Learning with Sparse Latent Structure

Vlad Niculae University of Amsterdam

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Gonçalo M. Correia, André Martins, Tsvetomila Mihaylova.

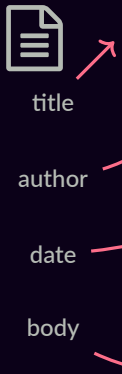
Rich Underlying Structure

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



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segmentation:
sentences,
words,
and so on

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relationships
e.g., dependency

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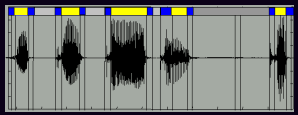
Most of this structure is **hidden**.

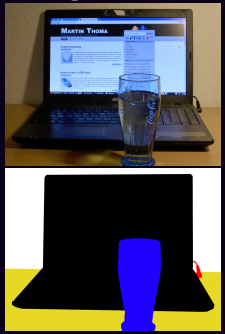
Rich Underlying Structure

Widely occuring pattern!

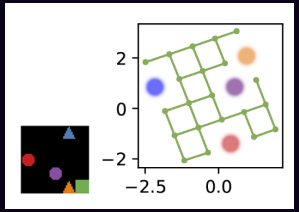
speech
(Andre-Obrecht, 1988)



objects
(Long et al., 2015)



transition graphs
(Kipf, Pol, et al., 2020)



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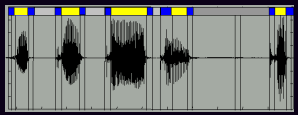

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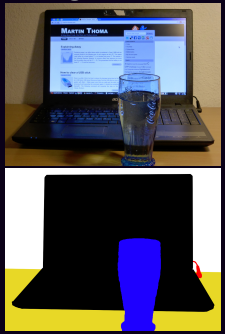

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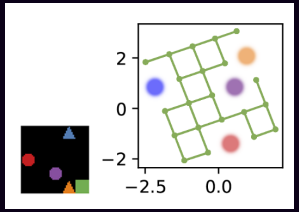
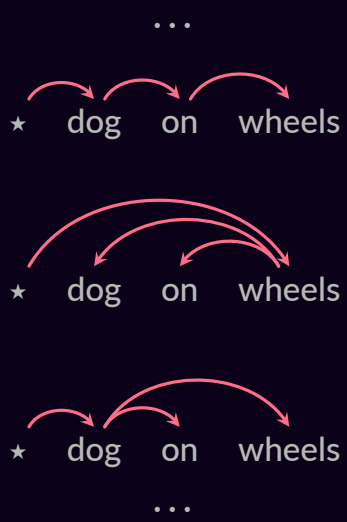


But we'll focus on NLP.

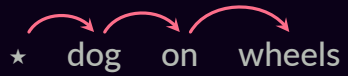
Structured Prediction

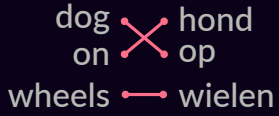


Structured Prediction

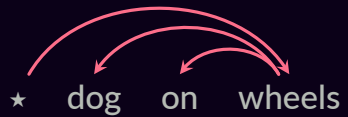
...

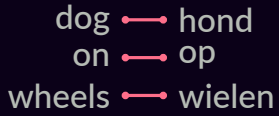
VERB PREP NOUN
dog on wheels



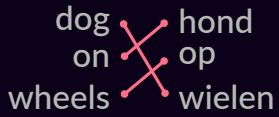


NOUN PREP NOUN
dog on wheels





NOUN DET NOUN
dog on wheels



...

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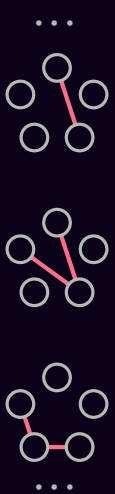
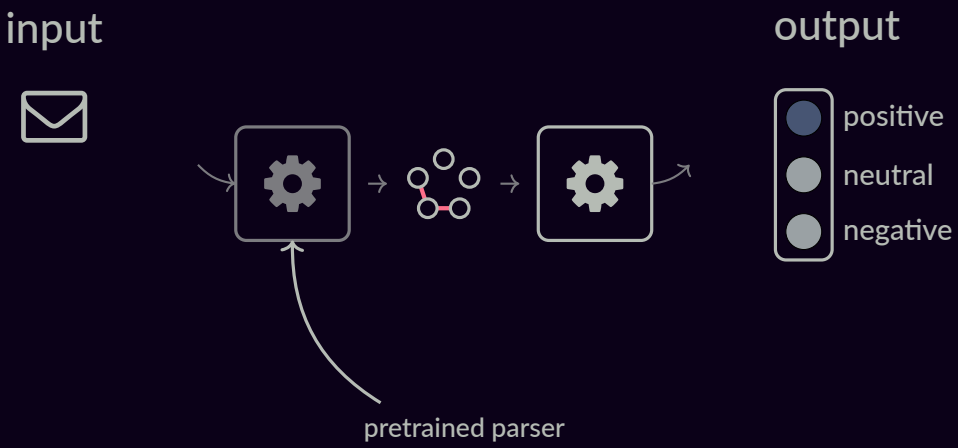


Traditional Pipeline Approach

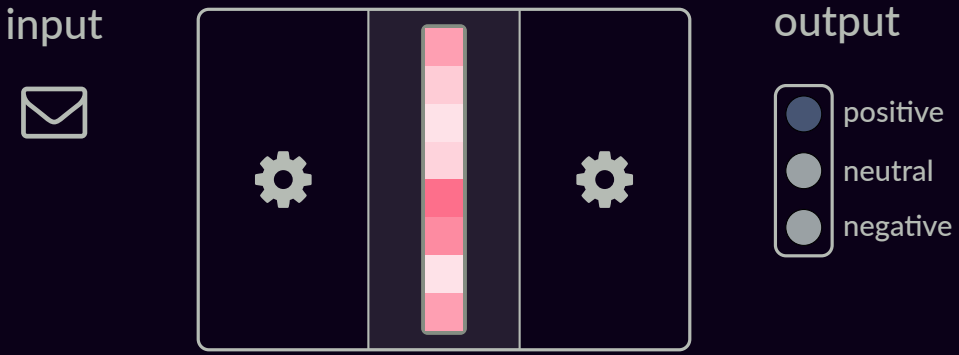
input

output

Traditional Pipeline Approach



Deep Learning & Hidden Representations



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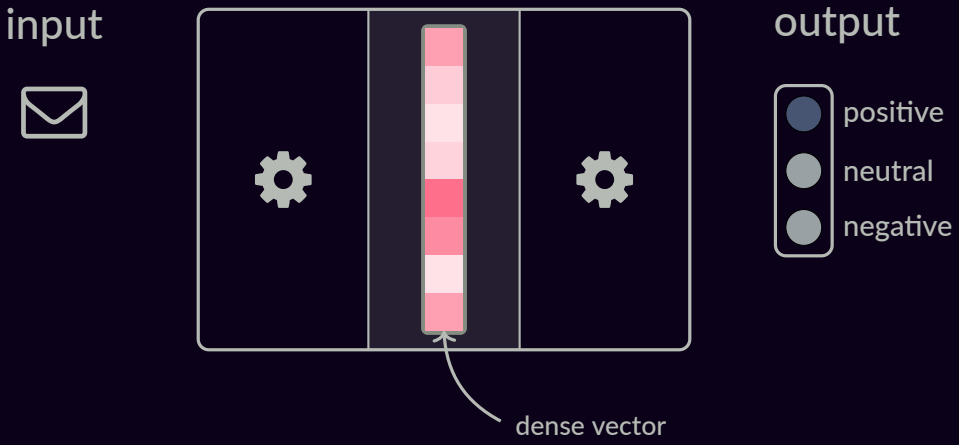
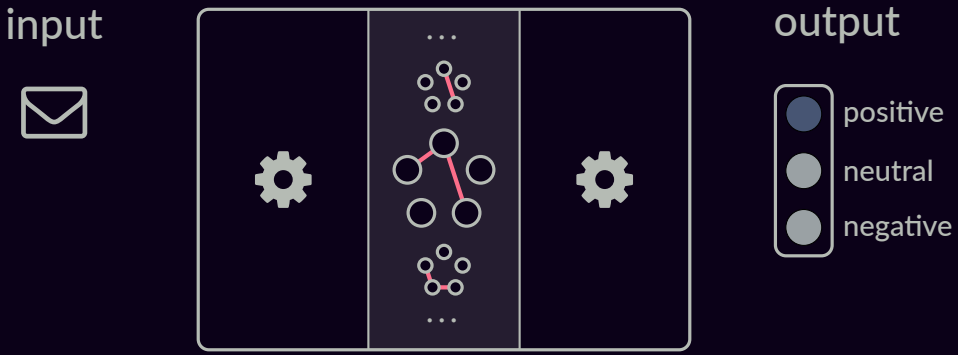


Latent Structure Models



record scratch

freeze frame

How to select an item from a set?

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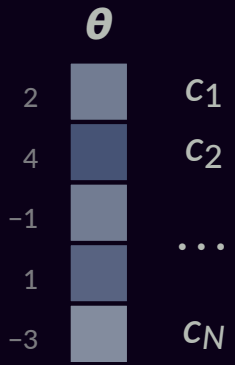
c_1

c_2

...

c_N

How to select an item from a set?



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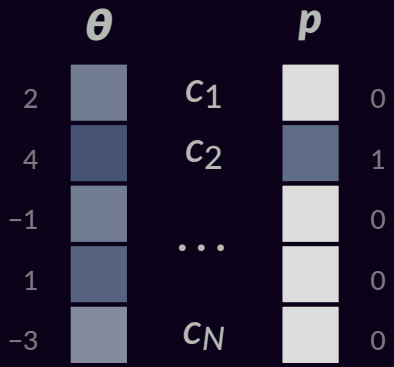

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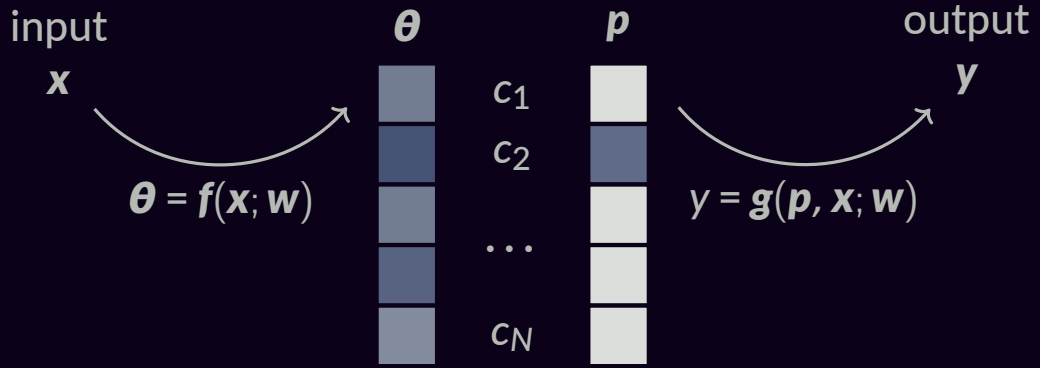

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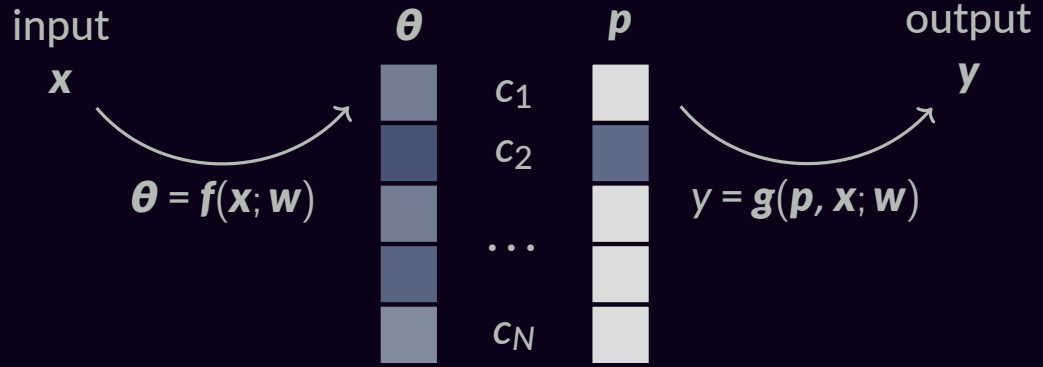

$$\frac{\partial y}{\partial \boldsymbol{w}} = ?$$

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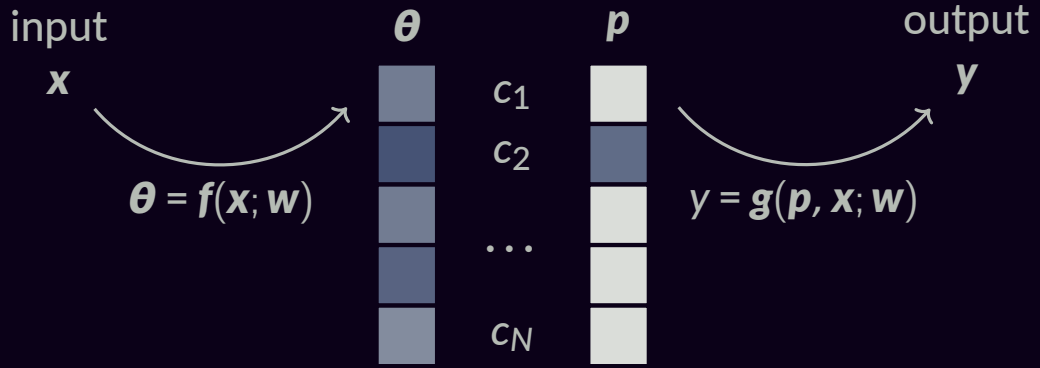
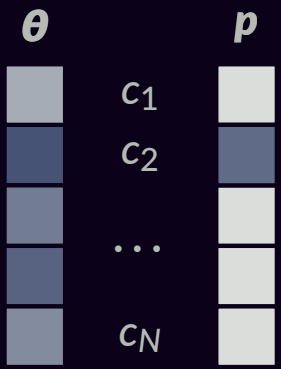


$\frac{\partial y}{\partial w}$=? or, essentially, $\frac{\partial p}{\partial \theta}$=?

