Learning with Sparse Latent Structure

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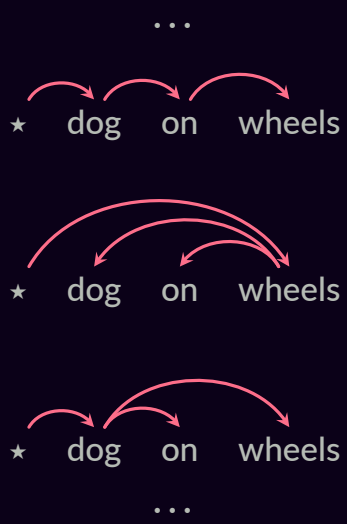
github.com/vene/sparsemap @vnfrombucharest

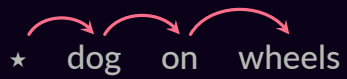
Structured Prediction

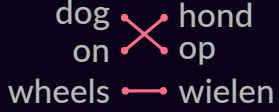


Structured Prediction

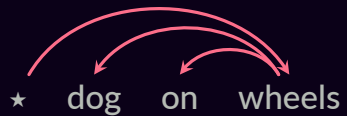
...

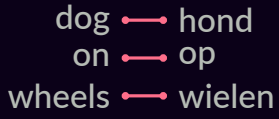
VERB PREP NOUN
dog on wheels



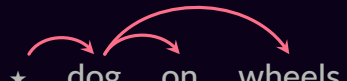


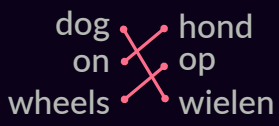
NOUN PREP NOUN
dog on wheels





NOUN DET NOUN
dog on wheels



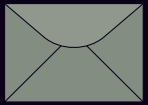


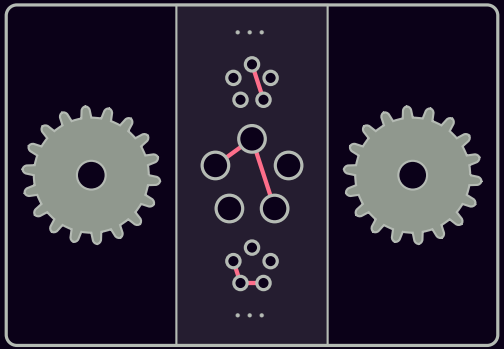
...

Structured Prediction

Latent Structure Models

input





output

positive

neutral

negative

record scratch

freeze frame

How to select an item from a set?

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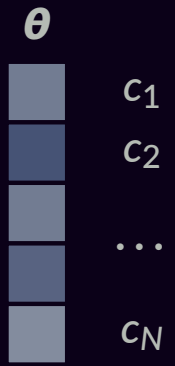
c_1

c_2

...

c_N

How to select an item from a set?



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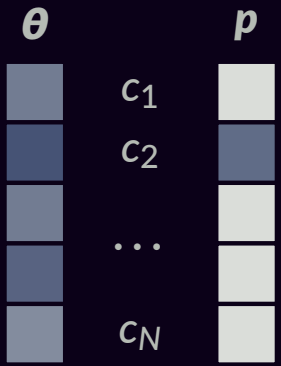

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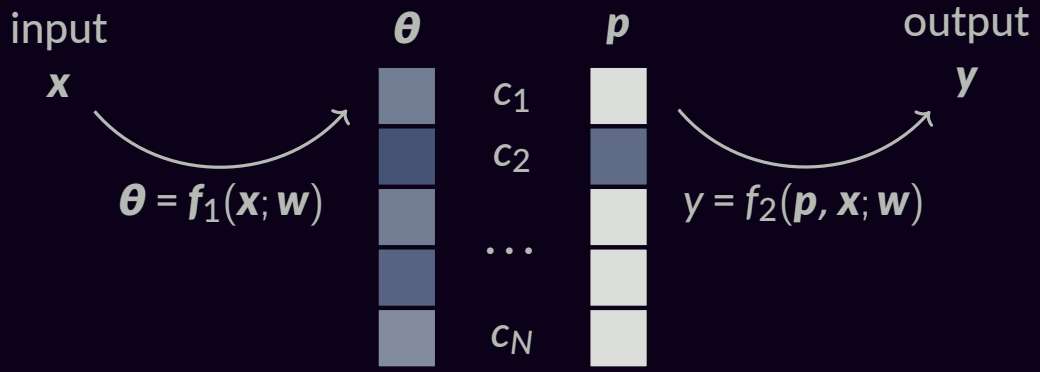

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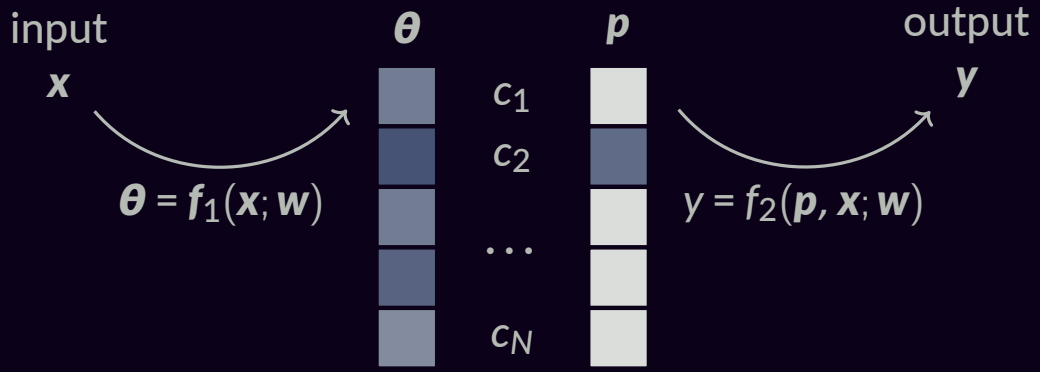

