Learning with Sparse Latent Structure

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Instituto de Telecomunicações

Work with: André Martins, Claire Cardie, Mathieu Blondel

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.

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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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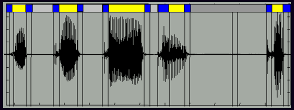
Most of this structure is **hidden**.

Rich Underlying Structure

Widely occuring pattern!

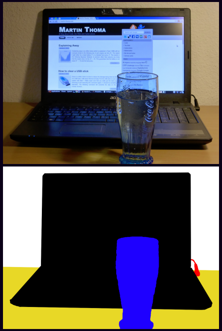
speech

(Andre-Obrecht, 1988)



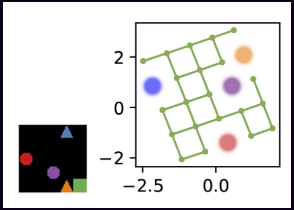
objects

(Long et al., 2015)



transition graphs

(Kipf, Pol, et al., 2020)



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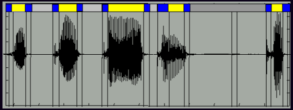

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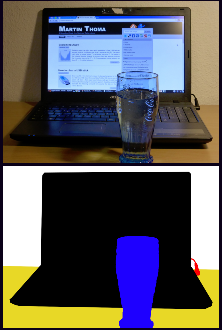

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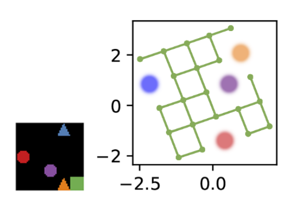
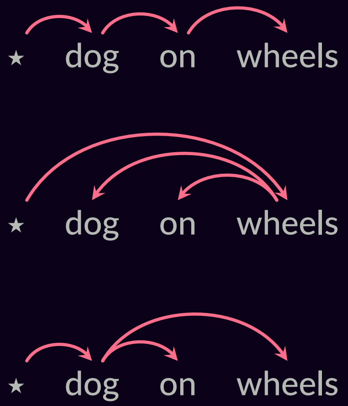


But we'll focus on NLP.

Structured Prediction

. . .



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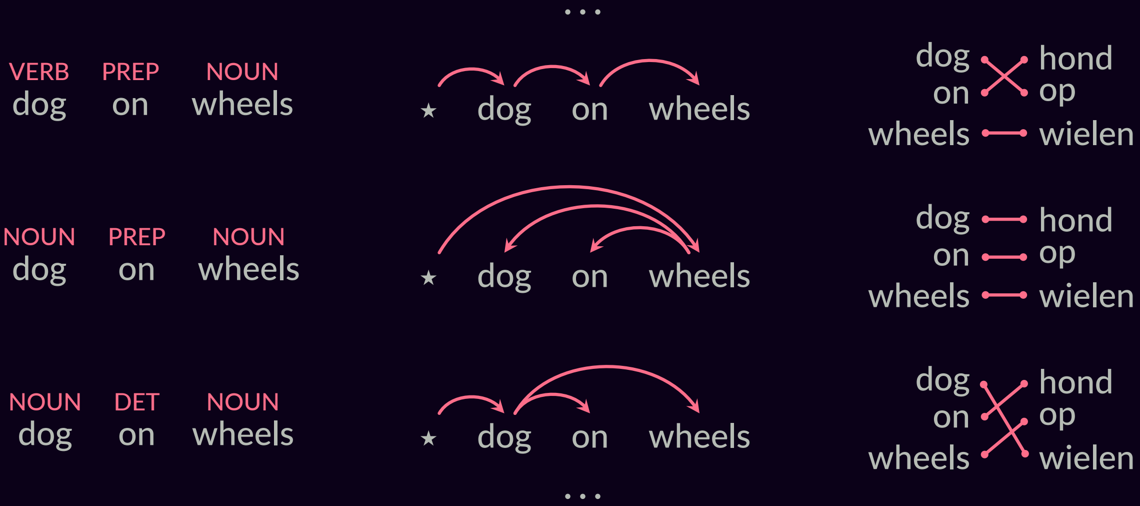

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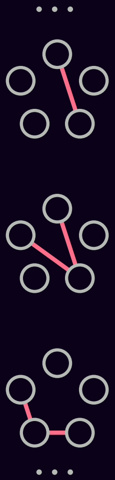


Traditional Pipeline Approach

input

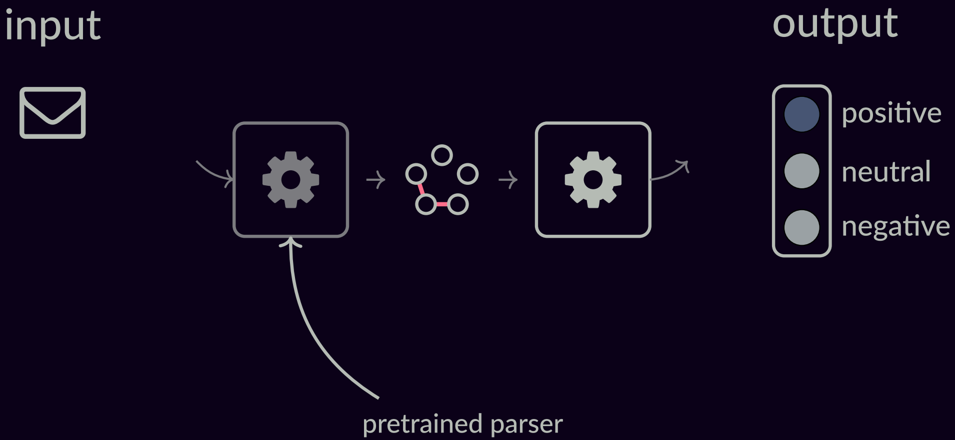
output

positive

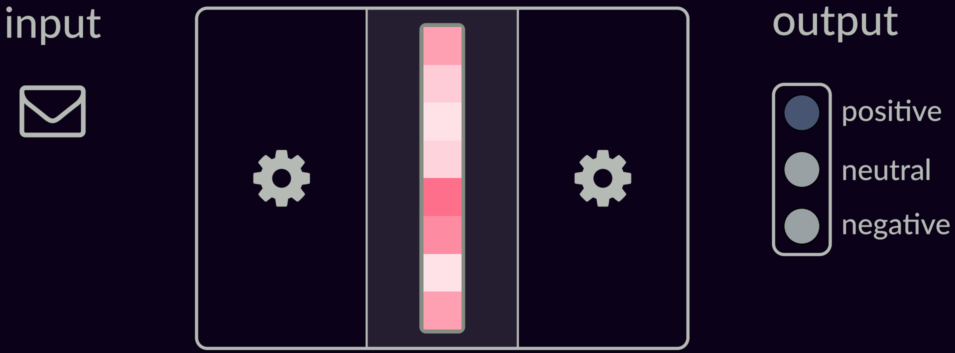
neutral

negative

Traditional Pipeline Approach



Deep Learning & Hidden Representations



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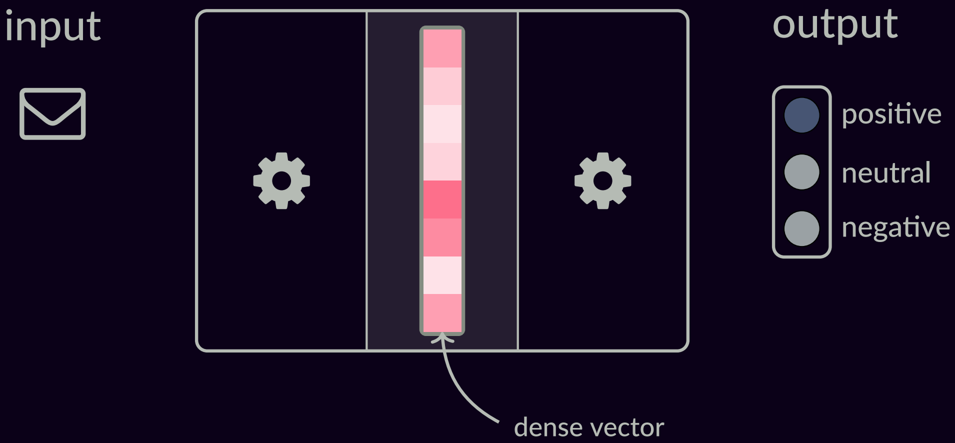
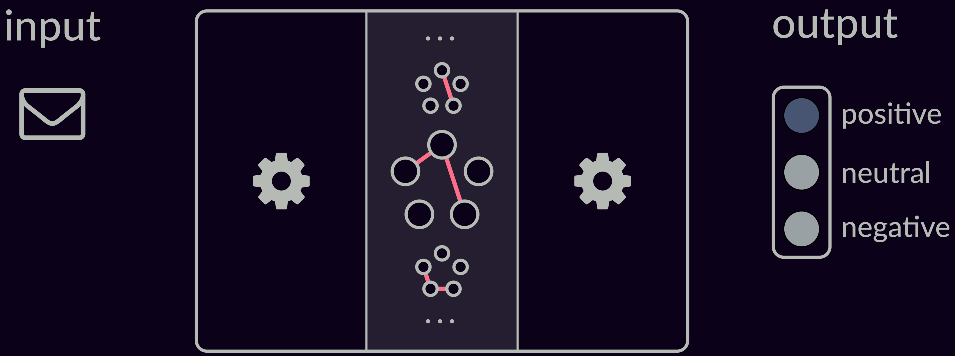


Latent Structure Models

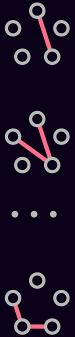


record scratch

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?

$$c_1$$

$$c_2$$

$$\cdots$$

$$c_N$$

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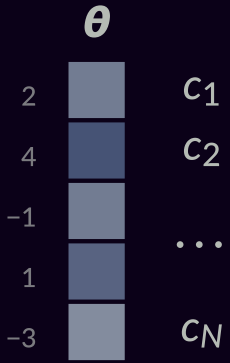

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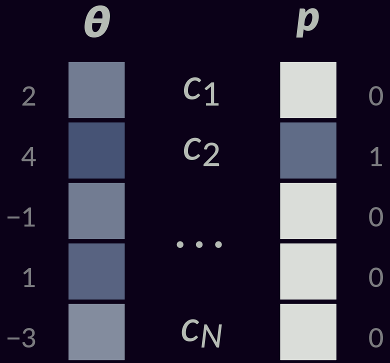

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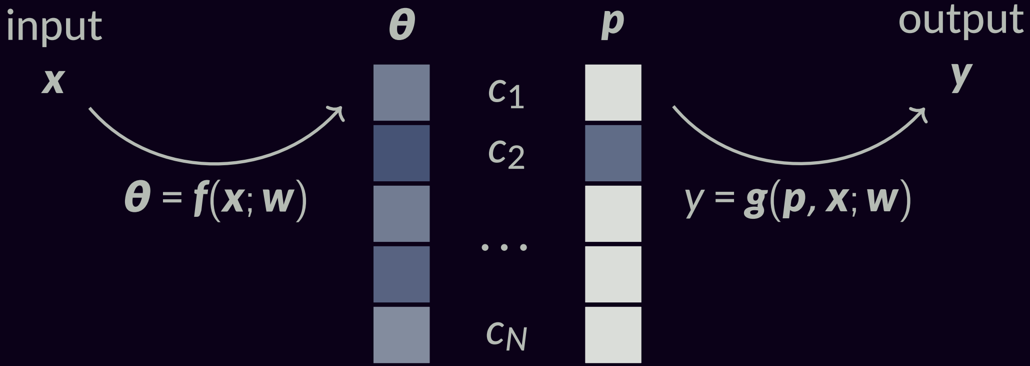

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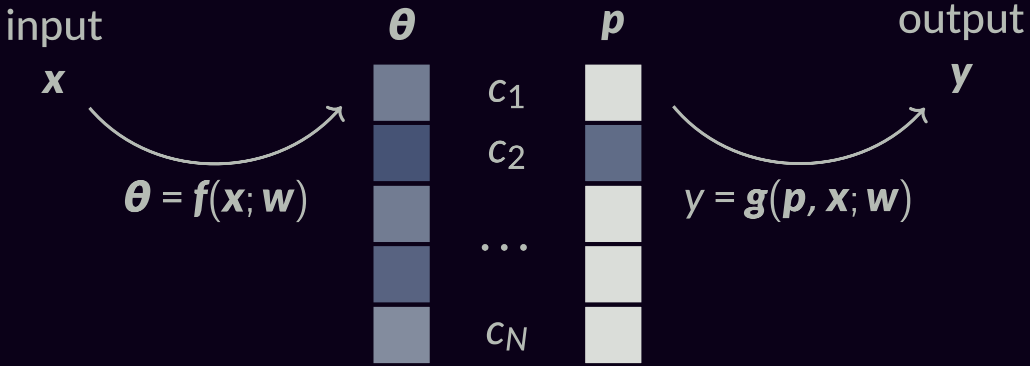

$$\frac{\partial y}{\partial \boldsymbol{w}} = ?$$

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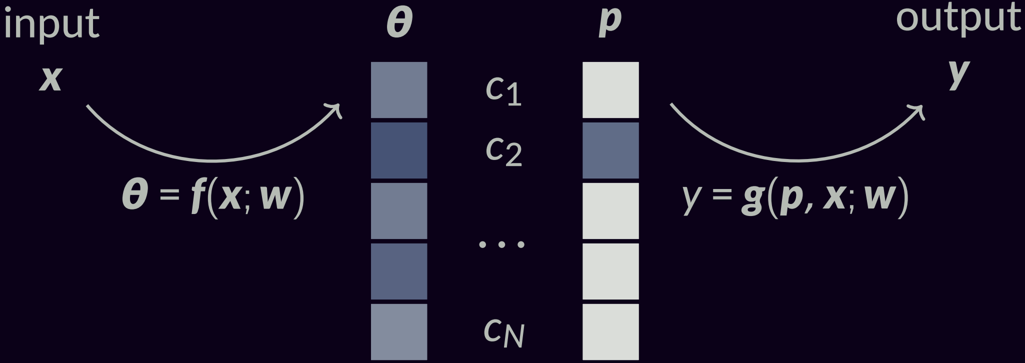
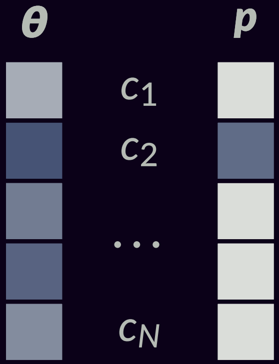


