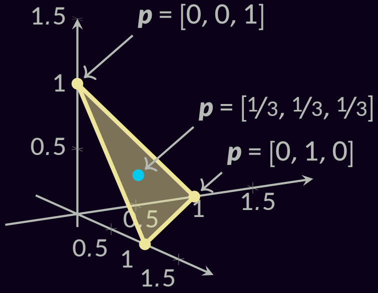


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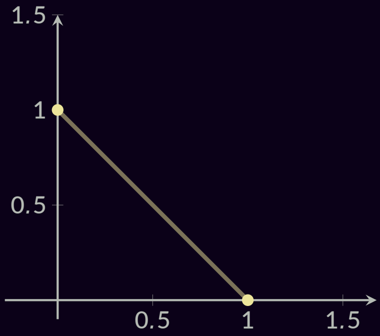
$$\max_j \theta_j = \max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{\theta}$$

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

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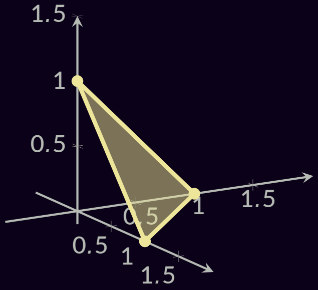


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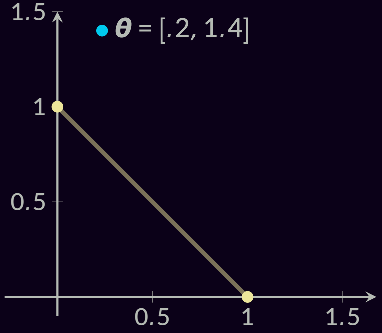


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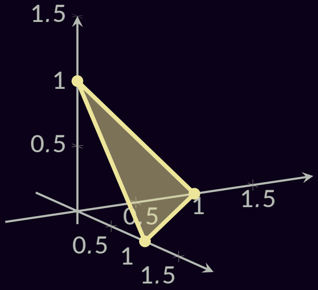


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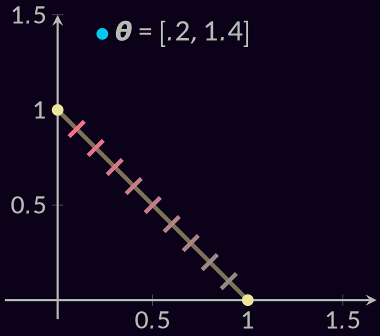


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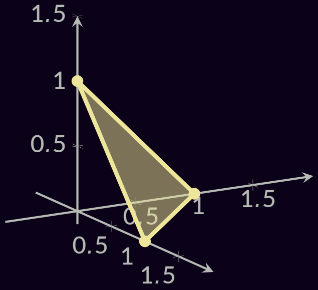


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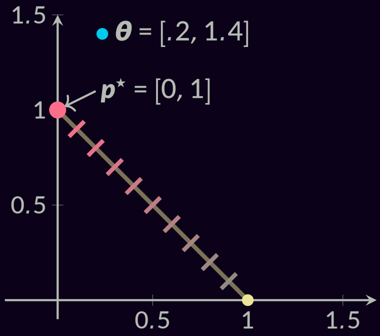
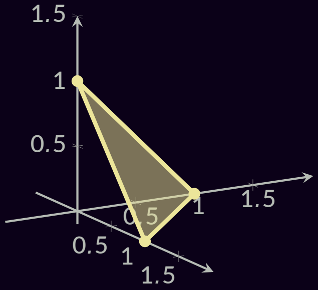



$N = 2$




$N = 3$

# A Softmax Origin Story 🦸🏽‍♀️

$$\max_j \theta_j = \max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top \boldsymbol{\theta}$$

Fundamental Thm. Lin. Prog.
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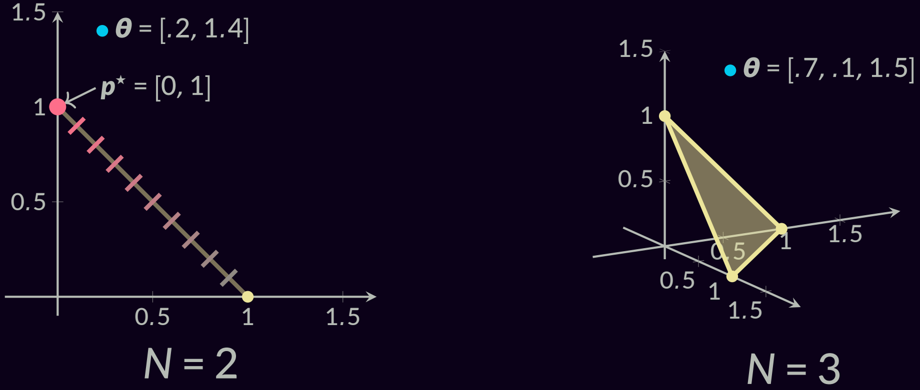

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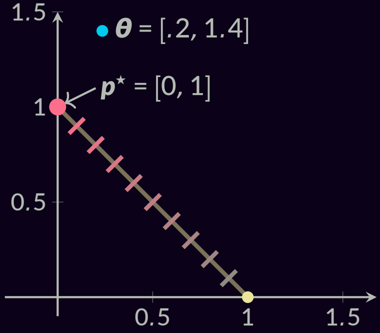
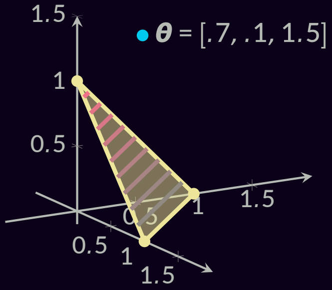



$N = 2$

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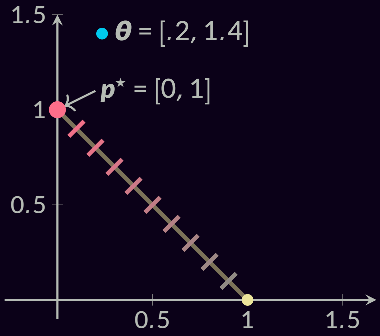


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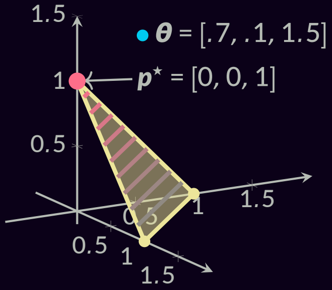
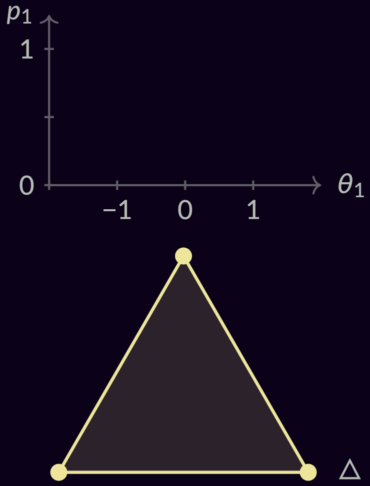



$N = 3$

(Niculae and Blondel, 2017)

# Smoothed Max Operators

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



(Niculae and Blondel, 2017)

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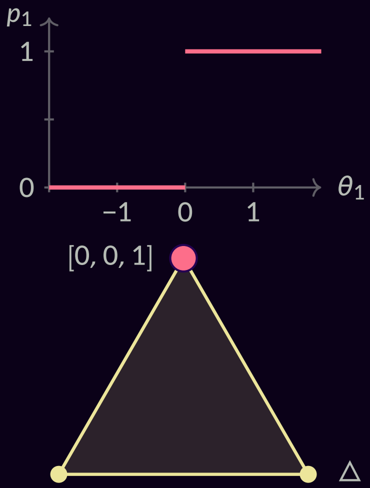

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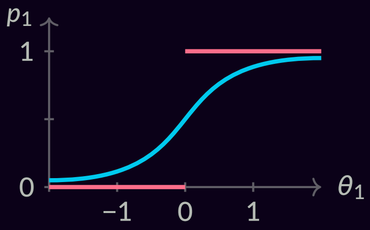


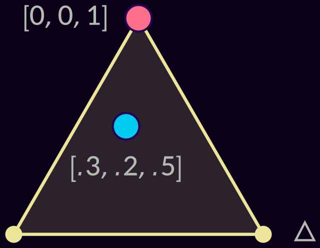

(Niculae and Blondel, 2017)

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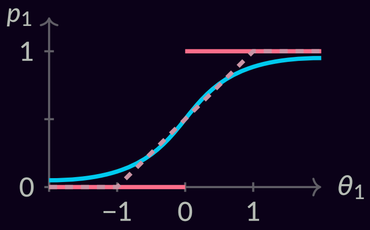


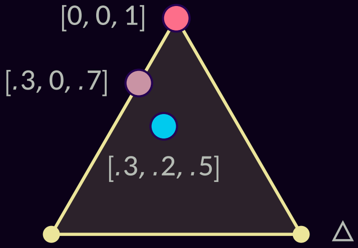


(Martins and Astudillo, 2016)

(Niculae and Blondel, 2017)

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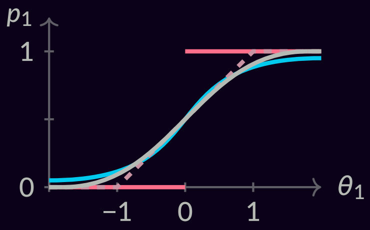
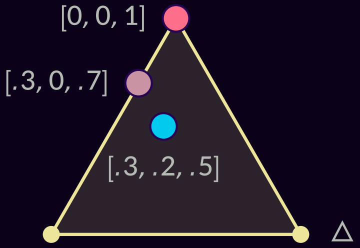
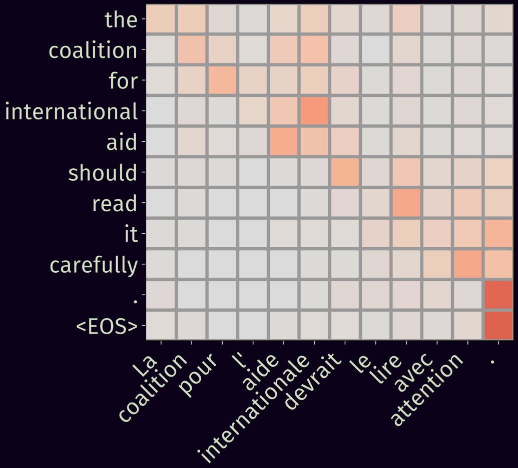



Tsallis (1988); a generalized entropy (Grünwald and Dawid, 2004)
(Blondel, Martins, and Niculae 2019a;
Peters, Niculae, and Martins 2019;
Correia, Niculae, and Martins 2019)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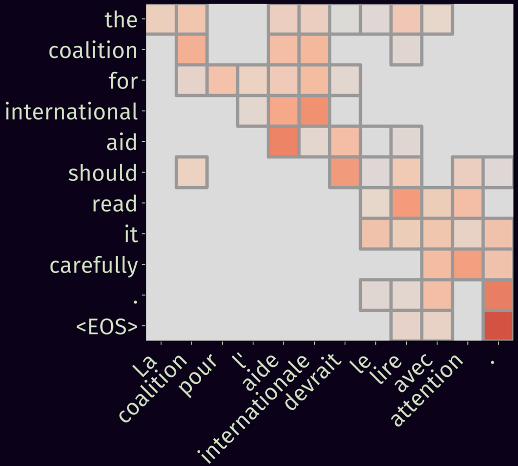
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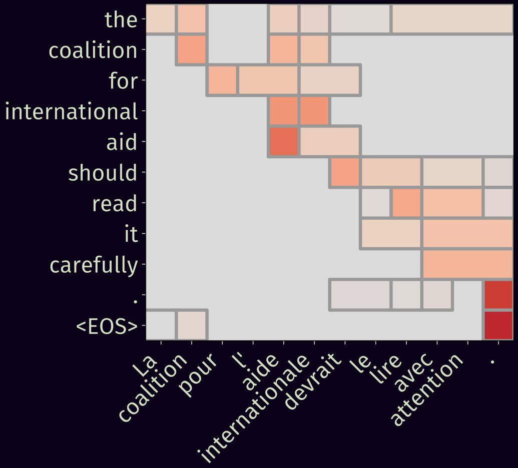
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fusedmax ?!