$$\frac{\partial y}{\partial w} = ?$$

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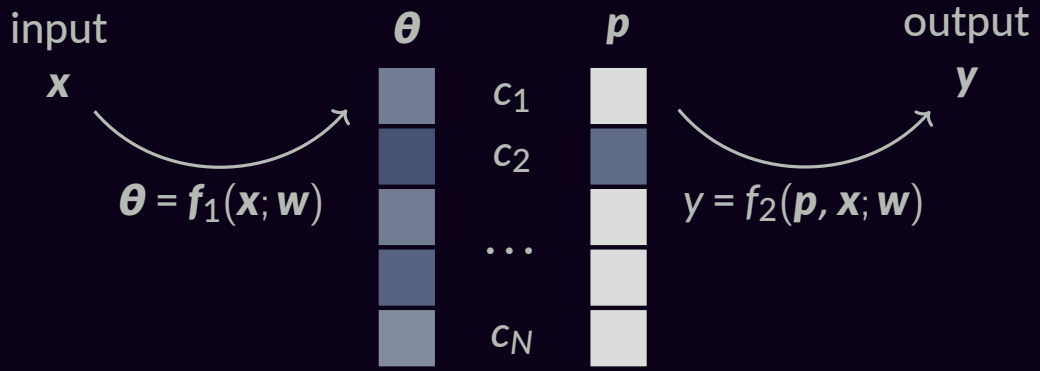
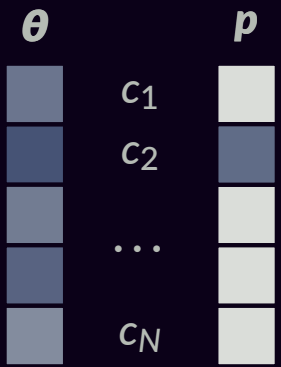


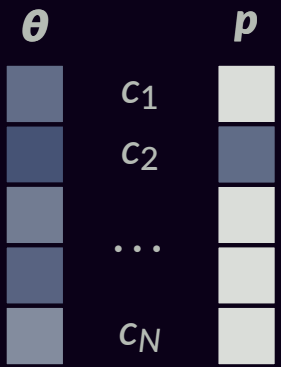
$\frac{\partial y}{\partial w}$=? or, essentially, $\frac{\partial p}{\partial \theta}$=?

Argmax



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

Argmax



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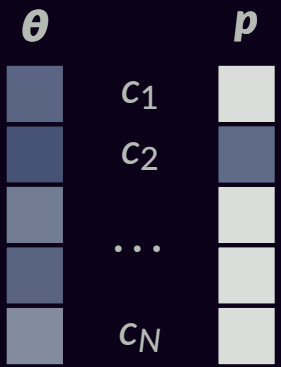

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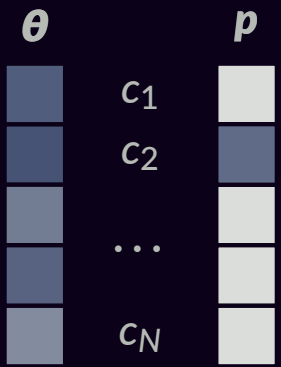

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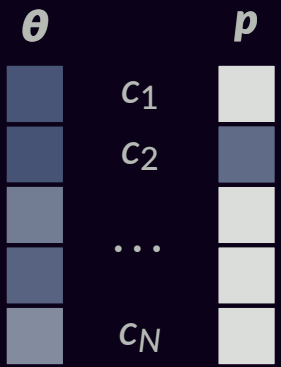

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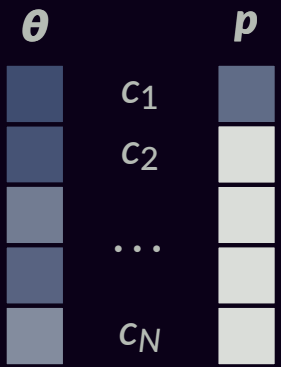

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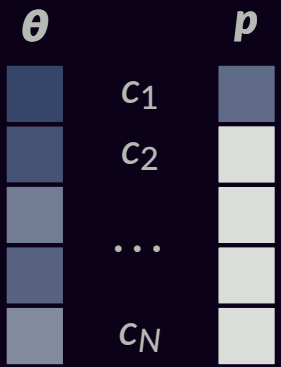

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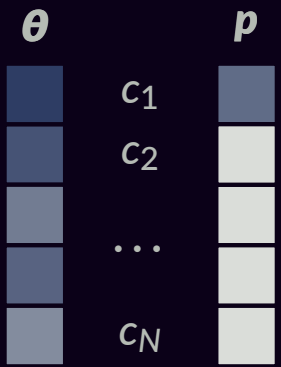

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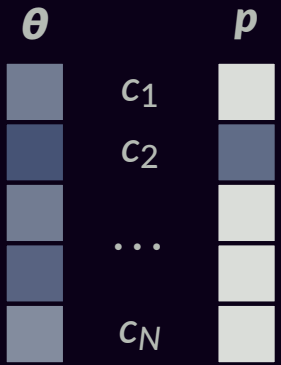
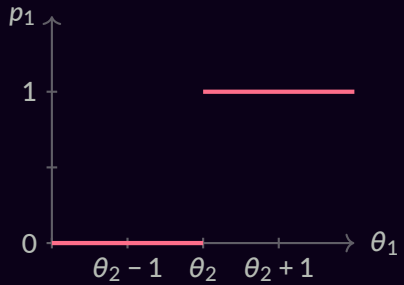
Argmax