$\frac{\partial y}{\partial \boldsymbol{w}} = ?$ or, essentially, $\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{\theta}} = ?$

Argmax



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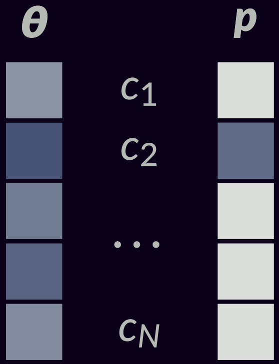

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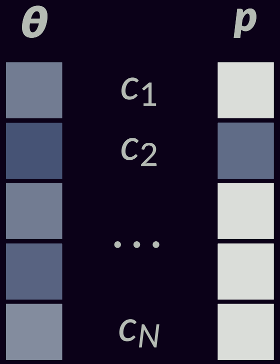

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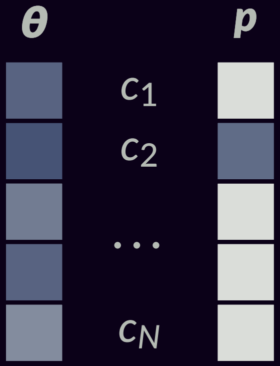

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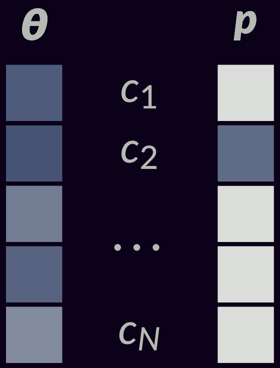

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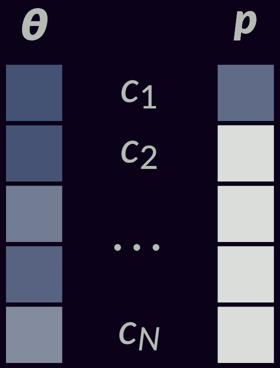

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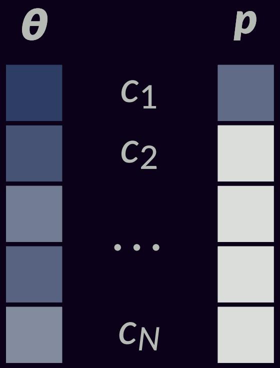

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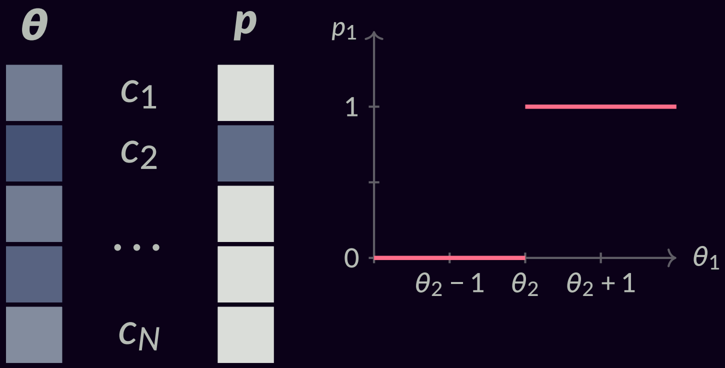
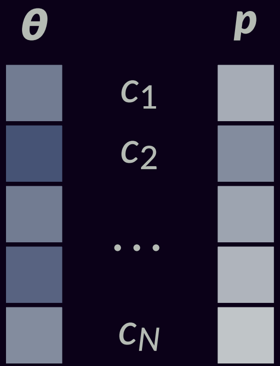
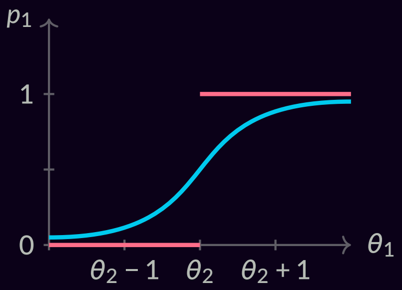


$$\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{\theta}} = \mathbf{0}$$

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 🦸🏽‍♀️

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

A Softmax Origin Story 🦸🏽‍♀️

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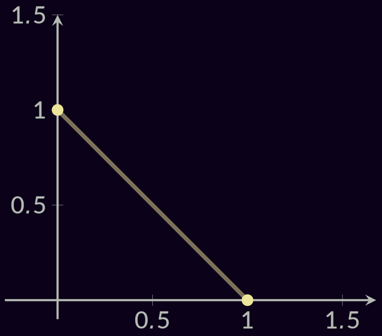

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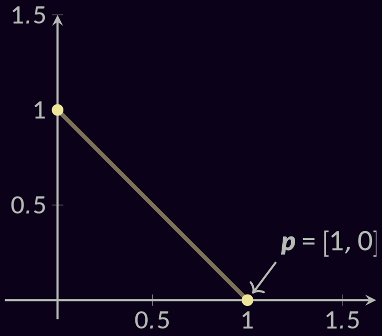

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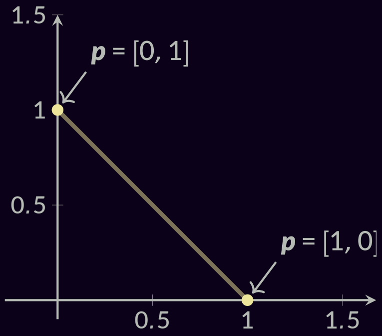

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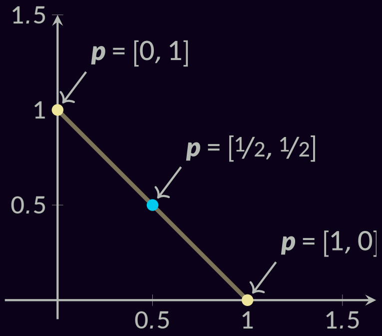

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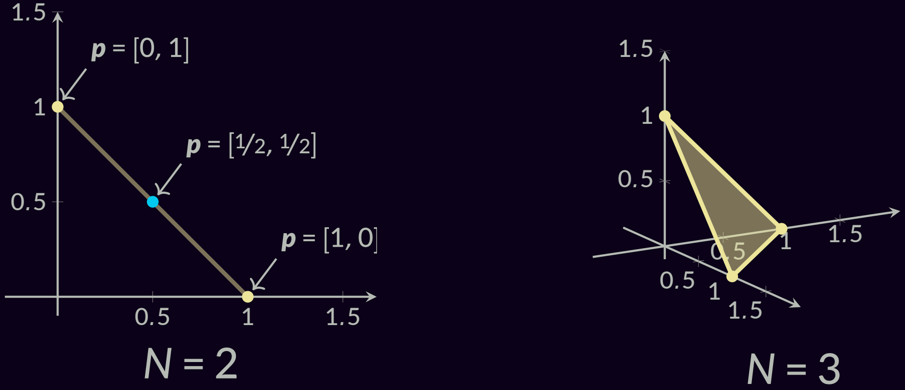

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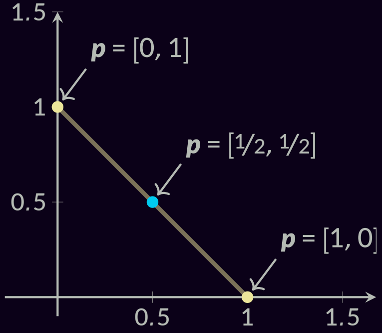

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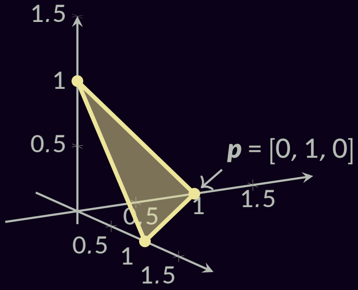

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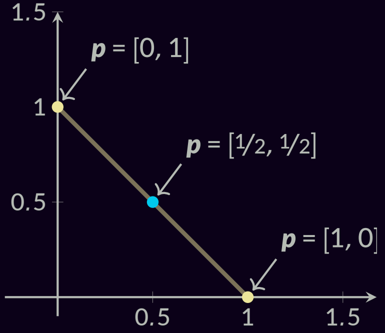

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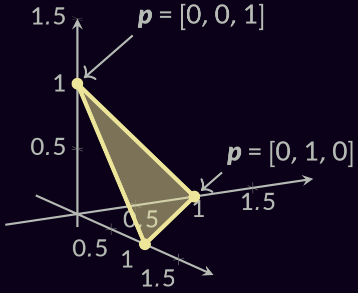

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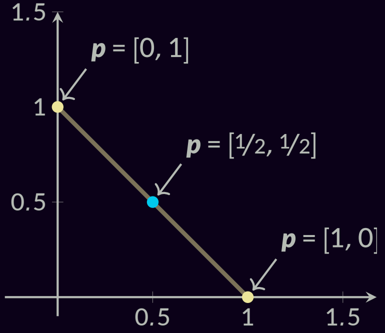

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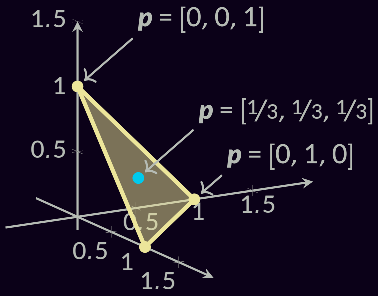

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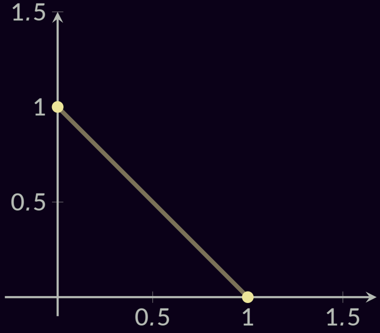
$$\max_j \theta_j = \max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top \boldsymbol{\theta}$$

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



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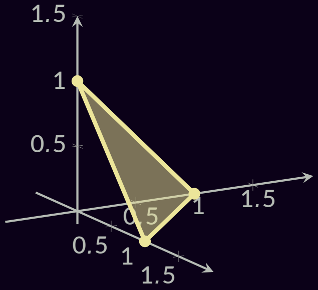

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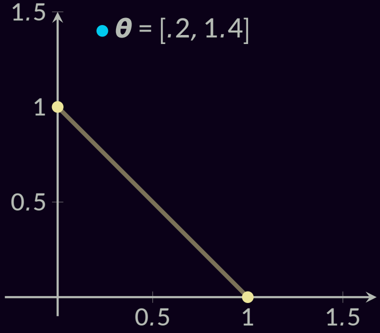

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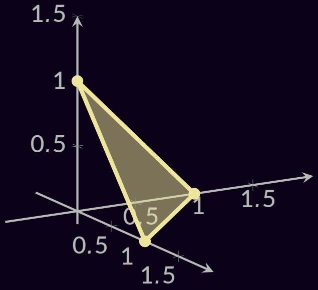

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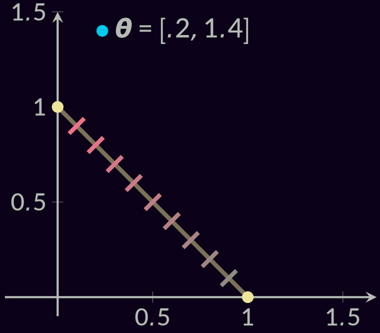

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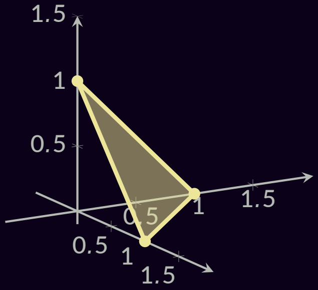

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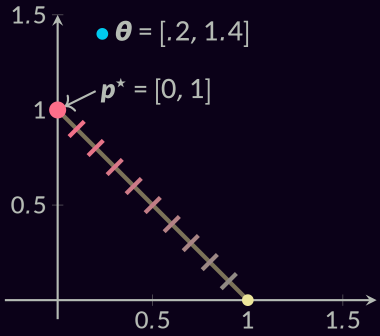