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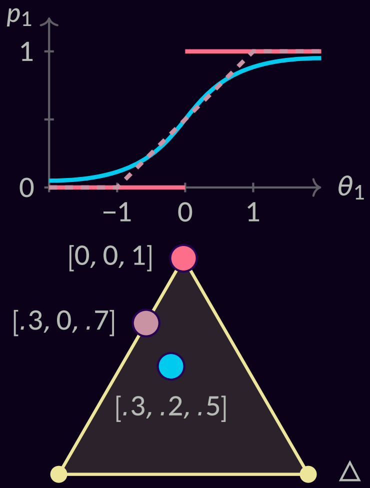

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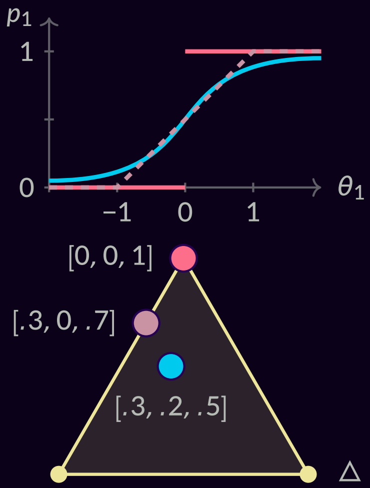

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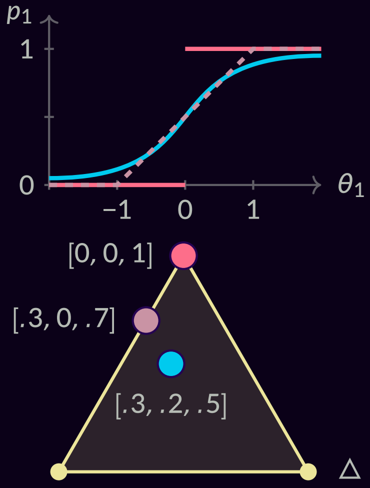

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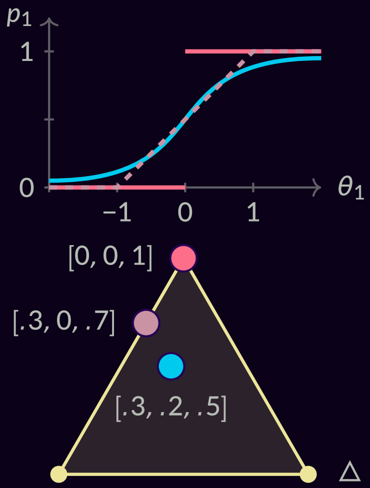
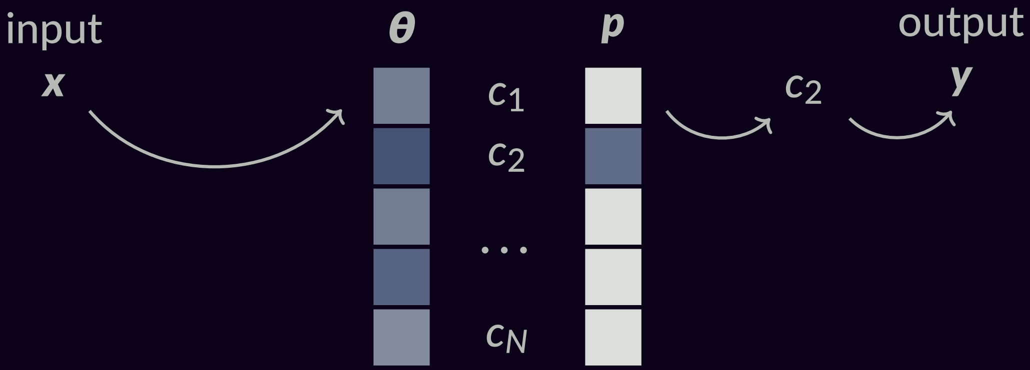


# Structured Prediction

**finally**

# Structured Prediction

is essentially a (very high-dimensional) argmax



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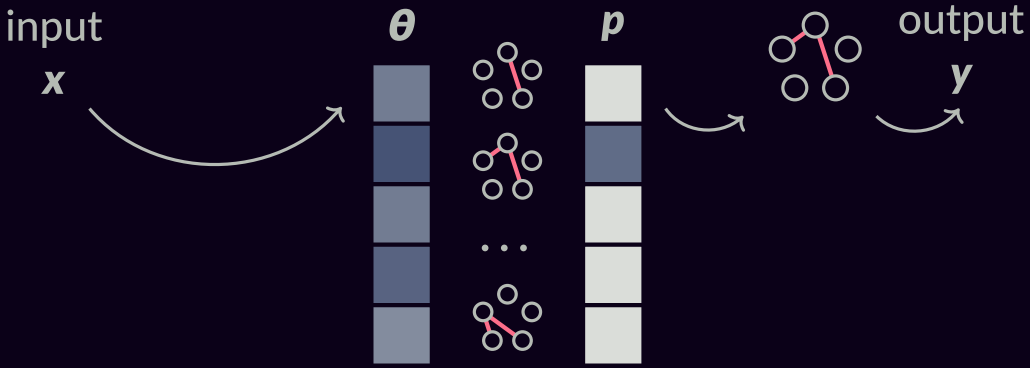

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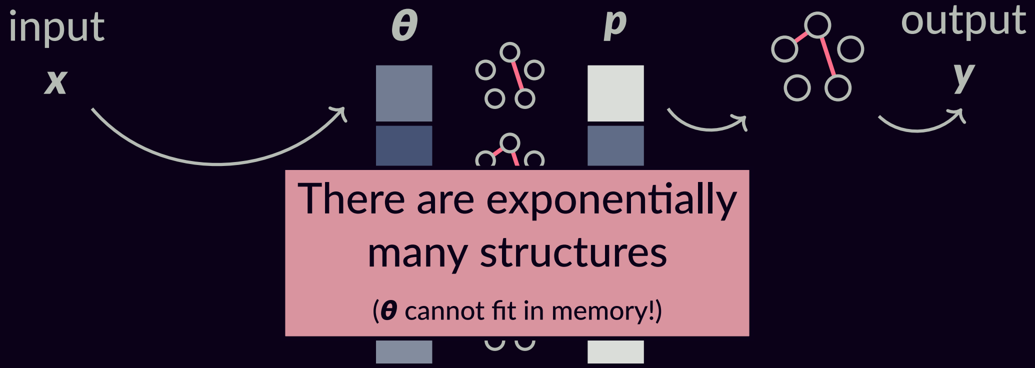



There are exponentially many structures

($\theta$ cannot fit in memory!)

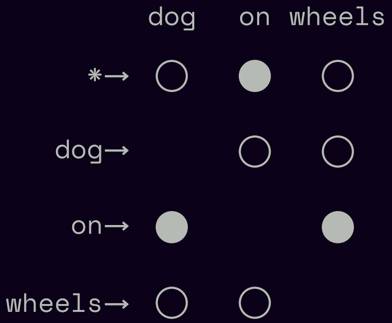
# Factorization Into Parts

$$\boldsymbol{\theta} = A^\top \boldsymbol{\eta}$$

$\star$ dog on wheels

# Factorization Into Parts

$$\boldsymbol{\theta} = A^{\top} \boldsymbol{\eta}$$

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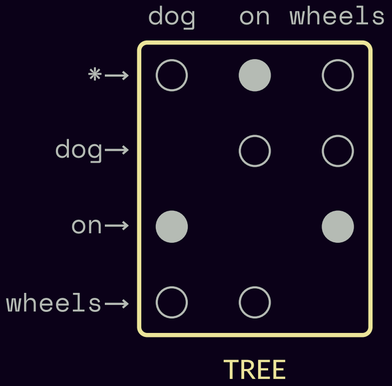

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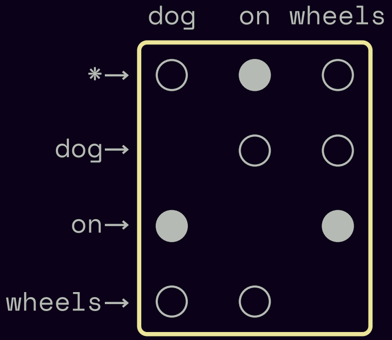


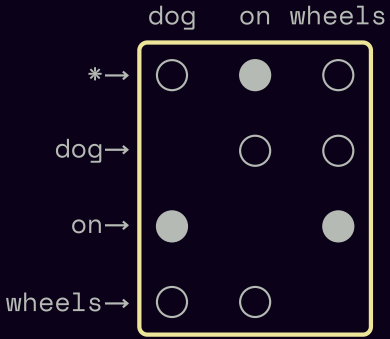

TREE

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

# Factorization Into Parts

$$\boldsymbol{\theta} = A^\top \boldsymbol{\eta}$$


$$\boldsymbol{A} = \begin{array}{r} \star\to\text{dog} \\ \text{on}\to\text{dog} \\ \text{wheels}\to\text{dog} \\ \star\to\text{on} \\ \text{dog}\to\text{on} \\ \text{wheels}\to\text{on} \\ \star\to\text{wheels} \\ \text{dog}\to\text{wheels} \\ \text{on}\to\text{wheels} \end{array} \left[\begin{array}{ccccc} 1 & & 0 & \boxed{0} & \\ 0 & & 1 & 1 & \\ 0 & & 0 & 0 & \\ \hline 0 & & 1 & 1 & \\ 1 & \dots & 0 & 0 & \dots \\ 0 & & 0 & 0 & \\ \hline 0 & & 0 & 0 & \\ 0 & & 1 & 0 & \\ 1 & & 0 & 1 & \end{array}\right] \quad \boldsymbol{\eta} = \left[\begin{array}{r} .1 \\ .2 \\ -.1 \\ \hline .3 \\ .8 \\ .1 \\ \hline -.3 \\ .2 \\ -.1 \end{array}\right]$$

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

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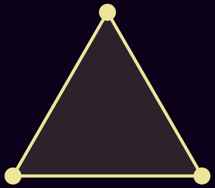
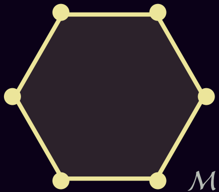
$$A = \begin{array}{r} \star\to\text{dog} \\ \text{on}\to\text{dog} \\ \text{wheels}\to\text{dog} \\ \star\to\text{on} \\ \text{dog}\to\text{on} \\ \text{wheels}\to\text{on} \\ \star\to\text{wheels} \\ \text{dog}\to\text{wheels} \\ \text{on}\to\text{wheels} \end{array} \left[\begin{array}{ccccc} 1 & & 0 & 0 & \\ 0 & & 1 & 1 & \\ 0 & & 0 & 0 & \\ \hline 0 & & 1 & 1 & \\ 1 & \dots & 0 & 0 & \dots \\ 0 & & 0 & 0 & \\ \hline 0 & & 0 & 0 & \\ 0 & & 1 & 0 & \\ 1 & & 0 & 1 & \end{array}\right] \quad \boldsymbol{\eta} = \left[\begin{array}{r} .1 \\ .2 \\ -.1 \\ \hline .3 \\ .8 \\ .1 \\ \hline -.3 \\ .2 \\ -.1 \end{array}\right]$$

$$A = \begin{array}{r} \text{dog—hond} \\ \text{dog—op} \\ \text{dog—wielen} \\ \text{on—hond} \\ \text{on—op} \\ \text{on—wielen} \\ \text{wheels—hond} \\ \text{wheels—op} \\ \text{wheels—wielen} \end{array} \left[\begin{array}{ccccc} 1 & & 0 & 0 & \\ 0 & & 1 & 1 & \\ 0 & & 0 & 0 & \\ \hline 0 & & 0 & 0 & \\ 1 & \dots & 0 & 0 & \dots \\ 0 & & 1 & 1 & \\ \hline 0 & & 1 & 0 & \\ 0 & & 0 & 0 & \\ 1 & & 0 & 1 & \end{array}\right] \quad \boldsymbol{\eta} = \left[\begin{array}{r} .1 \\ .2 \\ -.1 \\ \hline .3 \\ .8 \\ .1 \\ \hline -.3 \\ .2 \\ -.1 \end{array}\right]$$

