Learning with Sparse Latent Structure

Vlad Niculae University of Amsterdam (PhD opening!)

Work with: Wilker Aziz, Mathieu Blondel, Claire Cardie, Gonçalo M. Correia, André Martins.

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

Rich Underlying Structure

A disastrous show of pompous and inconsequential gibberish, garish visuals and tedious storytelling
themadmovieman 21 December 2019

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

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

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title

author

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segmentation:
sentences,
words,
and so on

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relationships
e.g., dependency

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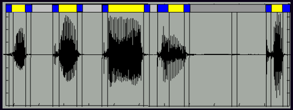
Most of this structure is **hidden**.

Rich Underlying Structure

Widely occuring pattern!

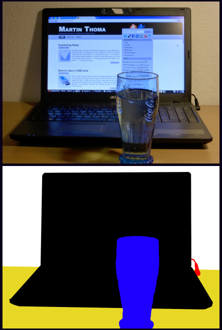
speech

(Andre-Obrecht, 1988)



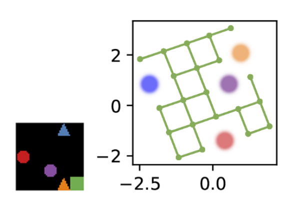
objects

(Long et al., 2015)



transition graphs

(Kipf, Pol, et al., 2020)



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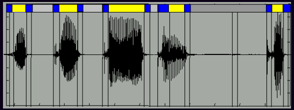

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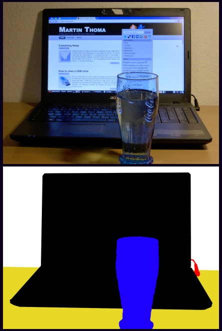

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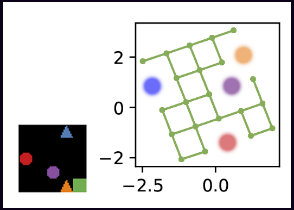


But we'll focus on NLP.

Structured Prediction

. . .

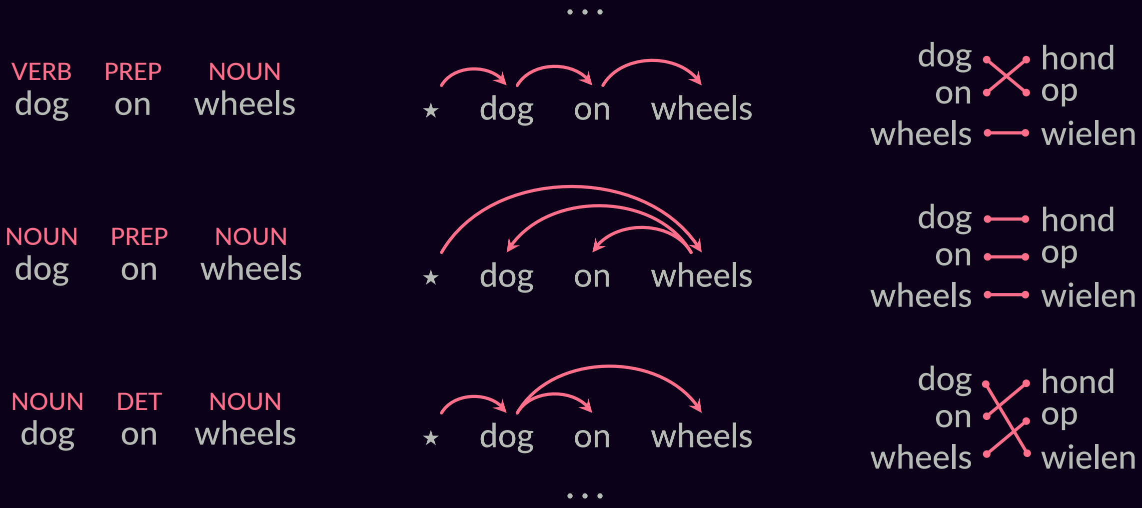
⋆ dog on wheels

⋆ dog on wheels

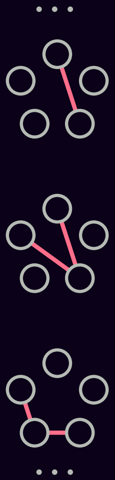
⋆ dog on wheels

. . .

Structured Prediction



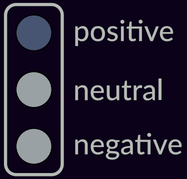
Structured Prediction



Traditional Pipeline Approach

input

output



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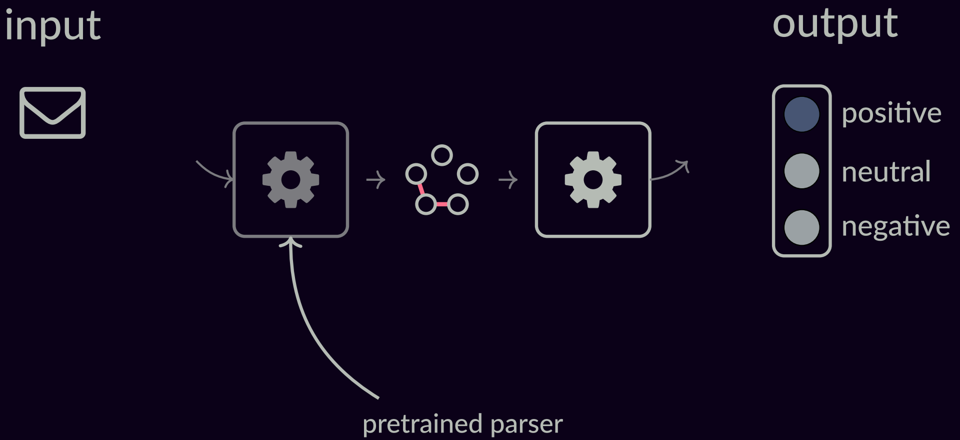
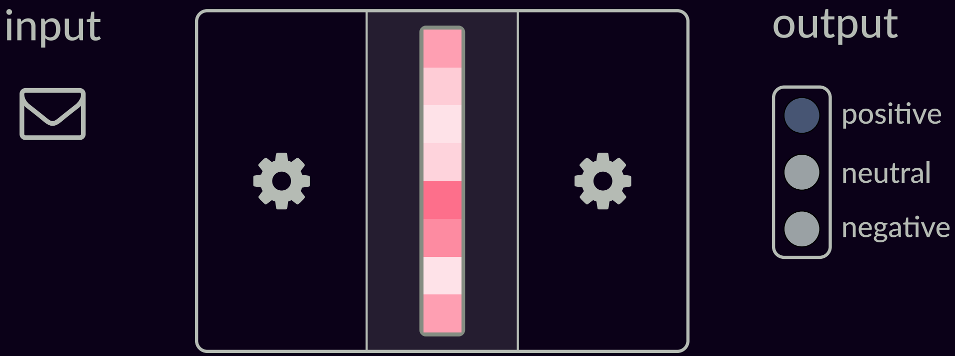


Deep Learning & Hidden Representations



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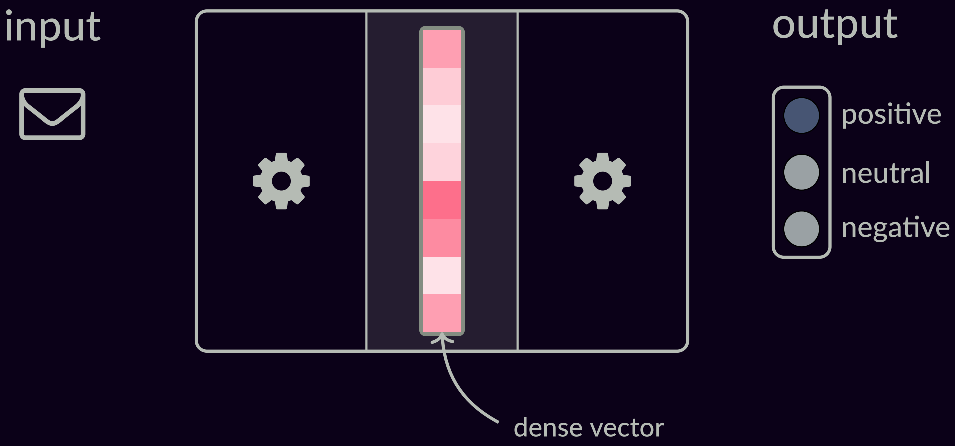
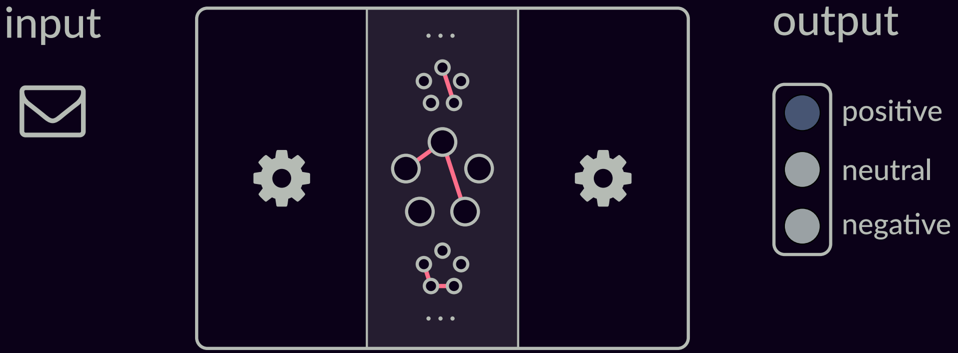


Latent Structure Models



record scratch

freeze frame

How to select an item from a set?

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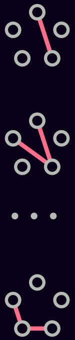

How to select an item from a set?

$$c_1$$

$$c_2$$

$$\cdots$$

$$c_N$$

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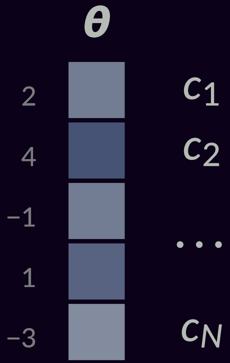

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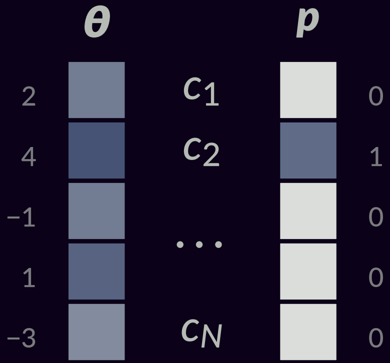

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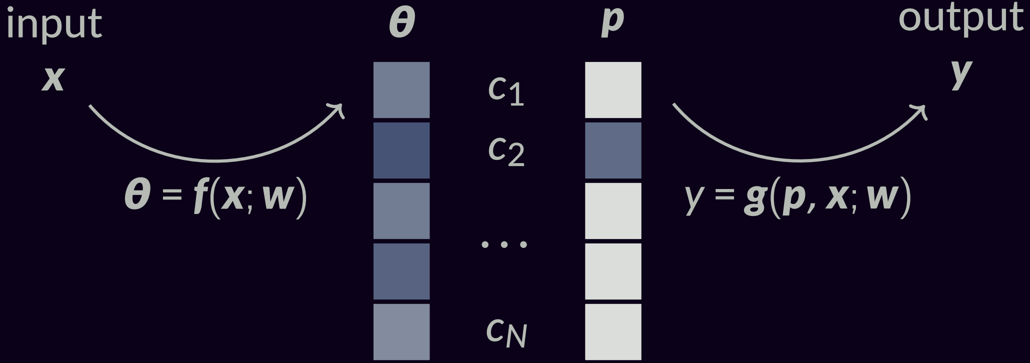

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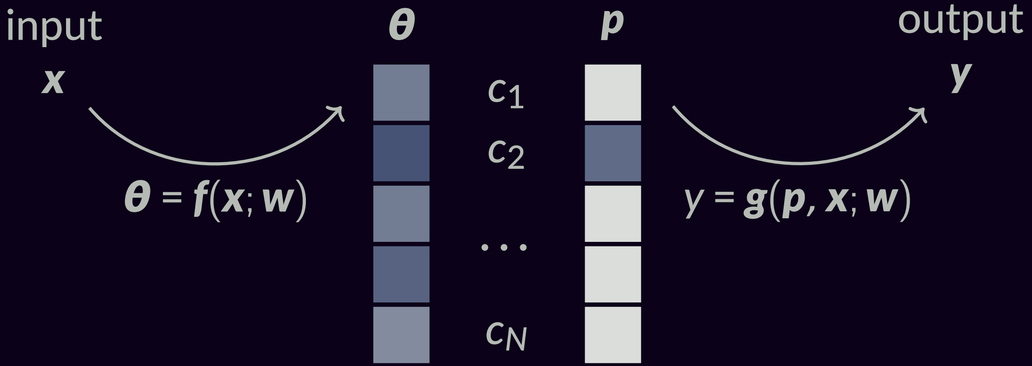

$$\frac{\partial y}{\partial \boldsymbol{w}} = ?$$

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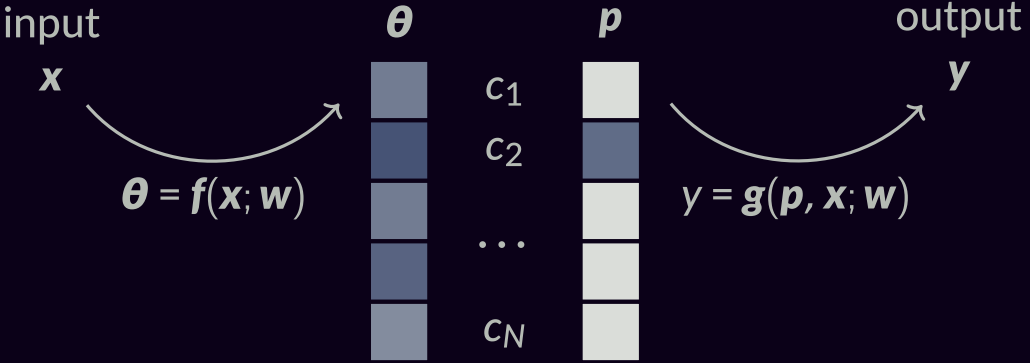
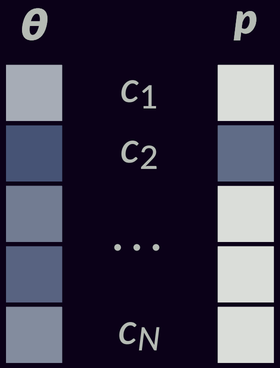