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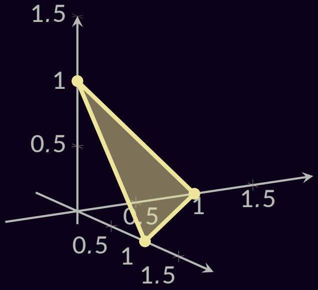

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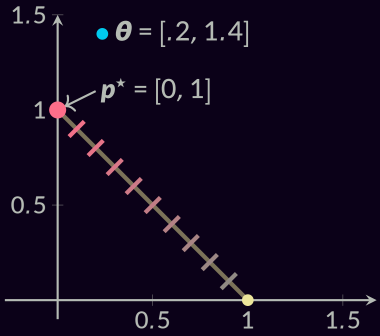
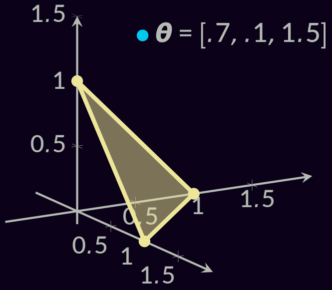


$N = 2$



$N = 3$

A Softmax Origin Story 🦸🏽‍♀️

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

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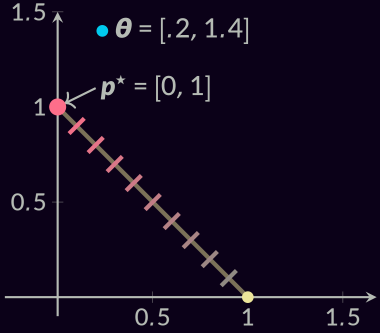

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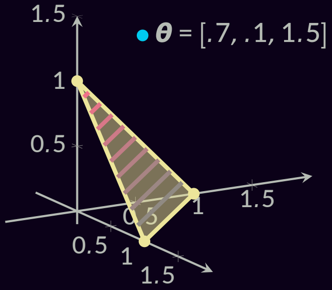

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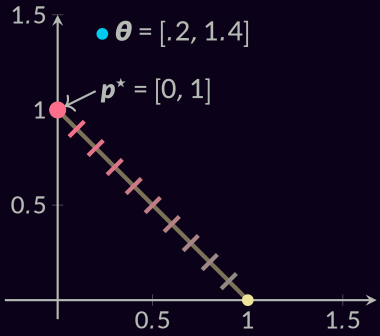

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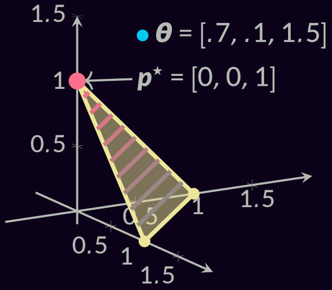

$N = 3$

(Niculae and Blondel, 2017)

Smoothed Max Operators

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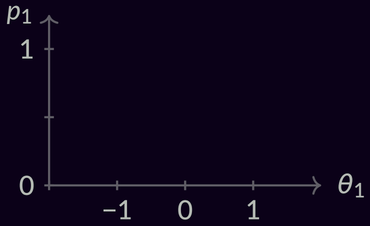

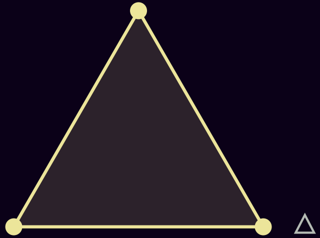

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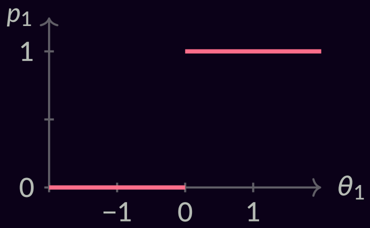

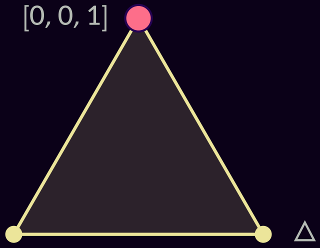

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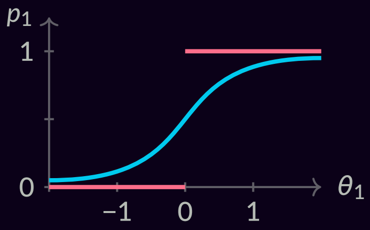

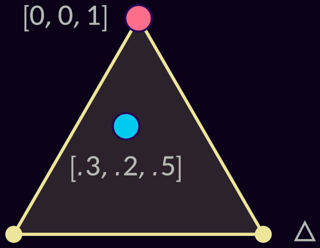

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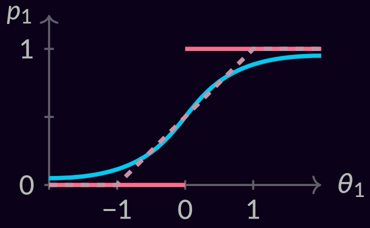

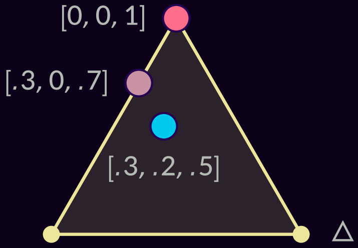

(Martins and Astudillo, 2016)

(Niculae and Blondel, 2017)

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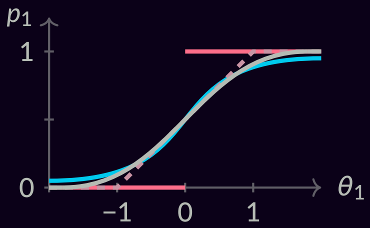
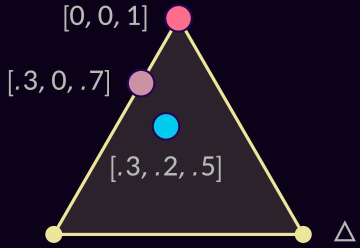
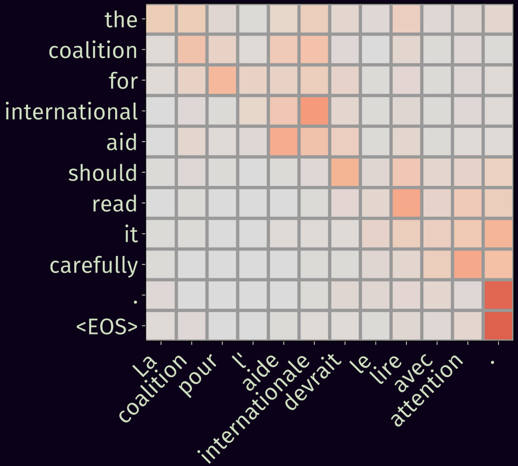




Tsallis (1988); a generalized entropy (Grünwald and Dawid, 2004)
(Blondel, Martins, and Niculae 2019a;
Peters, Niculae, and Martins 2019;
Correia, Niculae, and Martins 2019)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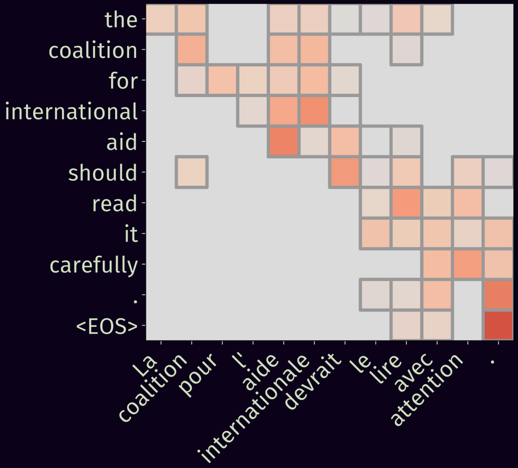
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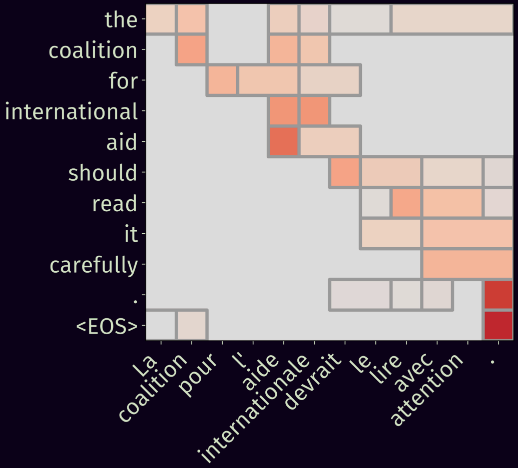
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fusedmax ?!

(Niculae and Blondel, 2017)

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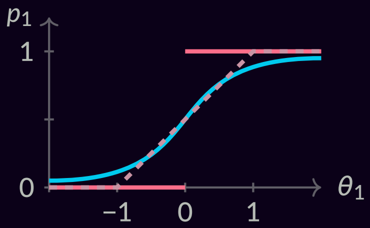

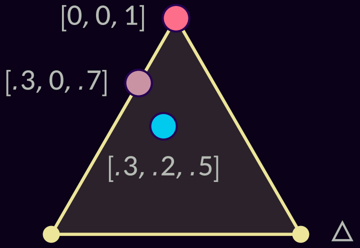

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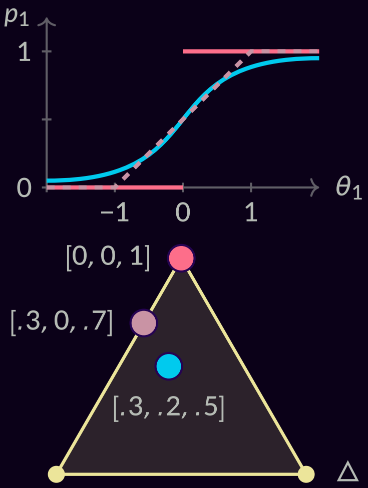

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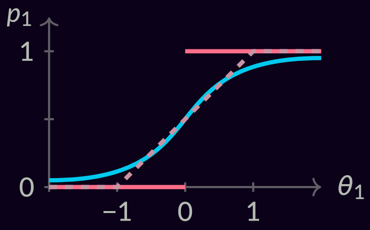

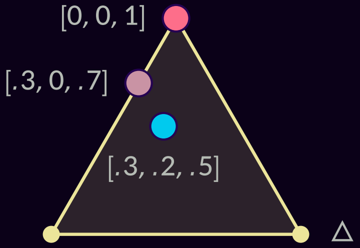

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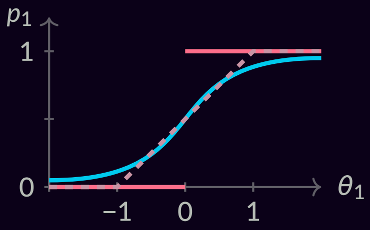
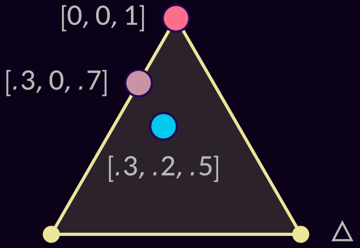


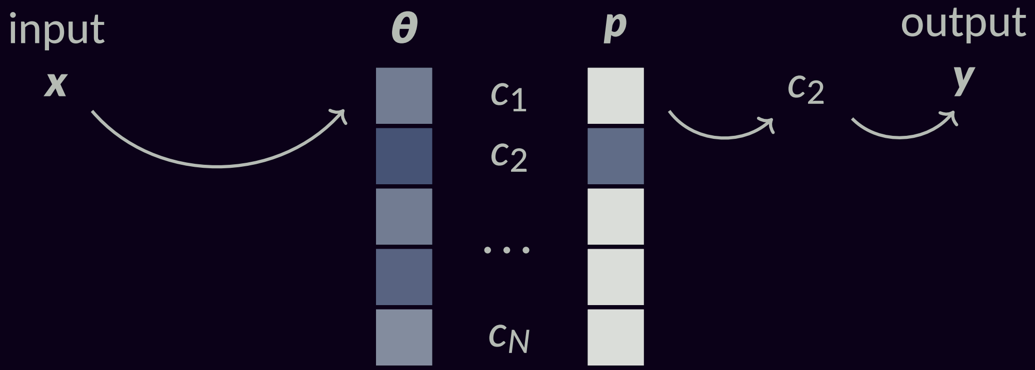


Structured Prediction

finally

Structured Prediction

is essentially a (very high-dimensional) argmax



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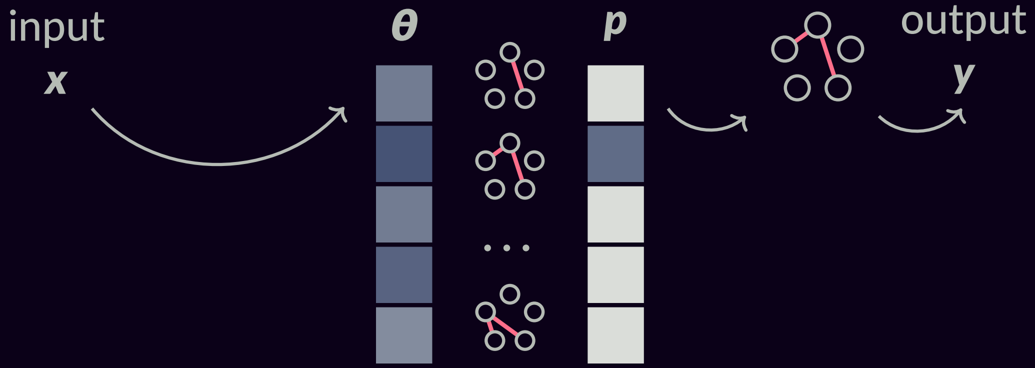

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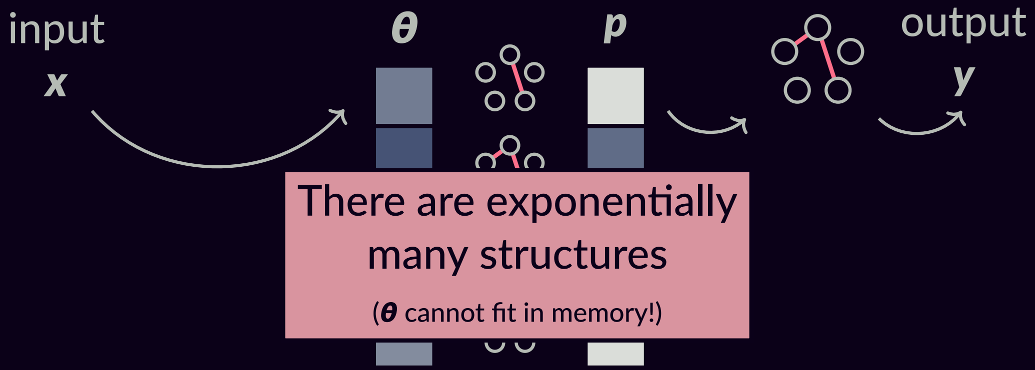

There are exponentially many structures

($\boldsymbol{\theta}$ cannot fit in memory!)