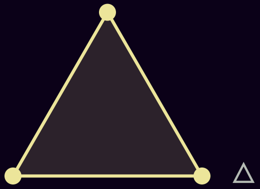


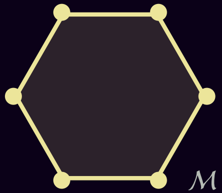
$\triangle$



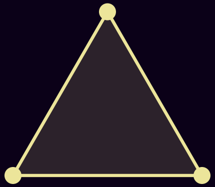
$\mathcal{M}$

$$\mathcal{M} := \operatorname{conv}\left\{\boldsymbol{a}_h : h \in \mathcal{H}\right\}$$

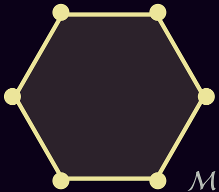


$$\mathcal{M} := \operatorname{conv}\left\{\boldsymbol{a}_h : h \in \mathcal{H}\right\}$$
$$= \left\{\boldsymbol{A}\boldsymbol{p} : \boldsymbol{p} \in \Delta\right\}$$

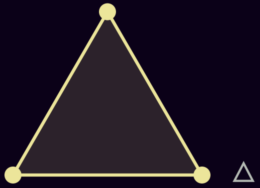


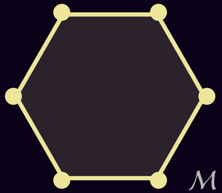
$\Delta$



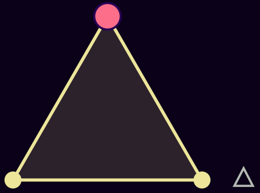
$\mathcal{M}$

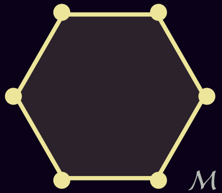
$$
\begin{aligned}
\mathcal{M} &:= \operatorname{conv}\left\{\boldsymbol{a}_h : h \in \mathcal{H}\right\} \\
&= \left\{\boldsymbol{A}\boldsymbol{p} : \boldsymbol{p} \in \Delta\right\} \\
&= \left\{\mathbb{E}_{H \sim \boldsymbol{p}}\, \boldsymbol{a}_H : \boldsymbol{p} \in \Delta\right\}
\end{aligned}
$$



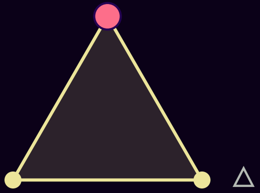



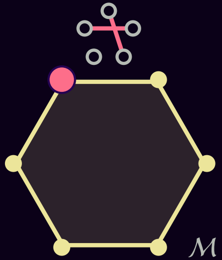
- **argmax** $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top \boldsymbol{\theta}$



- **argmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{\theta}$
- **MAP** $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta}$

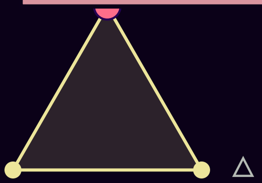


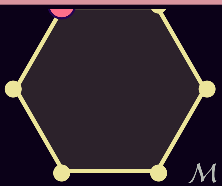



**argmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{\theta}$

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

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



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

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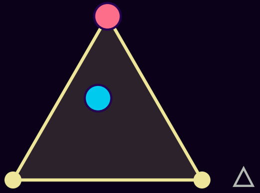
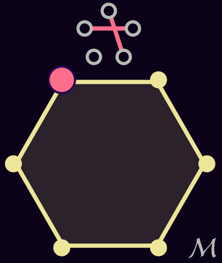
**softmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top\boldsymbol{\theta} + \mathrm{H}(\boldsymbol{p})$



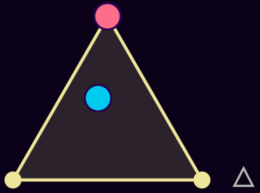



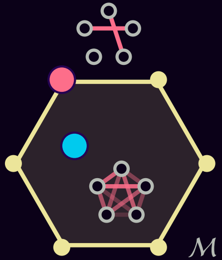
**argmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top\boldsymbol{\theta}$

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

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

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



- **argmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top\boldsymbol{\theta}$
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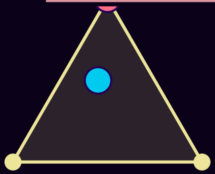
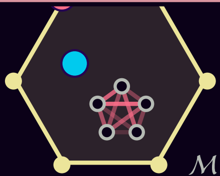
*e.g.* sequence labeling → forward-backward

(Rabiner, 1989)

As attention: (Kim et al., 2017)



$\triangle$



$\mathcal{M}$

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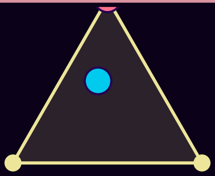
- **marginals** $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta} + \widetilde{\mathrm{H}}(\boldsymbol{\mu})$

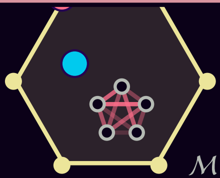
*e.g.* dependency parsing → **the Matrix-Tree theorem**

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

As attention: (Liu and Lapata, 2018)



$\triangle$



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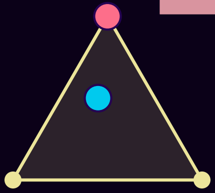
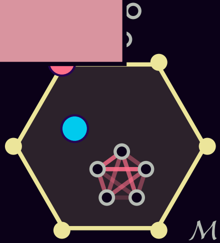
*e.g.* matchings → **#P-complete!**

(Taskar, 2004; Valiant, 1979)



$\triangle$



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

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

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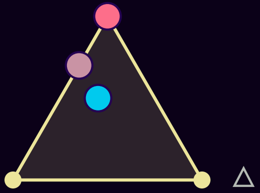


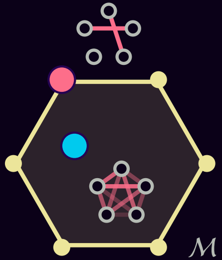

(Niculae, Martins, Blondel, and Cardie, 2018)

| | |
|---|---|
| **argmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top\boldsymbol{\theta}$ | **MAP** $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top\boldsymbol{\eta}$ |
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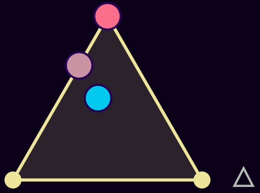
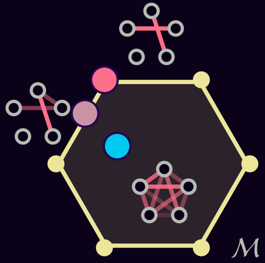
| **sparsemax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top\boldsymbol{\theta} - 1/2\|\boldsymbol{p}\|^2$ | **SparseMAP** $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top\boldsymbol{\eta} - 1/2\|\boldsymbol{\mu}\|^2$ |



# Algorithms for SparseMAP

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

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

linear constraints
*(alas, exponentially many!)*

quadratic objective

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**Conditional Gradient**

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

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

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- select a new corner of $\mathcal{M}$
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  - Update rules: vanilla, away-step, pairwise

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(Frank and Wolfe, 1956; Lacost

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  - Update rules: van
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    (Nocedal and Wright, 1999, Ch. 16.4 & 16.5)
    (Wolfe, 1976; Vinyes and Obozinski, 2017)

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

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**Backward pass**

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

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    (Wolfe, 1976; Vinyes and Obozinski, 2017)

## Backward pass

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

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

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

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    (Wolfe, 1976; Vinyes and Obozinski, 2017)

Completely modular: just add MAP

**pass**

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

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

# SparseMAP Applications

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

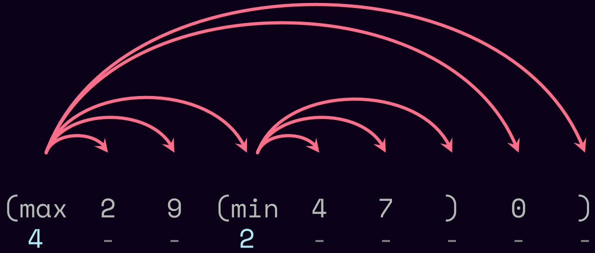
# Latent Dependency Trees

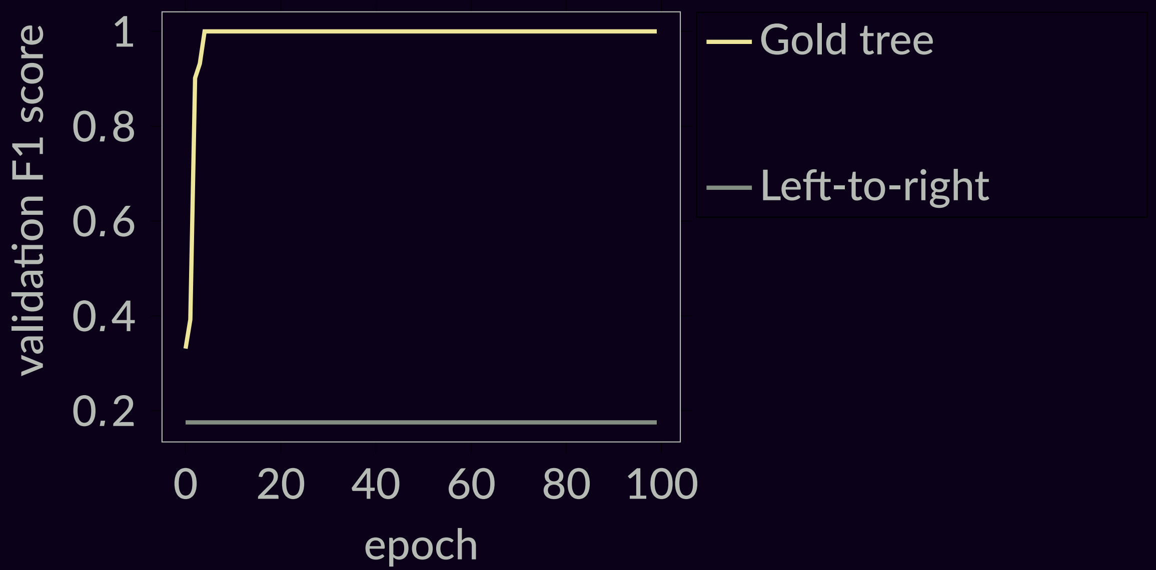
Arity tagging with latent GCN (Corro and Titov, 2019; Kipf and Welling, 2017)