$\frac{\partial y}{\partial \boldsymbol{w}} = ?$ or, essentially, $\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{\theta}} = ?$

Argmax



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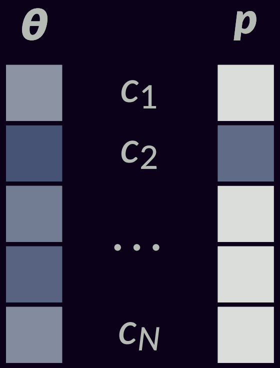

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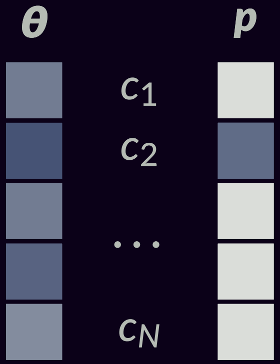

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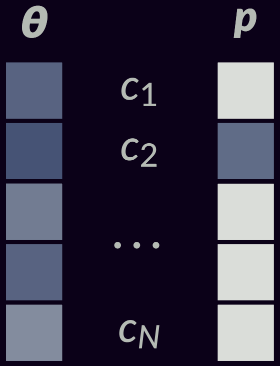

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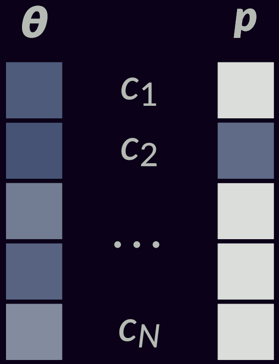

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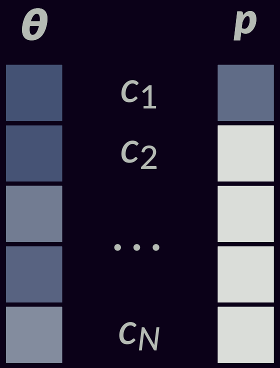

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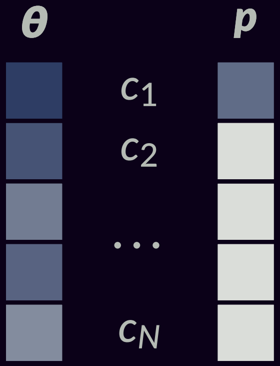

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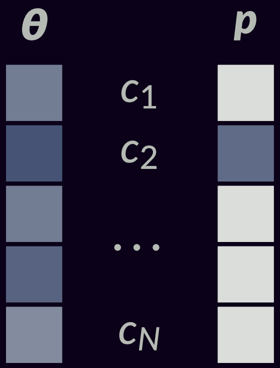
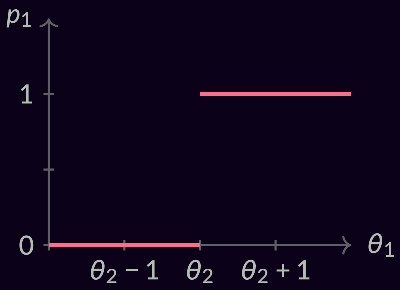
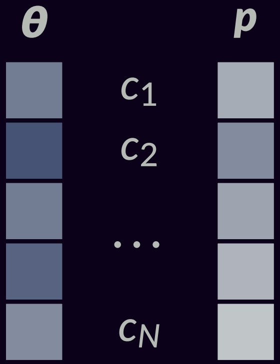


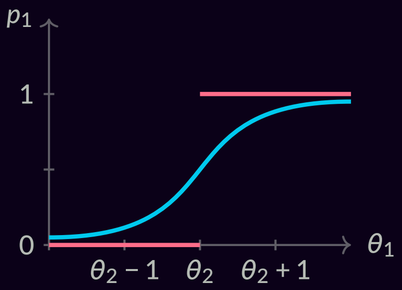


$$\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{\theta}} = \boldsymbol{0}$$

Argmax vs. Softmax

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





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

A Softmax Origin Story 🦸🏽‍♀️

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

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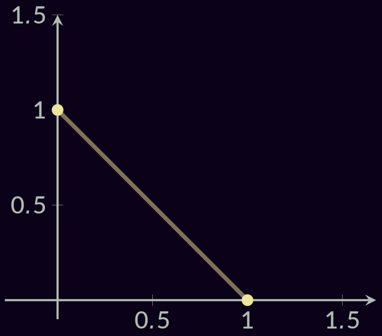

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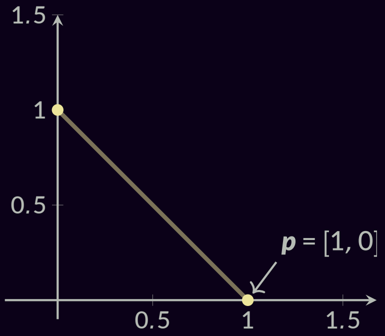

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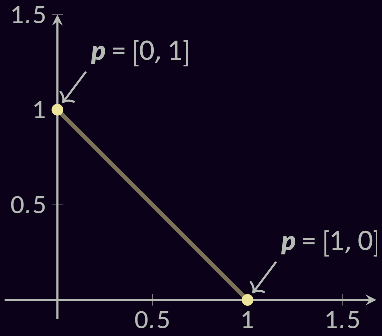

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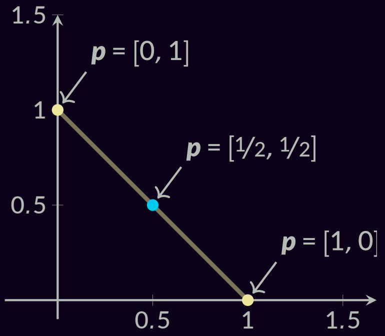

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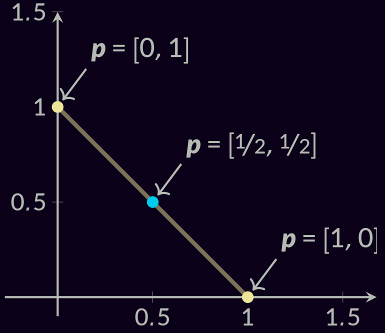

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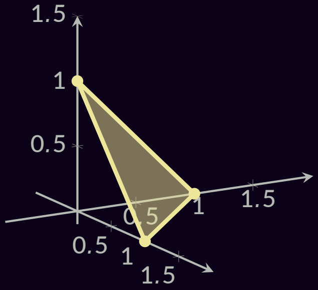

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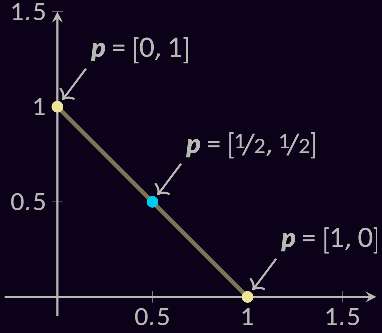

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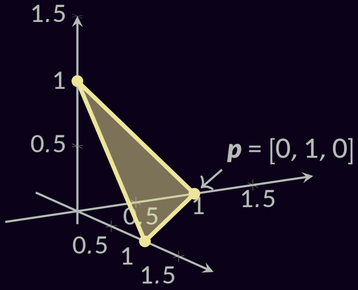

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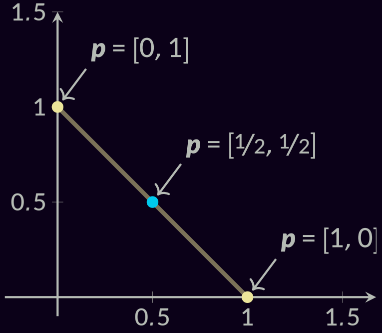

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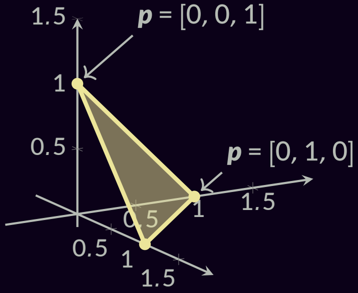

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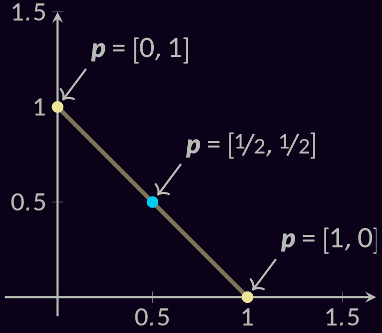

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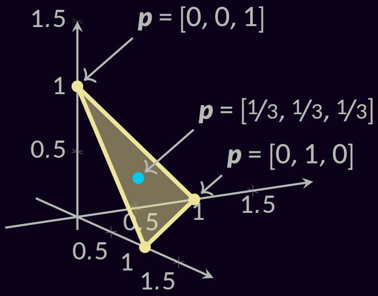

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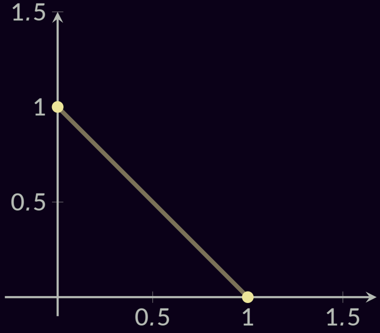
$$\max_j \theta_j = \max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top \boldsymbol{\theta}$$

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



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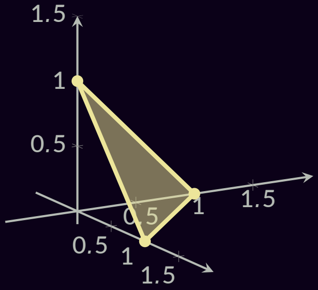

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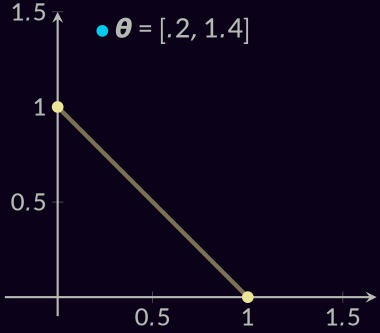

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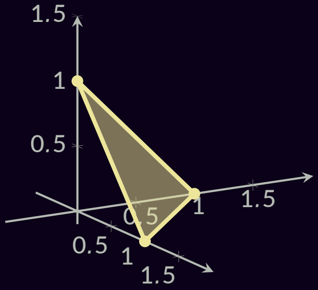

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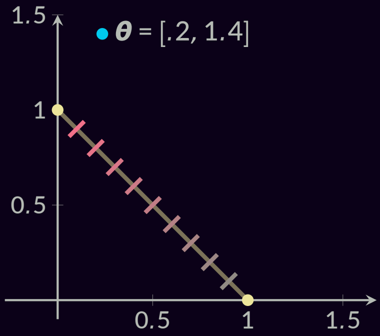

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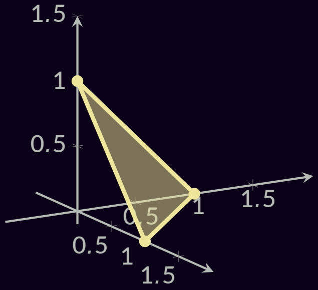

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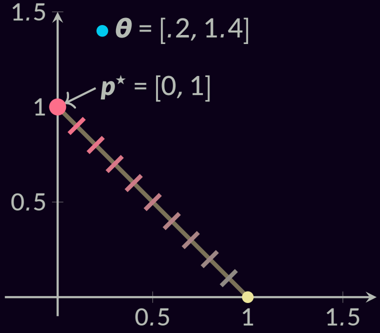

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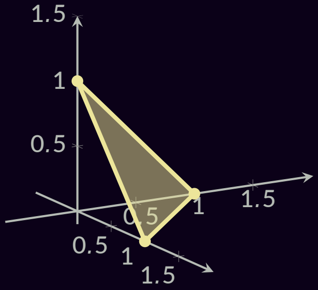

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A Softmax Origin Story 🦸🏽‍♀️