Argmax



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

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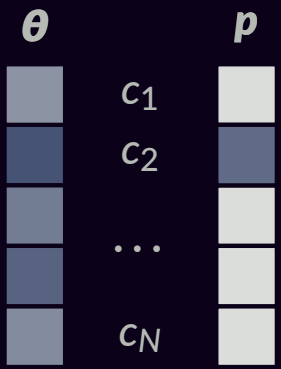

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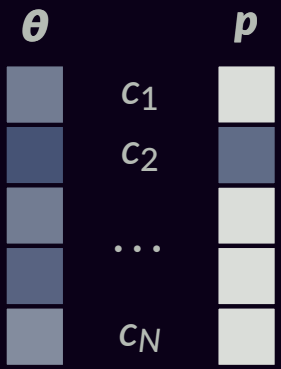

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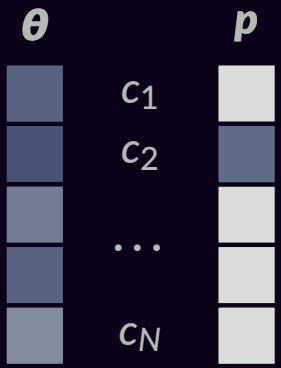

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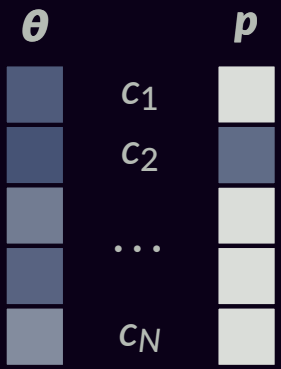

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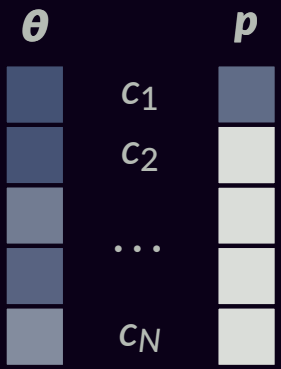

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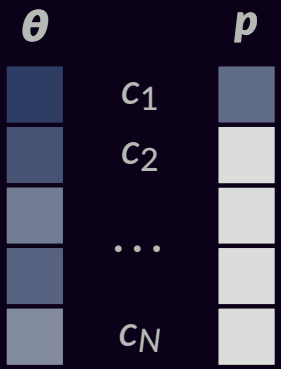

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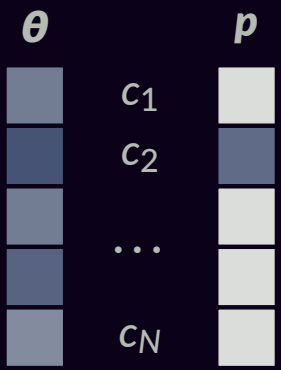

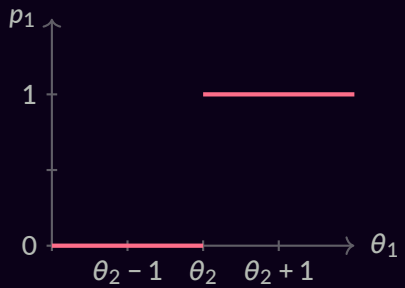

$$\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{\theta}} = \mathbf{0}$$

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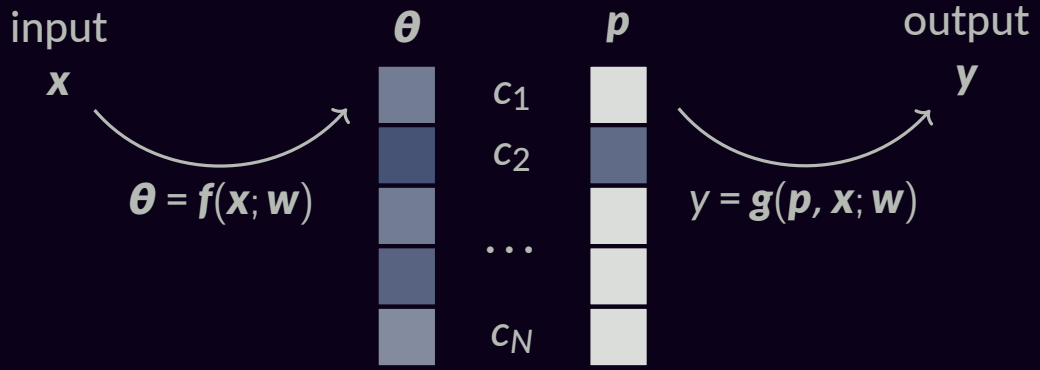

Ideas: sampling // fake gradients // relax p.

Gradients Through Choices

Three directions

- **sampling:** make $\boldsymbol{p}$ stochastic; $\boldsymbol{p} \sim \text{Cat}(\boldsymbol{\theta})$.
  then, $\frac{\partial \mathbb{E}[y]}{\partial \boldsymbol{\theta}} \neq 0$. (Mohamed et al., 2020)
  (but our model is now stochastic, high variance, …)

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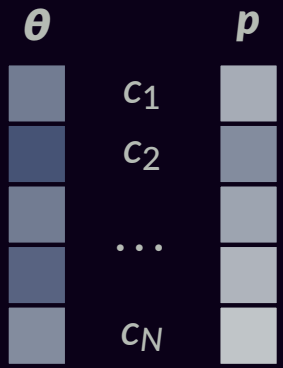
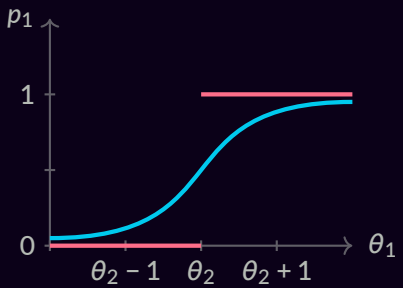
Argmax vs. Softmax

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





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

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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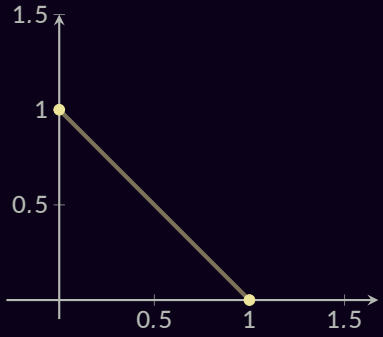

$N = 2$

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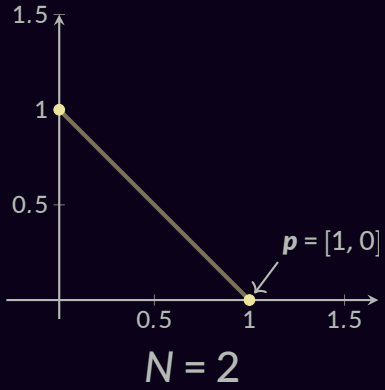

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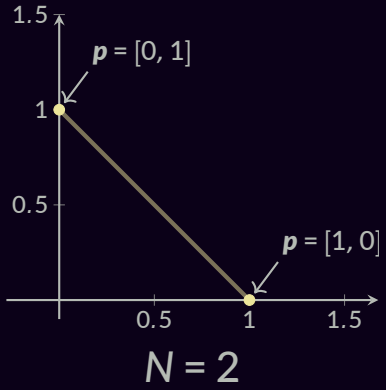

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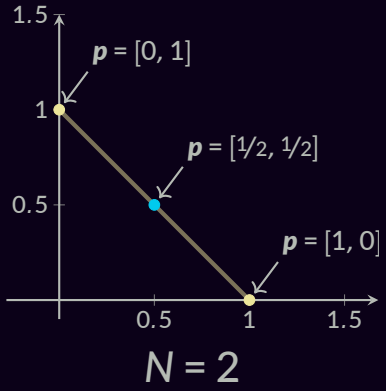

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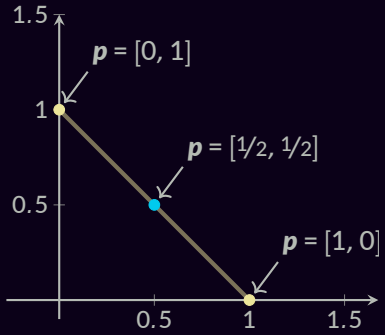

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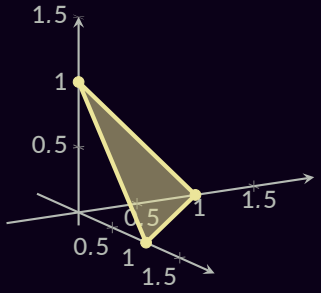
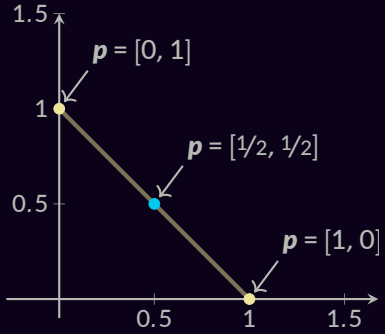


$N = 3$

A Softmax Origin Story

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



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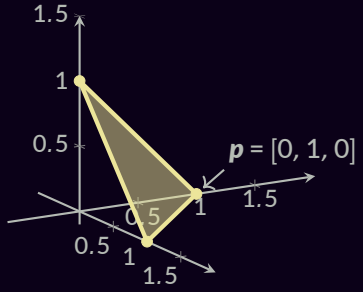

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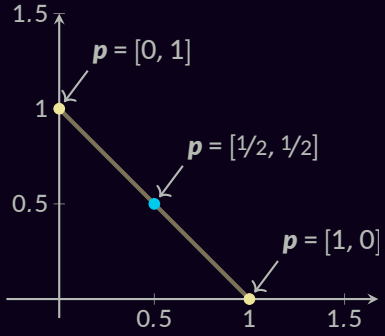

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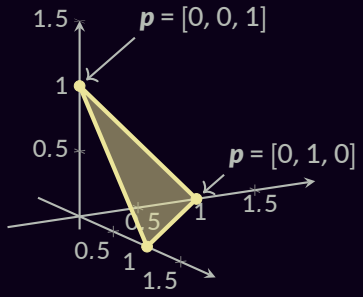

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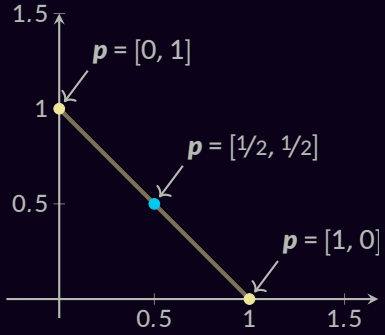

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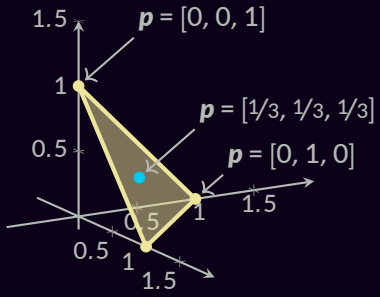

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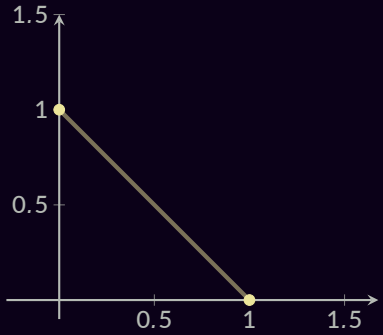
Fundamental Thm. Lin. Prog.
(Dantzig et al., 1955)



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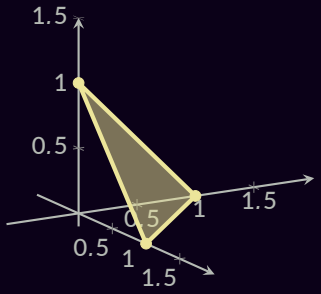

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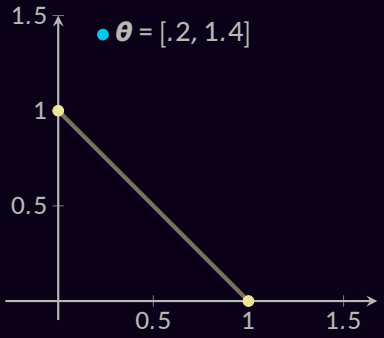

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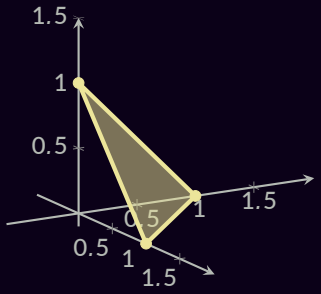

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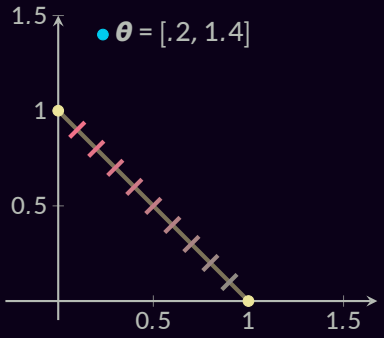

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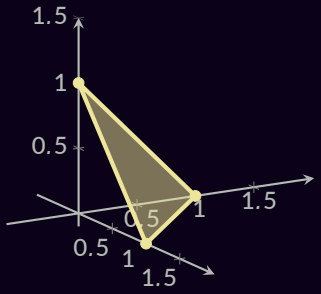

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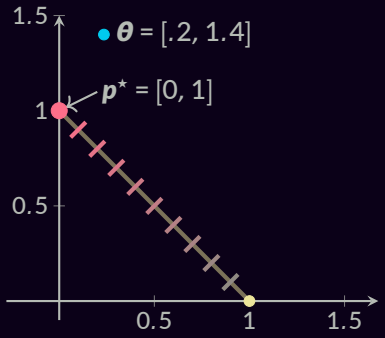

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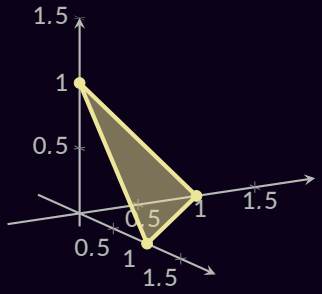