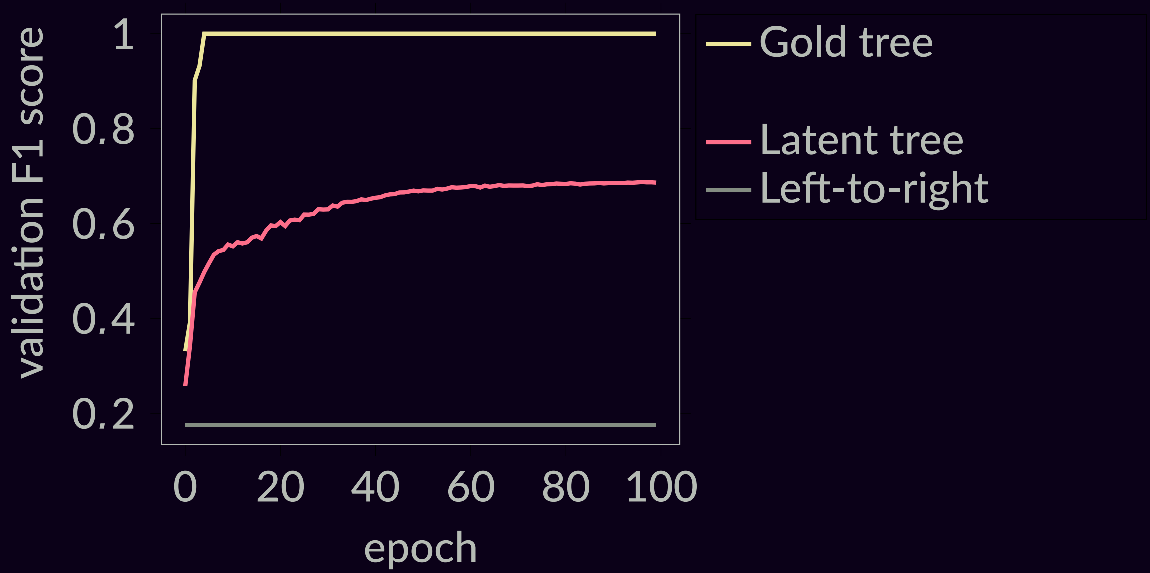
```
(max  2   9  (min  4   7   )   0   )
```

# Latent Dependency Trees

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

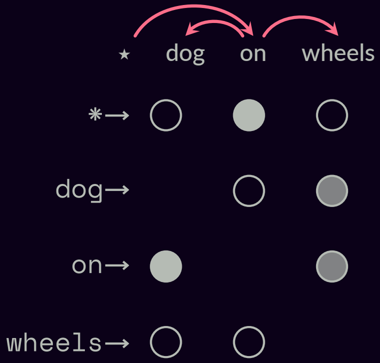



validation F1 score
1
0.8
0.6
0.4
0.2
0
20
40
60
80
100
epoch
Gold tree
Left-to-right


validation F1 score
1
0.8
0.6
0.4
0.2
0
20
40
60
80
100
epoch
Gold tree
Latent tree
Left-to-right

# What if MAP is not available?

# Multiple, Overlapping Factors



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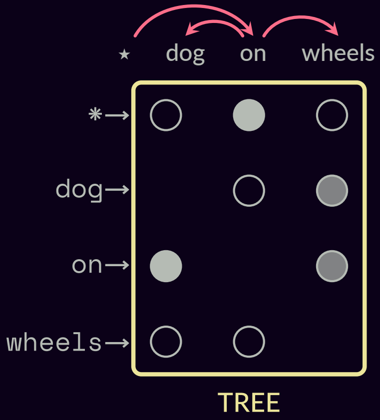

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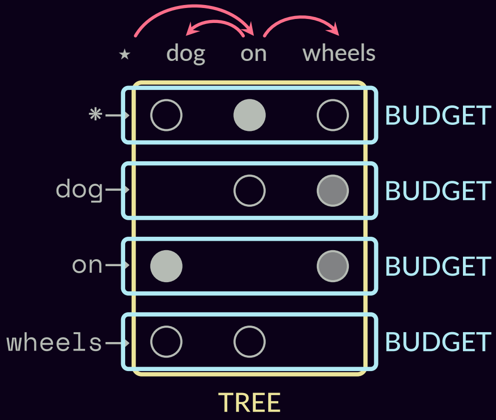
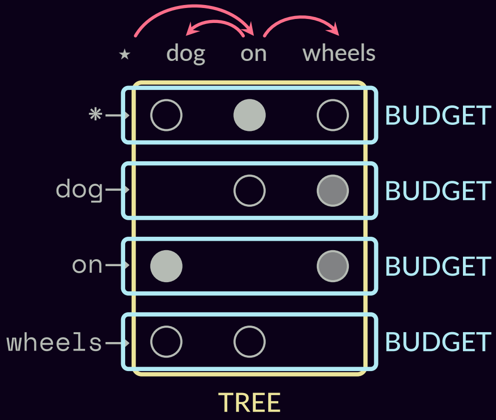
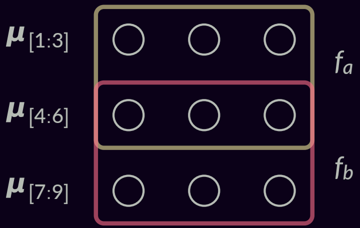


# Multiple, Overlapping Factors

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



# Optimization as Consensus-Seeking



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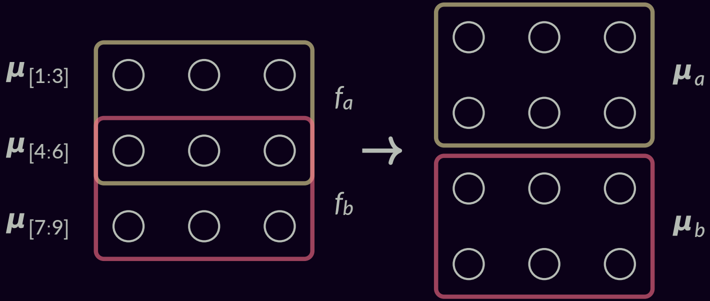

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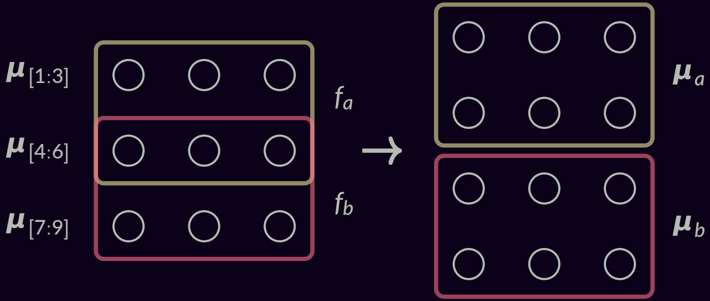


$$\max_{\boldsymbol{\mu}_f} \sum_{f \in \mathcal{F}} \boldsymbol{\eta}_f^\top \boldsymbol{\mu}_f \quad \text{s.t.} \quad \boldsymbol{\mu}_f \in \mathcal{M}_f \text{ for } f \in \mathcal{F}$$

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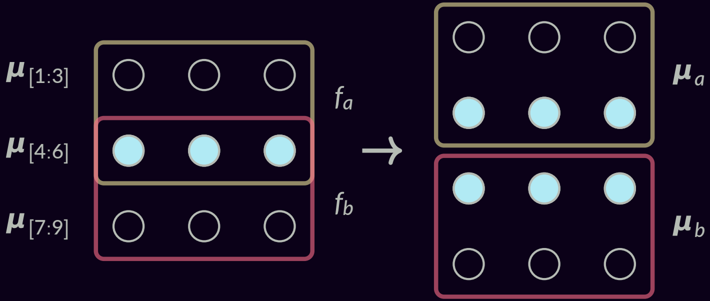


Agreement on overlap: $\boldsymbol{\mu}_{a,[4:6]} = \boldsymbol{\mu}_{b,[4:6]} = \boldsymbol{\mu}_{[4:6]}$

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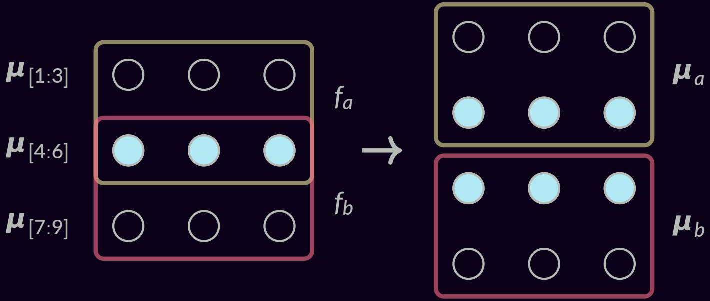


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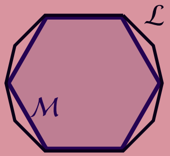
# Optim... ...eking

LP relaxation (Wainwright and Jordan, 2008)

the local polytope:

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




$\boldsymbol{\mu}_{[1:3}$ $\boldsymbol{\mu}_{[4:6}$ $\boldsymbol{\mu}_{[7:9}$

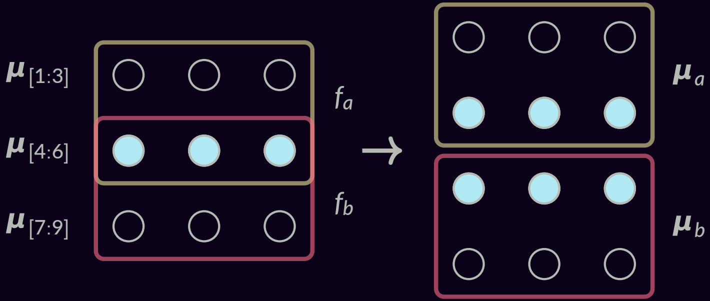
$\boldsymbol{\mu}_a$ $\boldsymbol{\mu}_b$

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

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

(Niculae and Martins, 2020)

# Optimization as Consensus-Seeking

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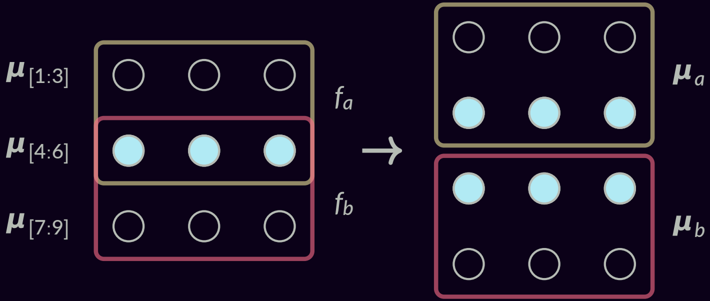


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$$\max_{\boldsymbol{\mu},\boldsymbol{\mu}_f} \Big( \sum_{f \in \mathcal{F}} \boldsymbol{\eta}_f^\top \boldsymbol{\mu}_f \Big) - \tfrac{1}{2} \|\boldsymbol{\mu}\|^2 \quad \text{s.t.} \quad \boldsymbol{C}_f \boldsymbol{\mu} = \boldsymbol{\mu}_f,\ \boldsymbol{\mu}_f \in \mathcal{M}_f \ \text{ for } f \in \mathcal{F}$$

# Algorithms for LP-SparseMAP

**Forward pass**

$$\operatorname*{arg\,max}_{\boldsymbol{C}_f\boldsymbol{\mu}=\boldsymbol{\mu}_f}\Big(\sum_{f\in\mathcal{F}}\boldsymbol{\eta}_f^\top\boldsymbol{\mu}_f\Big)-{}^1\!/_2\|\boldsymbol{\mu}\|^2$$

$$=\operatorname*{arg\,max}_{\boldsymbol{C}_f\boldsymbol{\mu}=\boldsymbol{\mu}_f}\sum_{f\in\mathcal{F}}\Big(\boldsymbol{\eta}_f^\top\boldsymbol{\mu}_f-{}^1\!/_2\|\boldsymbol{D}_f\boldsymbol{\mu}_f\|^2\Big)$$

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

(Niculae and Martins, 2020)

# Algorithms for LP-SparseMAP

### Forward pass

$$\arg\max_{C_f \boldsymbol{\mu} = \boldsymbol{\mu}_f} \Big( \sum_{f \in \mathcal{F}} \boldsymbol{\eta}_f^\top \boldsymbol{\mu}_f \Big) - 1/2 \|\boldsymbol{\mu}\|^2$$

$$= \arg\max_{C_f \boldsymbol{\mu} = \boldsymbol{\mu}_f} \sum_{f \in \mathcal{F}} \Big( \boldsymbol{\eta}_f^\top \boldsymbol{\mu}_f - 1/2 \|\boldsymbol{D}_f \boldsymbol{\mu}_f\|^2 \Big)$$

- Separable objective, agreement constraints

  ADMM in consensus form

- SparseMAP subproblem for each $f$

### Backward pass

- Jacobian fixed-point characterization

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

- 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 ≠ j]  # handwave

fg.add(Tree(var))

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

μ = fg.lp_sparsemap(η)
```

Factor graphs as a hidden-layer DSL!

(Niculae and Martins, 2020)

# Differentiable Sparse Structured Prediction


```
fg = FactorGraph()
var = [fg.variable() for i ≠ j]   # handwave

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

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# Differentiable Sparse Structured Prediction


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(ηf):   # abstract, private
        raise NotImplemented

    def sparsemap(ηf):
        # active set algo, uses self.map

    def backward(dμf):
        # analytic, uses active set result


class Budget(Factor):
    def sparsemap(ηf):
        # specialized

    def backward(dμf):
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```

(Niculae and Martins, 2020)

# Differentiable Sparse Structured Prediction


Factor graphs as a hidden-layer DSL!