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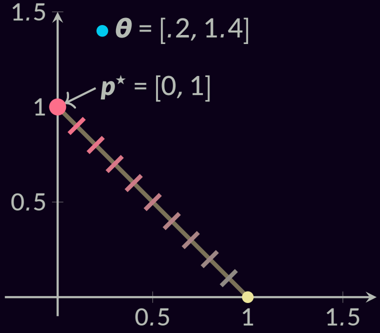

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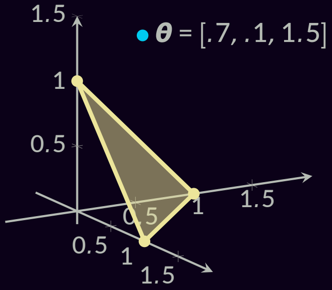

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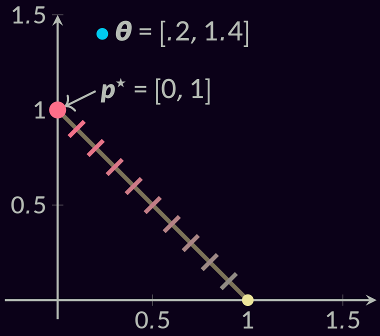

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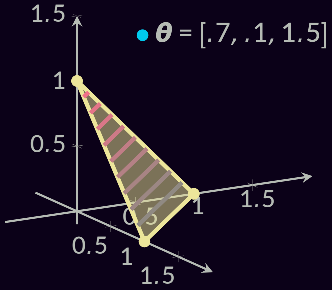

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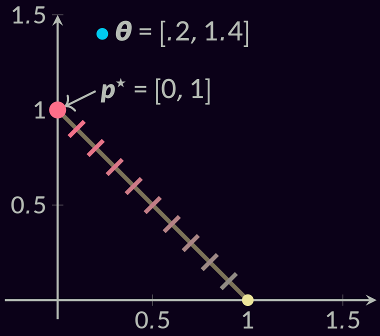

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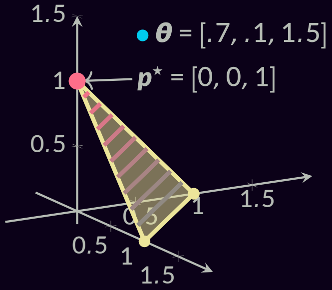

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(Niculae and Blondel, 2017)

Smoothed Max Operators

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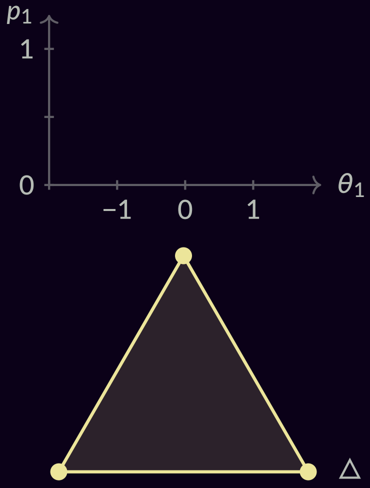

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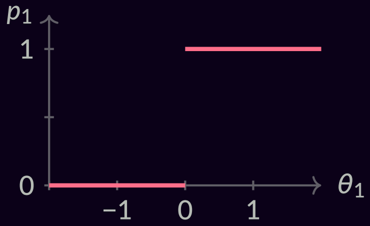

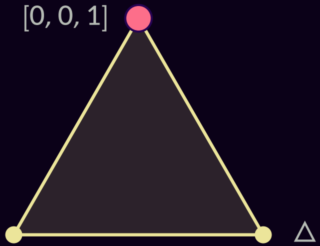

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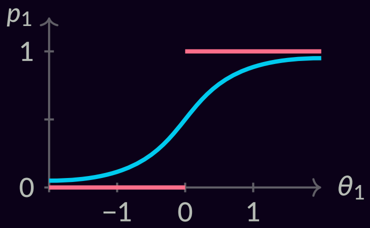

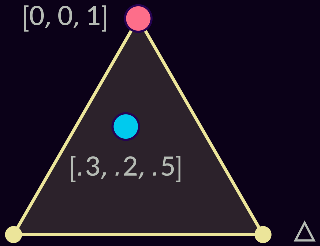

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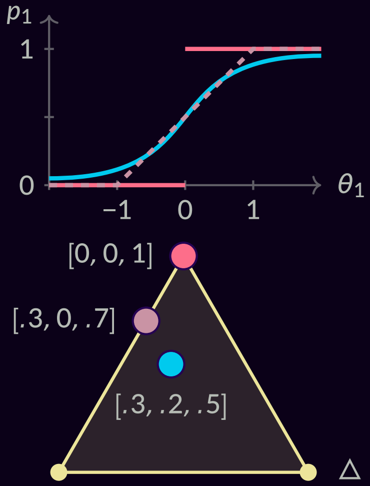

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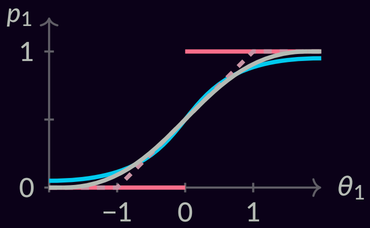

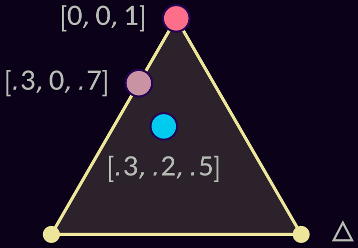

Tsallis (1988); a generalized entropy (Grünwald and Dawid, 2004)
(Blondel, Martins, and Niculae 2019a; Peters, Niculae, and Martins 2019; Correia, Niculae, and Martins 2019)

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

$\mathcal{O}(d)$ via partial sort

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

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Backward pass:

$$\boldsymbol{J}_{\text{sparsemax}} = \operatorname{diag}(\boldsymbol{s}) - \frac{1}{|\mathcal{S}|}\boldsymbol{s}\boldsymbol{s}^\top$$
$$\text{where } \mathcal{S} = \{j : p_j^\star > 0\},$$
$$s_j = [\![j \in \mathcal{S}]\!]$$

(Martins and Astudillo, 2016)

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argmin differentiation

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

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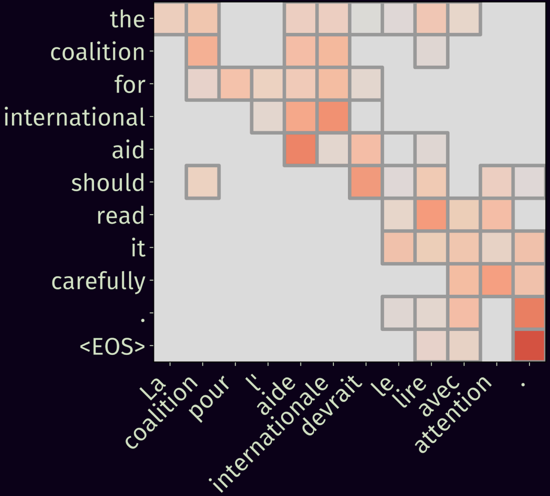
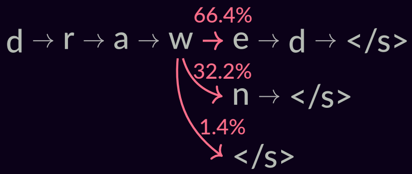
First applications:

sparse attention



sparse losses (& seq2seq)



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

Latent variable models!

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

- 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 $|\bar{\mathcal{H}}| \ll |\mathcal{H}|$.
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sum over all possible messages

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(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
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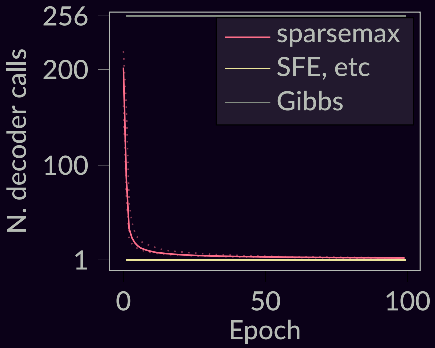

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$$k\text{-sparsemax}(\boldsymbol{\theta}) = \underset{\boldsymbol{p}\in\triangle,\, \|\boldsymbol{p}\|_0\leq k}{\arg\min} \|\boldsymbol{p}-\boldsymbol{\theta}\|_2^2$$

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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.

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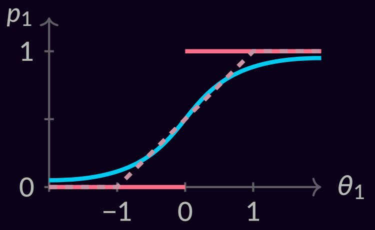

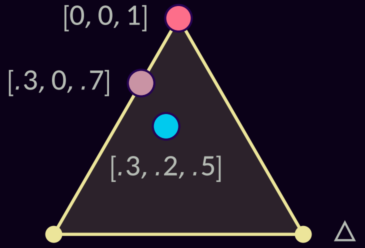

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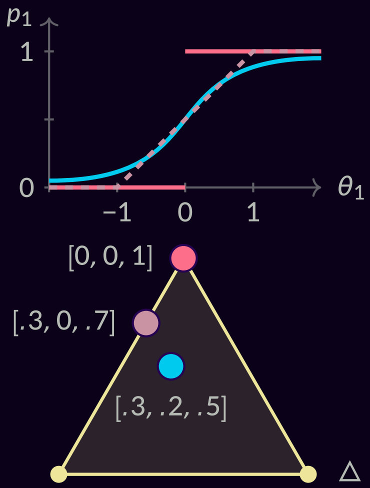
fusedmax: $\Omega(\boldsymbol{p}) = 1/2\|\boldsymbol{p}\|_2^2 + \sum_j |p_j - p_{j-1}|$

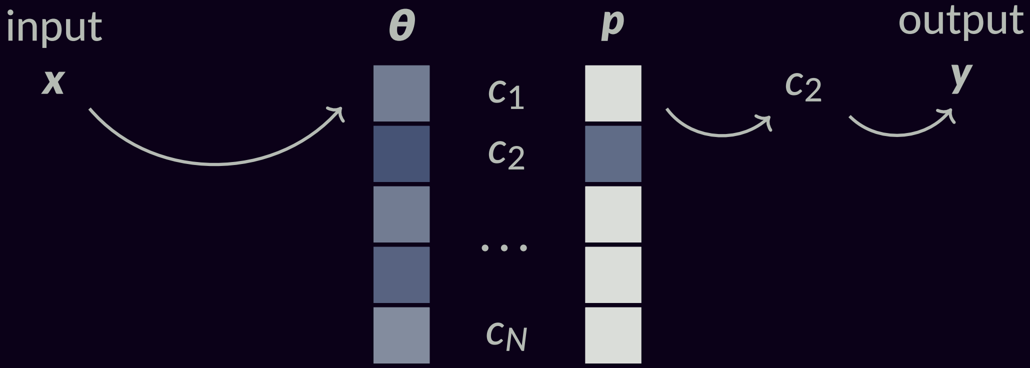


Structured Prediction

finally

Structured Prediction

is essentially a (very high-dimensional) argmax



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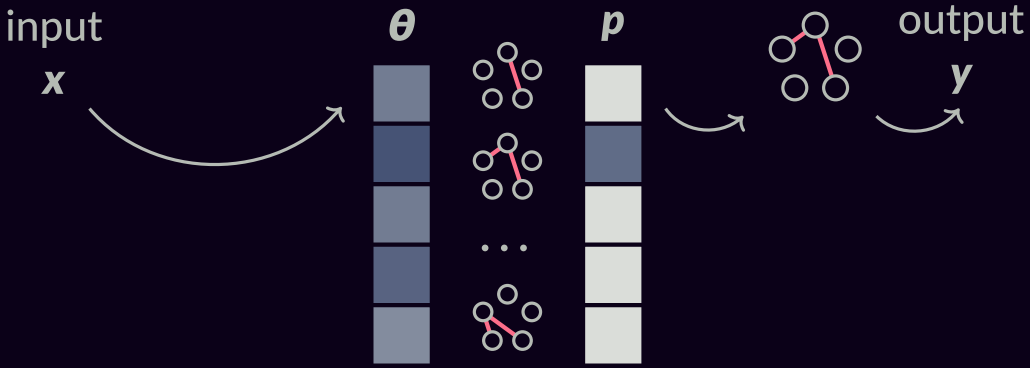

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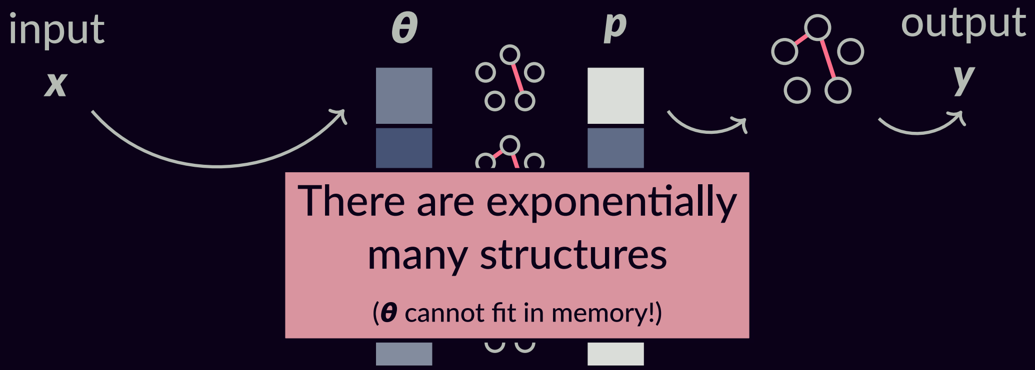