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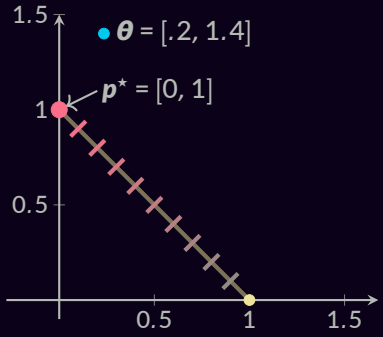

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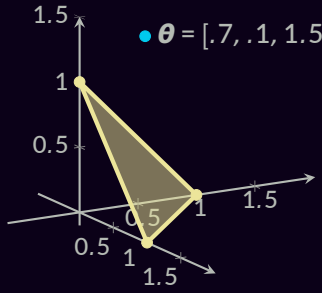

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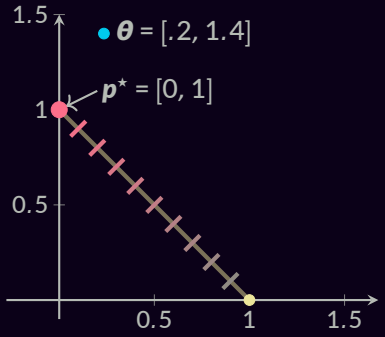

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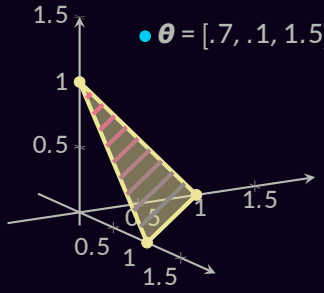

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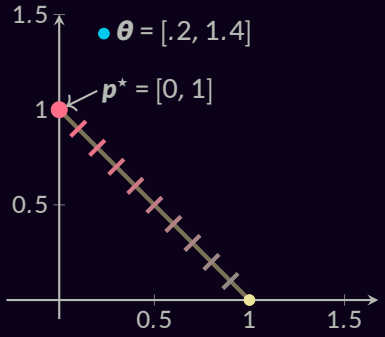

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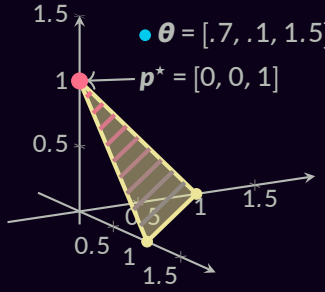

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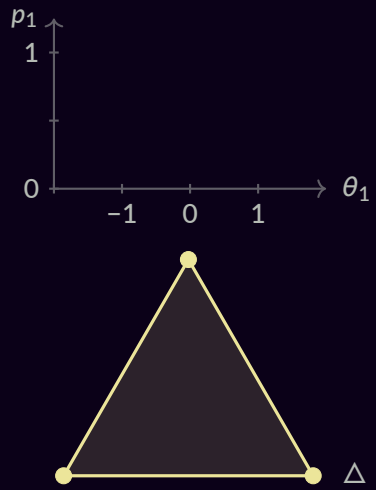
(Niculae and Blondel, 2017)

Smoothed Max Operators

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



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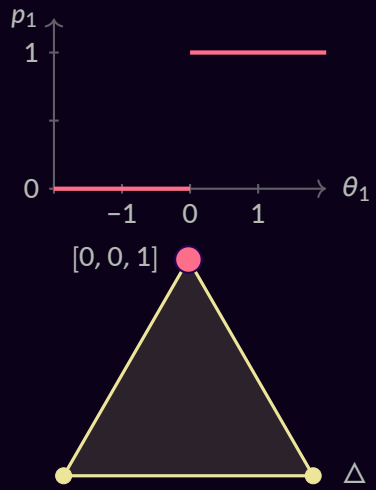

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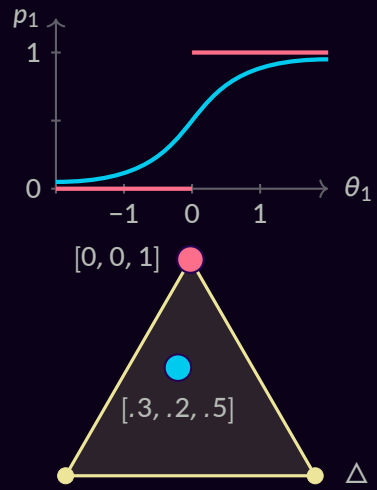

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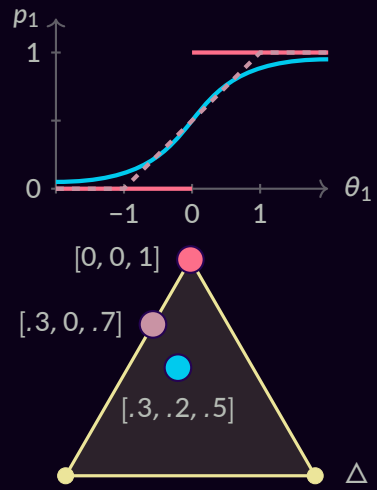

(Martins and Astudillo, 2016)

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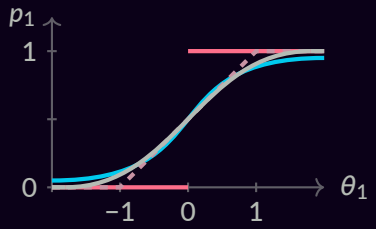
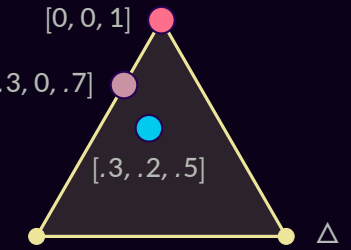
- α-entmax: $\Omega(\boldsymbol{p}) = \frac{1}{\alpha(\alpha-1)} \sum_j p_i^\alpha$





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

Sparsemax

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

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Computation:

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

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

$O(d)$ via partial sort

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

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Backward pass:

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

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

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

(Martins and Astudillo, 2016)

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

argmin differentiation

(Colson et al., 2007; Gould et al., 2016)

see also (Amos and Kolter, 2017)

Backward pass:

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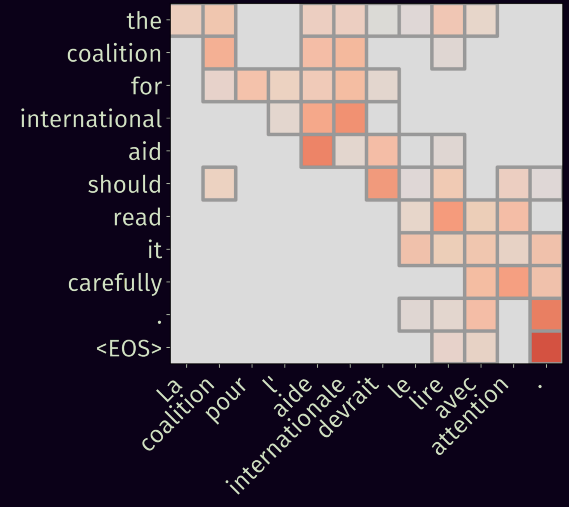
(Martins and Astudillo, 2016)

Some applications:

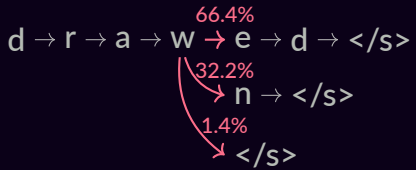
sparse attention

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



sparse losses (& seq2seq)

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

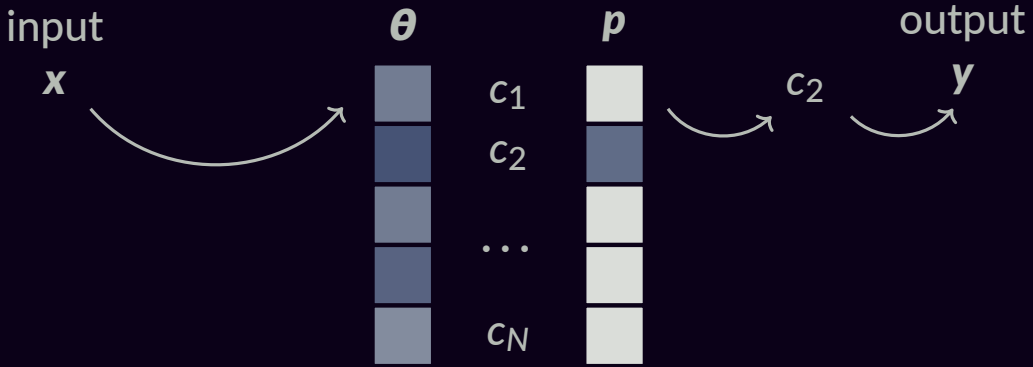


Structured Prediction

finally

Structured Prediction

is essentially a (very high-dimensional) argmax



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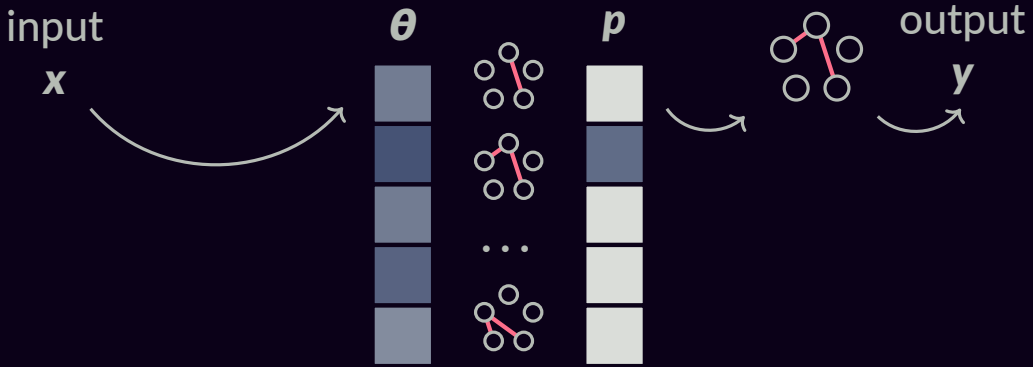

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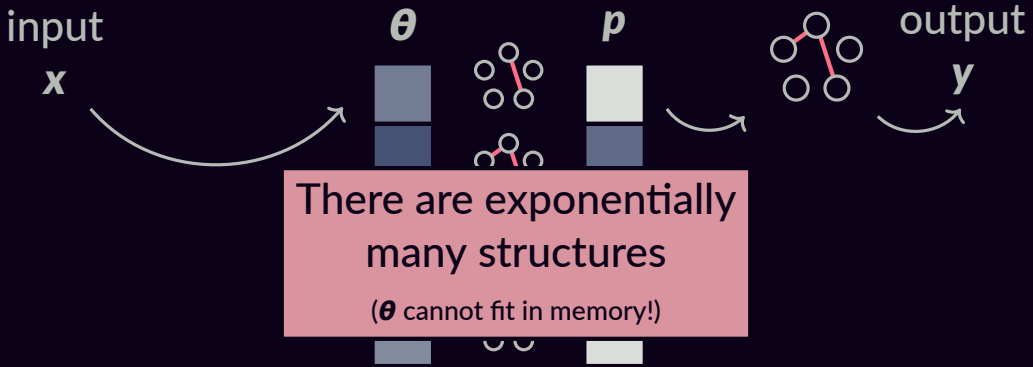

Factorization Into Parts

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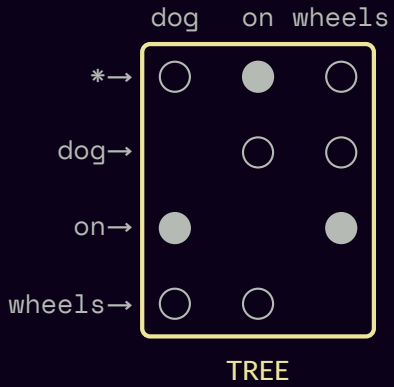

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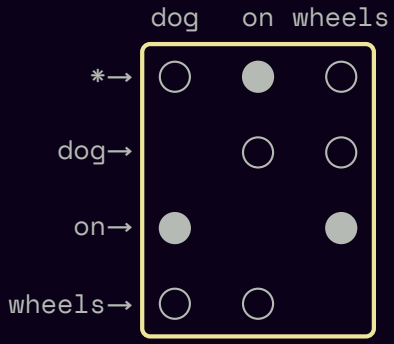
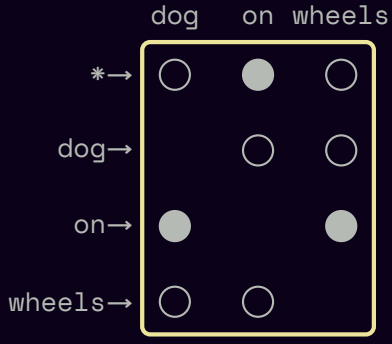


TREE

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

Factorization Into Parts

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



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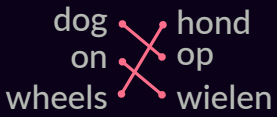

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\begin{bmatrix} 1 & 0 & \boxed{0} & \\ 0 & 1 & \boxed{1} & \\ 0 & 0 & \boxed{0} & \\ \hline 0 & 1 & \boxed{1} & \\ 1 & 0 & \boxed{0} & \cdots \\ 0 & 0 & \boxed{0} & \\ \hline 0 & 0 & \boxed{0} & \\ 0 & 1 & \boxed{0} & \\ 1 & 0 & \boxed{1} & \end{bmatrix}
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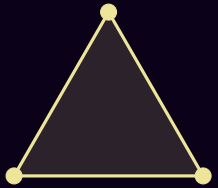
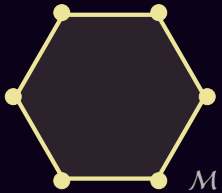
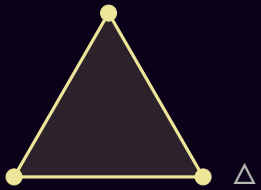
$$