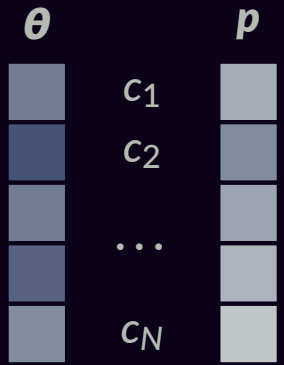


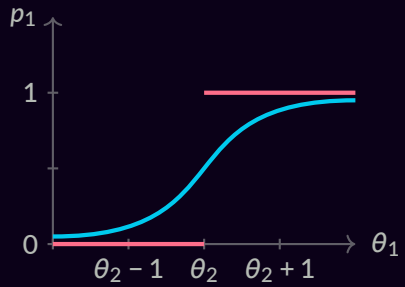


$$\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{\theta}} = \mathbf{0}$$

Argmax vs. Softmax

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





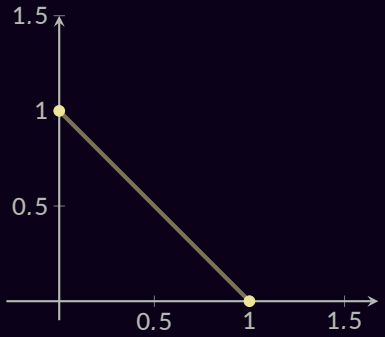
$$\frac{\partial \boldsymbol{p}}{\partial \boldsymbol{\theta}} = \text{diag}(\boldsymbol{p}) - \boldsymbol{p}\boldsymbol{p}^\top$$

Variational Form of Argmax

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

Variational Form of Argmax

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



$N = 2$

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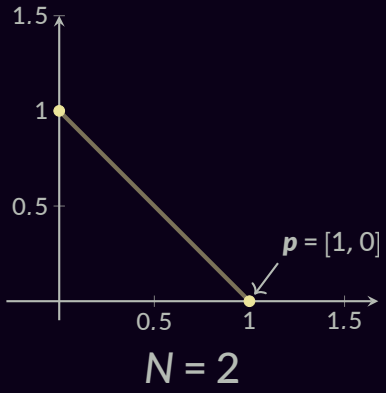

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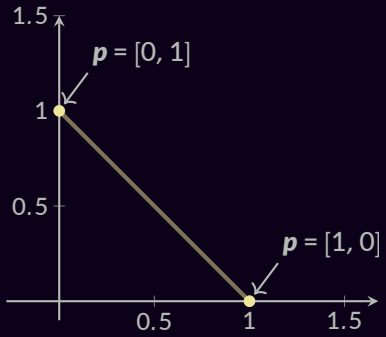

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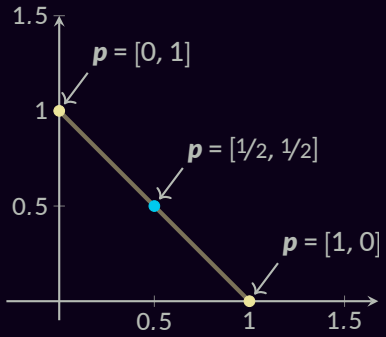

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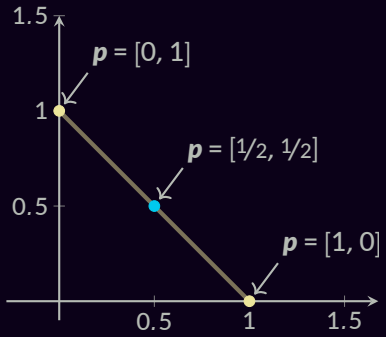

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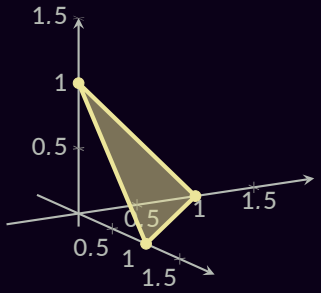

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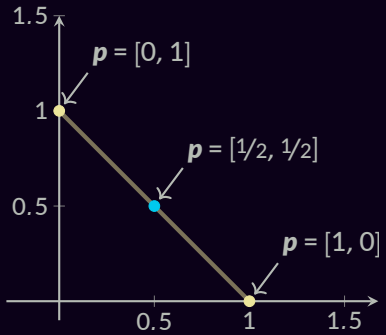

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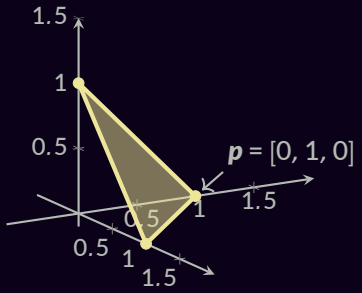

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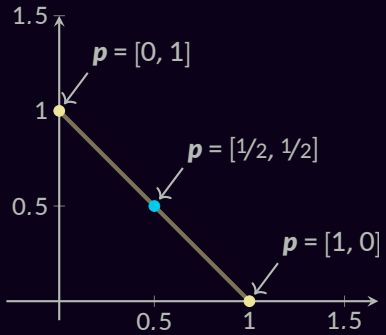

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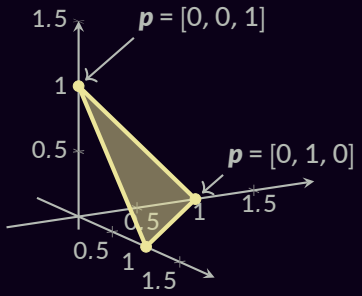