There are exponentially many structures

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

Factorization Into Parts

⋆ dog on wheels

Factorization Into Parts

★ dog on wheels

	dog	on	wheels
*→	○	●	○
dog→		○	○
on→	●		●
wheels→	○	○	

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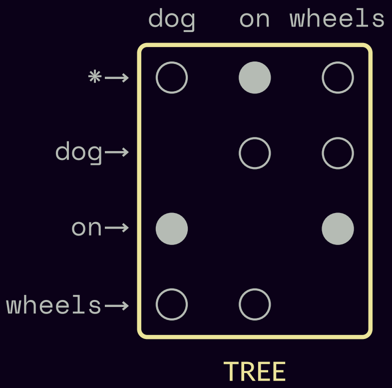

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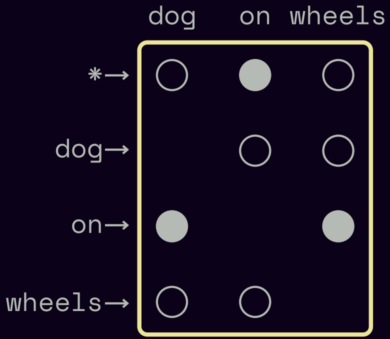

TREE

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

Factorization Into Parts

★ dog on wheels

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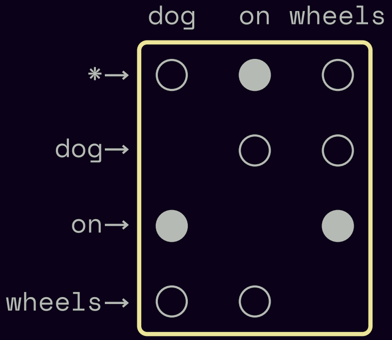
\end{array}
\begin{bmatrix}
1 & & 0 & 0 & \\
0 & & 1 & 1 & \\
0 & & 0 & 0 & \\ \hline
0 & & 1 & 1 & \\
1 & \dots & 0 & 0 & \dots \\
0 & & 0 & 0 & \\ \hline
0 & & 0 & 0 & \\
0 & & 1 & 0 & \\
1 & & 0 & 1 &
\end{bmatrix}
\quad
\boldsymbol{\eta} = \begin{bmatrix}
.1 \\ .2 \\ -.1 \\ \hline .3 \\ .8 \\ .1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



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\begin{bmatrix} 1 & & 0 & 0 & \\ 0 & & 1 & 1 & \\ 0 & & 0 & 0 & \\ 0 & & 1 & 1 & \\ 1 & \dots & 0 & 0 & \dots \\ 0 & & 0 & 0 & \\ 0 & & 0 & 0 & \\ 0 & & 1 & 0 & \\ 1 & & 0 & 1 & \end{bmatrix}
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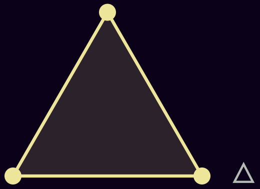
\boldsymbol{\eta} = \begin{bmatrix} .1 \\ .2 \\ -.1 \\ .3 \\ .8 \\ .1 \\ -.3 \\ .2 \\ -.1 \end{bmatrix}
$$

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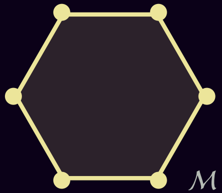
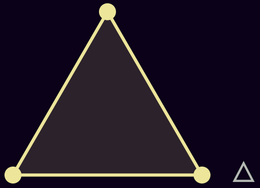
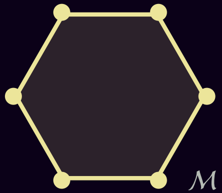
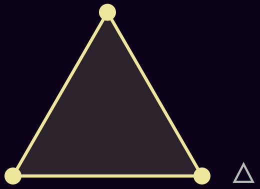

$\mathcal{M}$

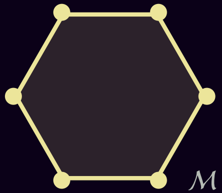
$$\mathcal{M} := \operatorname{conv}\left\{\boldsymbol{a}_h : h \in \mathcal{H}\right\}$$



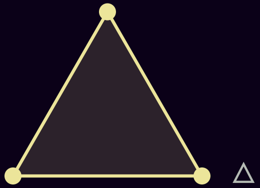


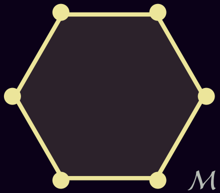
$$\mathcal{M} := \operatorname{conv}\left\{\boldsymbol{a}_h : h \in \mathcal{H}\right\}$$
$$= \left\{\boldsymbol{A}\boldsymbol{p} : \boldsymbol{p} \in \triangle\right\}$$





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

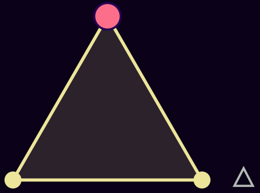


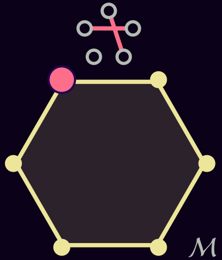


● **argmax** $\arg\max_{\boldsymbol{p}\in\triangle} \boldsymbol{p}^\top\boldsymbol{\theta}$

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

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



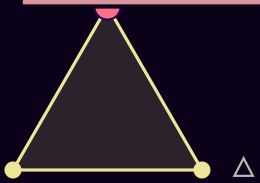


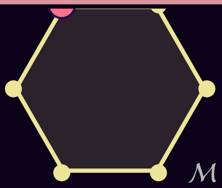
- **argmax** $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top \boldsymbol{\theta}$

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

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

matching → **Kuhn-Munkres**

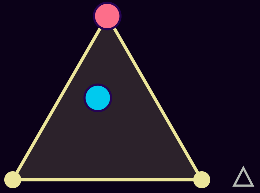


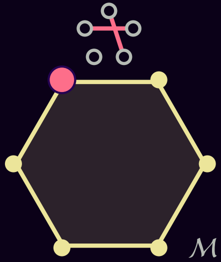


argmax $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top \boldsymbol{\theta}$

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

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





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

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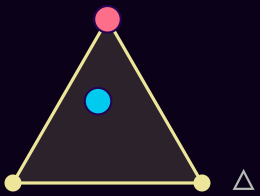
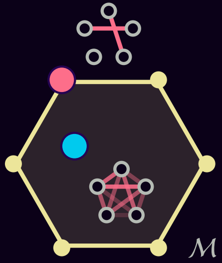
MAP $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta}$

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





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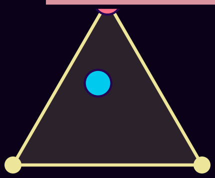
- **MAP** $\arg\max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta}$
- **marginals** $\arg\max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta} + \widetilde{\mathrm{H}}(\boldsymbol{\mu})$

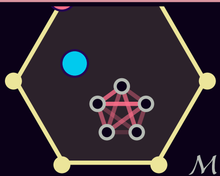
e.g. sequence labeling → forward-backward

(Rabiner, 1989)

As attention: (Kim et al., 2017)



$\triangle$



$\mathcal{M}$

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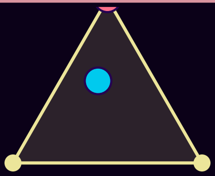
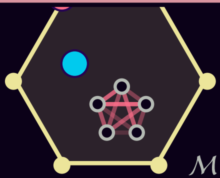
e.g. dependency parsing → **the Matrix-Tree theorem**

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

As attention: (Liu and Lapata, 2018)


$\triangle$


$\mathcal{M}$

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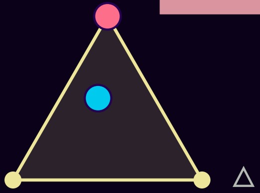
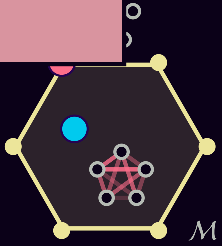
e.g. matchings → **#P-complete!**

(Taskar, 2004; Valiant, 1979)





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

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

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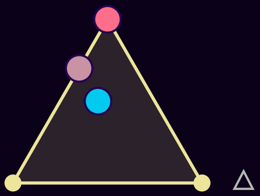

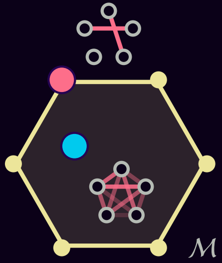

(Niculae, Martins, Blondel, and Cardie, 2018)

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

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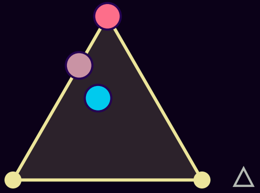
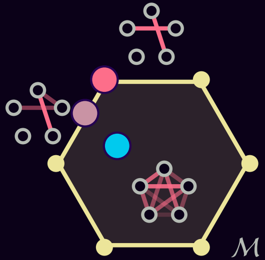
SparseMAP $\arg\max_{\boldsymbol{\mu}\in\mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta} - 1/2\|\boldsymbol{\mu}\|^2$





Algorithms for SparseMAP

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

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

linear constraints
(alas, exponentially many!)

quadratic objective

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Conditional Gradient

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

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

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

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

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

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

Algorithms for SparseMAP

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

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Conditional Gradient

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

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

Algorithms for SparseMAP

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

linear constraints
(alas, exponentially many!)

quadratic objective

Conditi

(Frank and Wolfe, 1956

Completely modular: just add MAP

pass

- select a new co...
- update the (sparse) coefficients of $\boldsymbol{p}$
  - Update rules: vanilla, away-step, pairwise
  - Quadratic objective: **Active Set**
    (Nocedal and Wright, 1999, Ch. 16.4 & 16.5)
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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)

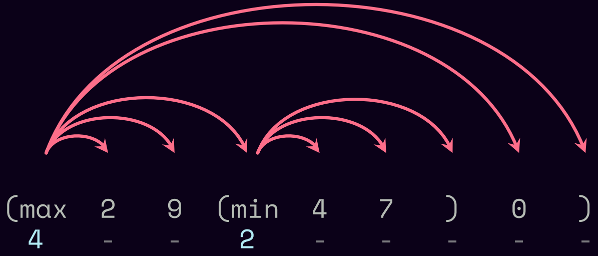
Latent Dependency Trees

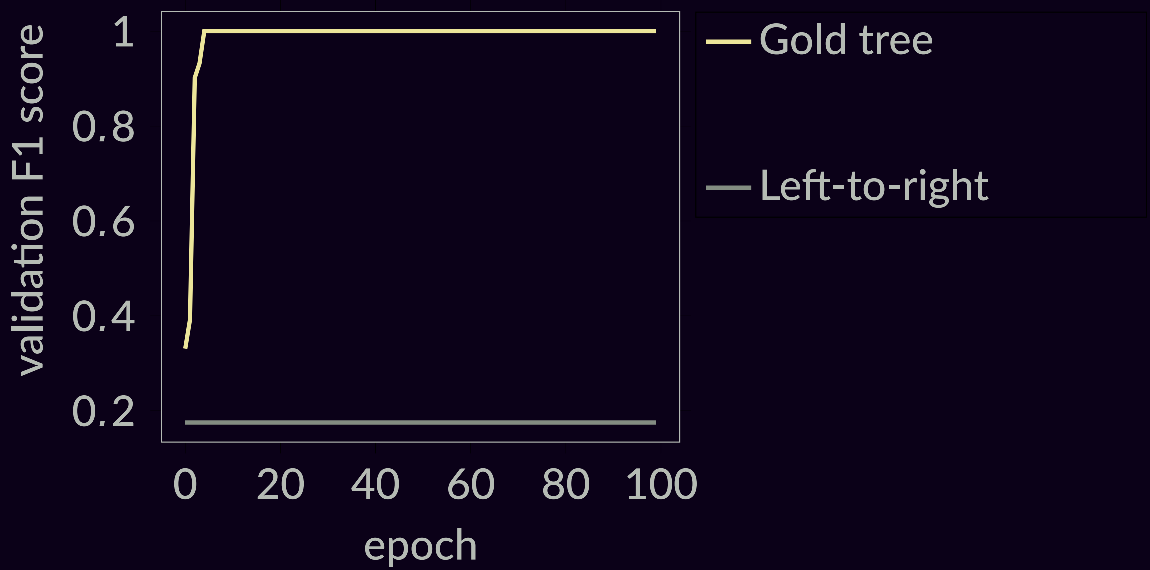
Arity tagging with latent GCN (Corro and Titov, 2019; Kipf and Welling, 2017)