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


Δ


$\mathcal{M}$

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



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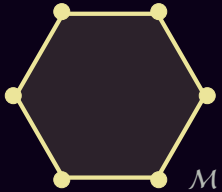
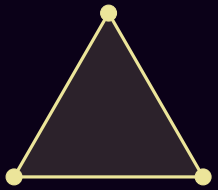


$\mathcal{M}$

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



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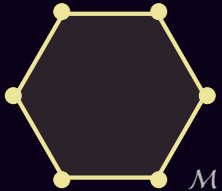

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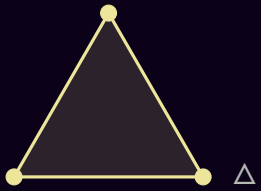
$$= \{\mathbb{E}_{H\sim\boldsymbol{p}}\, \boldsymbol{a}_H : \boldsymbol{p} \in \Delta\}$$



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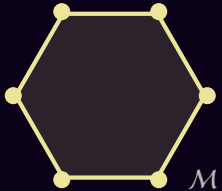
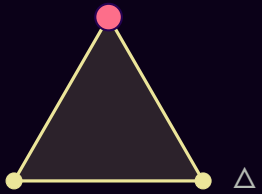
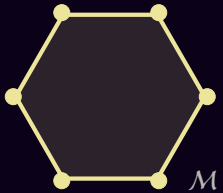


$\mathcal{M}$

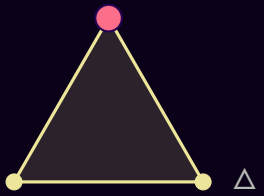
- **argmax** $\arg\max_{\boldsymbol{p} \in \Delta} \boldsymbol{p}^\top \boldsymbol{\theta}$

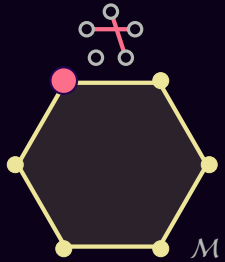




argmax $\arg\max_{\boldsymbol{p} \in \Delta} \boldsymbol{p}^\top \boldsymbol{\theta}$

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





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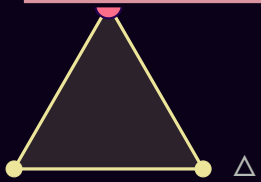
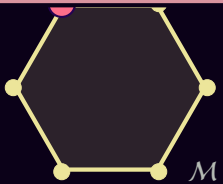
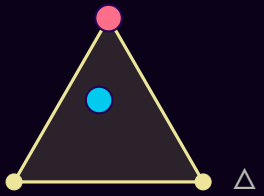
e.g. dependency parsing → **Chu-Liu/Edmonds**
matching → **Kuhn-Munkres**





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



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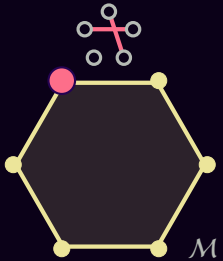

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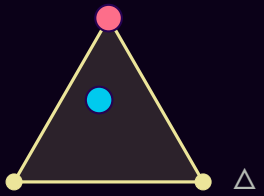

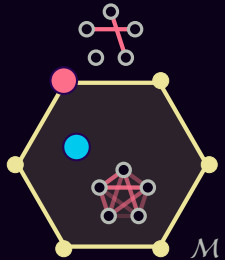

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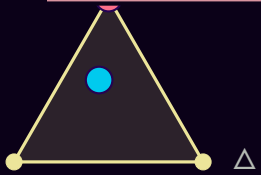
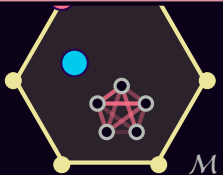
e.g. sequence labeling → forward-backward

(Rabiner, 1989)

As attention: (Kim et al., 2017)





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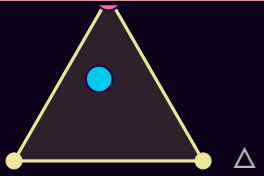
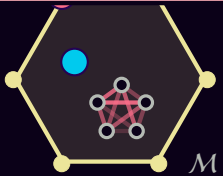
e.g. dependency parsing → **the Matrix-Tree theorem**

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

As attention: (Liu and Lapata, 2018)





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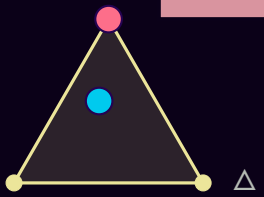
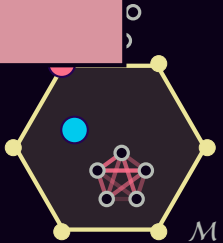
e.g. matchings → **#P-complete!**

(Taskar, 2004; Valiant, 1979)





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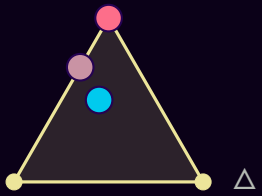
- **sparsemax** $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top \boldsymbol{\theta} - \frac{1}{2}\|\boldsymbol{p}\|^2$



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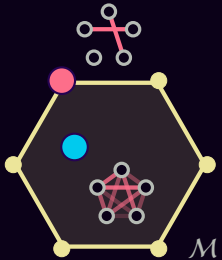

(Niculae, Martins, Blondel, and Cardie, 2018)

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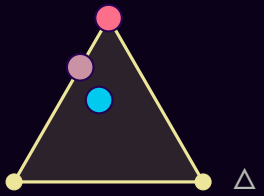

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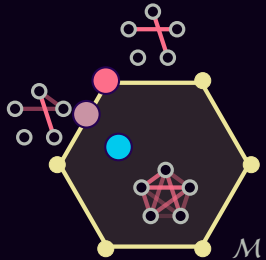
- **SparseMAP** $\arg\max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta} - \frac{1}{2}\|\boldsymbol{\mu}\|^2$



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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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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(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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    (Nocedal and Wright, 1999, Ch. 16.4 & 16.5)
    (Wolfe, 1976; Vinyes and Obozinski, 2017)

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

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

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Completely modular: just add MAP

Conditi **pass**

(Frank and Wolfe, 1956

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SparseMAP Applications

- Sparse alignment attention
  (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)

ListOps (Nangia and Bowman, 2018)

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)

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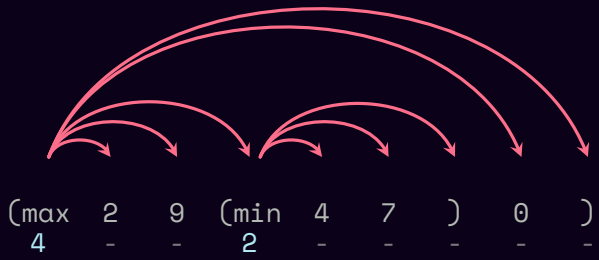
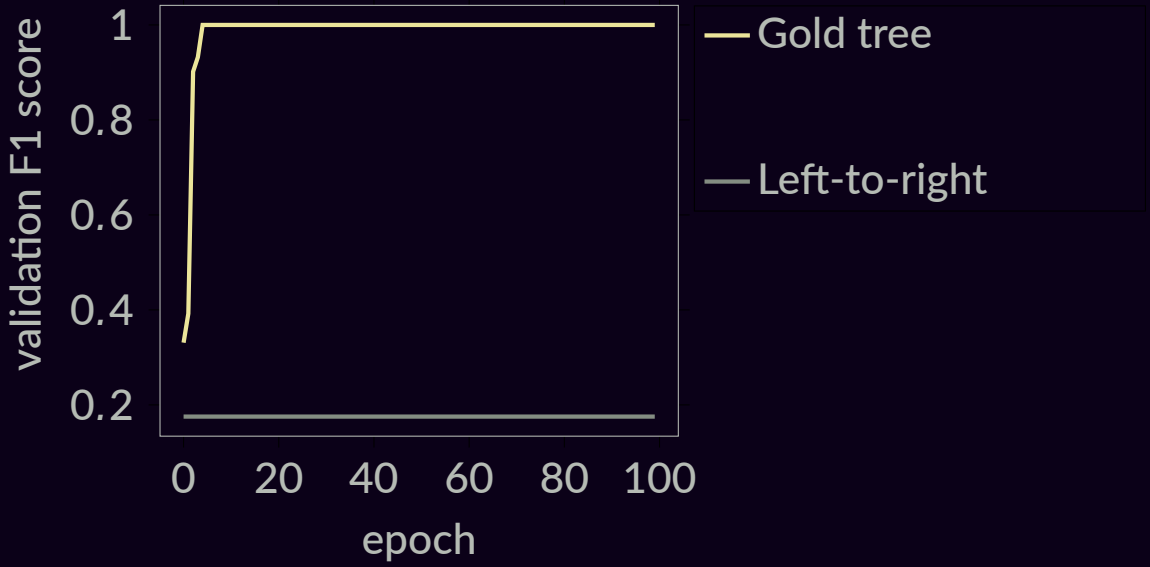
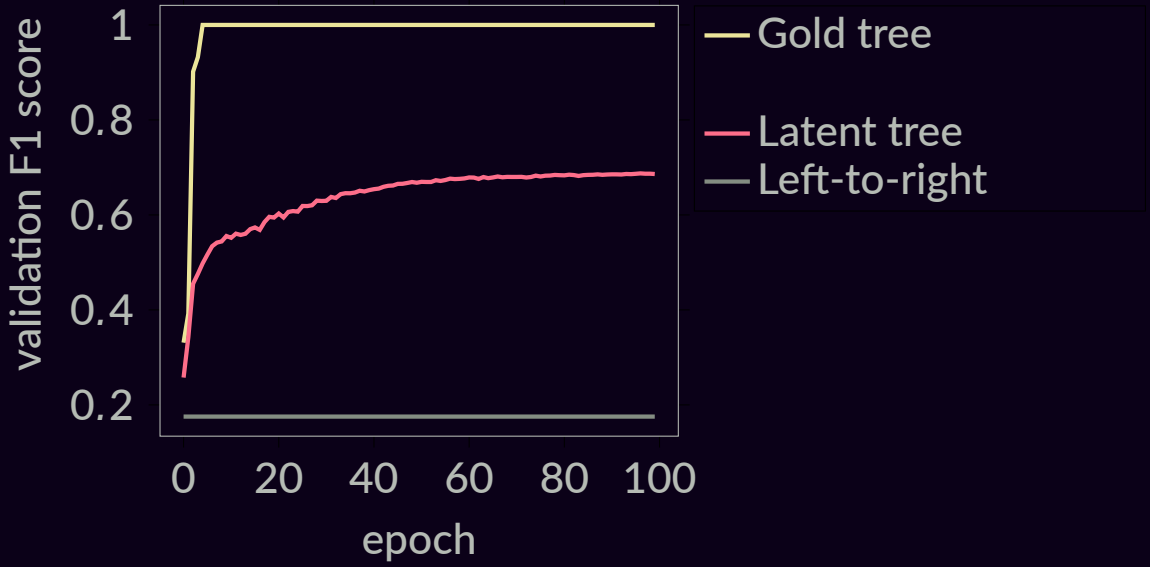



validation F1 score
1
0.8
0.6
0.4
0.2
0
20
40
60
80
100
epoch
Gold tree
Left-to-right


validation F1 score
1
0.8
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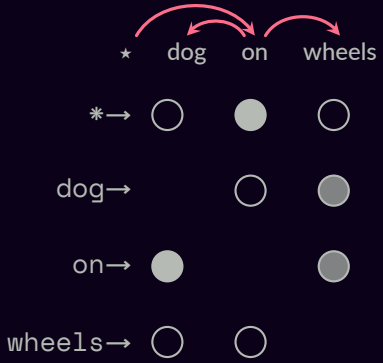
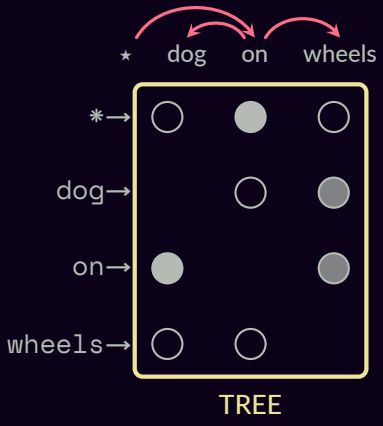
Gold tree
Latent tree
Left-to-right

What if MAP is not available?

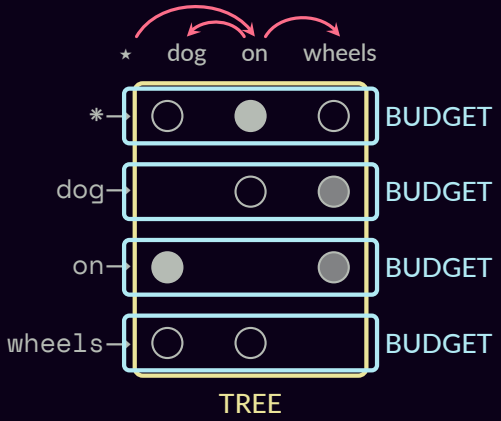
Multiple, Overlapping Factors



Multiple, Overlapping Factors

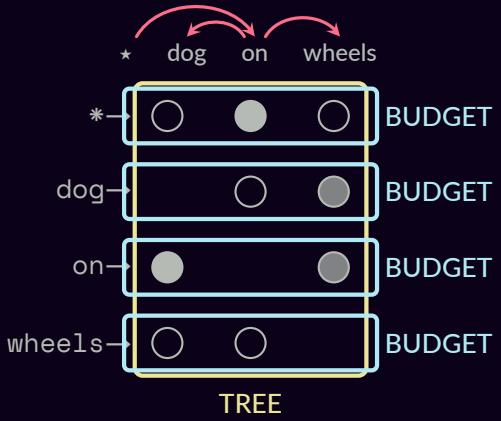


Multiple, Overlapping Factors

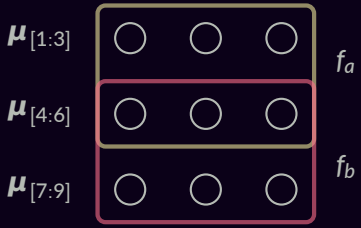


Multiple, Overlapping Factors

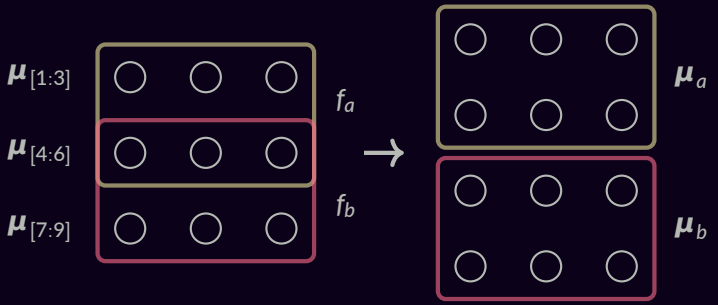
Maximization in factor graphs: NP-hard, even when each factor is tractable.