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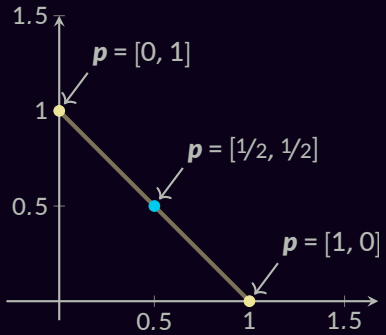

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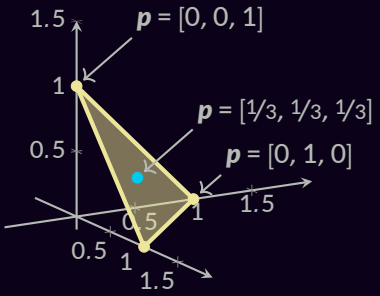

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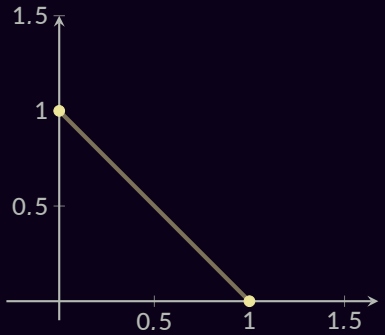
$$\max_j \theta_j = \max_{\boldsymbol{p} \in \Delta} \boldsymbol{p}^\top \boldsymbol{\theta}$$

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



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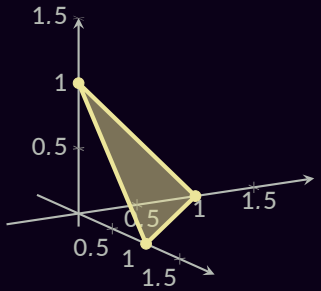

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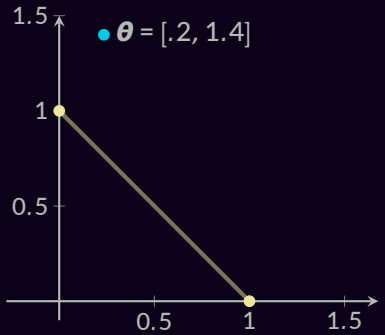

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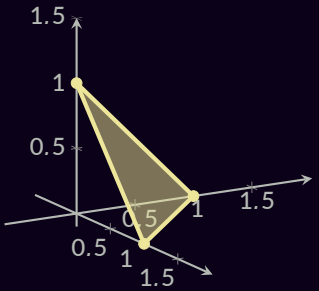

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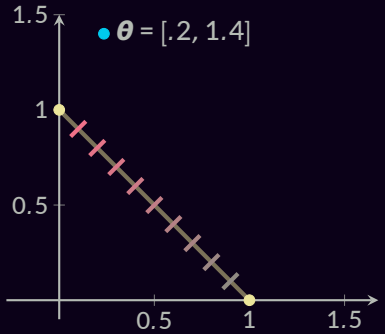

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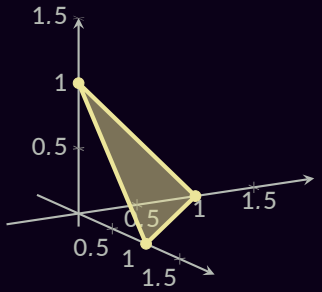

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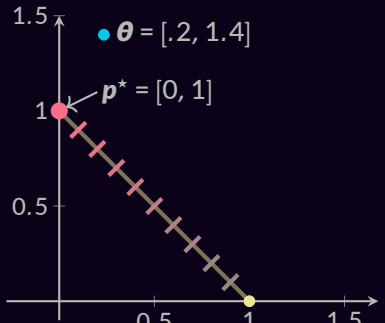

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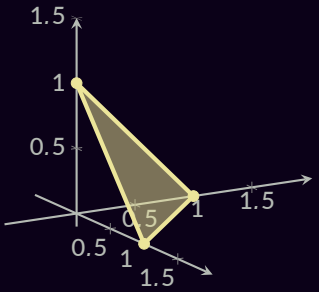

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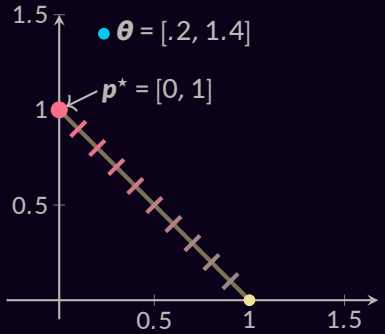

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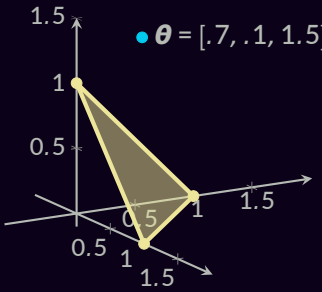

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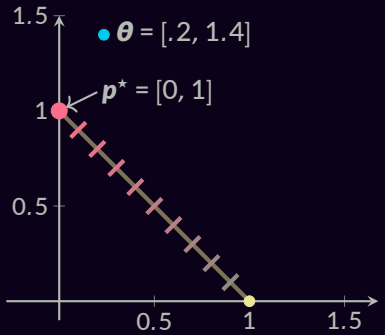