Factorization Into Parts

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

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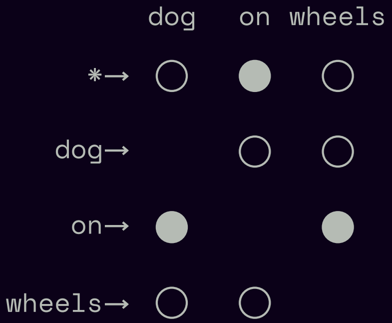

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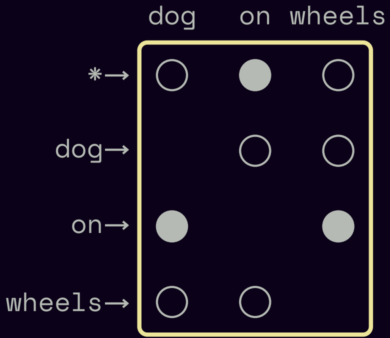
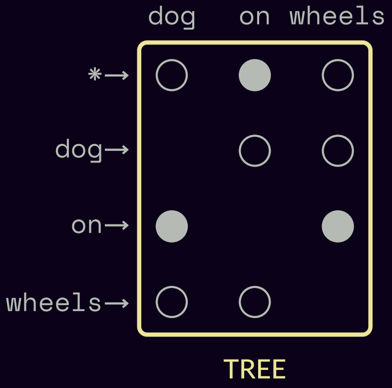


TREE

Factorization Into Parts

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



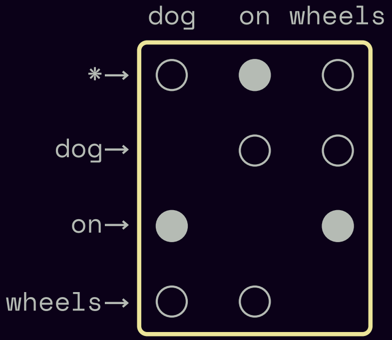
$\boldsymbol{a}_y$ = [010 100 001]

Factorization Into Parts

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

⋆ dog on wheels

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



TREE

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Factorization Into Parts

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⋆ dog on wheels

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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 & \boxed{0} & \\ 0 & & 1 & \boxed{1} & \\ 0 & & 0 & \boxed{0} & \\ \hline 0 & & 1 & \boxed{1} & \\ 1 & \dots & 0 & \boxed{0} & \dots \\ 0 & & 0 & \boxed{0} & \\ \hline 0 & & 0 & \boxed{0} & \\ 0 & & 1 & \boxed{0} & \\ 1 & & 0 & \boxed{1} & \end{array}\right]
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\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 & & \boxed{0} & 0 & \\ 0 & & \boxed{1} & 1 & \\ 0 & & \boxed{0} & 0 & \\ \hline 0 & & \boxed{0} & 0 & \\ 1 & \dots & \boxed{0} & 0 & \dots \\ 0 & & \boxed{1} & 1 & \\ \hline 0 & & \boxed{1} & 0 & \\ 0 & & \boxed{0} & 0 & \\ 1 & & \boxed{0} & 1 & \end{array}\right]
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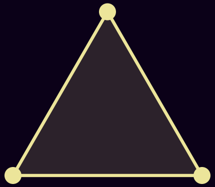

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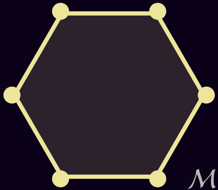
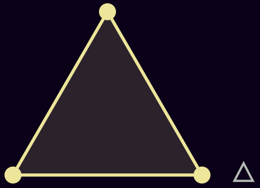
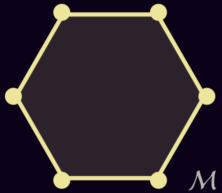


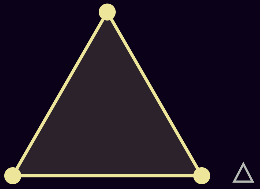
$\mathcal{M}$

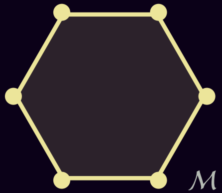
$$\mathcal{M} := \operatorname{conv}\left\{\boldsymbol{a}_h : h \in \mathcal{H}\right\}$$



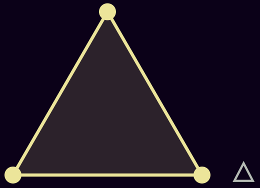


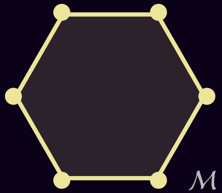
$$\mathcal{M} := \operatorname{conv}\left\{\boldsymbol{a}_h : h \in \mathcal{H}\right\}$$
$$= \left\{\boldsymbol{A}\boldsymbol{p} : \boldsymbol{p} \in \triangle\right\}$$



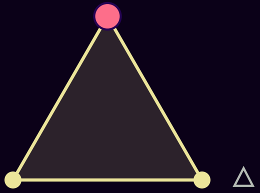


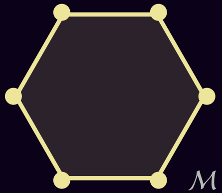
$$
\begin{aligned}
\mathcal{M} &:= \operatorname{conv}\left\{\boldsymbol{a}_h : h \in \mathcal{H}\right\} \\
&= \left\{\boldsymbol{A}\boldsymbol{p} : \boldsymbol{p} \in \Delta\right\} \\
&= \left\{\mathbb{E}_{H\sim \boldsymbol{p}}\, \boldsymbol{a}_H : \boldsymbol{p} \in \Delta\right\}
\end{aligned}
$$





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





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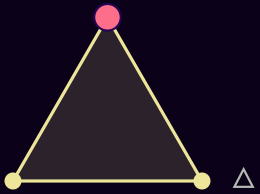
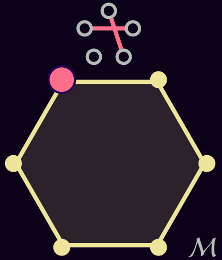
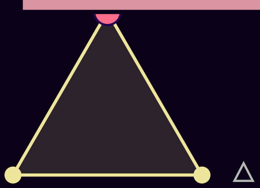
- **MAP** $\arg\max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta}$

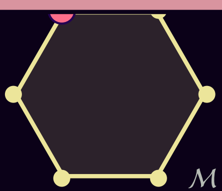




- **argmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{\theta}$
- **MAP** $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta}$

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

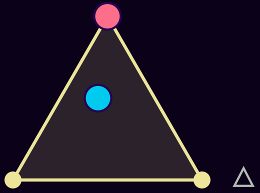


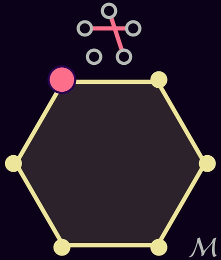


argmax $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top \boldsymbol{\theta}$

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

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





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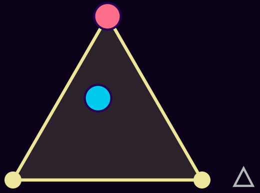
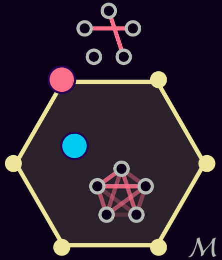
marginals $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta} + \widetilde{\mathrm{H}}(\boldsymbol{\mu})$





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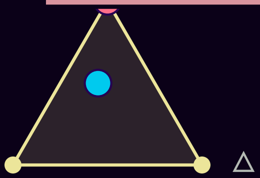
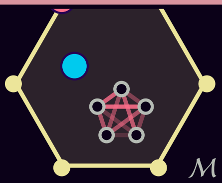
e.g. sequence labeling → forward-backward

(Rabiner, 1989)

As attention: (Kim et al., 2017)





- **argmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top \boldsymbol{\theta}$
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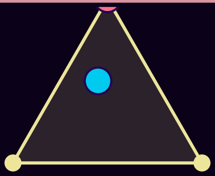
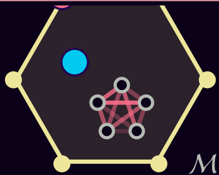
e.g. dependency parsing → **the Matrix-Tree theorem**

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

As attention: (Liu and Lapata, 2018)



$\triangle$



$\mathcal{M}$

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

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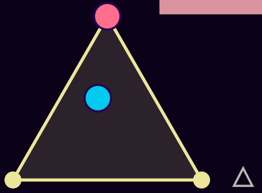
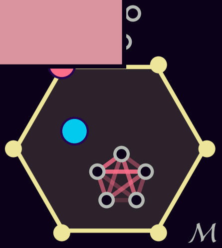
e.g. matchings → **#P-complete!**

(Taskar, 2004; Valiant, 1979)





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

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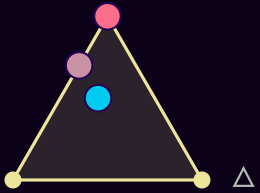

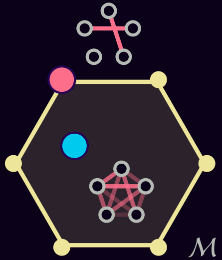

(Niculae, Martins, Blondel, and Cardie, 2018)

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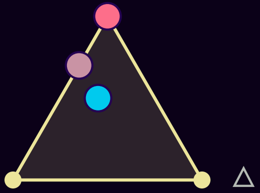
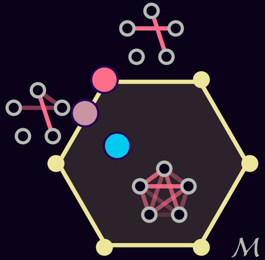
SparseMAP $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta} - 1/2\|\boldsymbol{\mu}\|^2$





Algorithms for SparseMAP

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

Algorithms for SparseMAP

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

linear constraints
(alas, exponentially many!)

quadratic objective

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Conditional Gradient

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

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

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

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

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

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

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

Algorithms for SparseMAP

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Backward pass

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

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Backward pass

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

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

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

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Conditi

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

    (Wolfe, 1976; Martins, Figueiredo, et al., 2015)

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

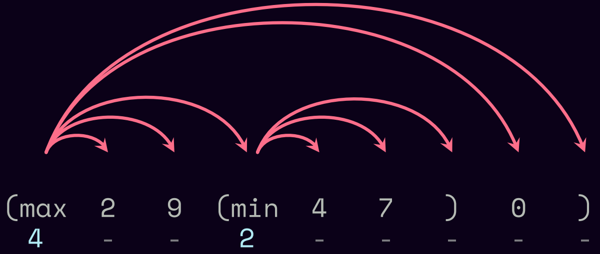
Arity tagging with latent GCN (Corro and Titov, 2019; Kipf and Welling, 2017)