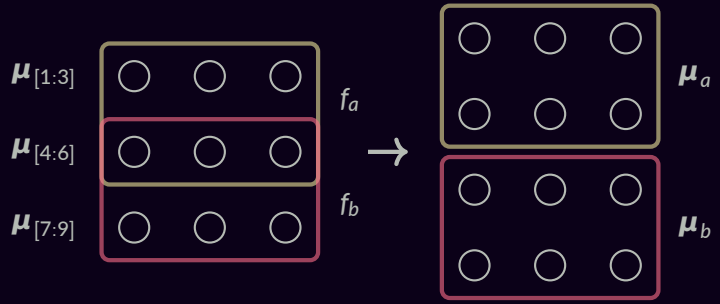
Optimization as Consensus-Seeking



Optimization as Consensus-Seeking

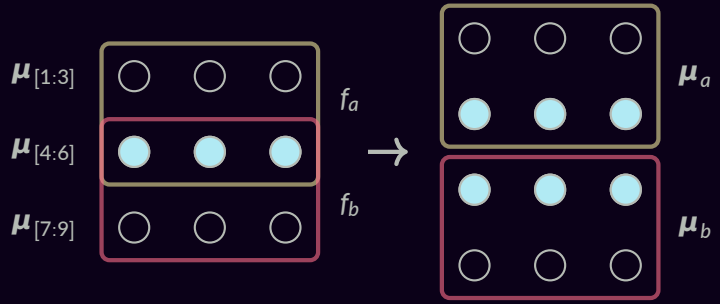


Optimization as Consensus-Seeking



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

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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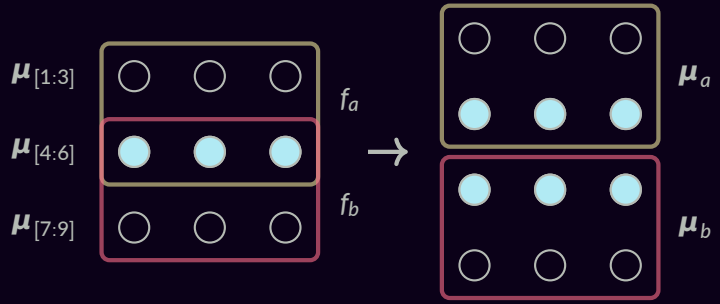

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$$\max_{\mu, \mu_f} \sum_{f \in \mathcal{F}} \eta_f^\top \mu_f \quad \text{s.t. } C_f \mu = \mu_f,\ \mu_f \in \mathcal{M}_f \text{ for } f \in \mathcal{F}$$

Optim eking

LP relaxation (Wainwright and Jordan, 2008)

the local polytope:

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

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

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

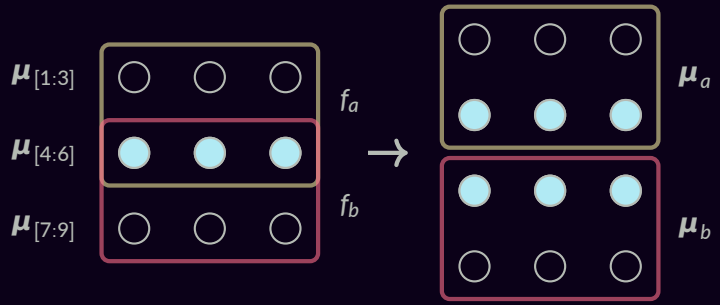
$\boldsymbol{\mu}_{[7:9}$ $\boldsymbol{\mu}_b$

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

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

(Niculae and Martins, 2020)

Optimization as Consensus-Seeking



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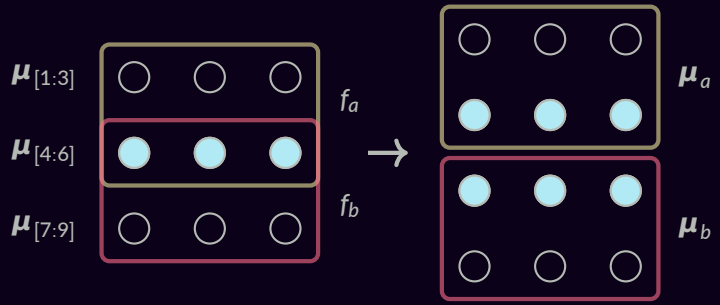

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$$\max_{\boldsymbol{\mu}, \boldsymbol{\mu}_f} \Big(\sum_{f \in \mathcal{F}} \boldsymbol{\eta}_f^\top \boldsymbol{\mu}_f \Big) - \tfrac{1}{2} \|\boldsymbol{\mu}\|^2 \quad \text{s.t.} \quad \boldsymbol{C}_f \boldsymbol{\mu} = \boldsymbol{\mu}_f, \ \boldsymbol{\mu}_f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

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Algorithms for LP-SparseMAP

Forward pass

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

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

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

(Niculae and Martins, 2020)

Algorithms for LP-SparseMAP

Forward pass

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

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

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.)

(Niculae and Martins, 2020)

Differentiable Sparse Structured Prediction

Factor graphs as a hidden-layer DSL!

```
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)
```

(Niculae and Martins, 2020)

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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(η_f):  # abstract, private
        raise NotImplemented