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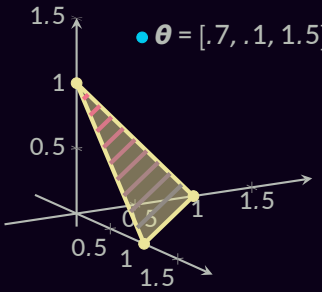

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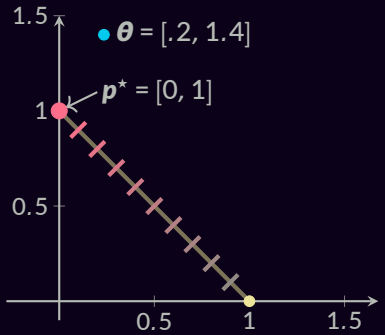
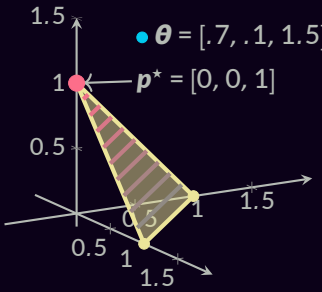
Fundamental Thm. Lin. Prog.
(Dantzig et al., 1955)



$N = 2$

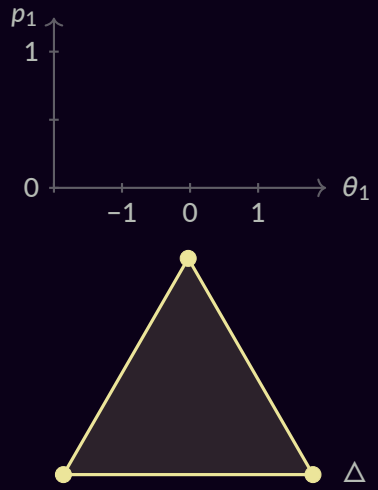


$N = 3$

(Niculae and Blondel, 2017)

Smoothed Max Operators

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



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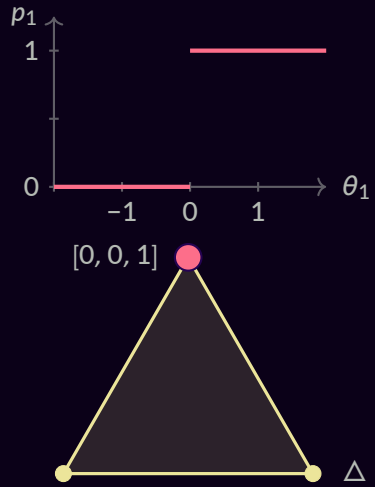

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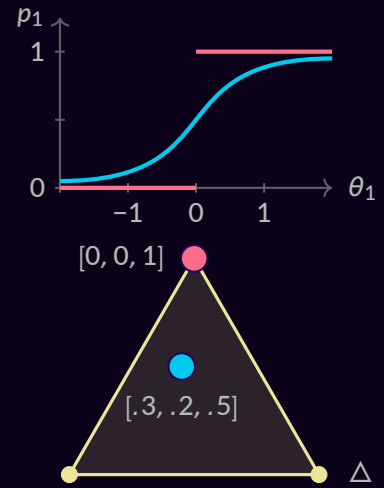

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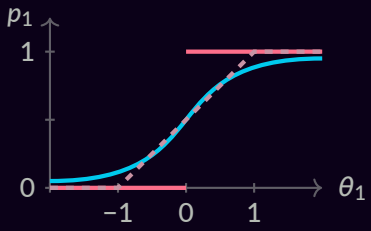
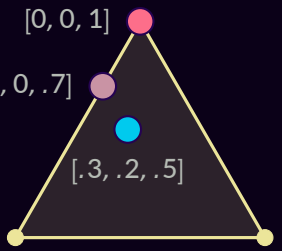
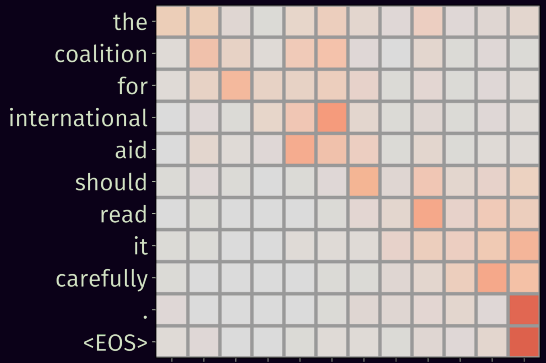




(Martins and Astudillo, 2016)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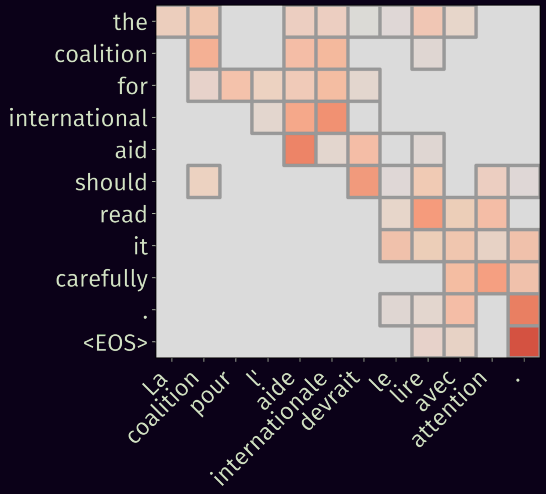
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sparsemax

Sparsemax

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

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

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Computation:

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

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

$O(d)$ via partial sort

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

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$O(d)$ via partial sort

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

Backward pass:

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

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

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

(Martins and Astudillo, 2016)