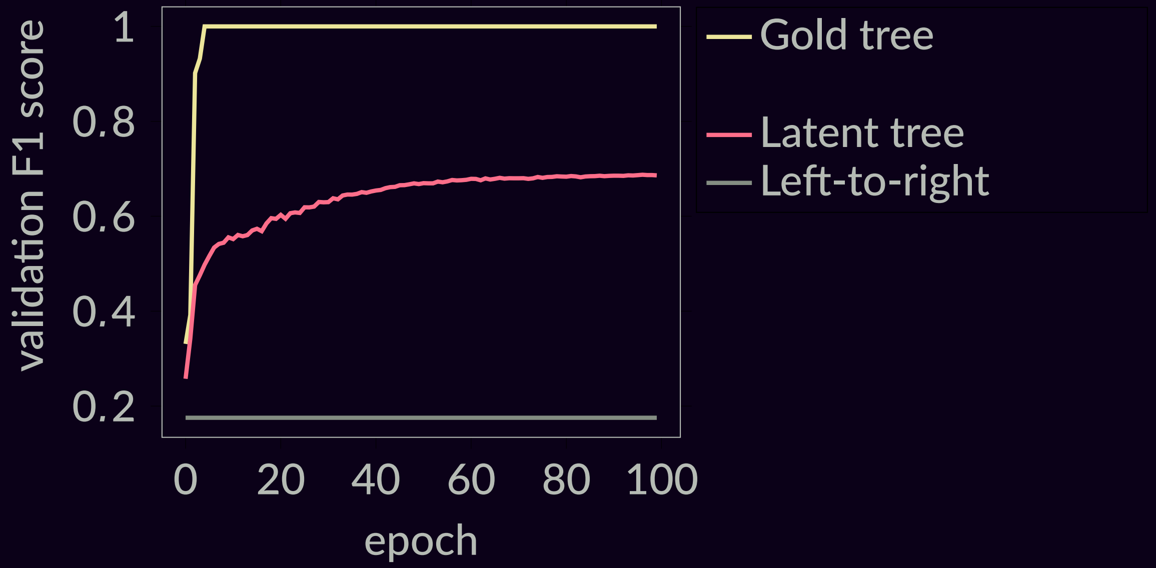
```
(max  2   9  (min  4   7   )   0   )
```

Latent Dependency Trees

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




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



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40
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80
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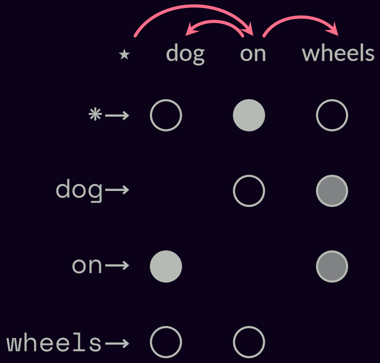
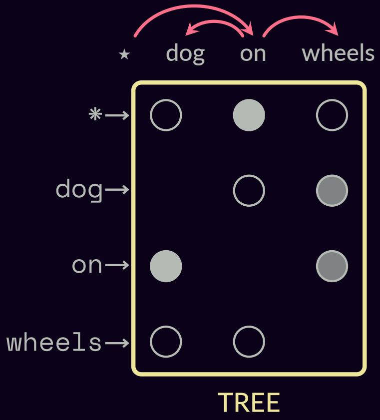
epoch
Gold tree
Latent tree
Left-to-right

What if MAP is not available?

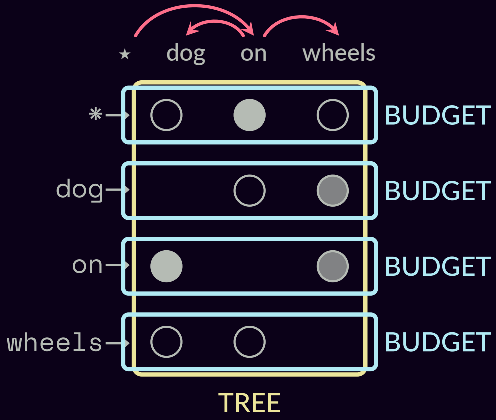
Multiple, Overlapping Factors



Multiple, Overlapping Factors

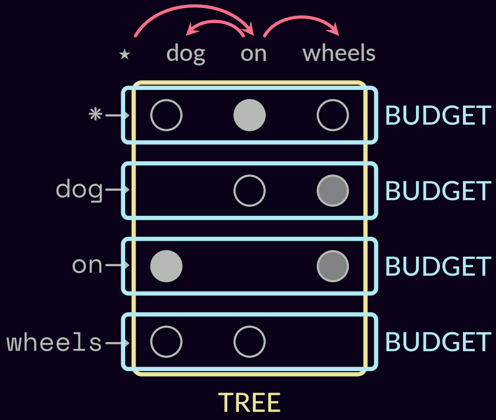


Multiple, Overlapping Factors

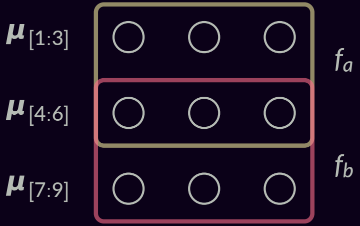


Multiple, Overlapping Factors

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



Optimization as Consensus-Seeking



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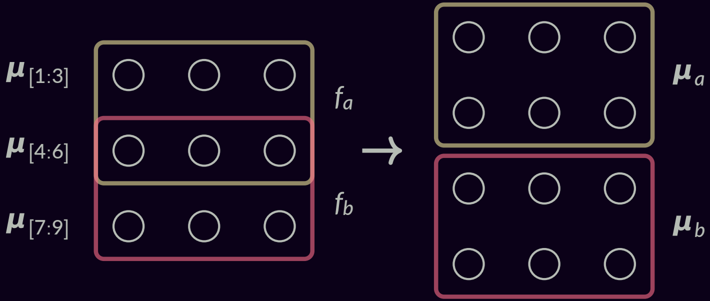
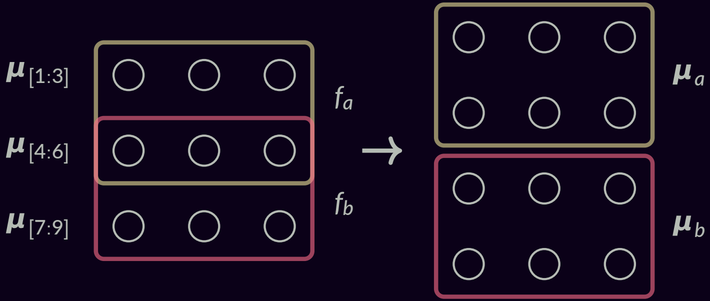
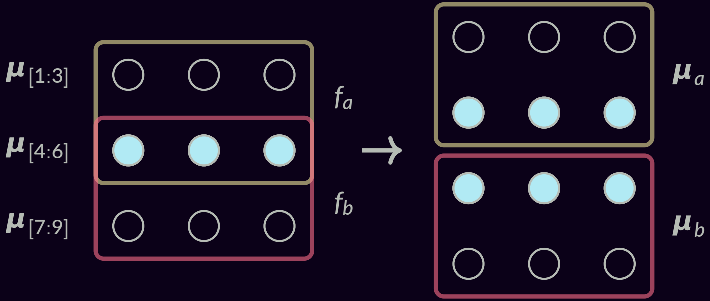


Optimization as Consensus-Seeking



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

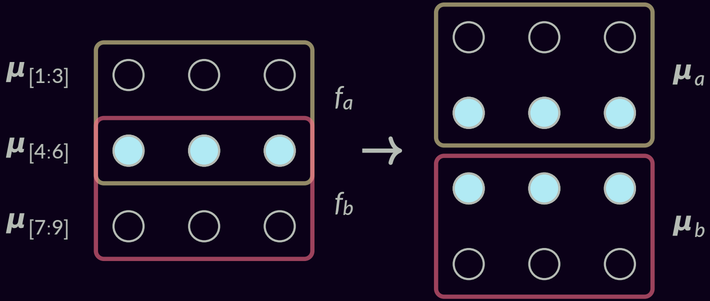
Optimization as Consensus-Seeking



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

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

Optimization as Consensus-Seeking



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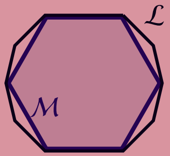
$$\max_{\boldsymbol{\mu},\boldsymbol{\mu}_f} \sum_{f\in\mathcal{F}} \boldsymbol{\eta}_f^\top \boldsymbol{\mu}_f \quad \text{s.t.} \quad \mathbf{C}_f \boldsymbol{\mu} = \boldsymbol{\mu}_f,\ \boldsymbol{\mu}_f \in \mathcal{M}_f \ \text{ for } f \in \mathcal{F}$$

Optim… …eking

LP relaxation (Wainwright and Jordan, 2008)

the local polytope:

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



$\boldsymbol{\mu}_{[1:…}$

$\boldsymbol{\mu}_{[4:…}$

$\boldsymbol{\mu}_{[7:…}$

$\boldsymbol{\mu}_a$

$\boldsymbol{\mu}_b$

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

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(Niculae and Martins, 2020)

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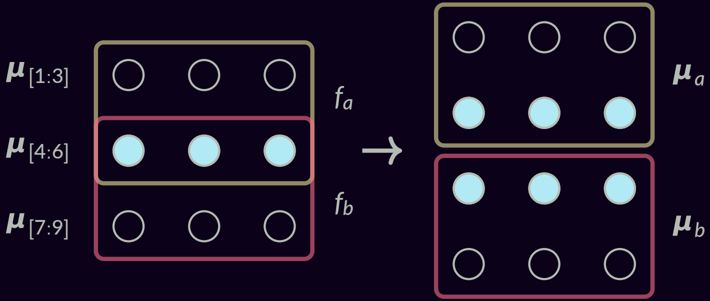

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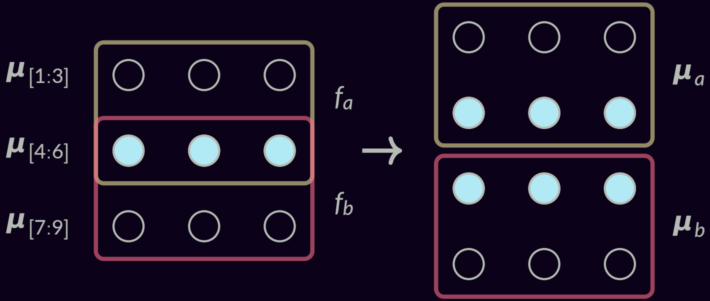

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$$\max_{\boldsymbol{\mu},\boldsymbol{\mu}_f} \left(\sum_{f \in \mathcal{F}} \boldsymbol{\eta}_f^\top \boldsymbol{\mu}_f \right) - \tfrac{1}{2}\|\boldsymbol{\mu}\|^2 \quad \text{s.t.} \quad \boldsymbol{C}_f \boldsymbol{\mu} = \boldsymbol{\mu}_f,\ \boldsymbol{\mu}_f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

(Niculae and Martins, 2020)

Algorithms for LP-SparseMAP

Forward pass

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

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

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

Algorithms for LP-SparseMAP

(Niculae and Martins, 2020)

Forward pass

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

- 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


```
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!

Differentiable Sparse Structured Prediction

(Niculae and Martins, 2020)


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

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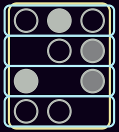


Factor graphs as a hidden-layer DSL!

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(η_f):   # abstract, private
        raise NotImplemented

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

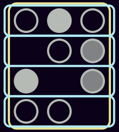
    def backward(dμ_f):
        # analytic, uses active set result


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

    def backward(dμ_f):
        # specialized
```

(Niculae and Martins, 2020)

Differentiable Sparse Structured Prediction



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New factors only require MAP.