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

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


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

    def backward(dμ_f):
        # specialized
```

(Niculae and Martins, 2020)

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New factors only require MAP.

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    def backward(dμ_f):
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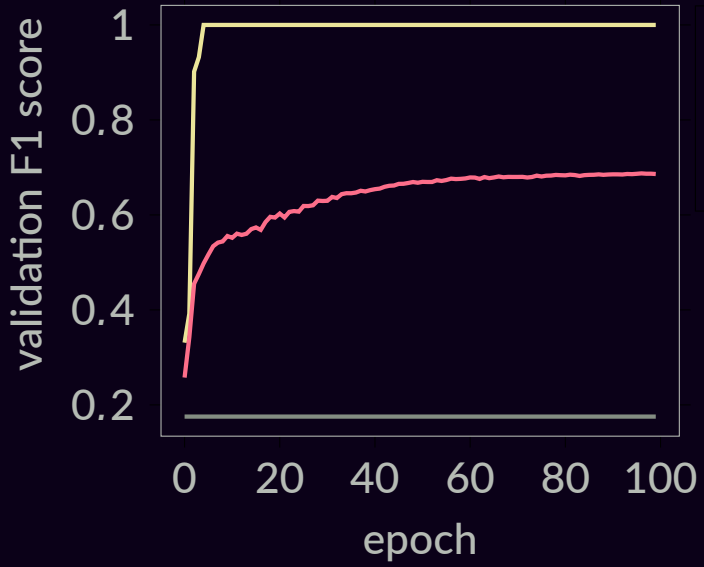
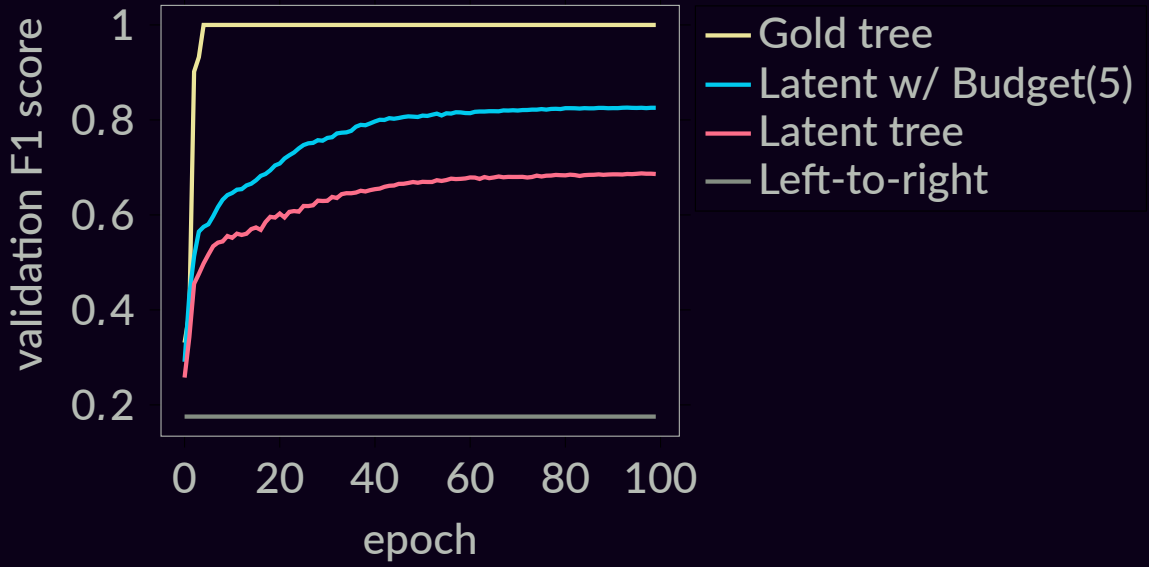
class Budget(Factor):
    def sparsemap(η_f):
        # specialized

    def backward(dμ_f):
        # 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
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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

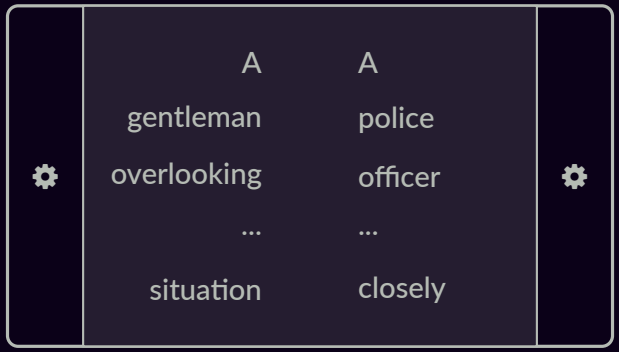
Structured Attention for Alignments

NLI

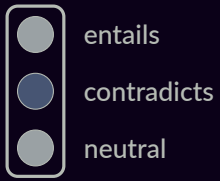
premise: A gentleman overlooking a neighborhood situation.
hypothesis: A police officer watches a situation closely.

input

(P, H)



output



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

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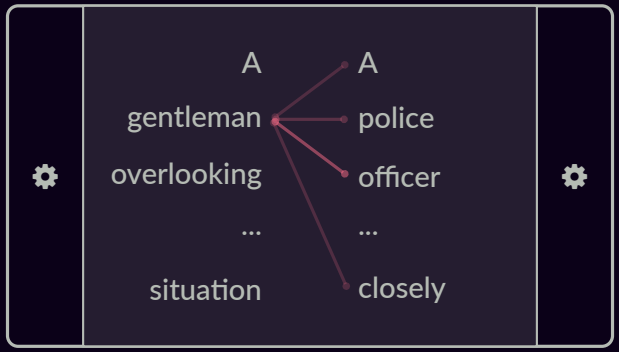
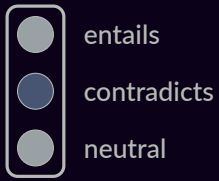


output



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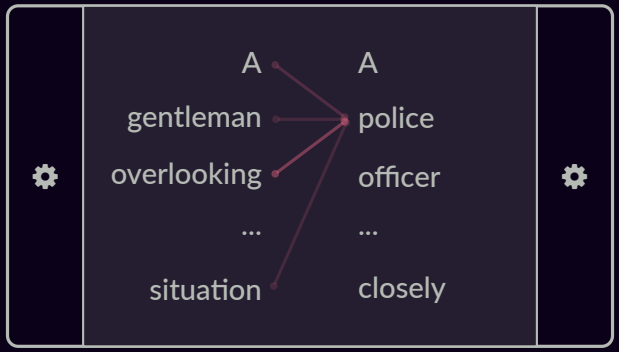
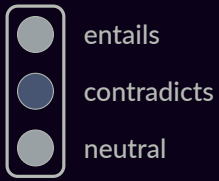


output



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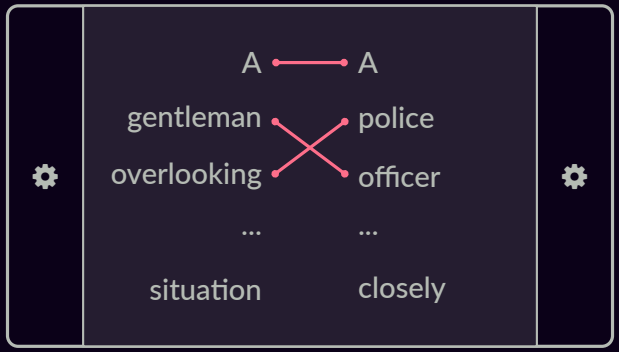
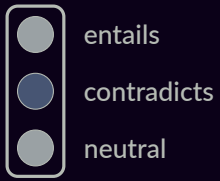


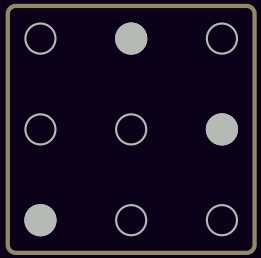
output



(Proposed model: global structured alignment.)

Structured Alignment Models

matching

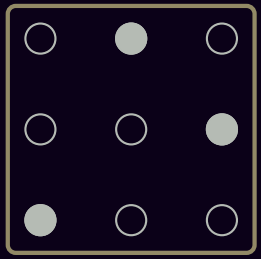


SparseMAP w/ Kuhn-Munkres

(Kuhn, 1955)

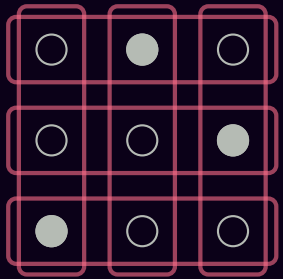
Structured Alignment Models

matching



SparseMAP w/ Kuhn-Munkres
(Kuhn, 1955)

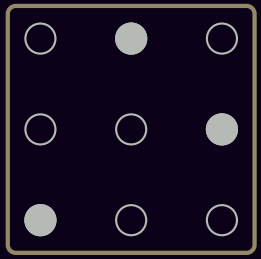
LP-matching



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

Structured Alignment Models

matching



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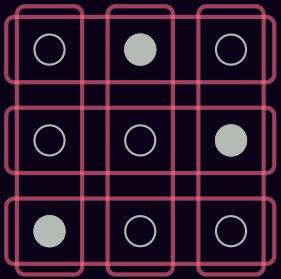
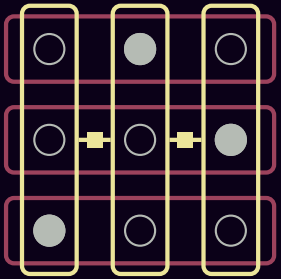


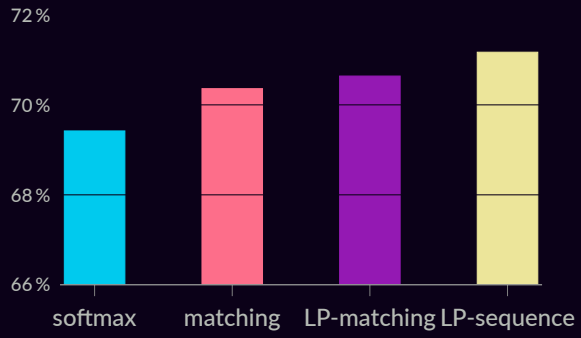
LP-SparseMAP w/ XORs
(equivalent; different solver)

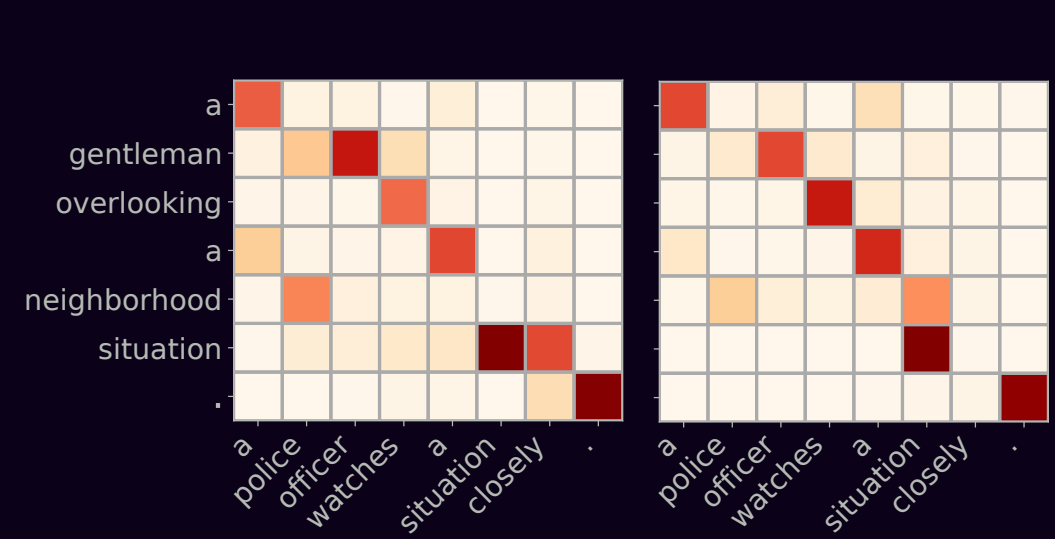
LP-sequence



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

MultiNLI (Williams et al., 2017)




a
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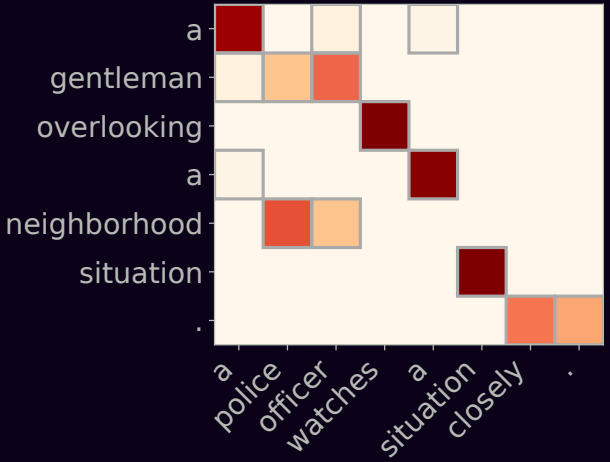
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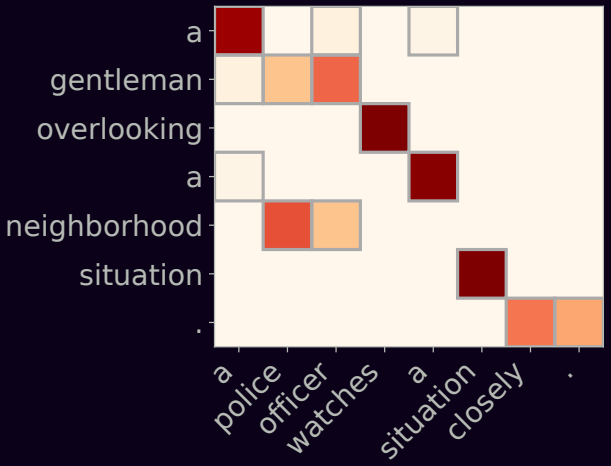
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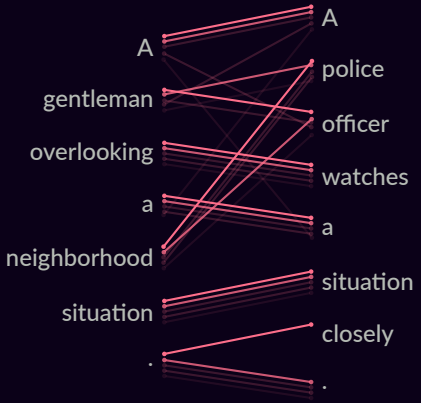
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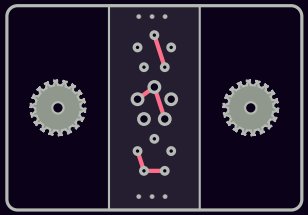
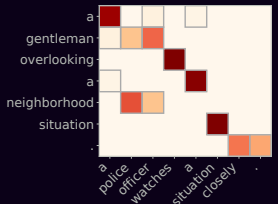
Conclusions

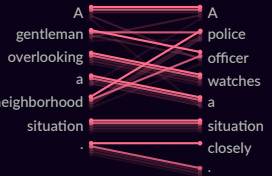


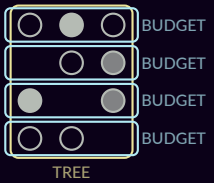
Differentiable & sparse
structured inference

Generic, extensible, efficient algorithms
for **any factor graph**

Decomposition into meaningful
coarse structures.







v.niculae@uva.nl github.com/deep-spin/lp-sparsemap
https://vene.ro @vnfrombucharest

Extra slides

Acknowledgements

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

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

Fusedmax

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

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

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

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

(Niculae and Blondel, 2017)

fusedmax(

$\text{prox}_{\text{fused}}($

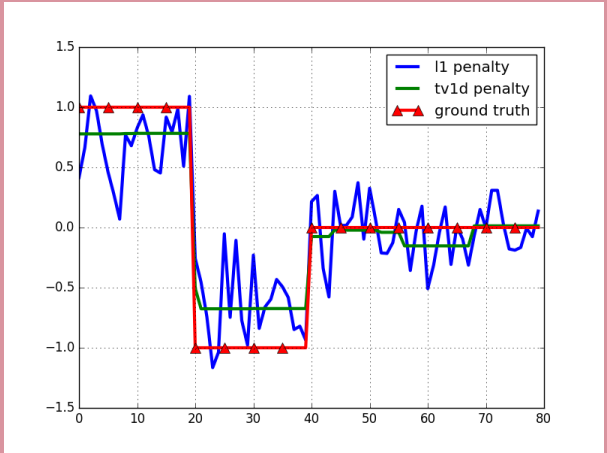
Proposi

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

$j-1|$

$j-1|$

$\text{used}(\boldsymbol{\theta})\big)$



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

(Tibshirani et al., 2005)

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

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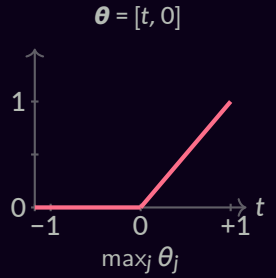