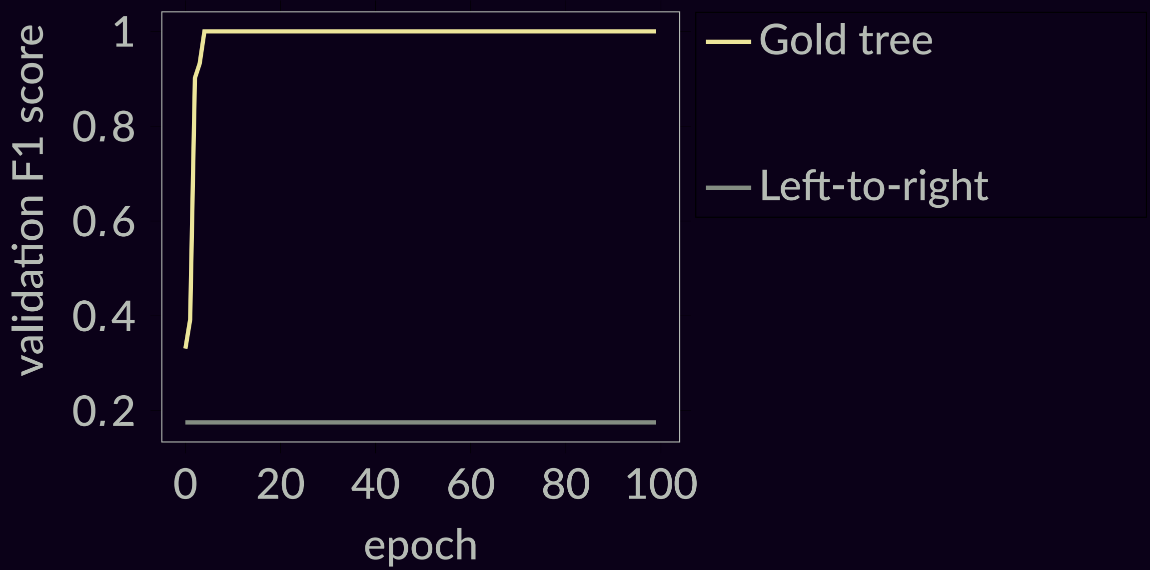
```
(max  2   9  (min  4   7   )   0   )
```

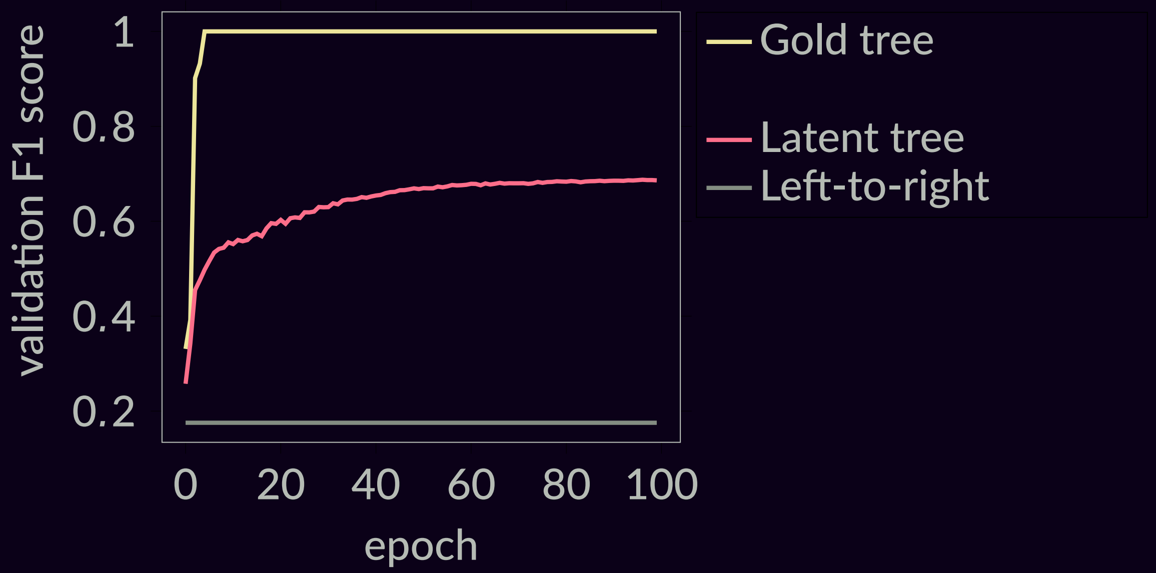
ListOps (Nangia and Bowman, 2018)

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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1
0.8
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0
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40
60
80
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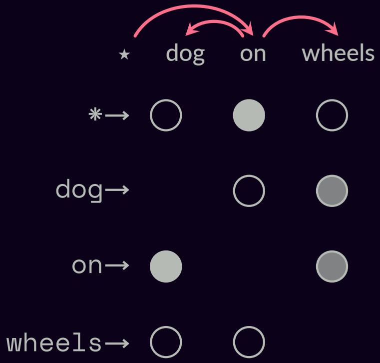
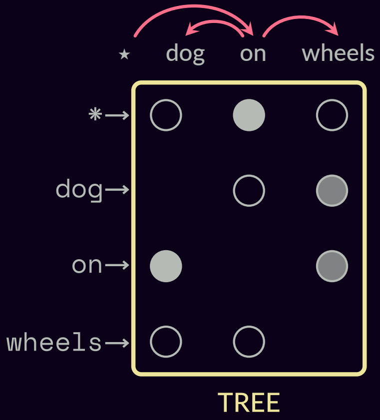
epoch
Gold tree
Latent tree
Left-to-right

What if MAP is not available?

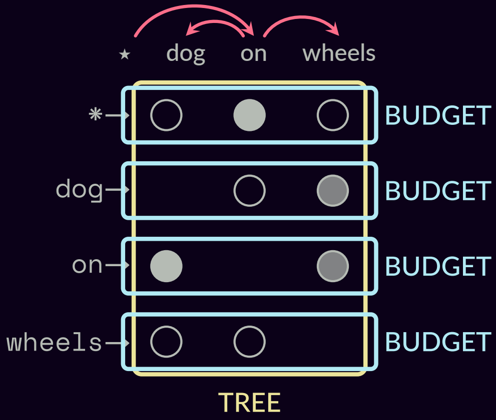
Multiple, Overlapping Factors



Multiple, Overlapping Factors

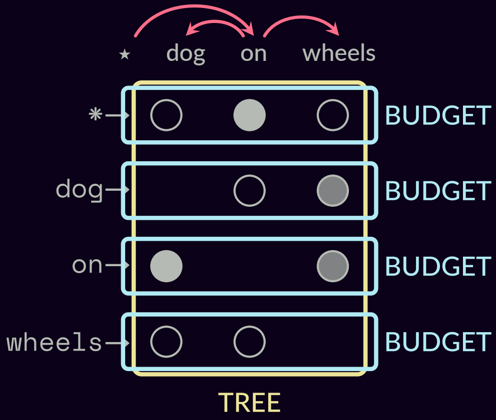


Multiple, Overlapping Factors

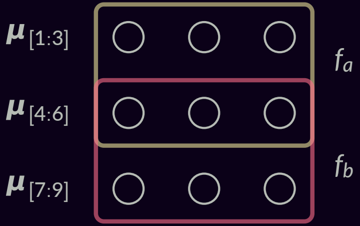


Multiple, Overlapping Factors

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



Optimization as Consensus-Seeking



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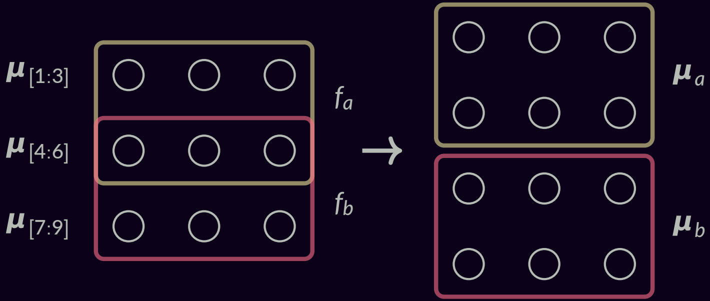
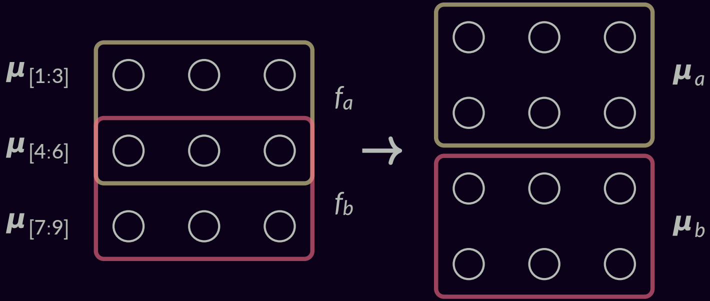
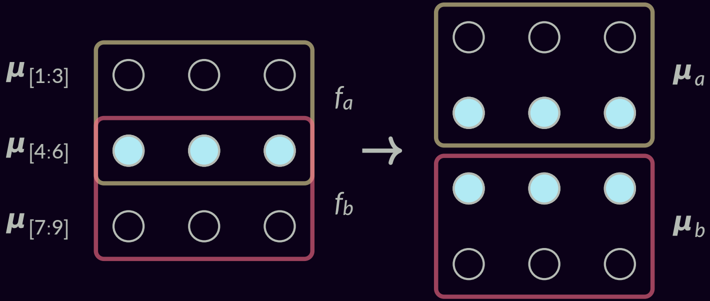


Optimization as Consensus-Seeking



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

Optimization as Consensus-Seeking



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

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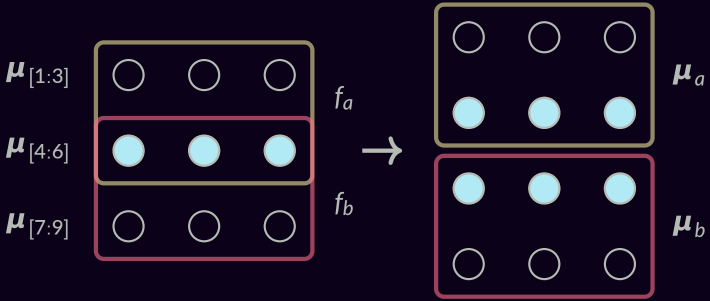

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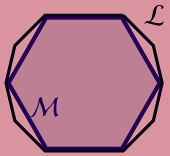
Optim… …eking

LP relaxation (Wainwright and Jordan, 2008)

the local polytope:

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



$\boldsymbol{\mu}_{[1:3}$ $\boldsymbol{\mu}_a$

$\boldsymbol{\mu}_{[4:6}$

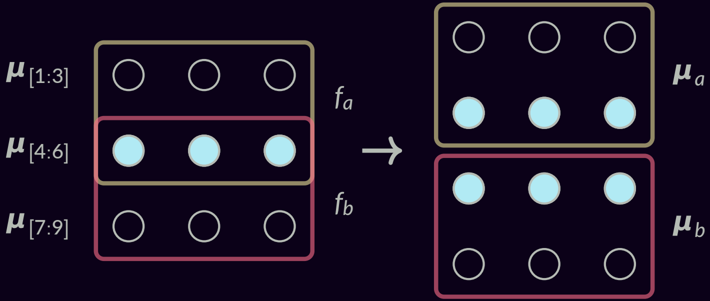
$\boldsymbol{\mu}_{[7:9}$ $\boldsymbol{\mu}_b$

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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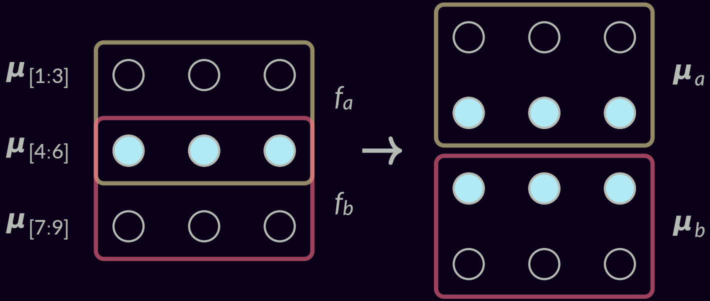


Agreement on overlap: $\boldsymbol{\mu}_{a,[4:6]} = \boldsymbol{\mu}_{b,[4:6]} = \boldsymbol{\mu}_{[4:6]}$

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

(Niculae and Martins, 2020)

Algorithms for LP-SparseMAP

Forward pass

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

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

(Niculae and Martins, 2020)

Algorithms for LP-SparseMAP

Forward pass

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

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

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

Backward pass

- Sparse fixed-point iteration
- Combines the SparseMAP Jacobians of each factor

Differentiable Sparse Structured Prediction


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

fg.add(Tree(var))

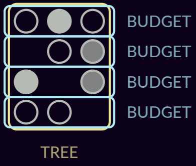
for i in range(n):
    fg.add(Budget(var[i, :], budget=5)

μ = fg.lp_sparsemap(η)
```

Factor graphs as a hidden-layer DSL!

(Niculae and Martins, 2020)

Differentiable Sparse Structured Prediction

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

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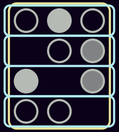


Factor graphs as a hidden-layer DSL!

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(ηf):   # abstract, private
        raise NotImplemented

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

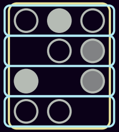
    def backward(dμf):
        # analytic, uses active set result


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

    def backward(dμf):
        # specialized
```

(Niculae and Martins, 2020)

Differentiable Sparse Structured Prediction



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New factors only require MAP.