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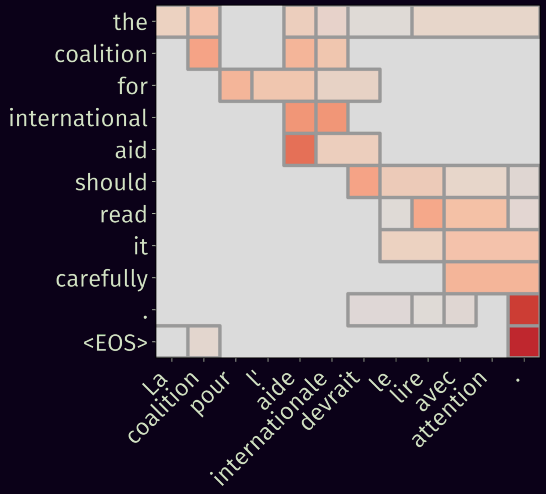
$: p_j^\star > 0\},$

$\equiv \mathcal{S}]]$

(Martins and Astudillo, 2016)

argmin differentiation

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

(Niculae and Blondel, 2017)

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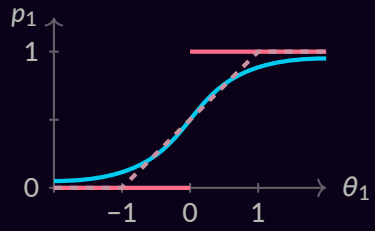

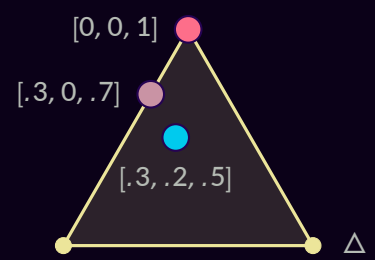

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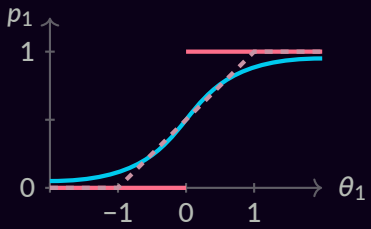
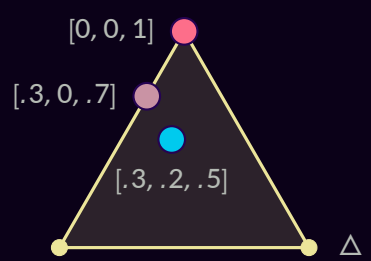
- csparsemax: $\Omega(\boldsymbol{p}) = \frac{1}{2}\|\boldsymbol{p}\|_2^2 + \iota(\boldsymbol{a} \le \boldsymbol{p} \le \boldsymbol{b})$





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(

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

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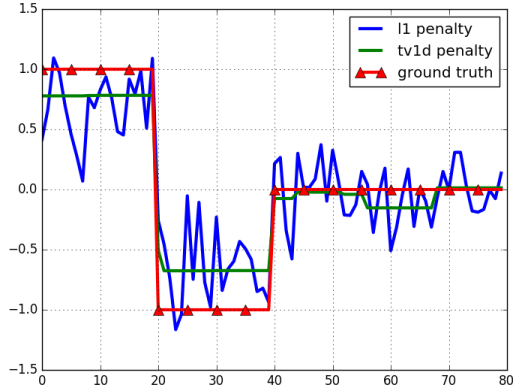
(Niculae and Blondel, 2017)



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

(Tibshirani et al., 2005)

(Niculae and Blondel, 2017)

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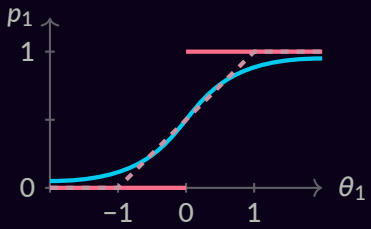
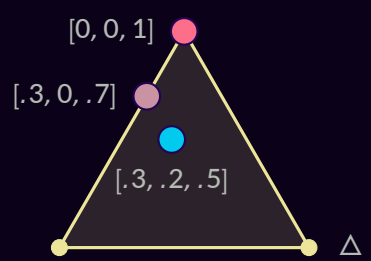