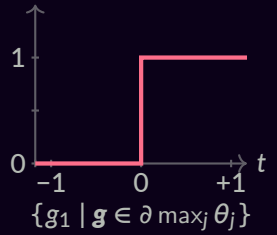




Discrete latent variables

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.

(Correia, Niculae, Aziz, and Martins, 2020)

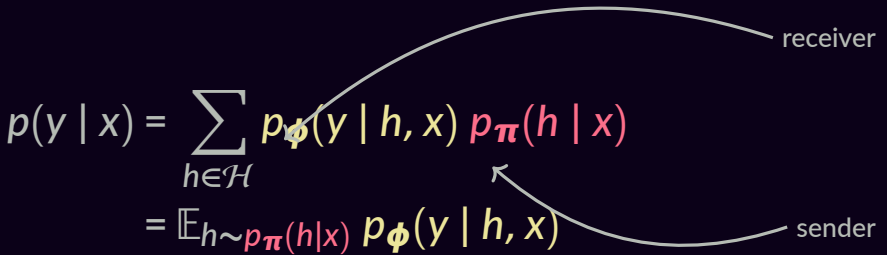
Latent variable models!

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

$$= \mathbb{E}_{h \sim p_{\boldsymbol{\pi}}(h \mid x)}\, p_{\boldsymbol{\phi}}(y \mid h, x)$$

(Correia, Niculae, Aziz, and Martins, 2020)

Latent variable models!



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

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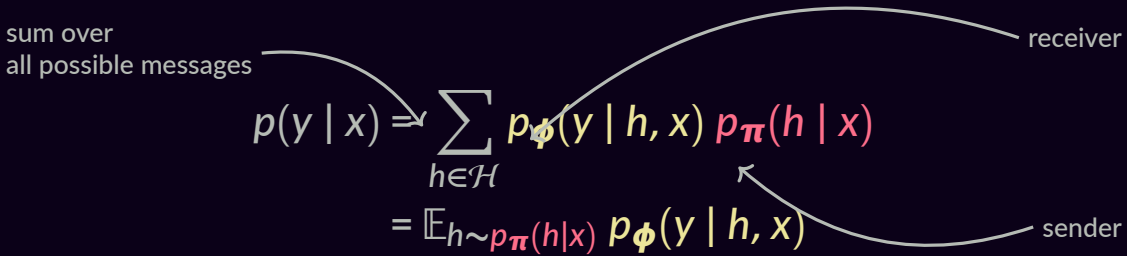

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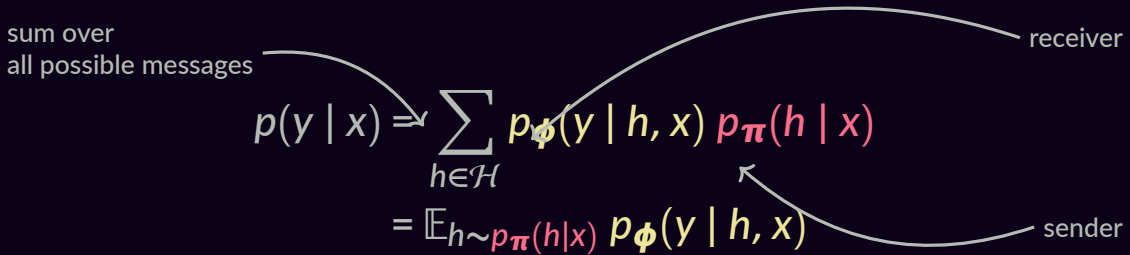

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- Standard: Monte Carlo gradient estimators (e.g. SFE, Gumbel)

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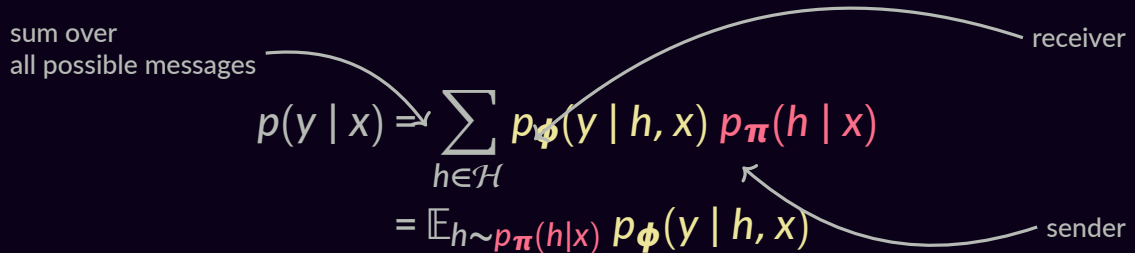

- Emergent communication: h is a word from a big vocabulary. $\boldsymbol{p_{\phi}(y \mid h)}$ **is expensive.**
- Standard: Monte Carlo gradient estimators (e.g. SFE, Gumbel)
- **Idea: parametrize $\boldsymbol{p_{\pi}(h \mid x)}$ using sparsemax!** Sum only over $|\bar{\mathcal{H}}| \ll |\mathcal{H}|$.
  No bias AND no variance by **changing the question**

(Lazaridou et al., 2017; Correia, Niculae, Aziz, et al., 2020)

Emergent Communication

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

Method	success (%)	Dec. calls
Monte Carlo		
SFE	33.05 ±2.84	1
NVIL	37.04 ±1.61	1
Gumbel	23.51 ±16.19	1
ST Gumbel	27.42 ±13.36	1
Marginalization		

(Lazaridou et al., 2017; Correia, Niculae, Aziz, et al., 2020)

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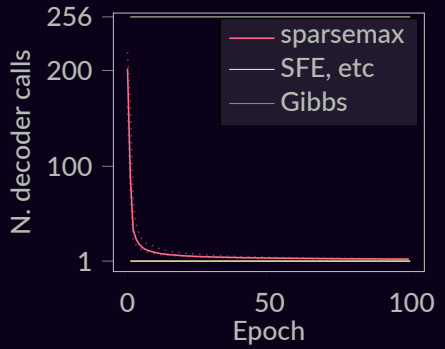

(Correia, Niculae, Aziz, and Martins, 2020)

Limitations

- Mostly (and eventually) very sparse.
  But $\text{sparsemax}(\mathbf{0}) = 1/d\,\mathbf{1}$: fully dense worst case.
- For the same reason, sparsemax cannot handle structured h.

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One solution: top-k sparsemax

$$k\text{-sparsemax}(\boldsymbol{\theta}) = \operatorname*{arg\,min}_{\boldsymbol{p} \in \triangle, \|\boldsymbol{p}\|_0 \leq k} \|\boldsymbol{p} - \boldsymbol{\theta}\|_2^2$$

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

Dependency TreeLSTM

(Tai et al., 2015)

Dependency TreeLSTM

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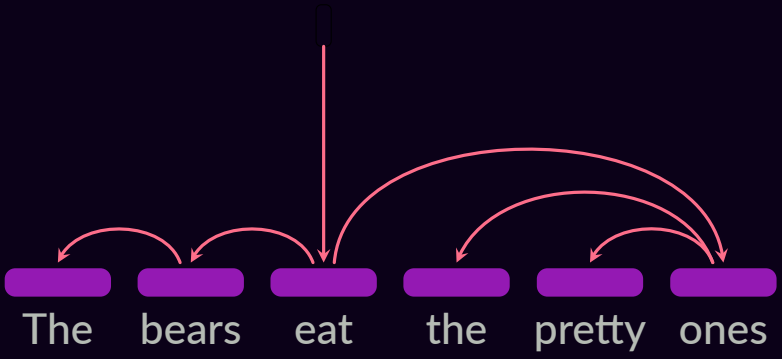

Dependency TreeLSTM

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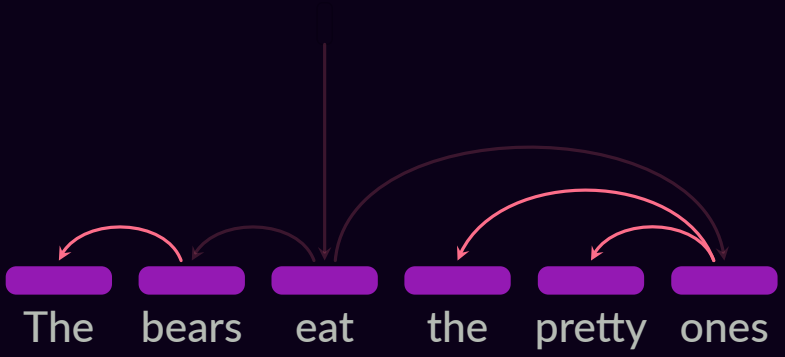

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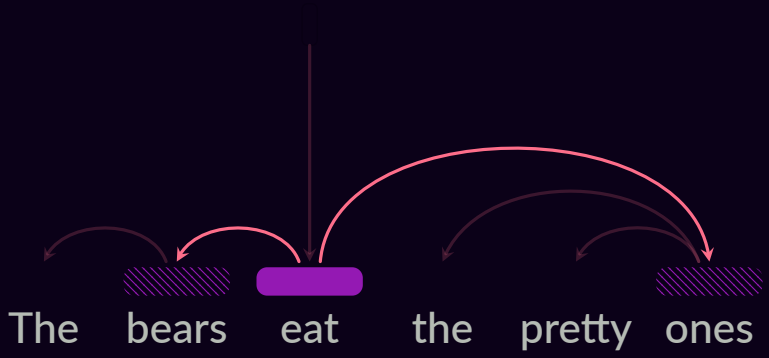

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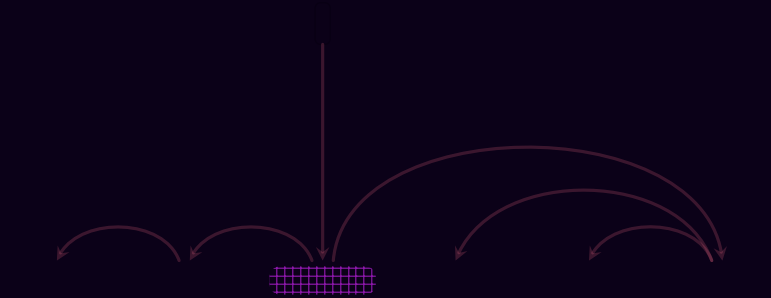

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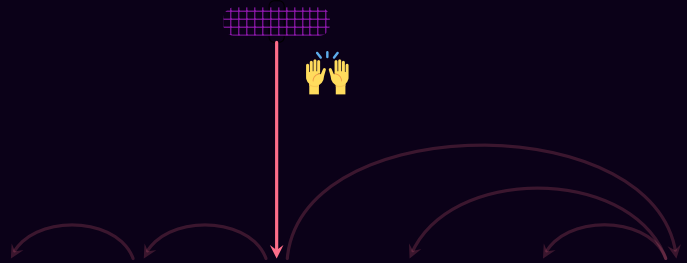
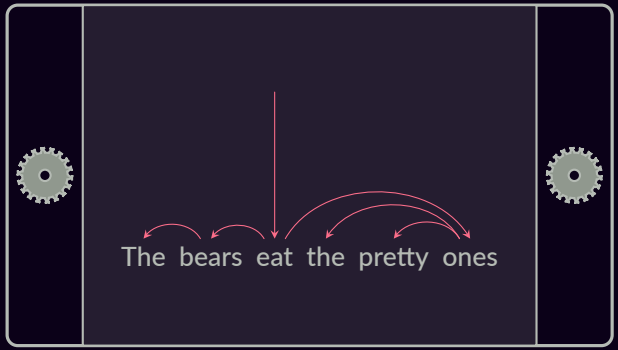


Latent Dependency TreeLSTM

(Niculae, Martins, and Cardie, 2018)

input

x



output

y

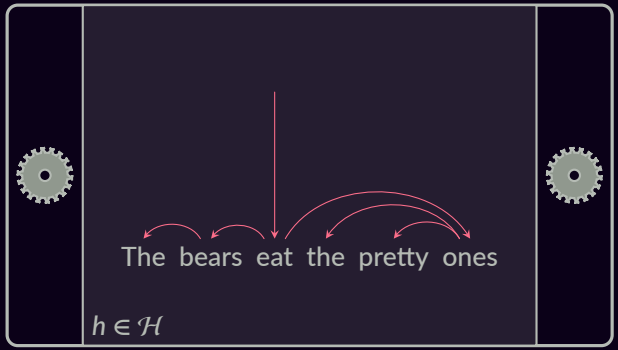
Latent Dependency TreeLSTM

(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

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

Structured Latent Variable Models

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Structured Latent Variable Models

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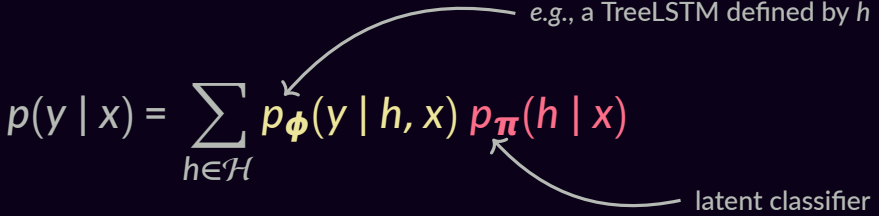
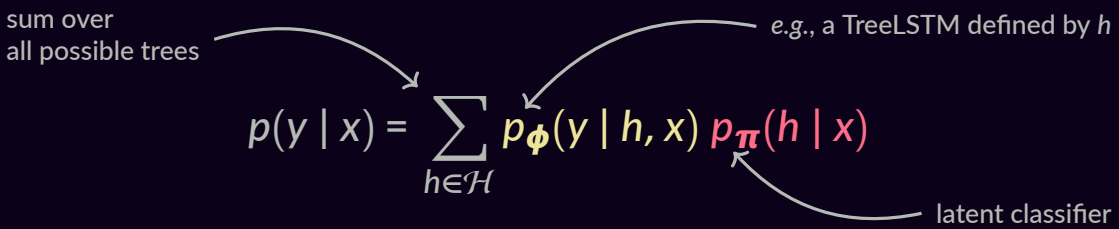


Structured Latent Variable Models



Exponentially large sum!

Structured Latent Variable Models

sum over
all possible trees

e.g., a TreeLSTM defined by h

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

latent classifier

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

idea 1
idea 2
idea 3

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idea 2

idea 3

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idea 2 $p_{\boldsymbol{\pi}}(h \mid x) \propto \exp\big(\text{score}_{\boldsymbol{\pi}}(h; x)\big)$ softmax

idea 3