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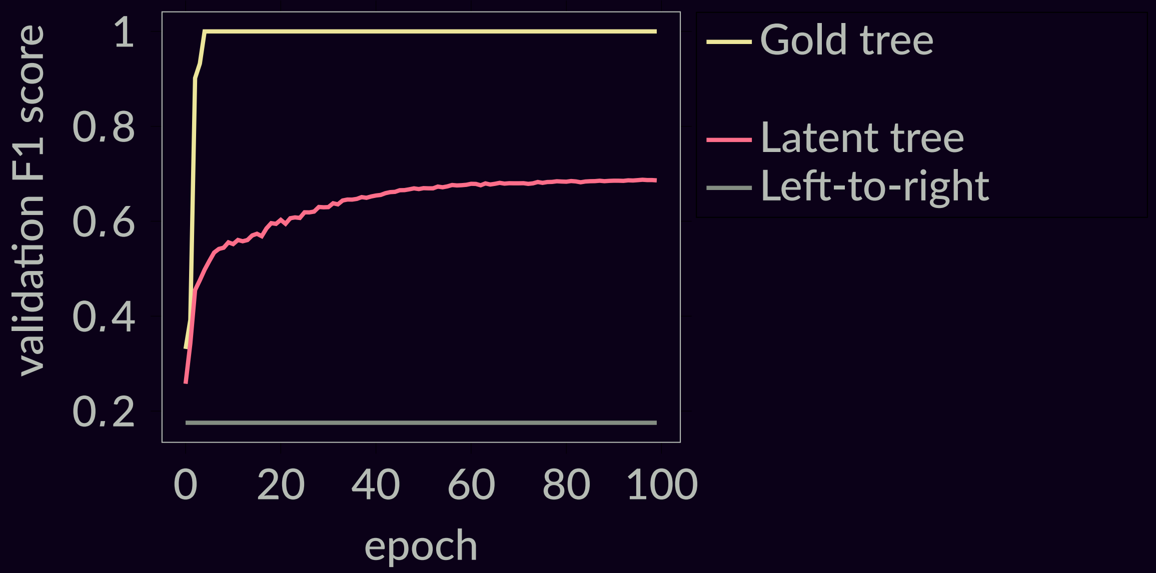
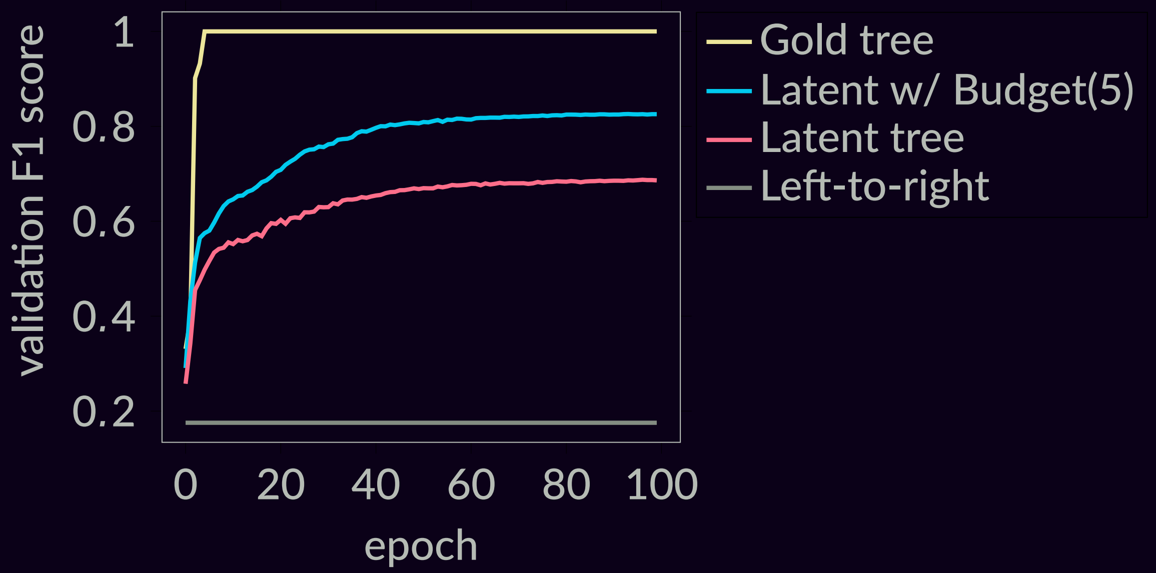
        # specialized

    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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Latent w/ Budget(5)
Latent tree
Left-to-right

Structured Attention for Alignments

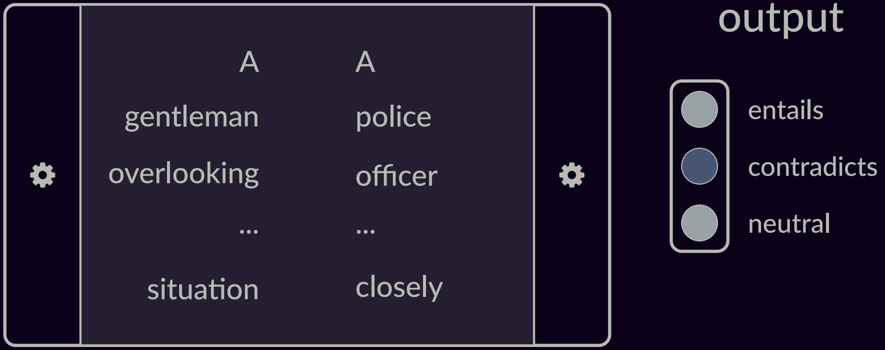
NLI

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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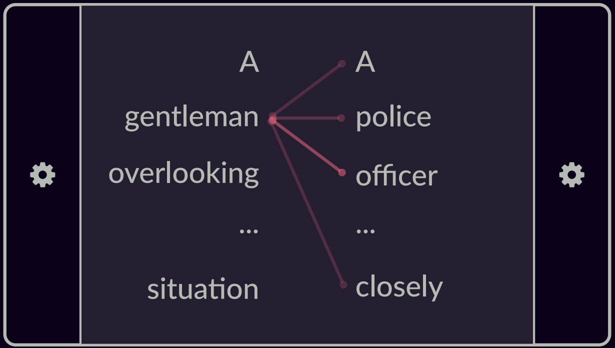
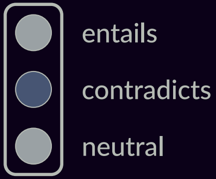


output



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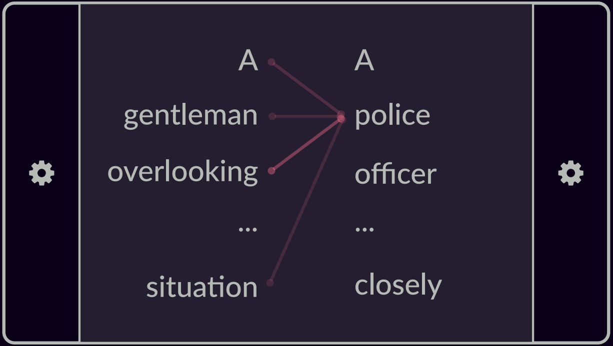
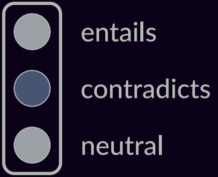


output



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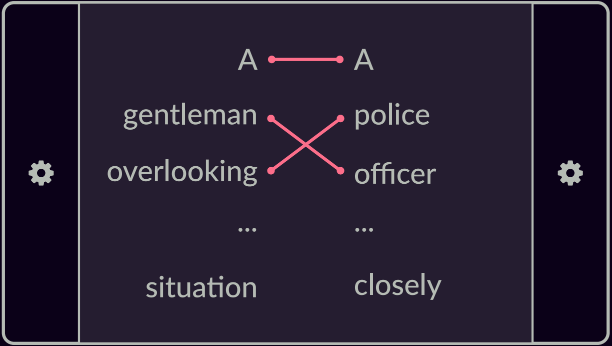
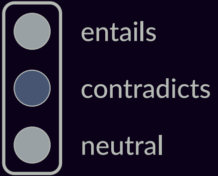


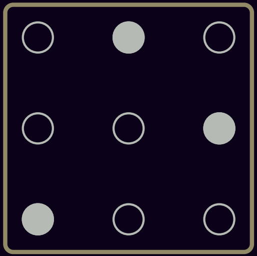
output



(Proposed model: global structured alignment.)

Structured Alignment Models

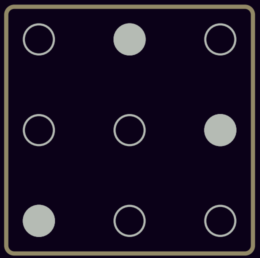
matching



SparseMAP w/ Kuhn-Munkres
(Kuhn, 1955)

Structured Alignment Models

matching



SparseMAP w/ Kuhn-Munkres
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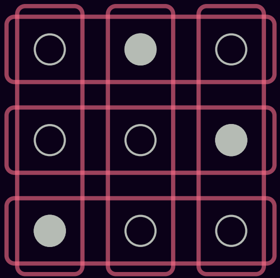
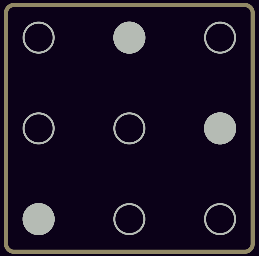
LP-matching



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

Structured Alignment Models

matching



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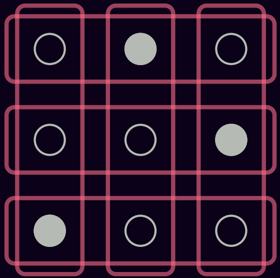
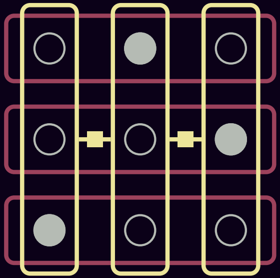


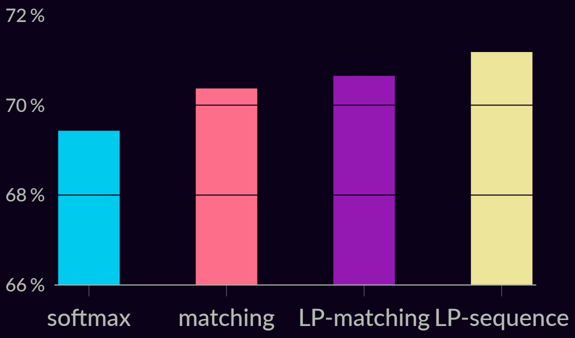
LP-SparseMAP w/ XORs
(equivalent; different solver)

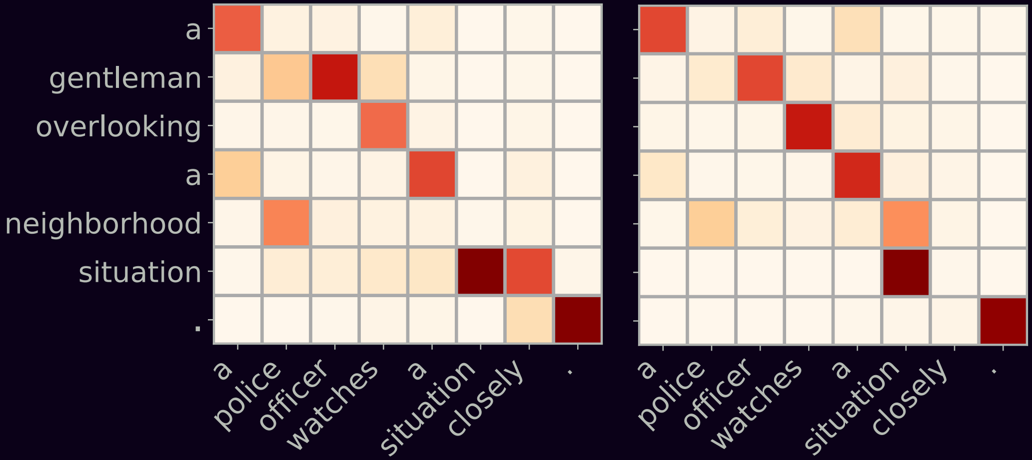
LP-sequence



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

MultiNLI (Williams et al., 2017)




a
gentleman
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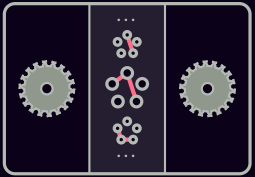
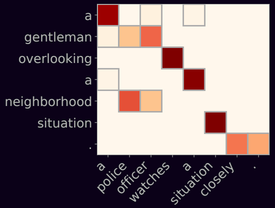
Conclusions

Differentiable & sparse
structured inference

Generic, extensible, efficient algorithms

Interpretable **structured attention**





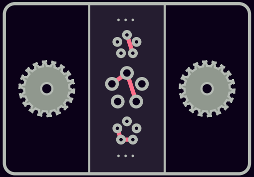
vlad@vene.ro
https://vene.ro
github.com/deep-spin/lp-sparsemap
@vnfrombucharest

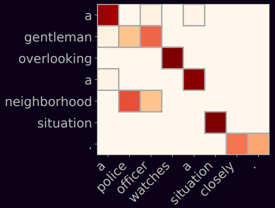
Conclusions

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

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

Sparsemax

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

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

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

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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Computation:

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

$\theta_i > \theta_j$

$\mathcal{O}(d)$ 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

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

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

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

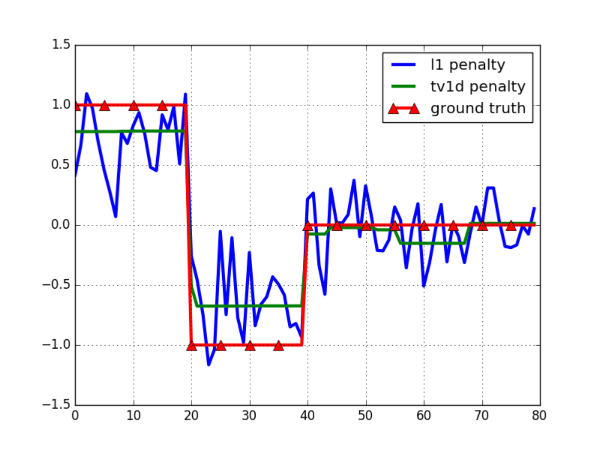
Proposition: $\text{fusedmax}(\boldsymbol{\theta}) = \text{sparsemax}\left(\text{prox}_{\text{fused}}(\boldsymbol{\theta})\right)$

(Niculae and Blondel, 2017)

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

$_{j-1}|$

prox$_{\text{fused}}$($_{j-1}|$



“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.