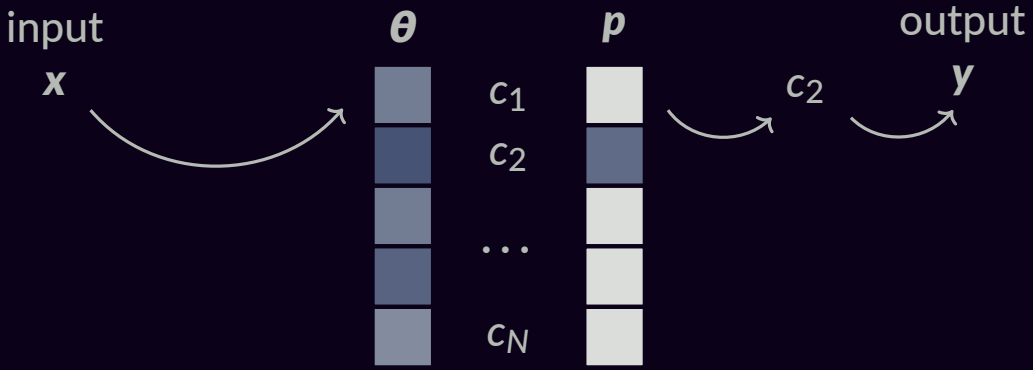


Structured Prediction

finally

Structured Prediction

is essentially a (very high-dimensional) argmax



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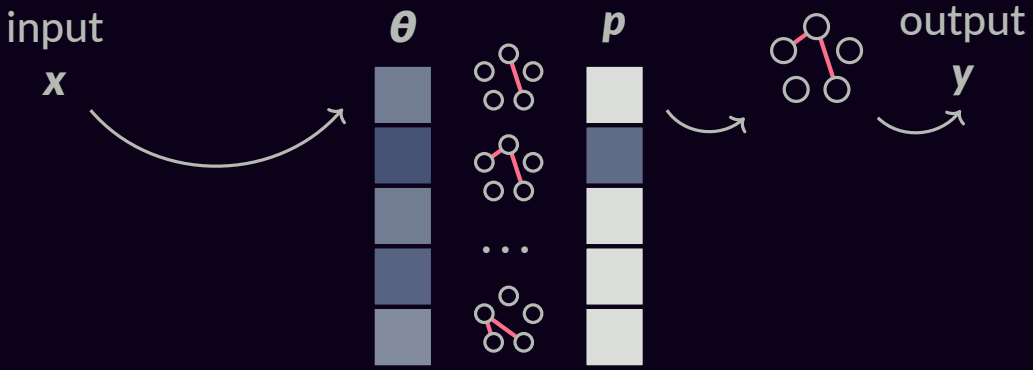

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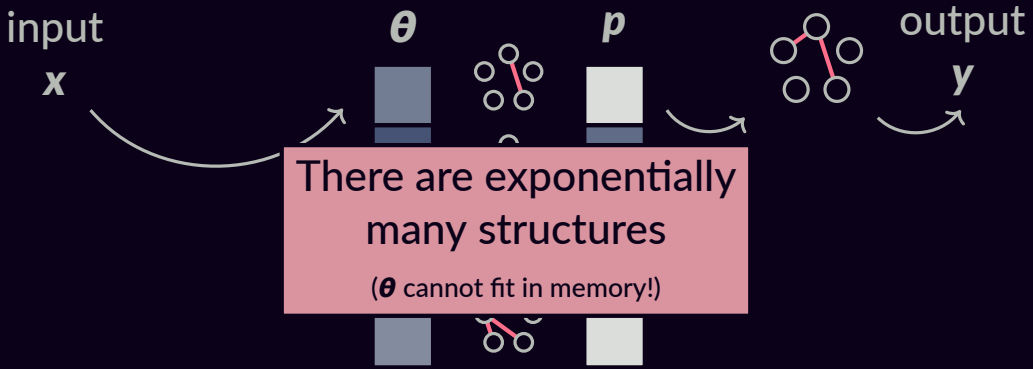

Factorization Into Parts

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

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

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

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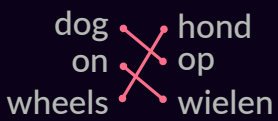
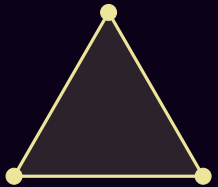


$$A = \begin{array}{r} \star\!\rightarrow\!\text{dog} \\ \text{on}\!\rightarrow\!\text{dog} \\ \text{wheels}\!\rightarrow\!\text{dog} \\ \hline \star\!\rightarrow\!\text{on} \\ \text{dog}\!\rightarrow\!\text{on} \\ \text{wheels}\!\rightarrow\!\text{on} \\ \hline \star\!\rightarrow\!\text{wheels} \\ \text{dog}\!\rightarrow\!\text{wheels}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

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



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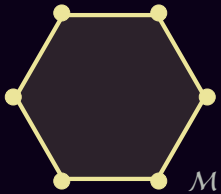
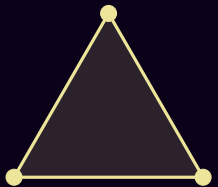


$\mathcal{M}$

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



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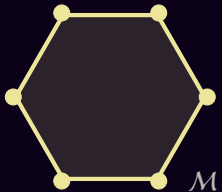

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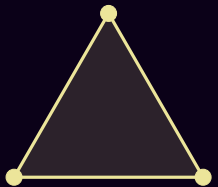
$$\mathcal{M} := \operatorname{conv}\{\boldsymbol{a}_h : h \in \mathcal{H}\}$$
$$= \{\boldsymbol{A}\boldsymbol{p} : \boldsymbol{p} \in \Delta\}$$



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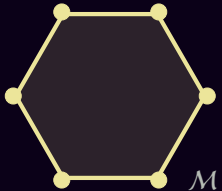
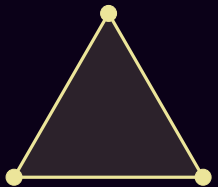


$\mathcal{M}$

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



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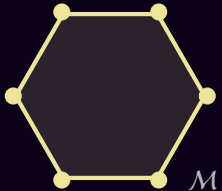
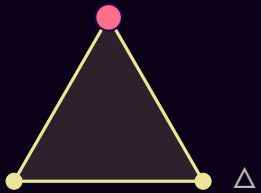
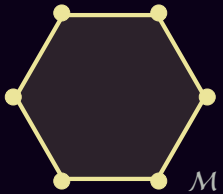


$\mathcal{M}$

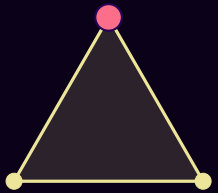
- **argmax** $\arg\max_{\boldsymbol{p} \in \Delta} \boldsymbol{p}^\top \boldsymbol{\theta}$





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

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



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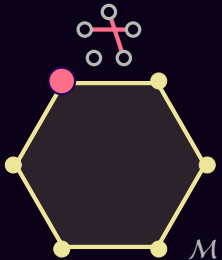
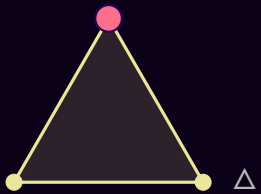