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

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New factors only require MAP.

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class Budget(Factor):
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        # specialized

    def backward(dμf):
        # specialized


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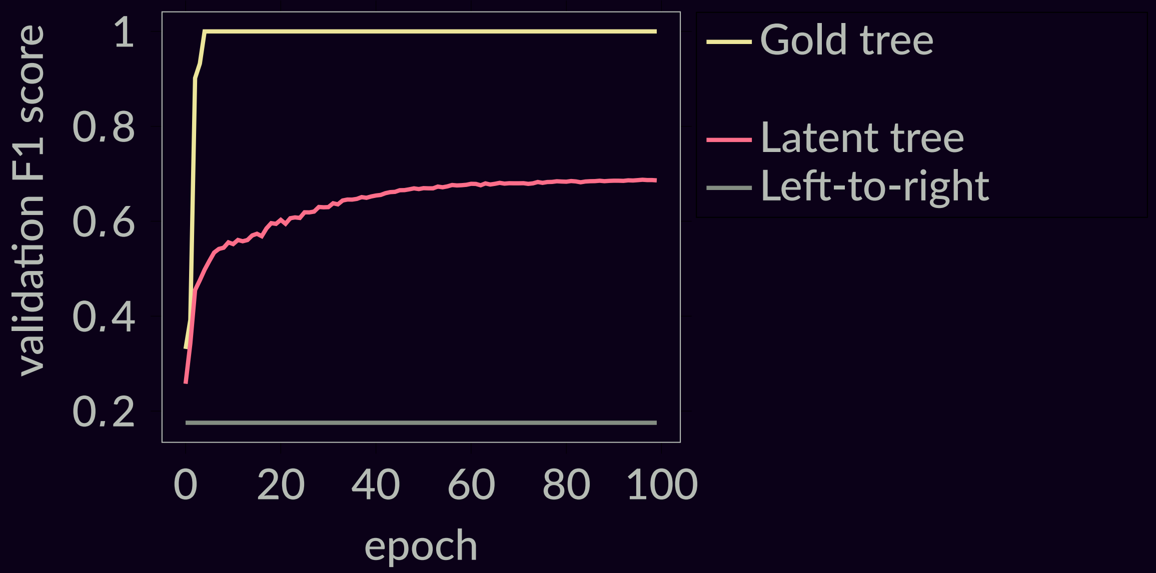
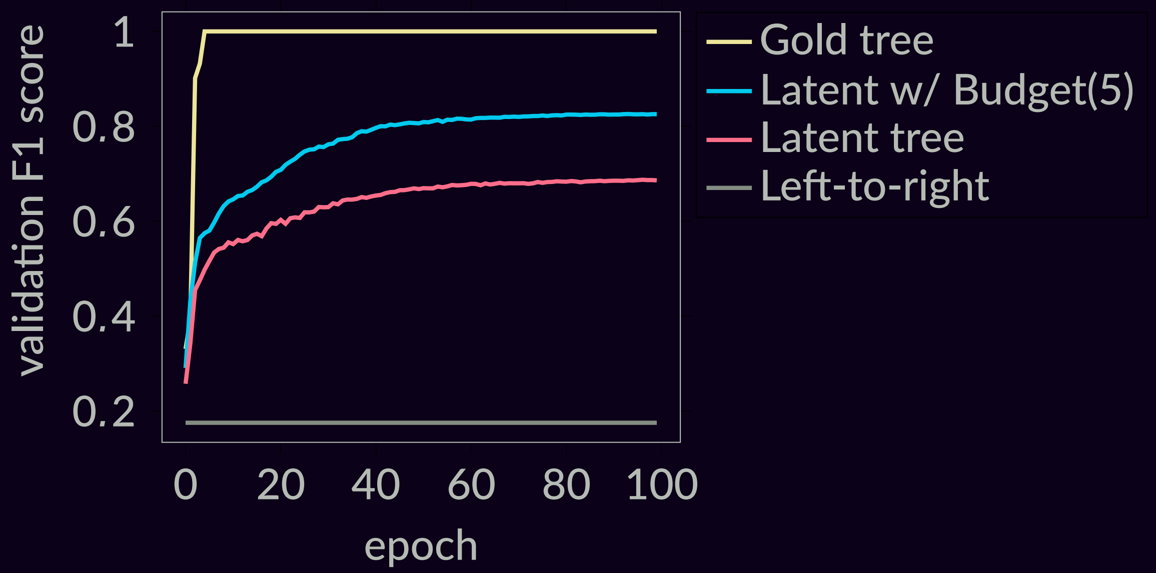


validation F1 score
1
0.8
0.6
0.4
0.2
0
20
40
60
80
100
epoch
Gold tree
Latent tree
Left-to-right


validation F1 score
1
0.8
0.6
0.4
0.2
0
20
40
60
80
100
epoch
Gold tree
Latent w/ Budget(5)
Latent tree
Left-to-right

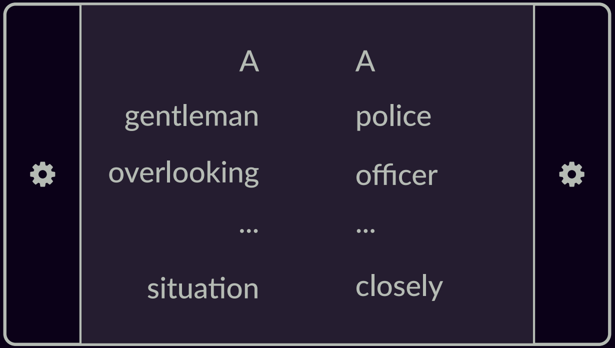
# Structured Attention for Alignments

NLI

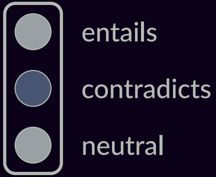
premise: A gentleman overlooking a neighborhood situation.
hypothesis: A police officer watches a situation closely.

input

(P, H)




output




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

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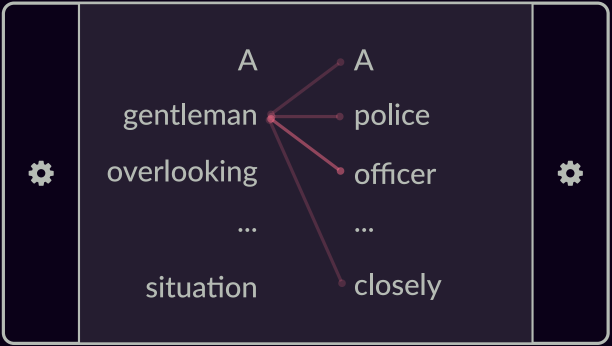


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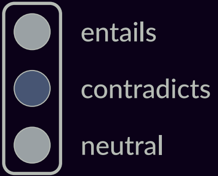


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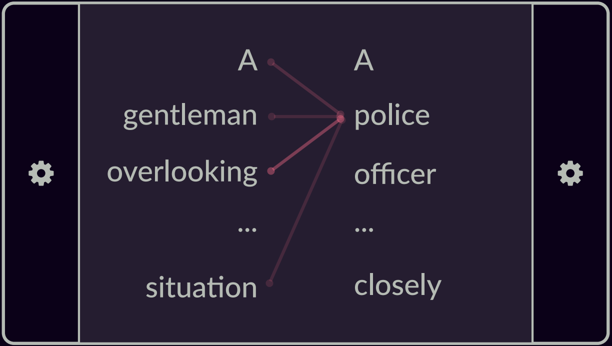
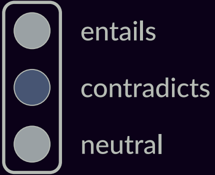



output

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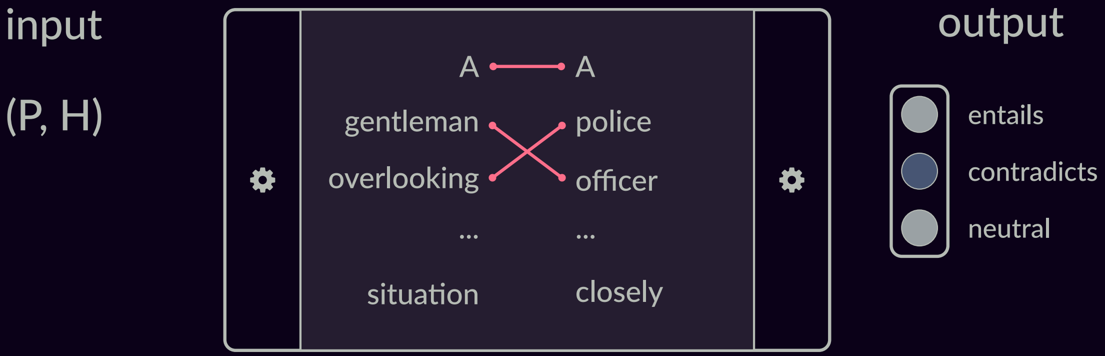
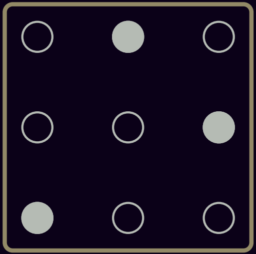



(Proposed model: global structured alignment.)