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

Example: maximum of a vector

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

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Example: maximum of a vector

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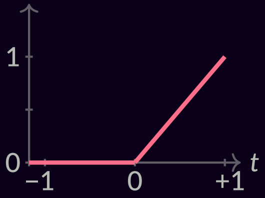
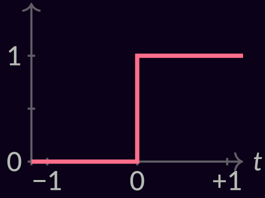
&= \operatorname{conv}\{\boldsymbol{p}^\star\}
\end{aligned}$$

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



$\max_j \theta_j$



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

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)

Dependency TreeLSTM

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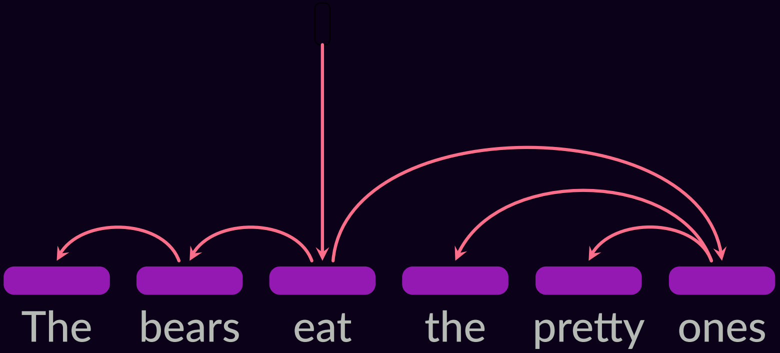

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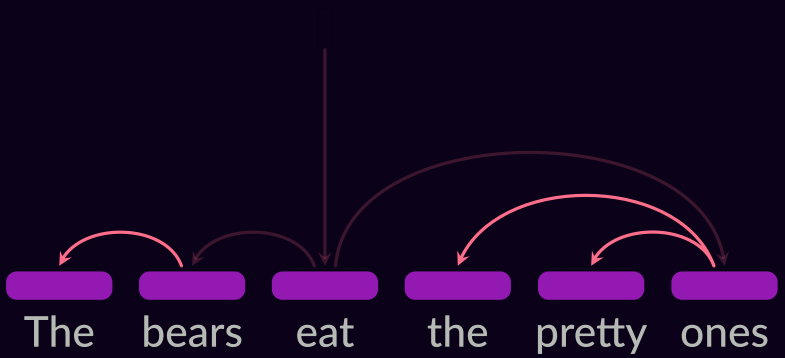
(Tai et al., 2015)



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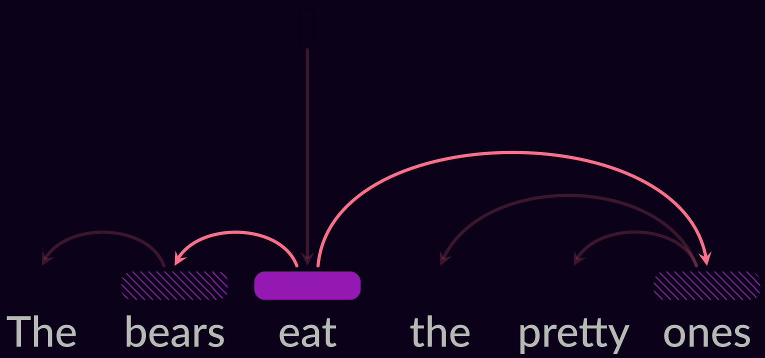

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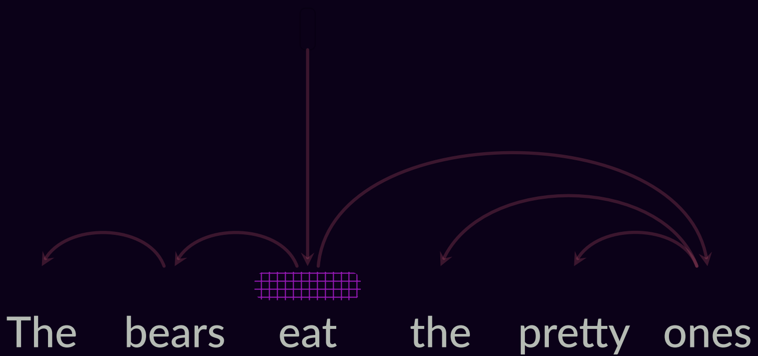

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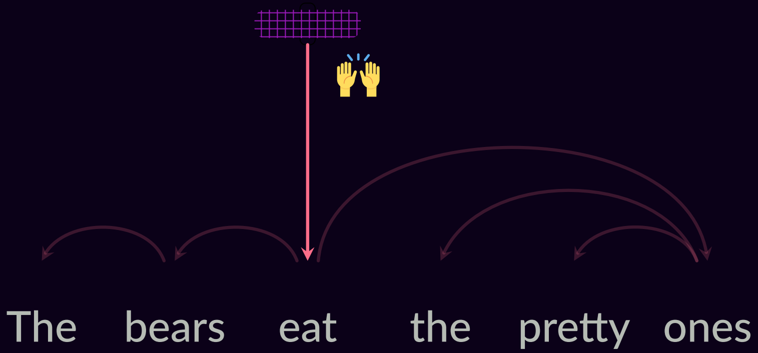
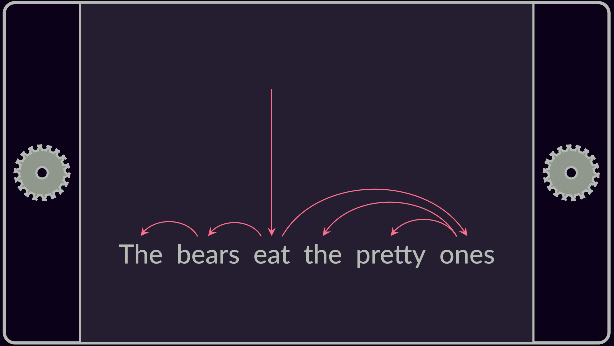


Latent Dependency TreeLSTM

(Niculae, Martins, and Cardie, 2018)

input

x



output

y

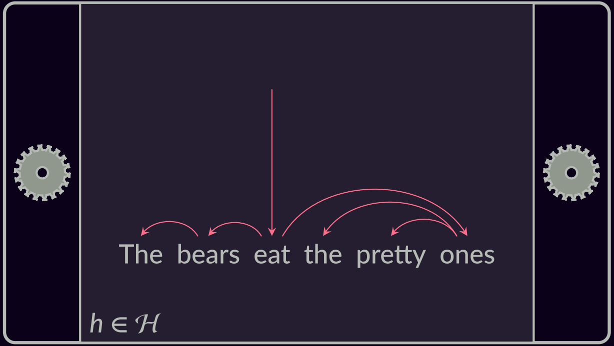
Latent Dependency TreeLSTM

(Niculae, Martins, and Cardie, 2018)

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

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

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

Structured Latent Variable Models

e.g., a TreeLSTM defined by h

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

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

Structured Latent Variable Models

sum over
all possible trees

e.g., a TreeLSTM defined by h

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

Exponentially large sum!

Structured Latent Variable Models

sum over
all possible trees

e.g., a TreeLSTM defined by h

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

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

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

idea 1

idea 2

idea 3

Structured Latent Variable Models

sum over
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How to define $\boldsymbol{p_{\pi}}$?

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

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Structured Latent Variable Models

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

$$\sum_{h \in \mathcal{H}} \qquad \frac{\partial p(y \mid x)}{\partial \boldsymbol{\pi}}$$

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Structured Latent Variable Models

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$\sum_{h \in \mathcal{H}}$ $\frac{\partial p(y \mid x)}{\partial \boldsymbol{\pi}}$

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$$\sum_{h \in \mathcal{H}} \qquad \frac{\partial p(y \mid x)}{\partial \boldsymbol{\pi}}$$

idea 1	$p_{\boldsymbol{\pi}}(h \mid x) = 1$ if $h = h^\star$ else 0	argmax	😊	😟
idea 2	$p_{\boldsymbol{\pi}}(h \mid x) \propto \exp\left(\text{score}_{\boldsymbol{\pi}}(h; x)\right)$	softmax		
idea 3				

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idea 1	$p_{\boldsymbol{\pi}}(h \mid x) = 1$ if $h = h^\star$ else 0	argmax	😊	😟
idea 2	$p_{\boldsymbol{\pi}}(h \mid x) \propto \exp\big(\mathrm{score}_{\boldsymbol{\pi}}(h; x)\big)$	softmax	😱	😊
idea 3		SparseMAP	😊	😊

SparseMAP

 = .7  + .3 

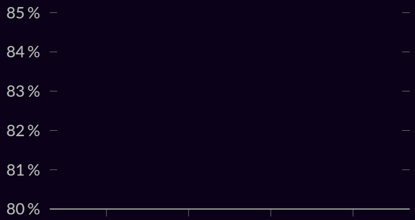
SparseMAP

 = .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 %
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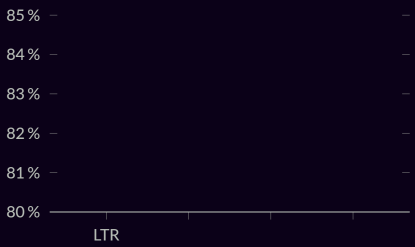
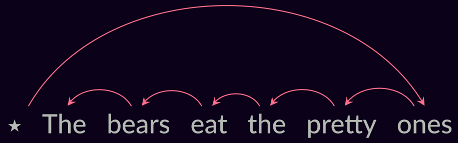
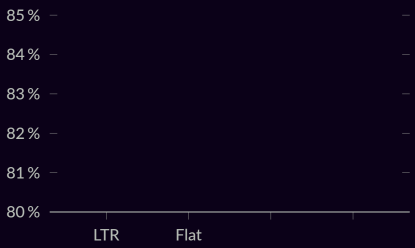
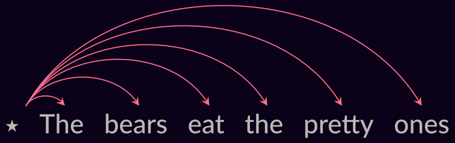
80 %



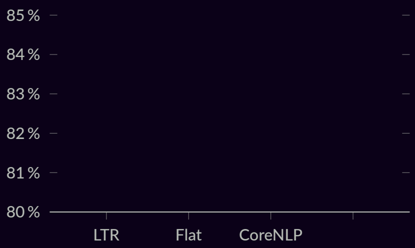


Left-to-right: regular LSTM

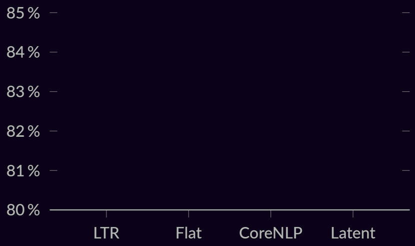




Flat: bag-of-words–like



CoreNLP: off-line parser


85 %
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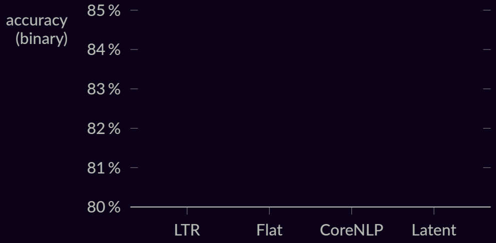
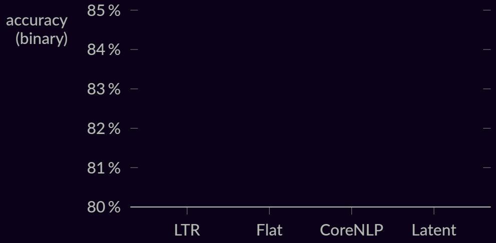
LTR
Flat
CoreNLP
Latent

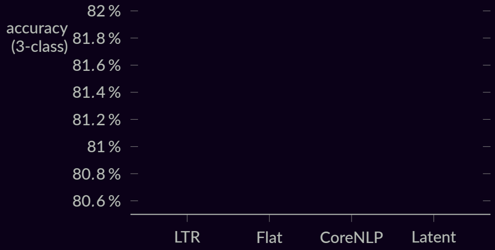
Sentiment classification (SST)



Sentiment classification (SST)



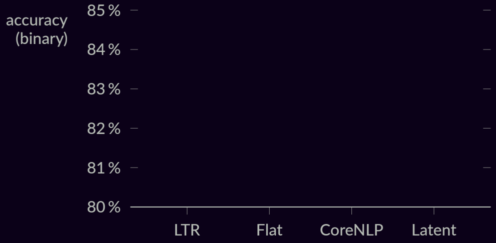
Natural Language Inference (SNLI)