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class Budget(Factor):
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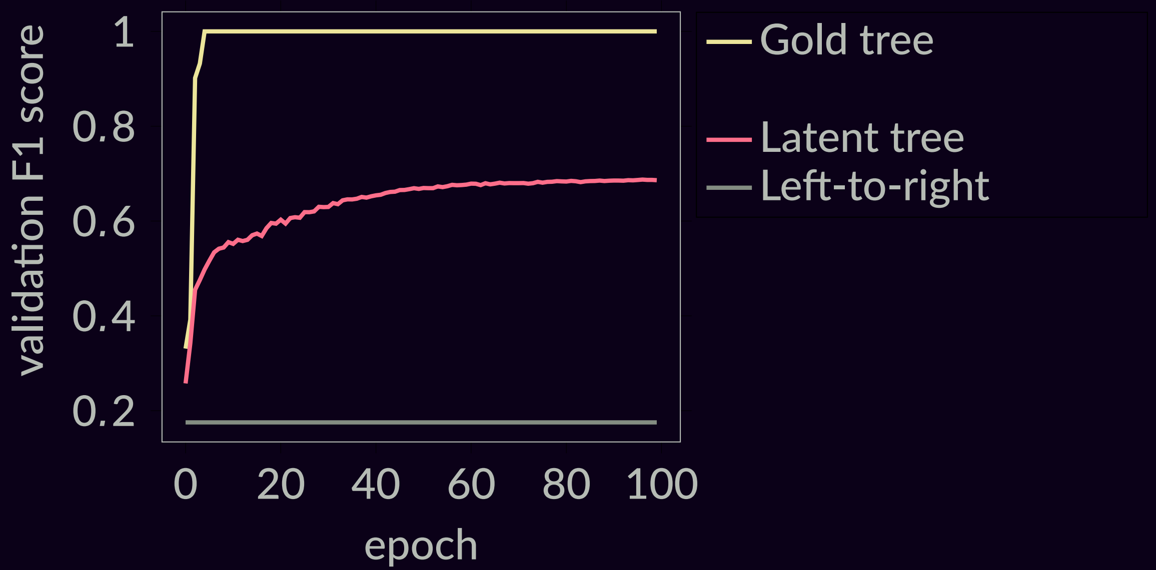
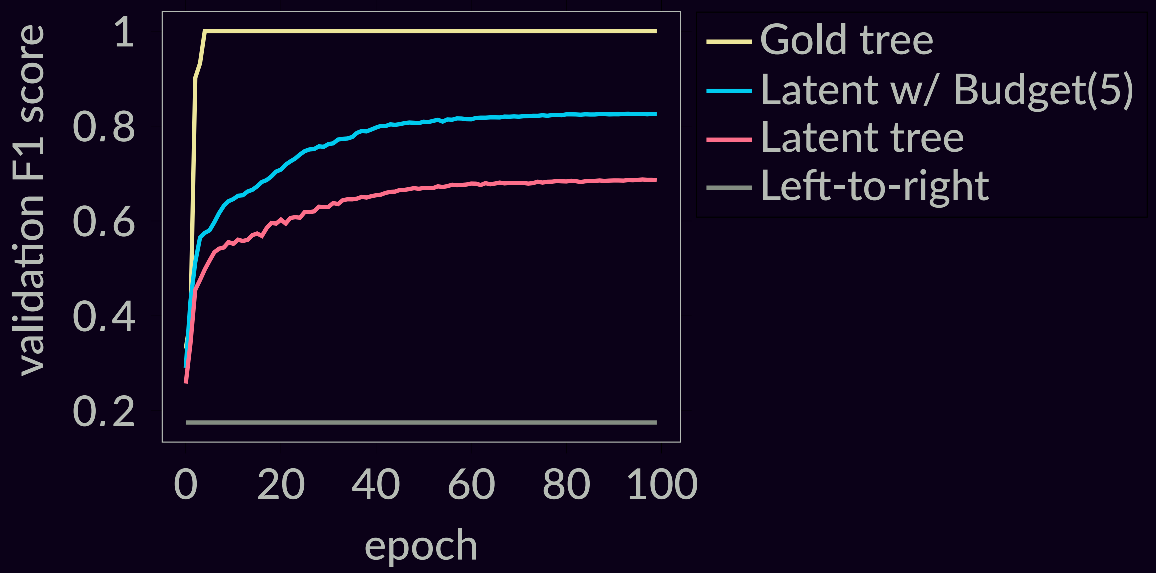
        # specialized

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

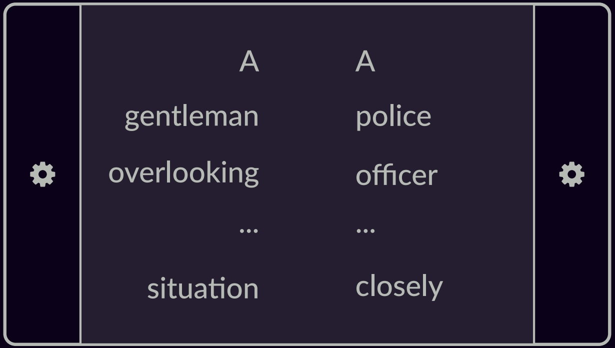
Structured Attention for Alignments

NLI

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

input

(P, H)



output

entails

contradicts

neutral

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

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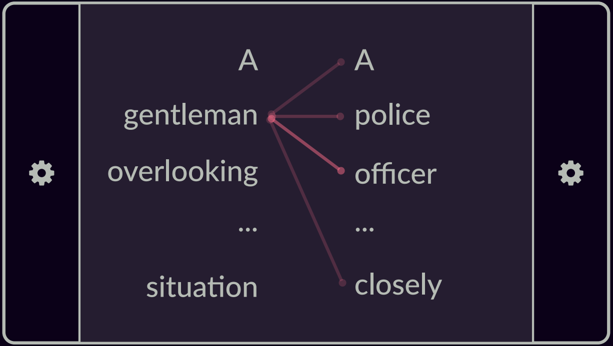
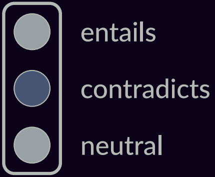


output



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

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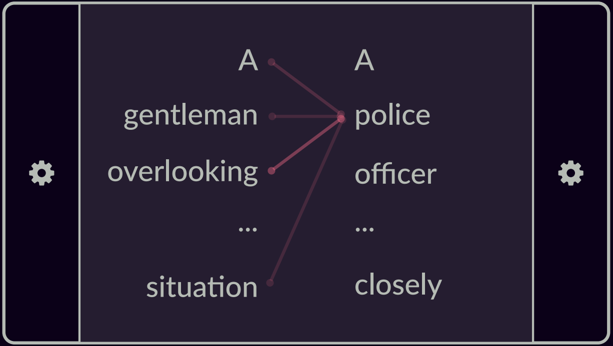
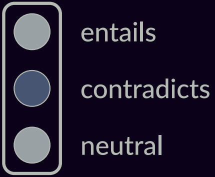


output



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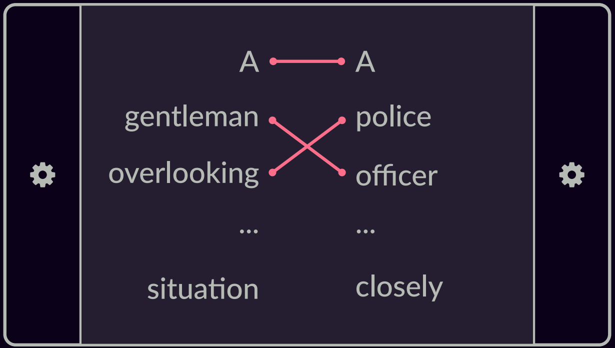


(Proposed model: global structured alignment.)

output

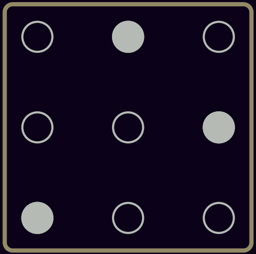
entails

contradicts

neutral

Structured Alignment Models

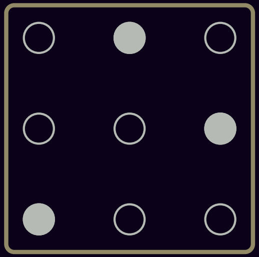
matching



SparseMAP w/ Kuhn-Munkres
(Kuhn, 1955)

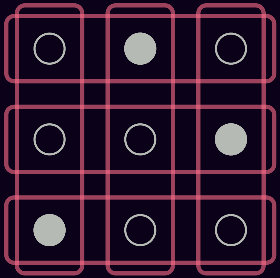
Structured Alignment Models

matching



SparseMAP w/ Kuhn-Munkres
(Kuhn, 1955)

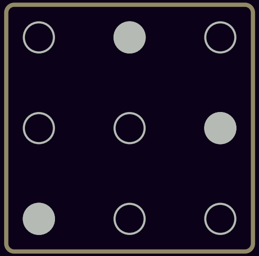
LP-matching



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

Structured Alignment Models

matching



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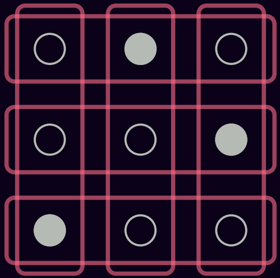
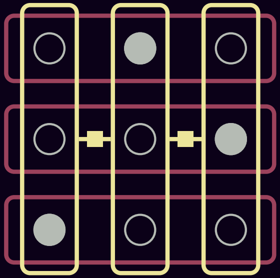


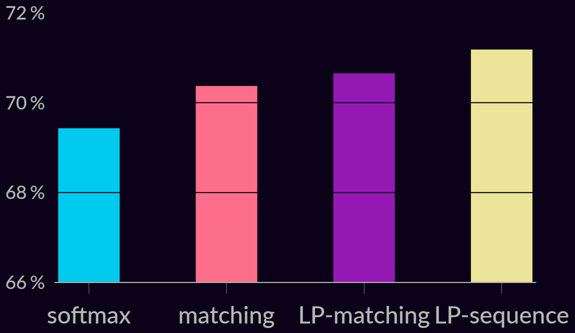
LP-SparseMAP w/ XORs
(equivalent; different solver)

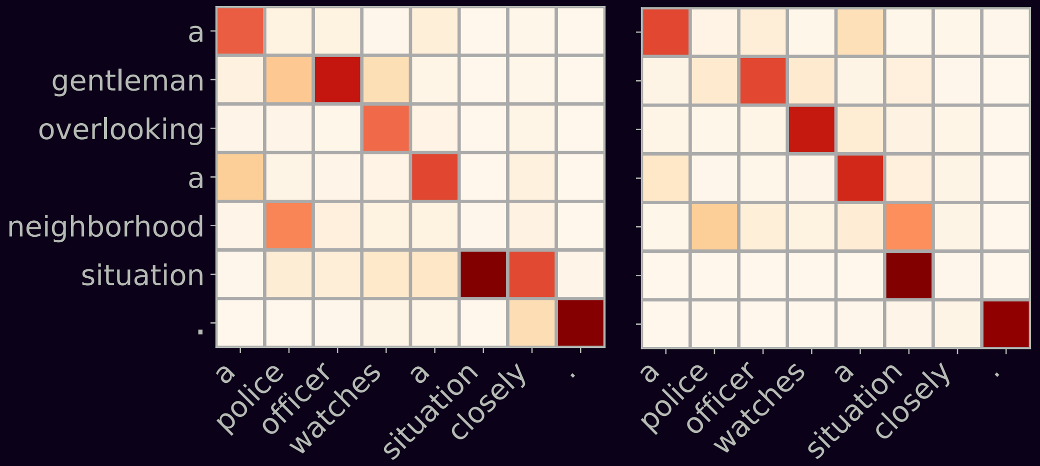
LP-sequence

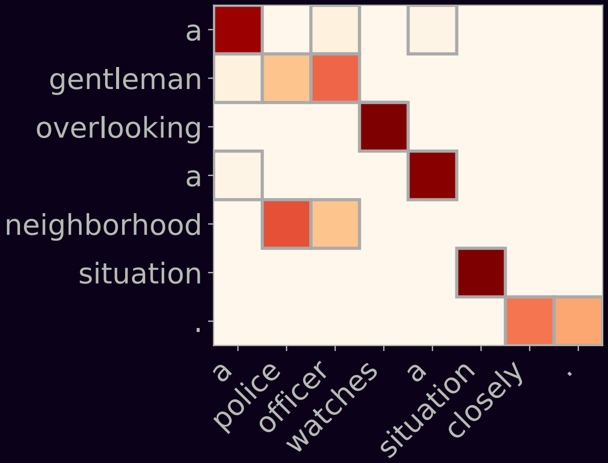


additional score
for *contiguous alignments*
$(i, j) - (i + 1, j \pm 1)$

MultiNLI (Williams et al., 2017)




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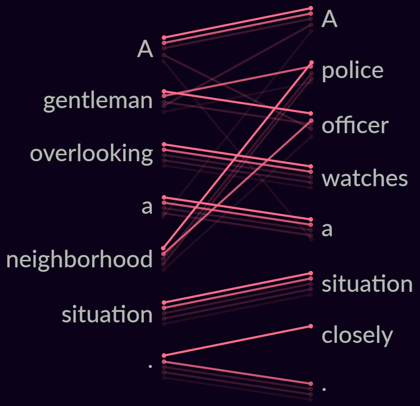
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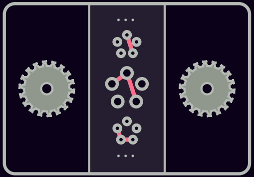
.

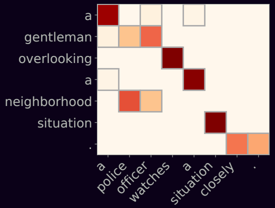
Conclusions

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

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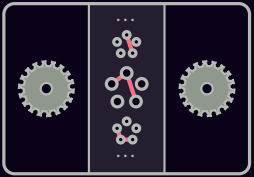
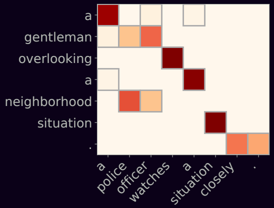
Interpretable **structured attention**



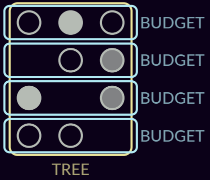


Future work

Structure beyond NLP

Weak & semi-supervision

Generative latent structure models



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Extra slides

Acknowledgements

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

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

Fusedmax

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

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

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

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

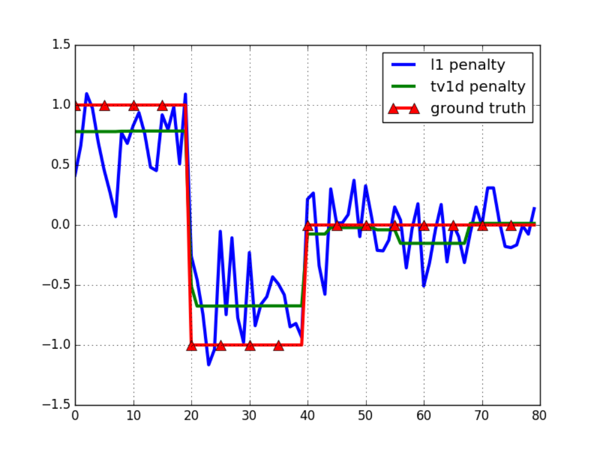
(Niculae and Blondel, 2017)

fusedmax(… $|p_j - p_{j-1}|$

prox$_{\text{fused}}$(… $_{j-1}|$

… $_{j-1}|$

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



"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.