# Structured Alignment Models

***matching***

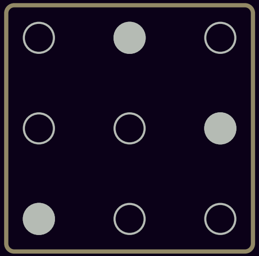


SparseMAP w/ Kuhn-Munkres

(Kuhn, 1955)

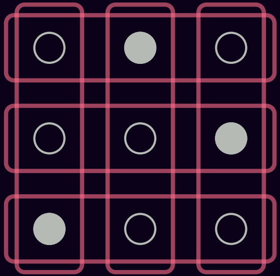
# Structured Alignment Models

***matching***



SparseMAP w/ Kuhn-Munkres
(Kuhn, 1955)

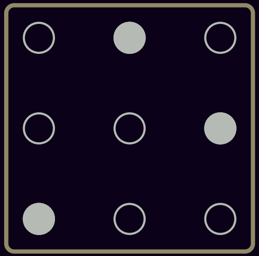
***LP-matching***



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

# Structured Alignment Models

### *matching*



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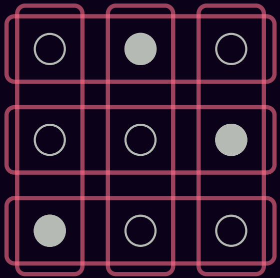
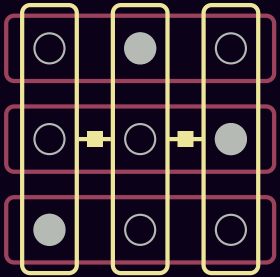


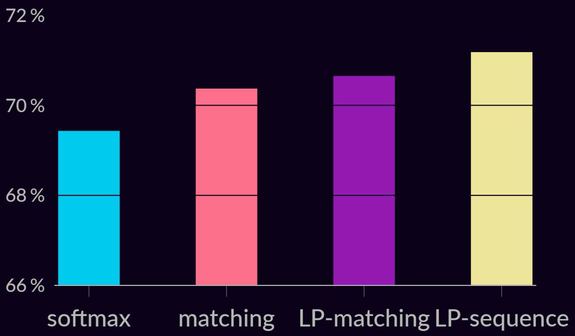
LP-SparseMAP w/ XORs
(equivalent; different solver)

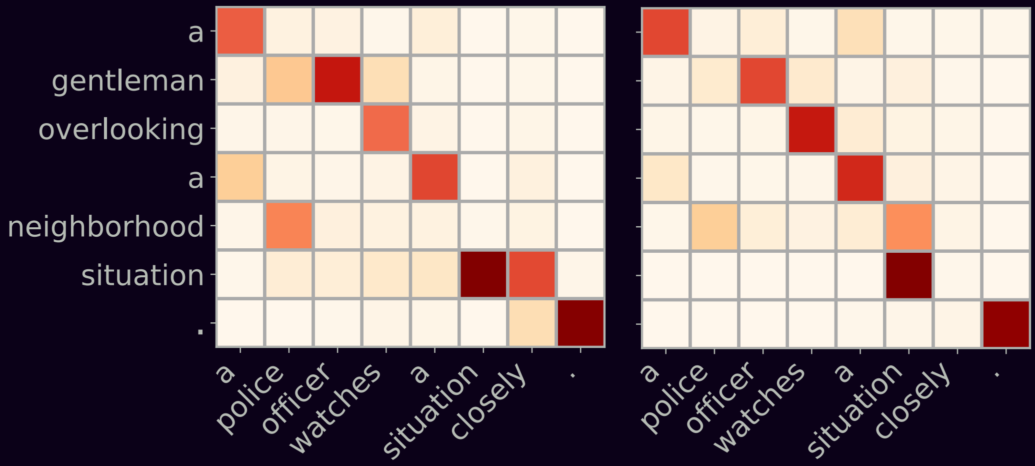
### *LP-sequence*



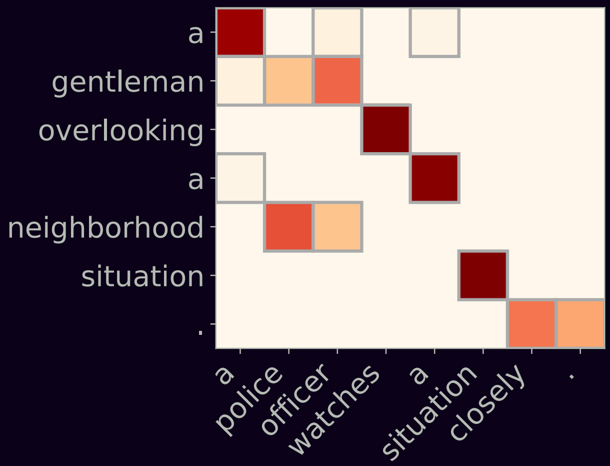
additional score
for *contiguous alignments*
$(i, j) - (i + 1, j \pm 1)$

## **MultiNLI** (Williams et al., 2017)





a
gentleman
overlooking
a
neighborhood
situation
.
a
police
officer
watches
a
situation
closely
.
a
police
officer
watches
a
situation
closely
.


a
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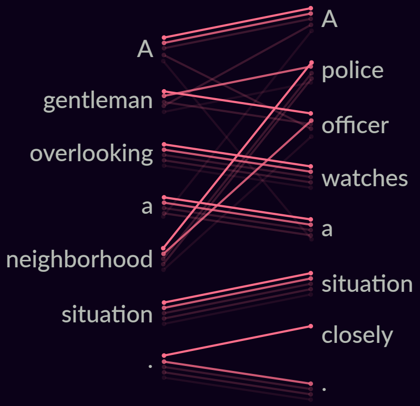
A
gentleman
overlooking
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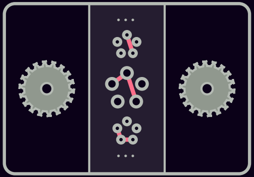
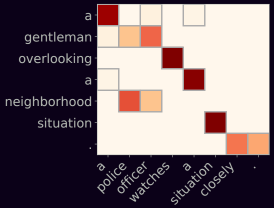
# Conclusions

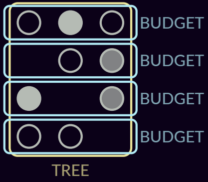
Differentiable & sparse
structured inference

Generic, extensible, efficient algorithms

Interpretable **structured attention**






vlad@vene.ro
https://vene.ro
github.com/deep-spin/lp-sparsemap
@vnfrombucharest

# Conclusions

Differentiable & sparse
structured inference

Generic, extensible, efficient algorithms

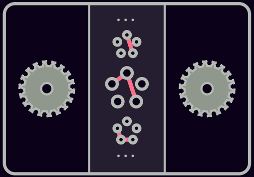
Interpretable **structured attention**

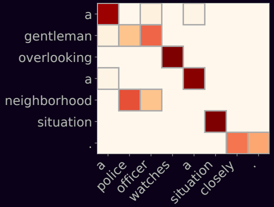
# Future work

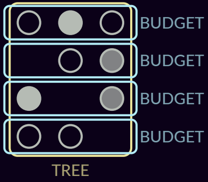
Structure beyond NLP

Weak & semi-supervision

Generative latent structure models



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# 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.

# Sparsemax

$$\operatorname{sparsemax}(\boldsymbol{\theta}) = \operatorname*{arg\,max}_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top \boldsymbol{\theta} - 1/2 \|\boldsymbol{p}\|_2^2$$

$$= \operatorname*{arg\,min}_{\boldsymbol{p} \in \triangle} \|\boldsymbol{p} - \boldsymbol{\theta}\|_2^2$$

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**Computation:**

$$\boldsymbol{p}^\star = [\boldsymbol{\theta} - \tau\mathbf{1}]_+$$
$$\theta_i > \theta_j \Rightarrow p_i \geq p_j$$
$\mathcal{O}(d)$ via partial sort

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

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**Backward pass:**

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

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

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

(Martins and Astudillo, 2016)

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$\boldsymbol{p}^\star = [($

$\theta_i > \theta_j$

$\mathcal{O}(d)$ via

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

**argmin differentiation**

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

**Backward pass:**

$g(\boldsymbol{s}) - \frac{1}{|\mathcal{S}|}\boldsymbol{s}\boldsymbol{s}^\top$

$: p_j^\star > 0\},$

$\in \mathcal{S}]$

(Martins and Astudillo, 2016)

# Fusedmax

$$\mathrm{fusedmax}(\boldsymbol{\theta}) = \underset{\boldsymbol{p}\in\triangle}{\arg\max}\, \boldsymbol{p}^\top\boldsymbol{\theta} - 1/2\|\boldsymbol{p}\|_2^2 - \sum_{2\le j\le d} |p_j - p_{j-1}|$$

$$= \underset{\boldsymbol{p}\in\triangle}{\arg\min}\, \|\boldsymbol{p} - \boldsymbol{\theta}\|_2^2 + \sum_{2\le j\le d} |p_j - p_{j-1}|$$

$$\mathrm{prox}_{\mathrm{fused}}(\boldsymbol{\theta}) = \underset{\boldsymbol{p}\in\mathbb{R}^d}{\arg\min}\, \|\boldsymbol{p} - \boldsymbol{\theta}\|_2^2 + \sum_{2\le j\le d} |p_j - p_{j-1}|$$

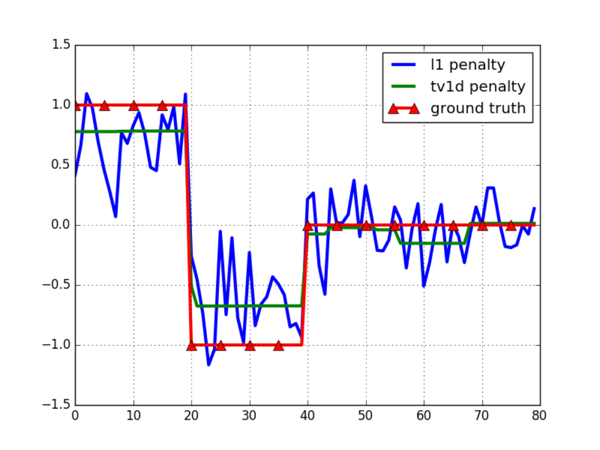
**Proposition:** $\mathrm{fusedmax}(\boldsymbol{\theta}) = \mathrm{sparsemax}\left(\mathrm{prox}_{\mathrm{fused}}(\boldsymbol{\theta})\right)$

(Niculae and Blondel, 2017)

fusedmax( … $|p_j - p_{j-1}|$

prox$_{\text{fused}}$( … $_{j-1}|$

… $_{j-1}|$




"Fused Lasso" a.k.a. 1-d Total Variation

(Tibshirani et al., 2005)

**Proposi** … $_{\text{used}}(\boldsymbol{\theta}))$

(Niculae and Blondel, 2017)

(Danskin, 1966; Prop. B.25 in Bertsekas, 1999)

# Danskin's Theorem

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

$$\partial \max_{\boldsymbol{z} \in \mathcal{Z}} \phi(\boldsymbol{x}, \boldsymbol{z}) = \operatorname{conv}\{\nabla_{\boldsymbol{x}} \phi(\boldsymbol{x}, \boldsymbol{z}^\star) \mid \boldsymbol{z}^\star \in \arg\max_{\boldsymbol{z} \in \mathcal{Z}} \phi(\boldsymbol{x}, \boldsymbol{z})\}.$$

**Example: maximum of a vector**

(Danskin, 1966; Prop. B.25 in Bertsekas, 1999)

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**Example: maximum of a vector**

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

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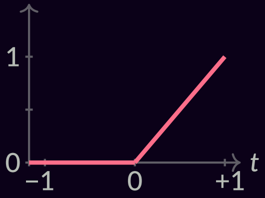
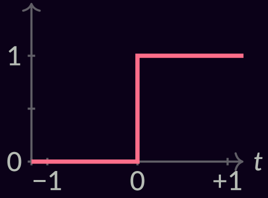
&= \operatorname{conv}\left\{ \boldsymbol{p}^\star \right\}
\end{aligned}$$

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



$\max_j \theta_j$



$\{ g_1 \mid \boldsymbol{g} \in \partial \max_j \theta_j \}$

# Dynamically inferring the computation graph

So far: a structured hidden layer

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

Network must handle “soft” combinations of structures.

Fine for attention, but can be limiting.