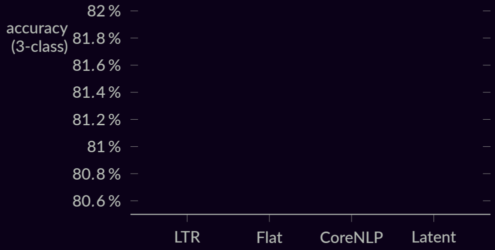
Sentence pair classification (P, H)

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

Sentiment classification (SST)



Natural Language Inference (SNLI)

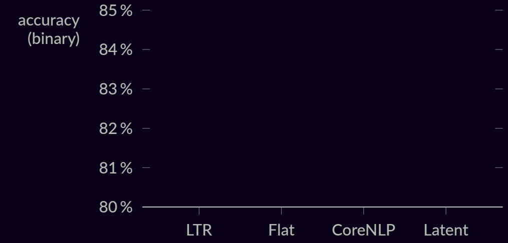


Reverse dictionary lookup

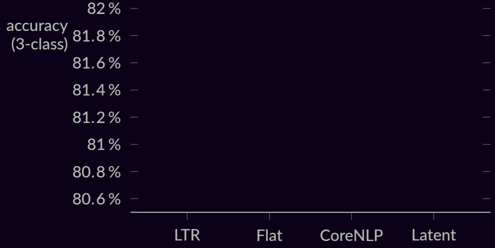
given word description, predict word embedding (Hill et al., 2016)

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)

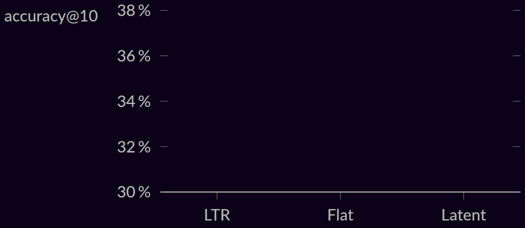


Natural Language Inference (SNLI)

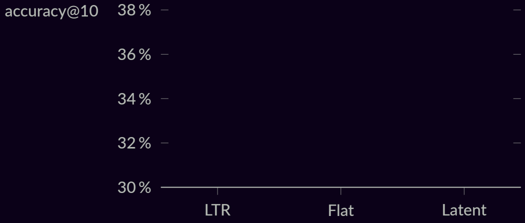


Reverse dictionary lookup

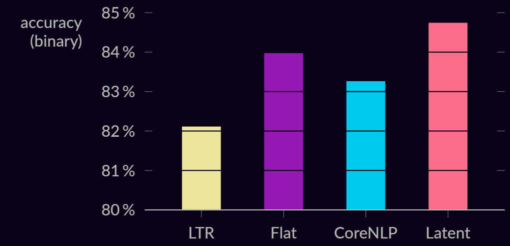
(definitions)



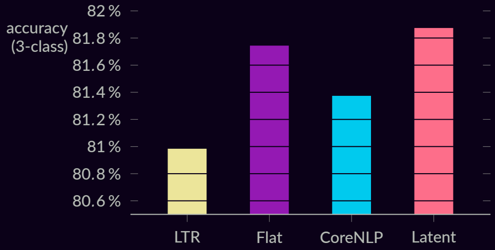
(concepts)



Sentiment classification (SST)

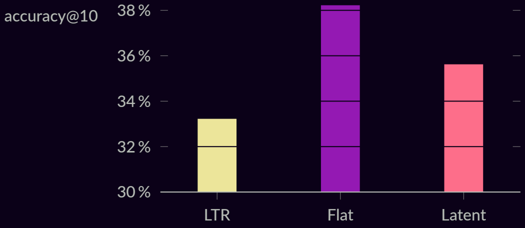


Natural Language Inference (SNLI)

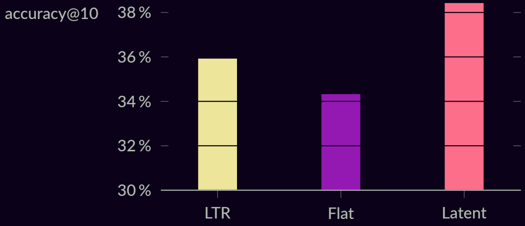


Reverse dictionary lookup

(definitions)

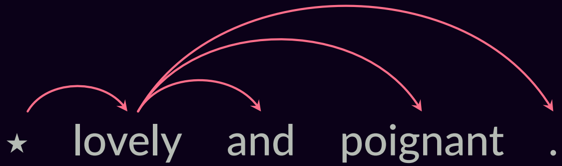


(concepts)



Syntax vs. Composition Order

CoreNLP parse, $p = 21.4\%$



Syntax vs. Composition Order

$p = 22.6\%$

★ lovely and poignant .

CoreNLP parse, $p = 21.4\%$

★ lovely and poignant .

. . .

Syntax vs. Composition Order

$p = 22.6\%$

⋆ lovely and poignant .

CoreNLP parse, $p = 21.4\%$

⋆ lovely and poignant .

. . .

$p = 15.33\%$

⋆ a deep and meaningful film .

$p = 15.27\%$

⋆ a deep and meaningful film .

. . .

CoreNLP parse, $p = 0\%$

⋆ a deep and meaningful film .

Structured Output Prediction

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

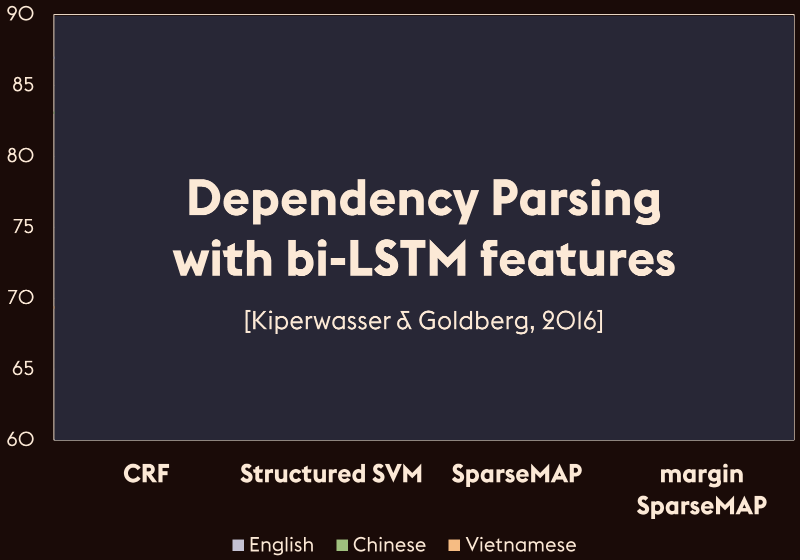
Instance of a structured Fenchel-Young loss, like CRF, SVM, etc. (Blondel, Martins, and Niculae, 2019b)

Structured Output Prediction

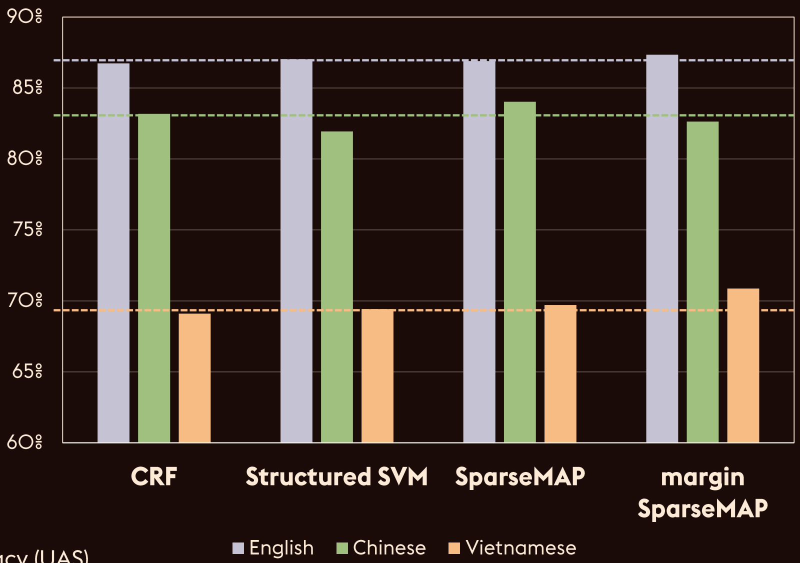
SparseMAP
$$L_{A}(\boldsymbol{\eta}, \bar{\boldsymbol{\mu}}) = \max_{\boldsymbol{\mu} \in \mathcal{M}} \left\{ \boldsymbol{\eta}^\top \boldsymbol{\mu} - 1/2 \|\boldsymbol{\mu}\|^2 \right\} - \boldsymbol{\eta}^\top \bar{\boldsymbol{\mu}} + 1/2 \|\bar{\boldsymbol{\mu}}\|^2$$

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)



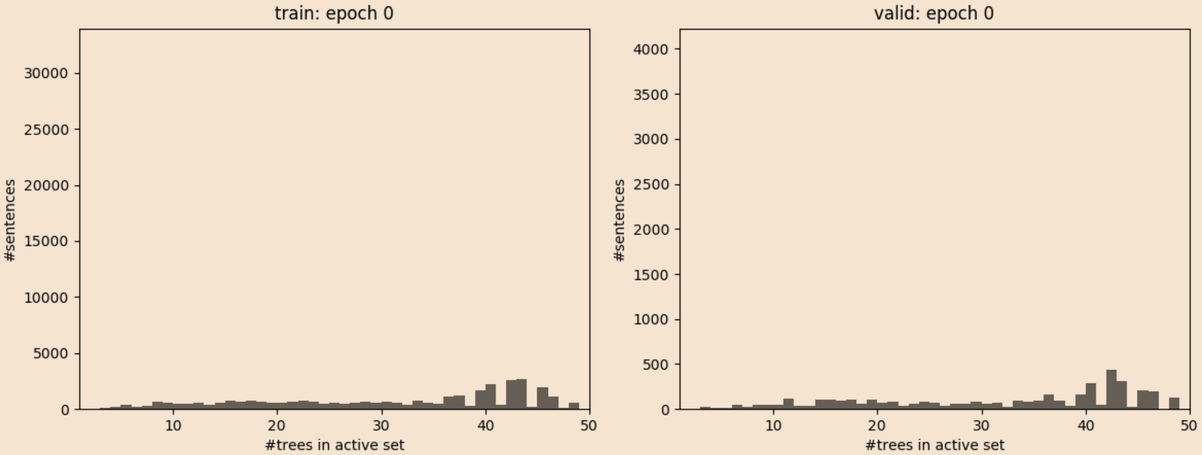
Dependency Parsing
with bi-LSTM features
[Kiperwasser & Goldberg, 2016]
90
85
80
75
70
65
60
CRF
Structured SVM
SparseMAP
margin SparseMAP
English
Chinese
Vietnamese



Unlabeled Accuracy (UAS)
Universal Dependencies dataset

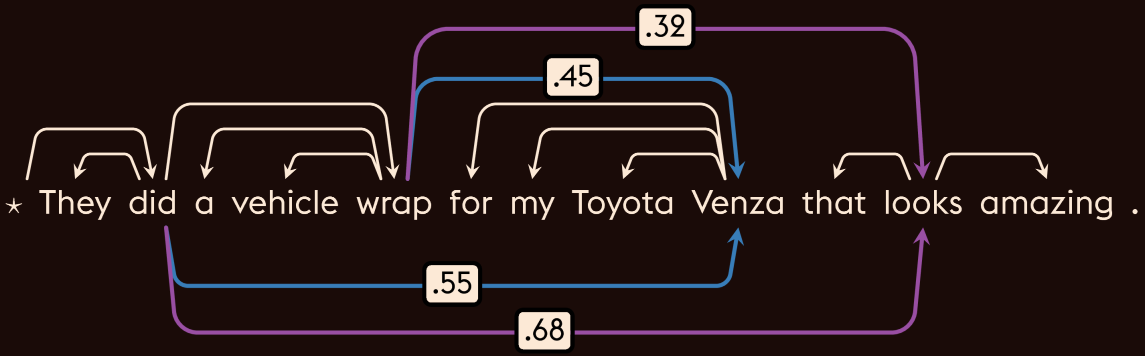
Sparse Structured Output Prediction

As models train, inference gets sparser!



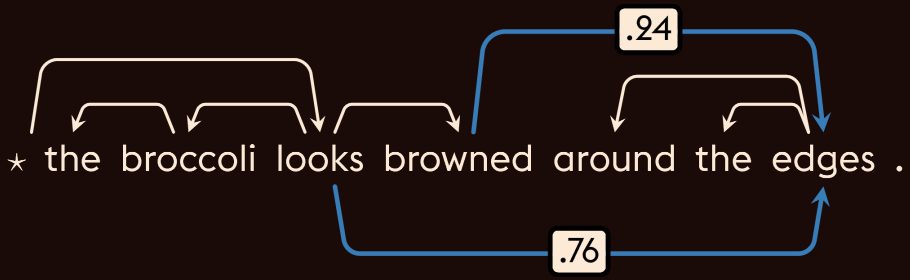
Sparse Structured Output Prediction

Inference captures linguistic ambiguity!



Sparse Structured Output Prediction

Inference captures linguistic ambiguity!



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