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

Example: maximum of a vector

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

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Example: maximum of a vector

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

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Example: maximum of a vector

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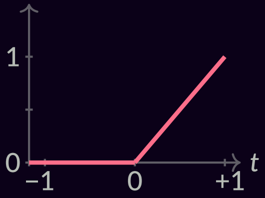
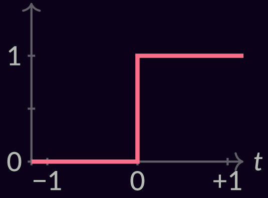
&= \partial \max_{\boldsymbol{p} \in \triangle} \phi(\boldsymbol{p}, \boldsymbol{\theta}) \\
&= \operatorname{conv}\{\nabla_{\boldsymbol{\theta}} \phi(\boldsymbol{p}^\star, \boldsymbol{\theta})\} \\
&= \operatorname{conv}\{\boldsymbol{p}^\star\}
\end{aligned}$$

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



$\max_j \theta_j$



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

Dynamically inferring the computation graph

So far: a structured hidden layer

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

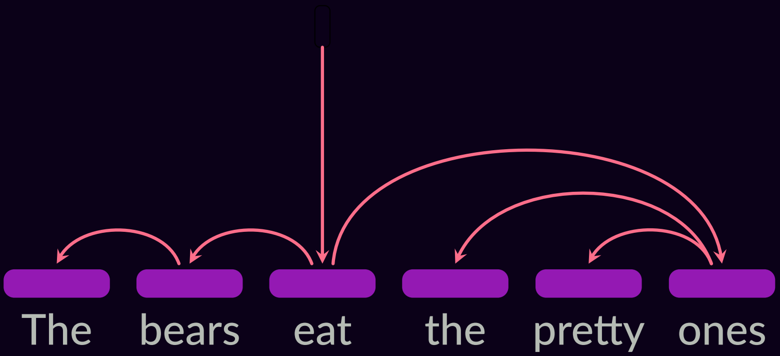
Network must handle "soft" combinations of structures.
Fine for attention, but can be limiting.

Dependency TreeLSTM

(Tai et al., 2015)

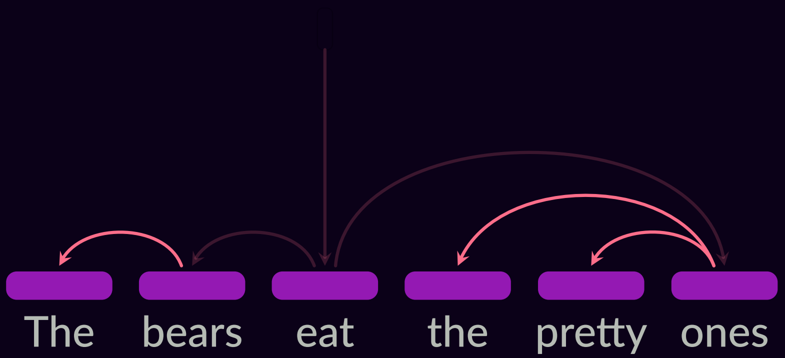
Dependency TreeLSTM

(Tai et al., 2015)



Dependency TreeLSTM

(Tai et al., 2015)



Dependency TreeLSTM

(Tai et al., 2015)

Dependency TreeLSTM

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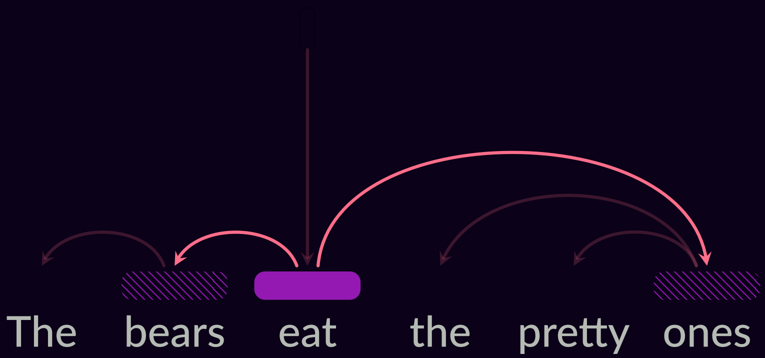

Dependency TreeLSTM

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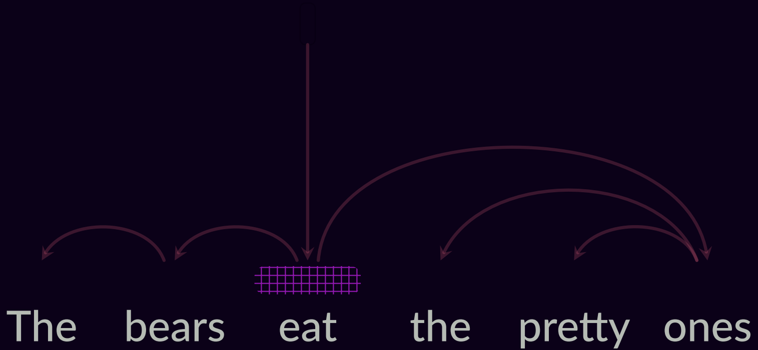

Dependency TreeLSTM

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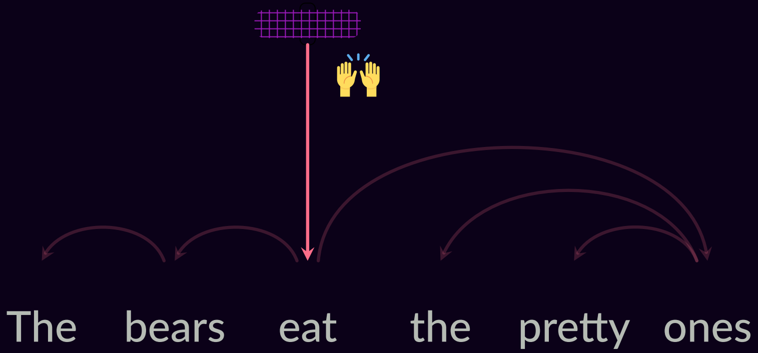
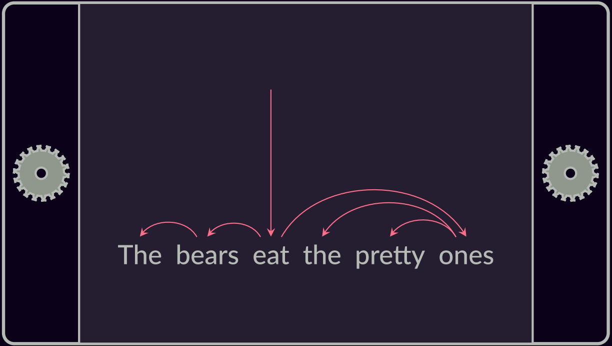


Latent Dependency TreeLSTM

(Niculae, Martins, and Cardie, 2018)

input

x



output

y

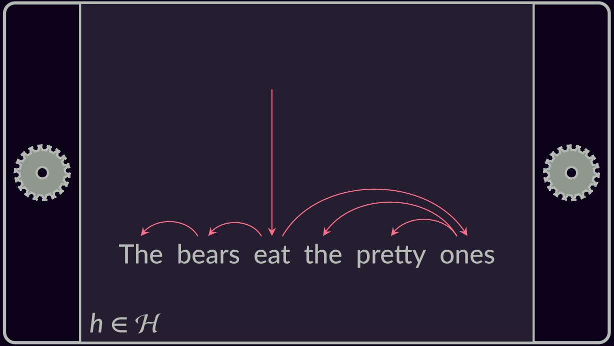
Latent Dependency TreeLSTM

(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

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

latent classifier

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

Exponentially large sum!

Structured Latent Variable Models

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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

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 $\boldsymbol{p_{\pi}}$?

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

idea 1

idea 2

idea 3

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 $p_{\boldsymbol{\pi}}$?

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

idea 1

idea 2

idea 3

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 $p_{\boldsymbol{\pi}}$?

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

idea 1 $p_{\boldsymbol{\pi}}(h \mid x) = 1$ if $h = h^\star$ else 0 argmax

idea 2

idea 3

Structured Latent Variable Models

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latent classifier

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

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latent classifier

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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	$p_{\boldsymbol{\pi}}(h \mid x) \propto \exp\left(\mathrm{score}_{\boldsymbol{\pi}}(h; x)\right)$	softmax		
idea 3				

Structured Latent Variable Models

sum over
all possible trees

e.g., a TreeLSTM defined by h

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latent classifier

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

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

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Structured Latent Variable Models

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			$\sum_{h \in \mathcal{H}}$	$\frac{\partial p(y \mid x)}{\partial \boldsymbol{\pi}}$
idea 1	$p_{\boldsymbol{\pi}}(h \mid x) = 1$ if $h = h^\star$ else 0	argmax	😊	😟
idea 2	$p_{\boldsymbol{\pi}}(h \mid x) \propto \exp\big(\text{score}_{\boldsymbol{\pi}}(h; x)\big)$	softmax	😱	😊
idea 3		SparseMAP	😊	😊

SparseMAP

 = .7  + .3 

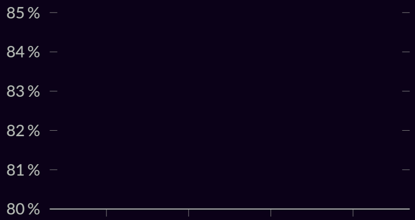
SparseMAP

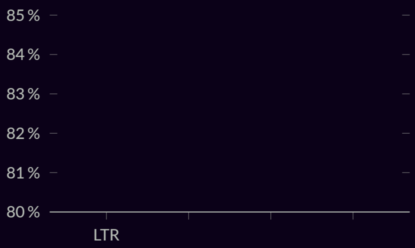
 = .7  + .3  + 0  + ...

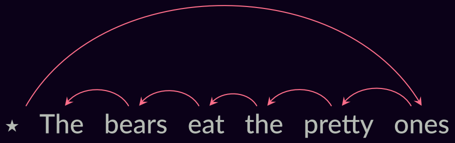
SparseMAP

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

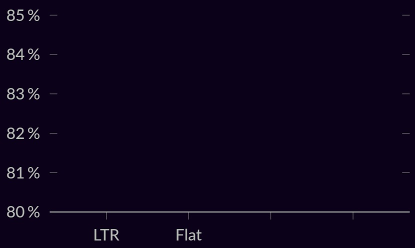
$p(y \mid x) = .7\, p_{\boldsymbol{\phi}}(y \mid$  $) + .3\, p_{\boldsymbol{\phi}}(y \mid$  $)$

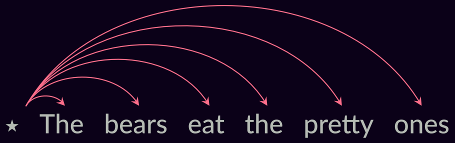

85 %
84 %
83 %
82 %
81 %
80 %



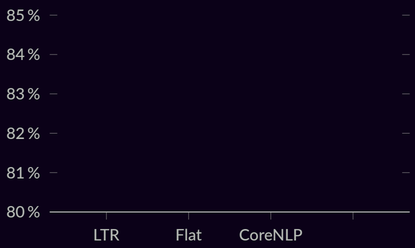


Left-to-right: regular LSTM

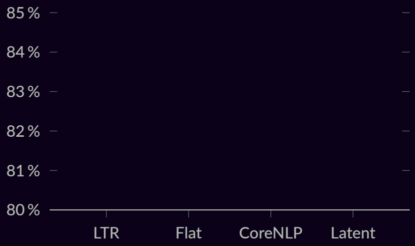




Flat: bag-of-words–like



CoreNLP: off-line parser


85 %
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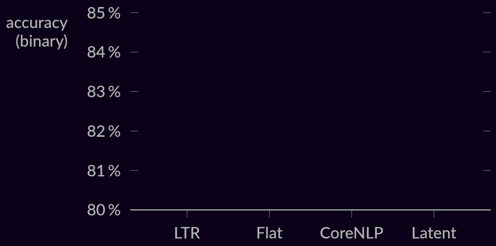
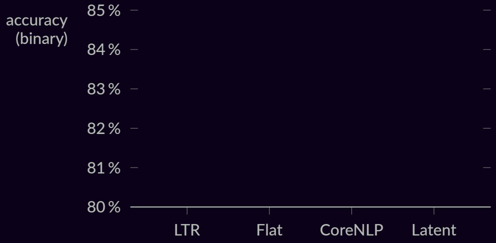
LTR
Flat
CoreNLP
Latent

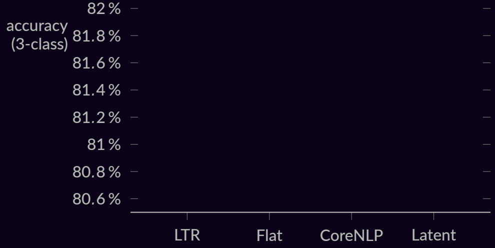
Sentiment classification (SST)



Sentiment classification (SST)