# Dependency TreeLSTM

(Tai et al., 2015)

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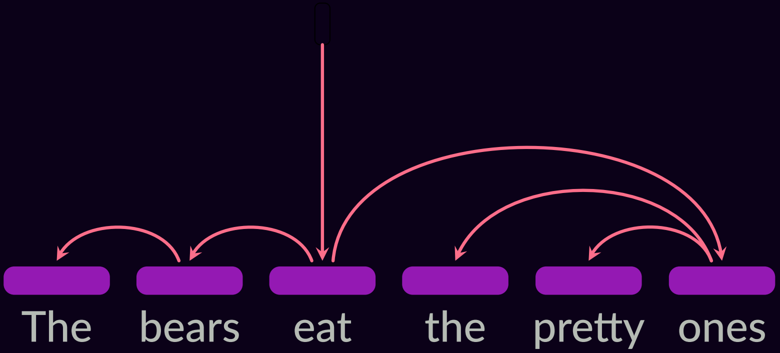
(Tai et al., 2015)



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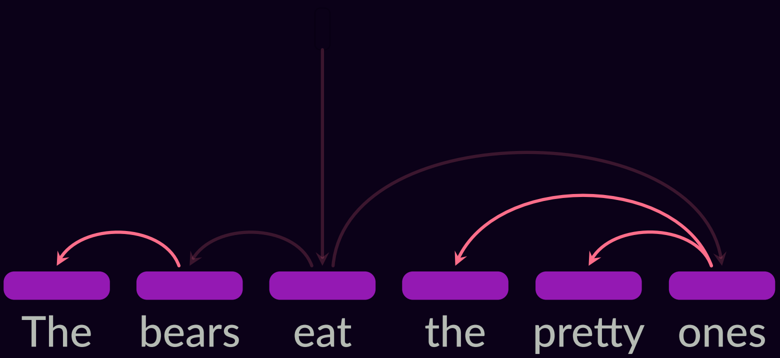

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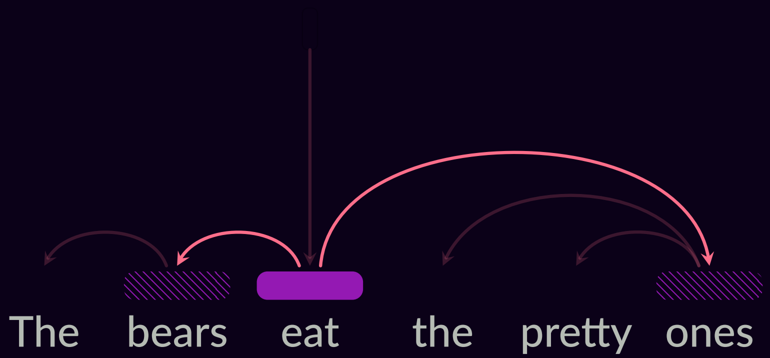

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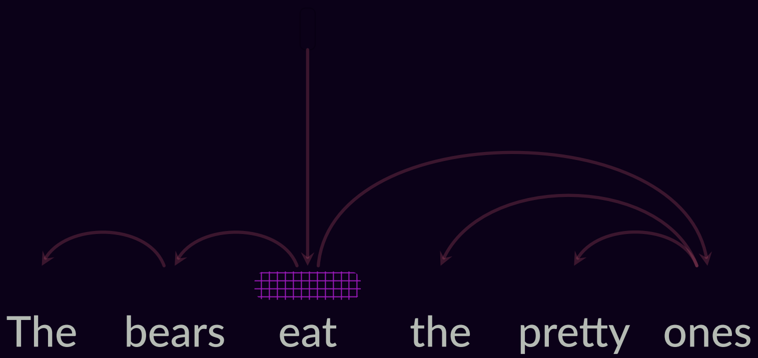

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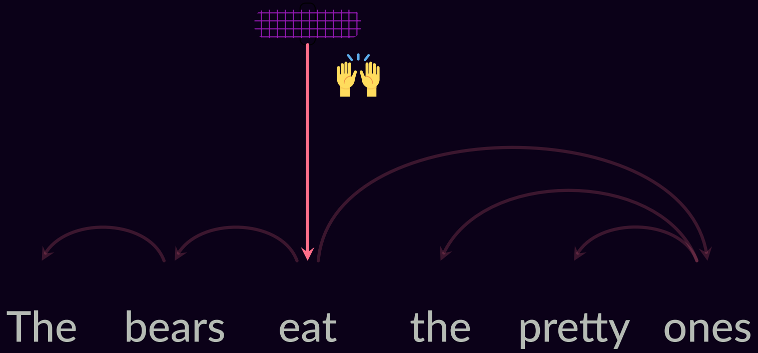
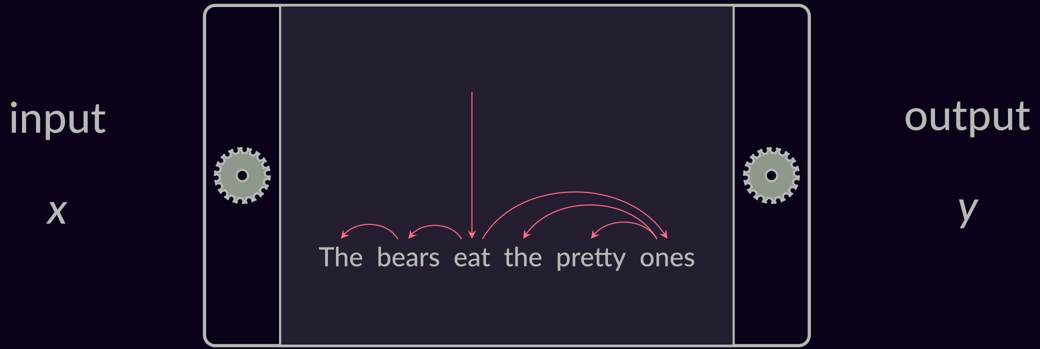


# Latent Dependency TreeLSTM

(Niculae, Martins, and Cardie, 2018)



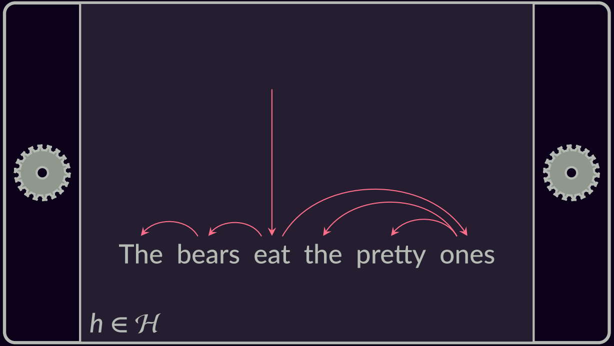
# Latent Dependency TreeLSTM

(Niculae, Martins, and Cardie, 2018)

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

input

$x$




output

$y$

# Structured Latent Variable Models

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

# Structured Latent Variable Models

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

# Structured Latent Variable Models

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

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parsing model,
using some $\text{score}_{\boldsymbol{\pi}}(h; x)$

# Structured Latent Variable Models

sum over
all possible trees

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Exponentially large sum!

# Structured Latent Variable Models

sum over
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*e.g.*, a TreeLSTM defined by $h$

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**How to define $p_{\boldsymbol{\pi}}$?**

idea 1

idea 2

idea 3

# Structured Latent Variable Models

sum over
all possible trees

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

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😊 😟

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| | | | | |
|---|---|---|---|---|
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| idea 3 | | | | |

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| idea 3 | | SparseMAP | 😊 | 😊 |

# SparseMAP

 = .7  + .3 

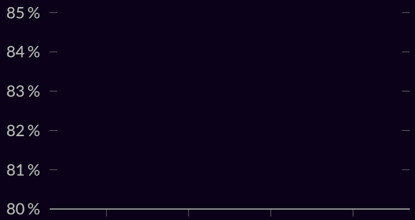
# SparseMAP

 = .7  + .3  + 0  + ...

# SparseMAP

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

$p(y \mid x) = \ .7 \ p_{\boldsymbol{\phi}}(y \mid$  $) + .3 \ p_{\boldsymbol{\phi}}(y \mid$  $)$


85 %
84 %
83 %
82 %
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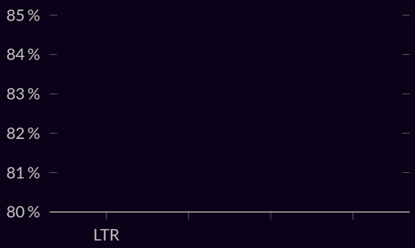
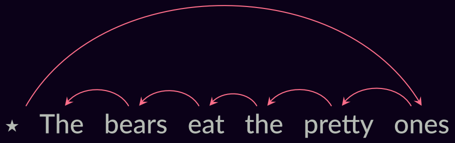
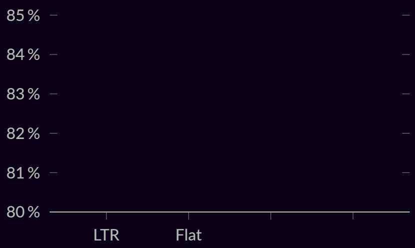
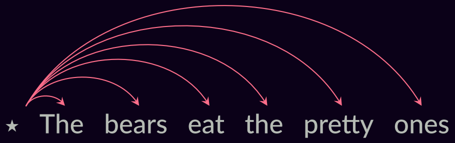
80 %



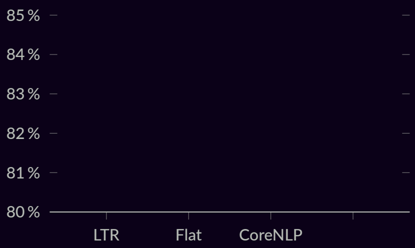




Left-to-right: regular LSTM



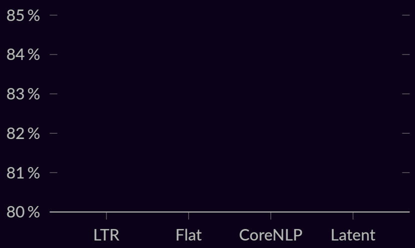




Flat: bag-of-words–like

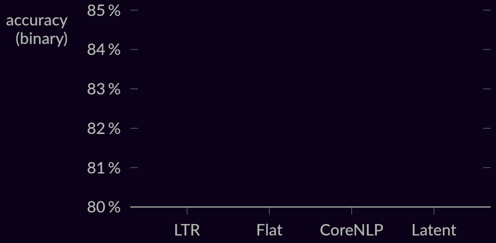




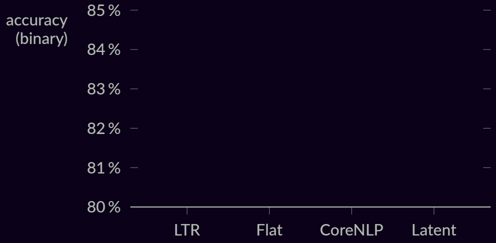
CoreNLP: off-line parser


85 %
84 %
83 %
82 %
81 %
80 %
LTR
Flat
CoreNLP
Latent

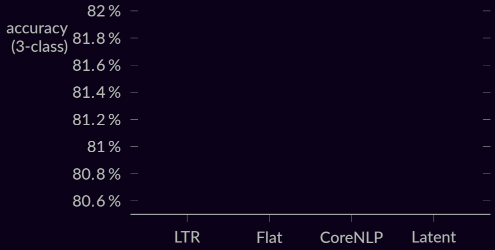
# **Sentiment classification** (SST)



**Sentiment classification** (SST)



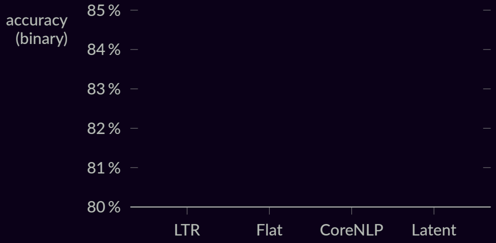

**Natural Language Inference** (SNLI)




Sentence pair classification $(P, H)$

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

**Sentiment classification** (SST)

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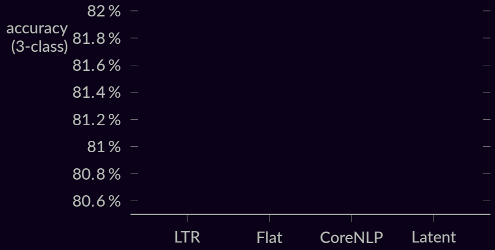
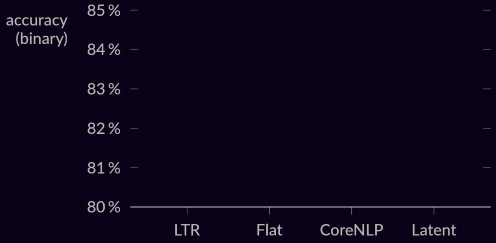