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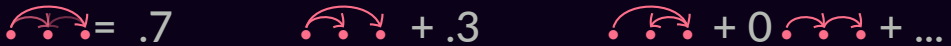
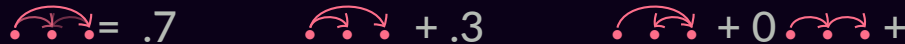
idea 3		SparseMAP	😊	😊

SparseMAP

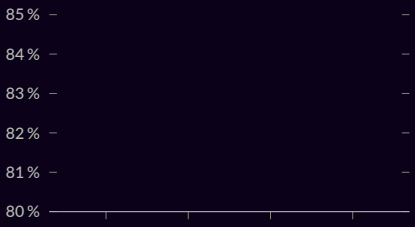
SparseMAP



SparseMAP



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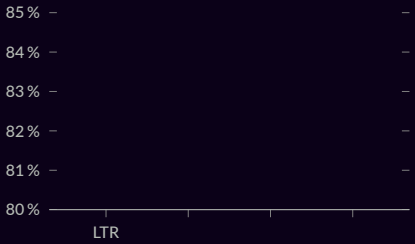
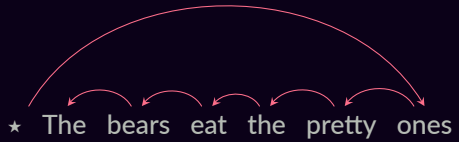
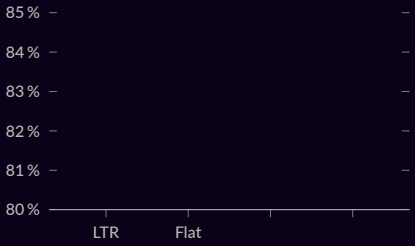
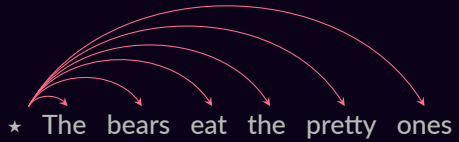


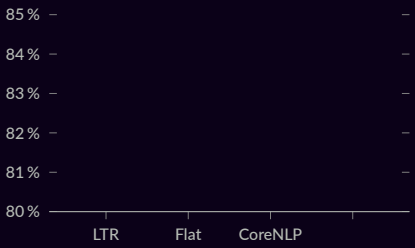


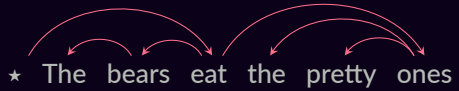
Left-to-right: regular LSTM



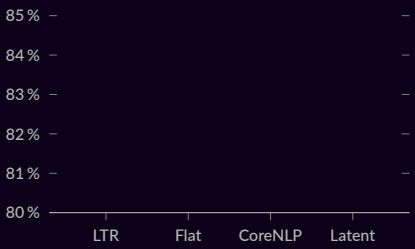


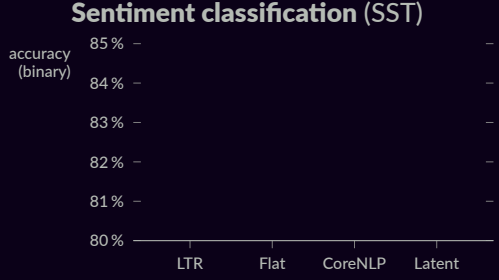
Flat: bag-of-words–like

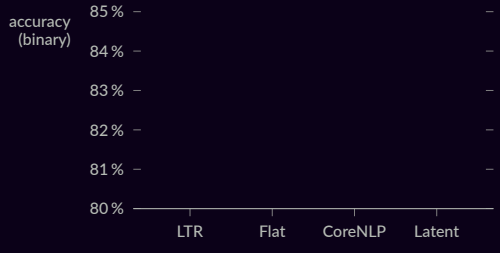


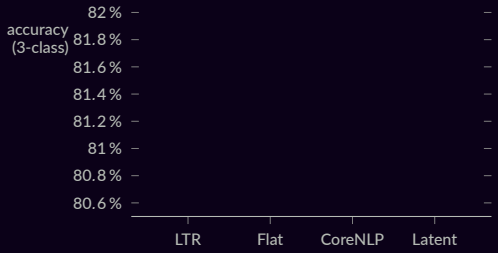


CoreNLP: off-line parser


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


Sentiment classification (SST)
accuracy (binary)
85 %
84 %
83 %
82 %
81 %
80 %
LTR
Flat
CoreNLP
Latent

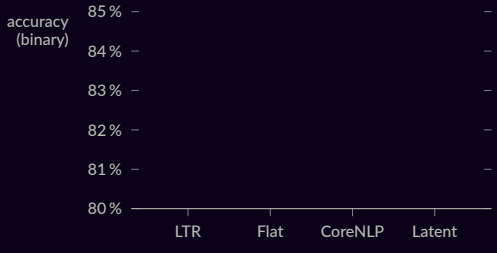




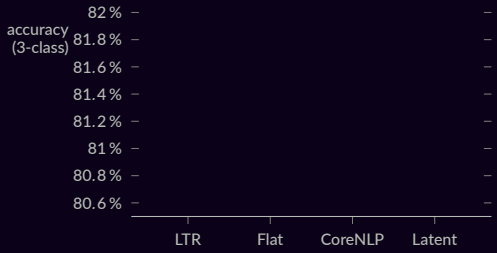
Sentence pair classification (P, H)

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

Sentiment classification (SST)



Natural Language Inference (SNLI)

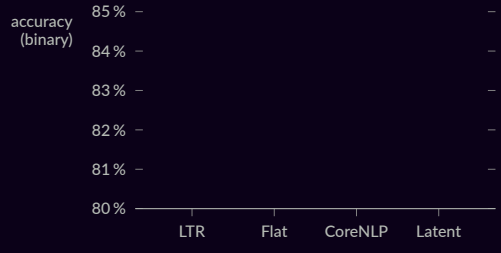


Reverse dictionary lookup

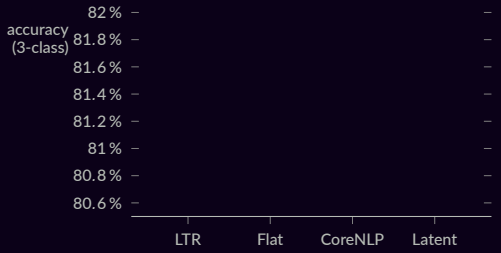
given word description, predict word embedding (Hill et al., 2016)

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

Sentiment classification (SST)

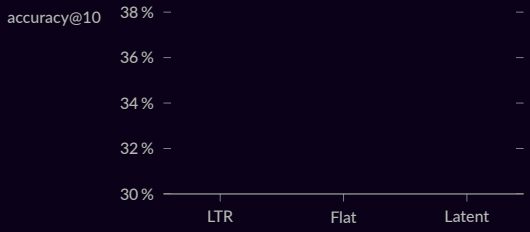


Natural Language Inference (SNLI)

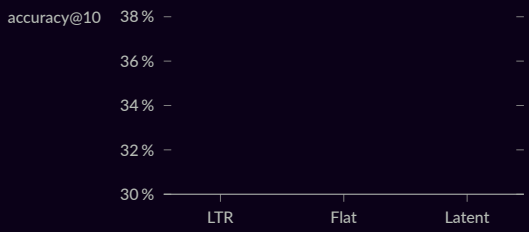


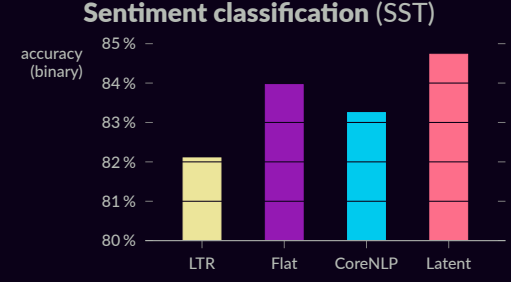
Reverse dictionary lookup

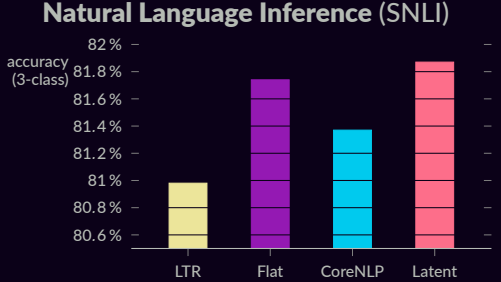
(definitions)

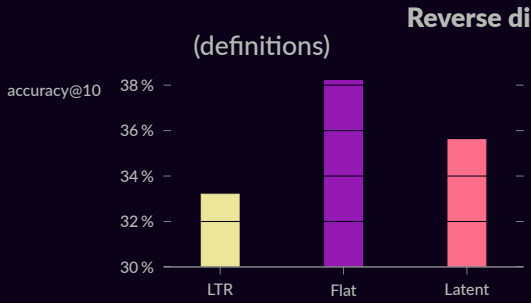


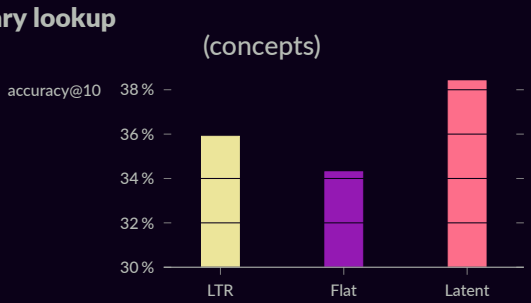
(concepts)




Sentiment classification (SST)
accuracy (binary)
85 %
84 %
83 %
82 %
81 %
80 %
LTR
Flat
CoreNLP
Latent

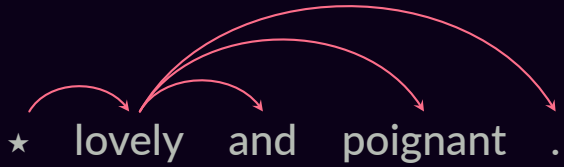

Natural Language Inference (SNLI)
accuracy (3-class)
82 %
81.8 %
81.6 %
81.4 %
81.2 %
81 %
80.8 %
80.6 %
LTR
Flat
CoreNLP
Latent


Reverse dictionary lookup
(definitions)
accuracy@10
38 %
36 %
34 %
32 %
30 %
LTR
Flat
Latent


(concepts)
accuracy@10
38 %
36 %
34 %
32 %
30 %
LTR
Flat
Latent

Syntax vs. Composition Order

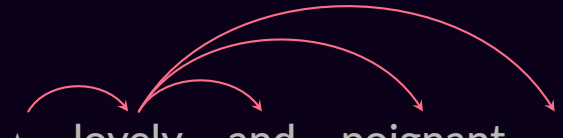
CoreNLP parse, $p = 21.4\%$



Syntax vs. Composition Order

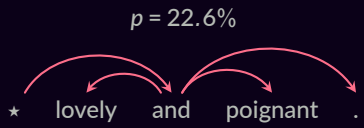
$p = 22.6\%$

CoreNLP parse, $p = 21.4\%$

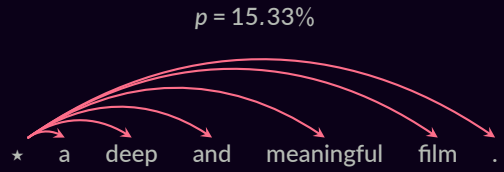


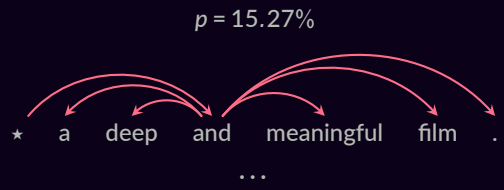
. . .

Syntax vs. Composition Order

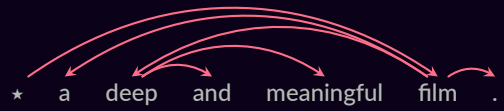


CoreNLP parse, $p = 21.4\%$





CoreNLP parse, $p = 0\%$



Structured Output Prediction

SparseMAP

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

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

Structured Output Prediction

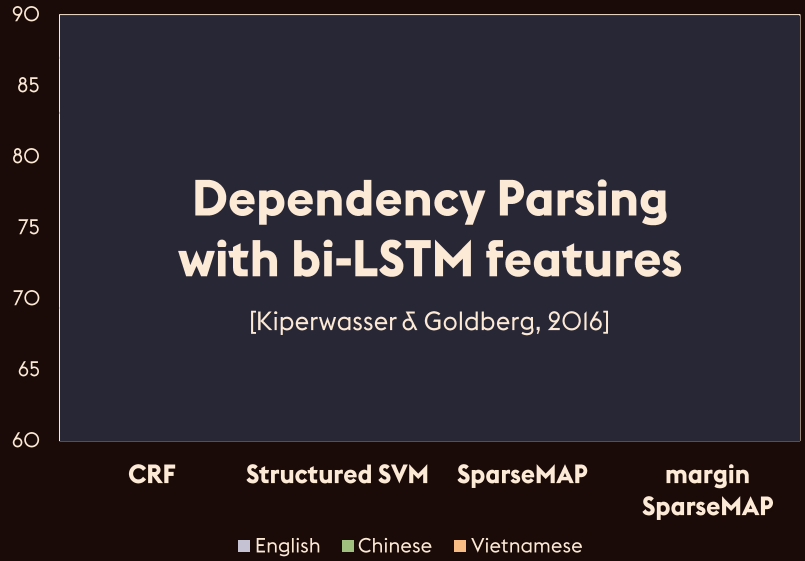
SparseMAP

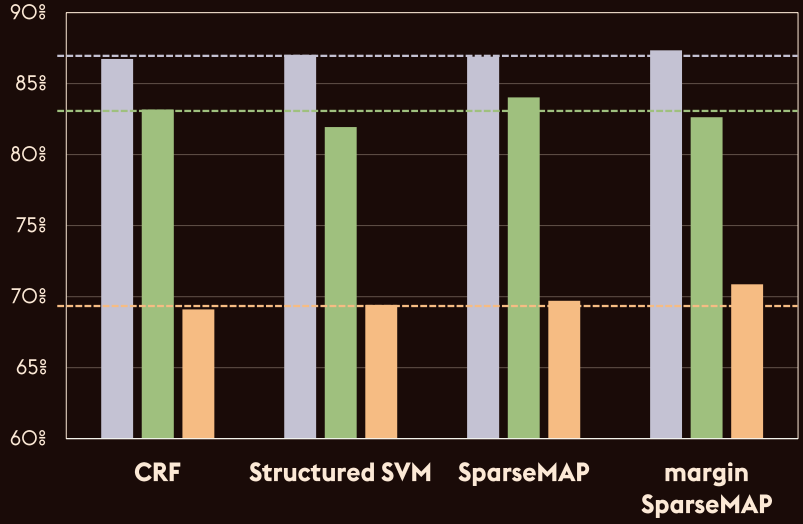
$$L_{\boldsymbol{A}}(\boldsymbol{\eta}, \bar{\boldsymbol{\mu}}) = \max_{\boldsymbol{\mu} \in \mathcal{M}} \left\{ \boldsymbol{\eta}^\top \boldsymbol{\mu} - 1/2 \|\boldsymbol{\mu}\|^2 \right\} - \boldsymbol{\eta}^\top \bar{\boldsymbol{\mu}} + 1/2 \|\bar{\boldsymbol{\mu}}\|^2$$

cost-SparseMAP

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

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

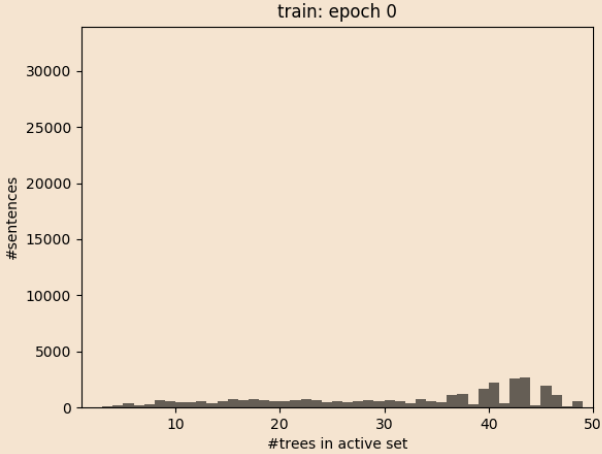

90
85
80
75
70
65
60
Dependency Parsing with bi-LSTM features
[Kiperwasser & Goldberg, 2016]
CRF
Structured SVM
SparseMAP
margin SparseMAP
English
Chinese
Vietnamese



Unlabeled Accuracy (UAS)
Universal Dependencies dataset

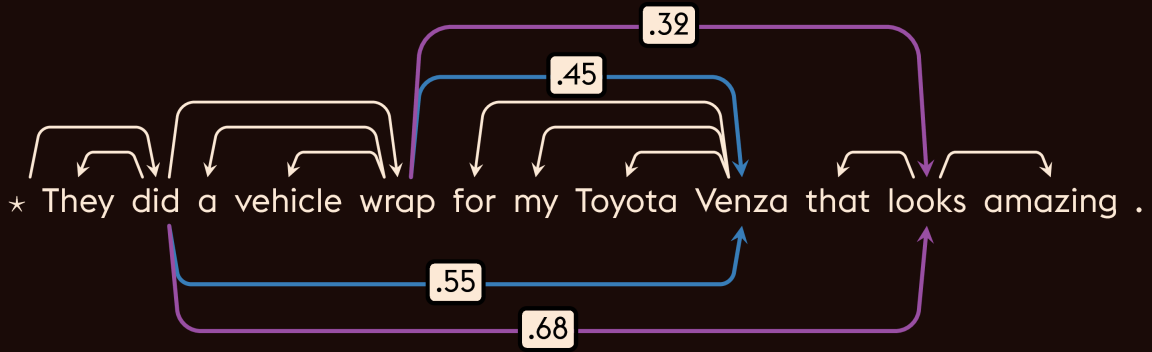
Sparse Structured Output Prediction

As models train, inference gets sparser!



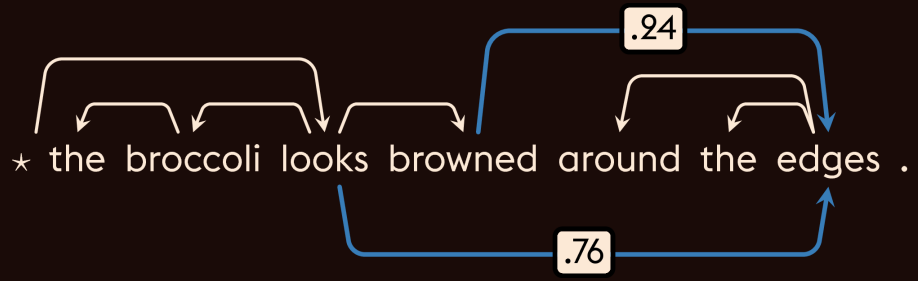
Sparse Structured Output Prediction

Inference captures linguistic ambiguity!



Sparse Structured Output Prediction

Inference captures linguistic ambiguity!



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