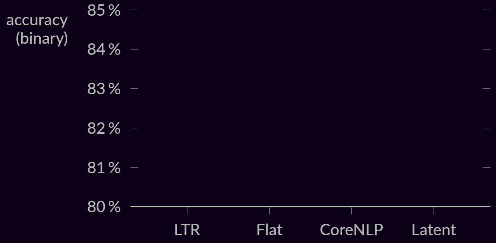
Natural Language Inference (SNLI)



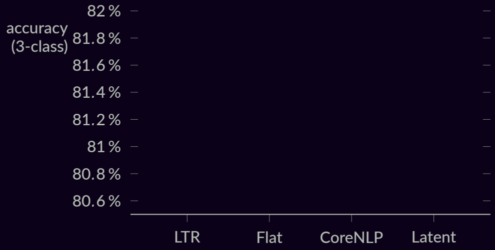
Sentence pair classification (P, H)

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

Sentiment classification (SST)



Natural Language Inference (SNLI)

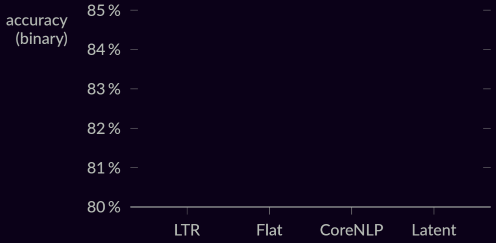


Reverse dictionary lookup

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)



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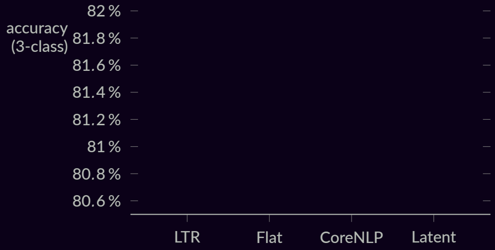
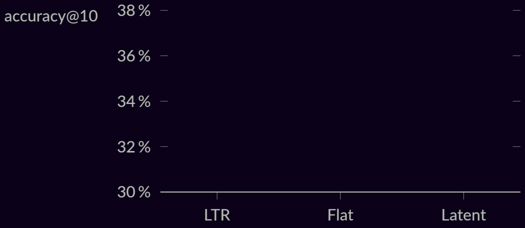
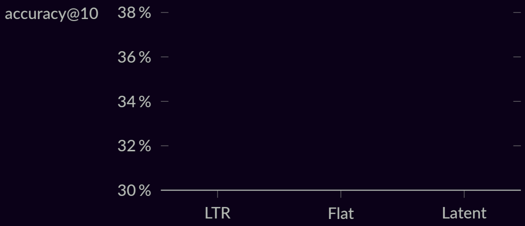


Reverse dictionary lookup

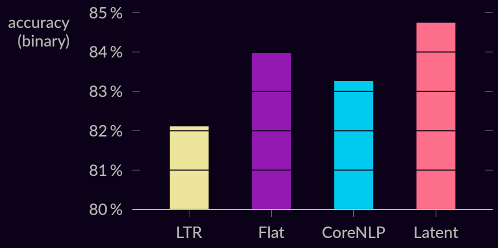
(definitions)



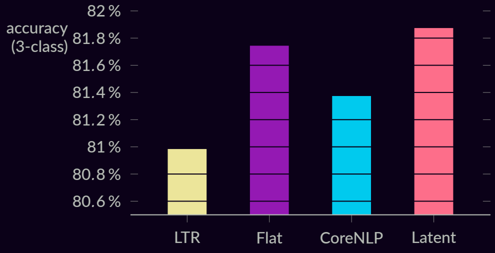
(concepts)



Sentiment classification (SST)



Natural Language Inference (SNLI)



Reverse dictionary lookup

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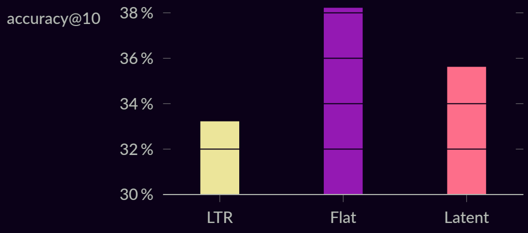
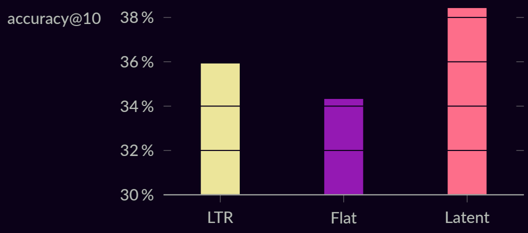


(concepts)



Syntax vs. Composition Order

CoreNLP parse, $p = 21.4\%$

★ lovely and poignant .

Syntax vs. Composition Order

$p = 22.6\%$

★ lovely and poignant .

CoreNLP parse, $p = 21.4\%$

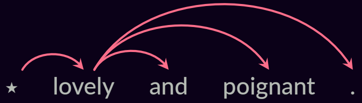
★ lovely and poignant .

. . .

Syntax vs. Composition Order

$p = 22.6\%$

CoreNLP parse, $p = 21.4\%$



. . .

$p = 15.33\%$

$p = 15.27\%$

. . .

CoreNLP parse, $p = 0\%$

Structured Output Prediction

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

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

Structured Output Prediction

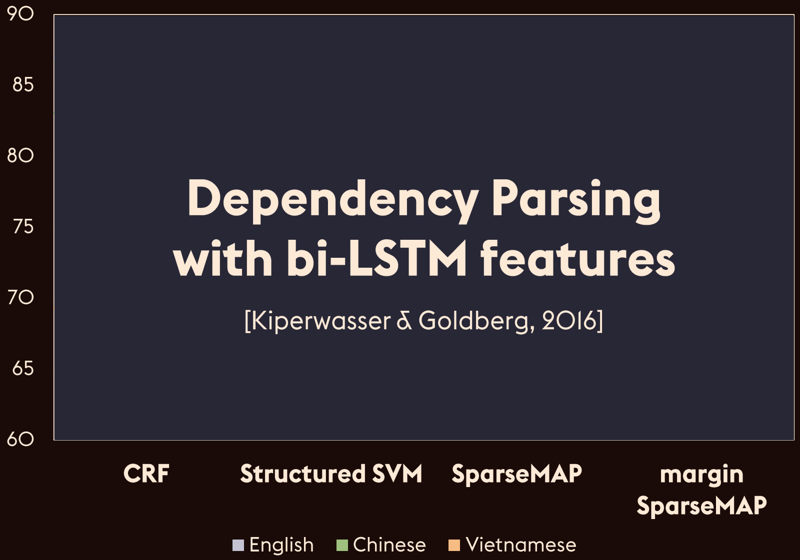
SparseMAP
$$L_A(\boldsymbol{\eta}, \bar{\boldsymbol{\mu}}) = \max_{\boldsymbol{\mu} \in \mathcal{M}} \left\{ \boldsymbol{\eta}^\top \boldsymbol{\mu} - \tfrac{1}{2}\|\boldsymbol{\mu}\|^2 \right\} - \boldsymbol{\eta}^\top \bar{\boldsymbol{\mu}} + \tfrac{1}{2}\|\bar{\boldsymbol{\mu}}\|^2$$

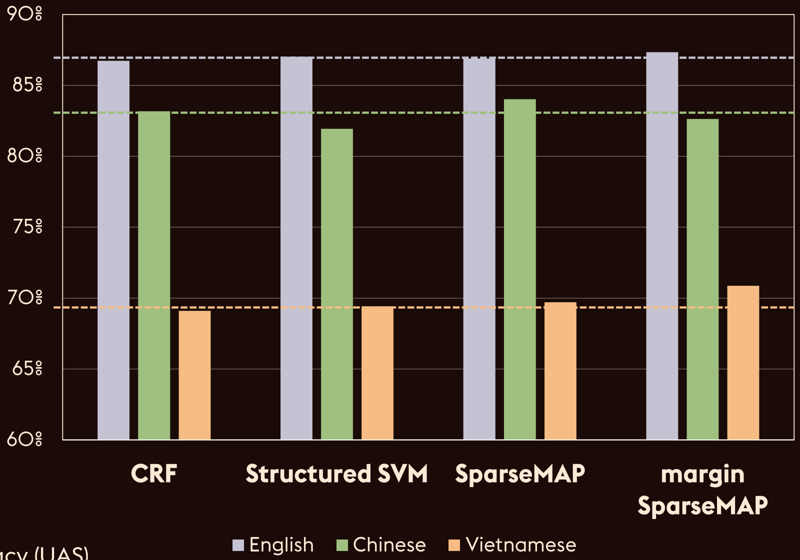
cost-SparseMAP
$$L_A^\rho(\boldsymbol{\eta}, \bar{\boldsymbol{\mu}}) = \max_{\boldsymbol{\mu} \in \mathcal{M}} \left\{ \boldsymbol{\eta}^\top \boldsymbol{\mu} - \tfrac{1}{2}\|\boldsymbol{\mu}\|^2 + \rho(\boldsymbol{\mu}, \bar{\boldsymbol{\mu}}) \right\} - \boldsymbol{\eta}^\top \bar{\boldsymbol{\mu}}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

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

Dependency Parsing with bi-LSTM features

[Kiperwasser & Goldberg, 2016]

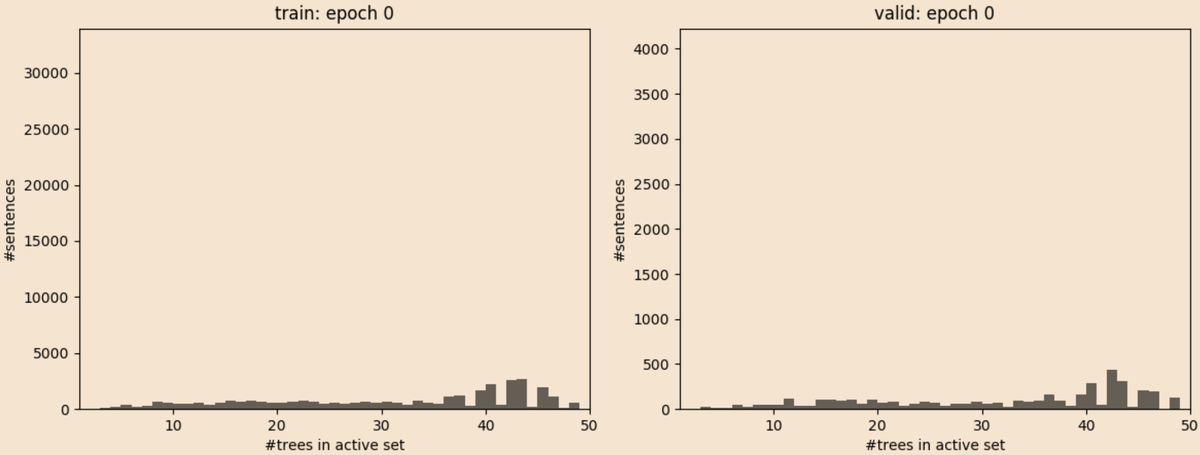




Unlabeled Accuracy (UAS)
Universal Dependencies dataset

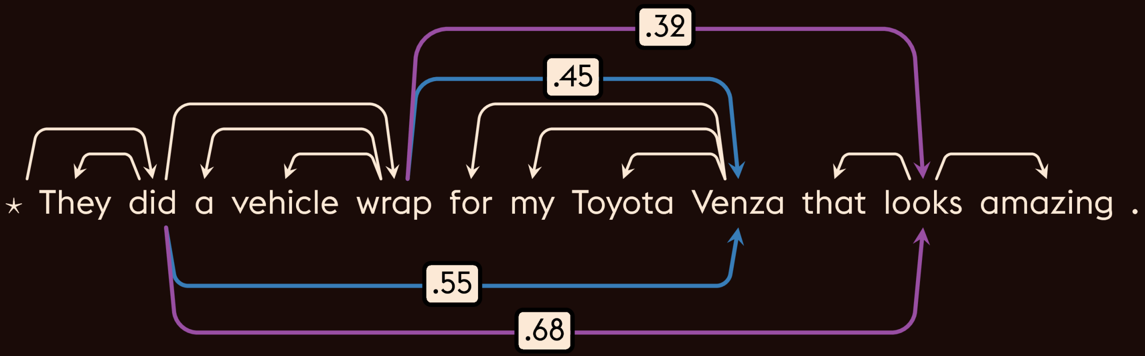
Sparse Structured Output Prediction

As models train, inference gets sparser!



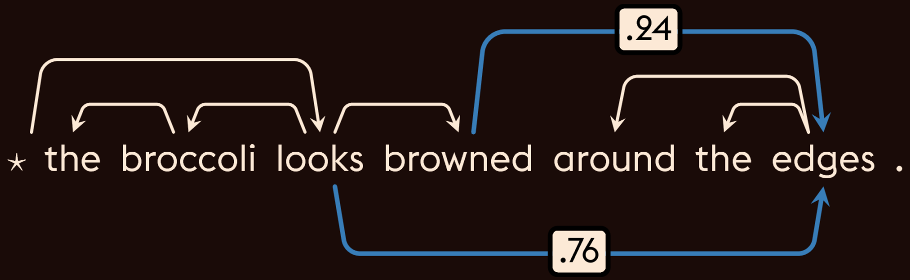
Sparse Structured Output Prediction

Inference captures linguistic ambiguity!



Sparse Structured Output Prediction

Inference captures linguistic ambiguity!



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