## Reverse dictionary lookup

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

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

## **Sentiment classification** (SST)

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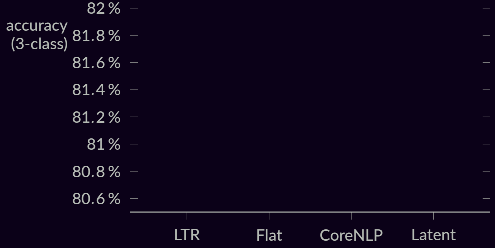
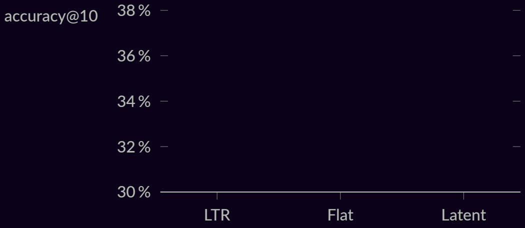
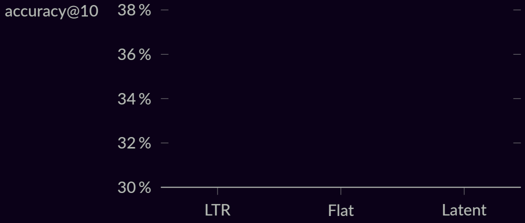



## **Reverse dictionary lookup**

(definitions)




(concepts)



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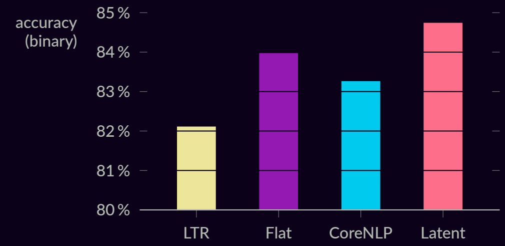


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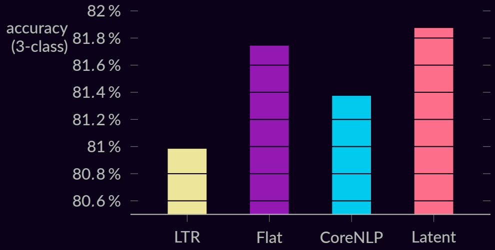


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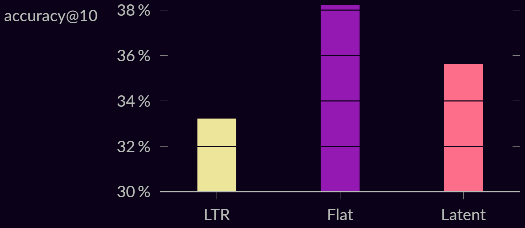
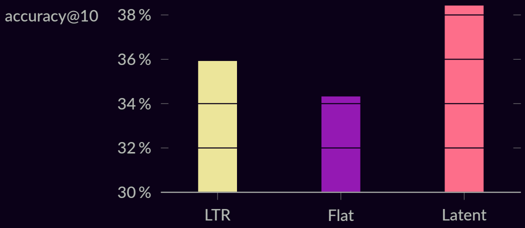



(concepts)



# Syntax vs. Composition Order

CoreNLP parse, $p = 21.4\%$

# Syntax vs. Composition Order

$p = 22.6\%$

⋆ lovely and poignant .

CoreNLP parse, $p = 21.4\%$

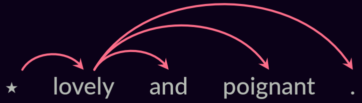
⋆ lovely and poignant .

. . .

# Syntax vs. Composition Order

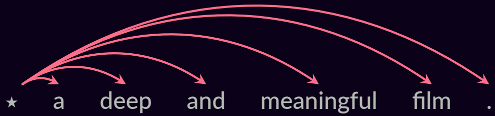
$p = 22.6\%$


CoreNLP parse, $p = 21.4\%$




. . .

$p = 15.33\%$




$p = 15.27\%$


. . .

CoreNLP parse, $p = 0\%$

# Structured Output Prediction

SparseMAP

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

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

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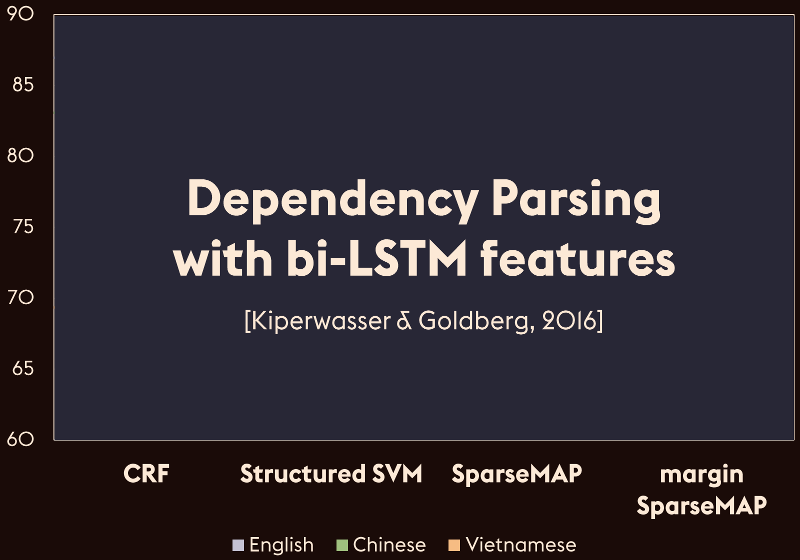
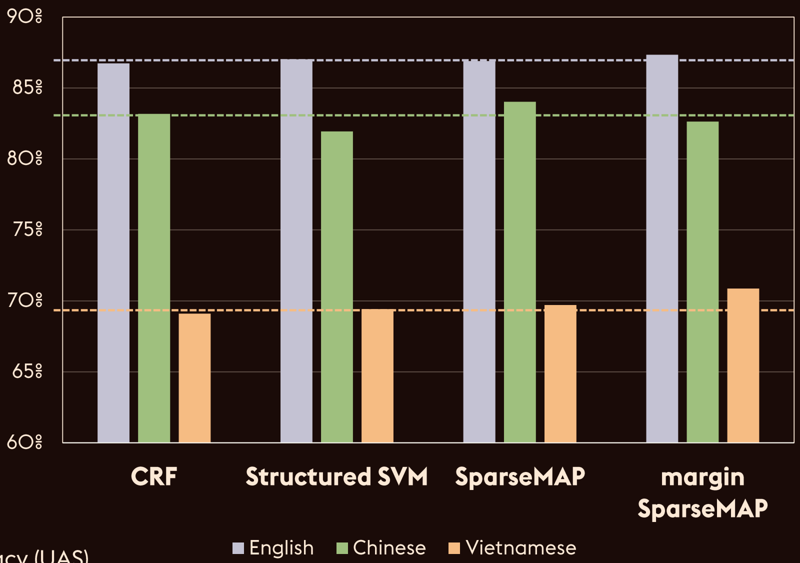
cost-SparseMAP
$$L_A^\rho(\boldsymbol{\eta}, \bar{\boldsymbol{\mu}}) = \max_{\boldsymbol{\mu} \in \mathcal{M}} \left\{ \boldsymbol{\eta}^\top \boldsymbol{\mu} - 1/2 \|\boldsymbol{\mu}\|^2 + \rho(\boldsymbol{\mu}, \bar{\boldsymbol{\mu}}) \right\} - \boldsymbol{\eta}^\top \bar{\boldsymbol{\mu}} + 1/2 \|\bar{\boldsymbol{\mu}}\|^2$$

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



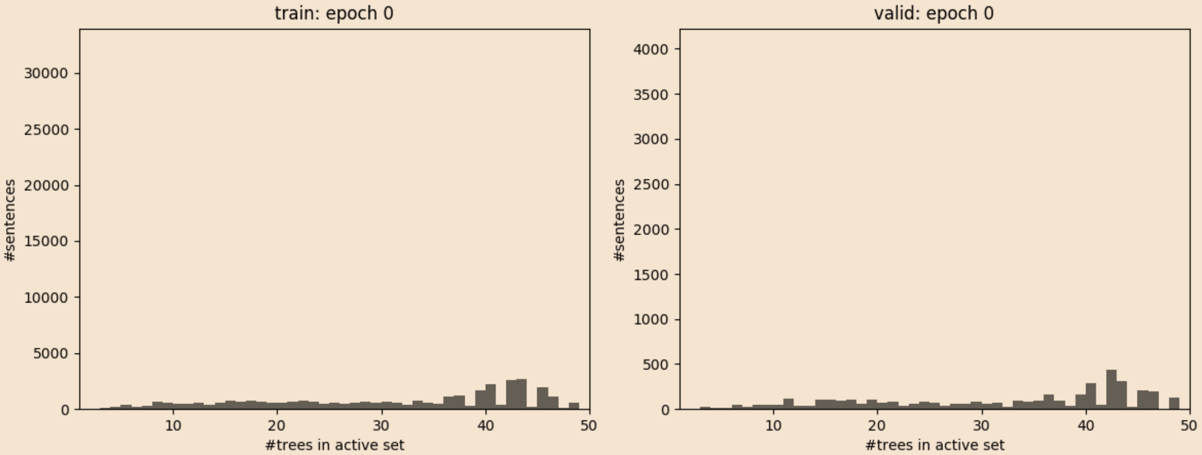
90
85
80
75
70
65
60
Dependency Parsing
with bi-LSTM features
[Kiperwasser & Goldberg, 2016]
CRF
Structured SVM
SparseMAP
margin SparseMAP
English
Chinese
Vietnamese




Unlabeled Accuracy (UAS)
Universal Dependencies dataset

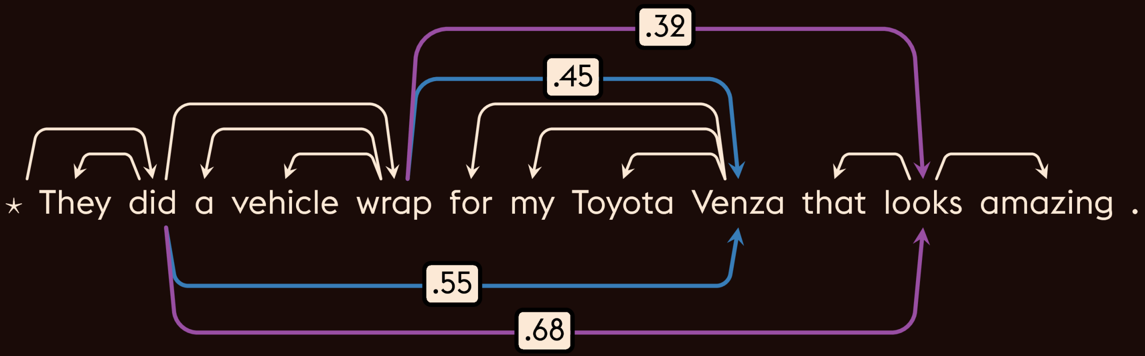
# Sparse Structured Output Prediction

## As models train, inference gets sparser!



# Sparse Structured Output Prediction

**Inference captures linguistic ambiguity!**



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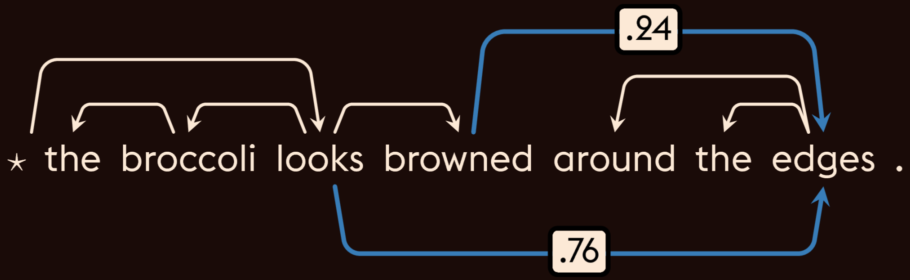

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