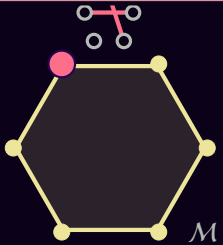
$\mathcal{M}$

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

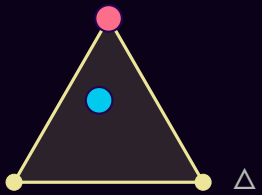
MAP $\arg\max_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^\top \boldsymbol{\eta}$

e.g. dependency parsing → **max. spanning tree**
matching → **the Hungarian algorithm**

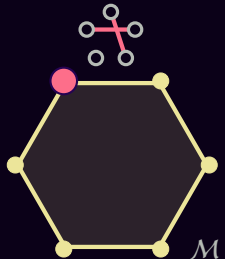




- **argmax** $\arg\max_{\boldsymbol{p} \in \Delta} \boldsymbol{p}^\top \boldsymbol{\theta}$
- **softmax** $\arg\max_{\boldsymbol{p} \in \Delta} \boldsymbol{p}^\top \boldsymbol{\theta} + \mathrm{H}(\boldsymbol{p})$



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



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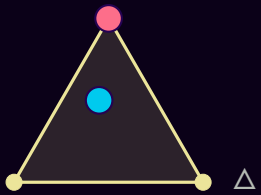

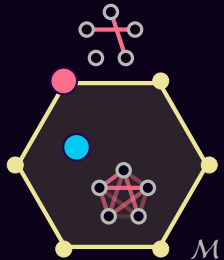

- **argmax** $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top \boldsymbol{\theta}$
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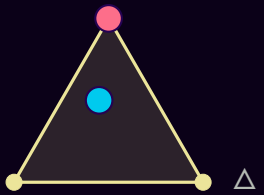
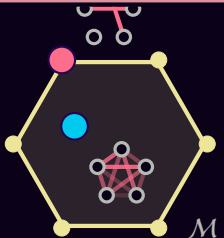
e.g. sequence labelling → forward-backward

(Rabiner, 1989)

As attention: (Kim et al., 2017)





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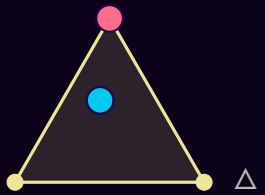
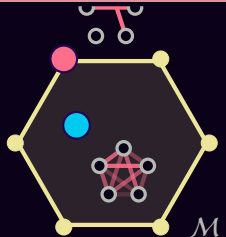
e.g. dependency parsing → **the Matrix-Tree theorem**

(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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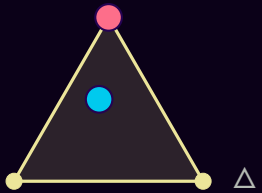
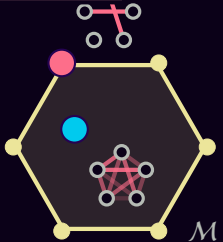
e.g. matchings → **#P-complete!**

(Taskar, 2004; Valiant, 1979)





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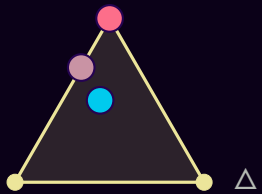
- **sparsemax** $\arg\max_{\boldsymbol{p} \in \triangle} \boldsymbol{p}^\top \boldsymbol{\theta} - \frac{1}{2}\|\boldsymbol{p}\|^2$



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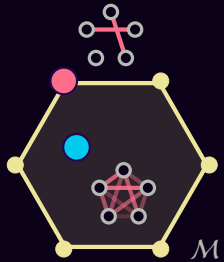

(Niculae, Martins, Blondel, and Cardie, 2018)

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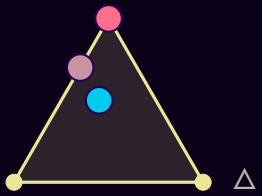

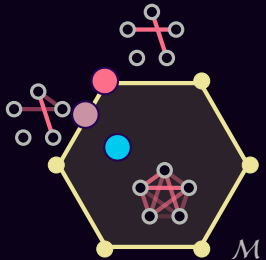

SparseMAP Solution

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

=  = .6 + .4

$$= \boldsymbol{A}\boldsymbol{p}^\star \text{ with very sparse } \boldsymbol{p}^\star \in \triangle^N$$

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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- 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

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

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

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

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

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

(Frank and Wolfe, 1956

Completely modular: just add MAP

pass

- select a new corner of $\mathcal{M}$
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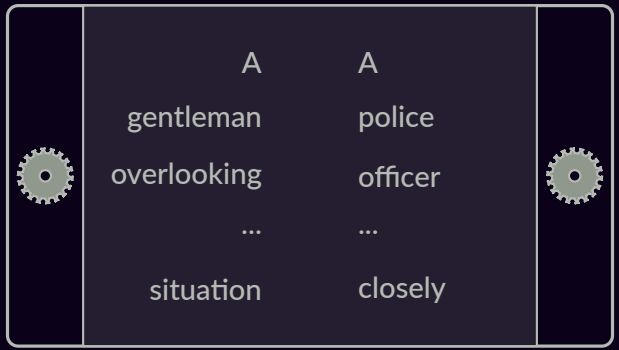
Structured Attention for Alignments

NLI

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

input

(P, H)



output

entails
contradicts
neutral

(Model: ESIM (Chen et al., 2017))

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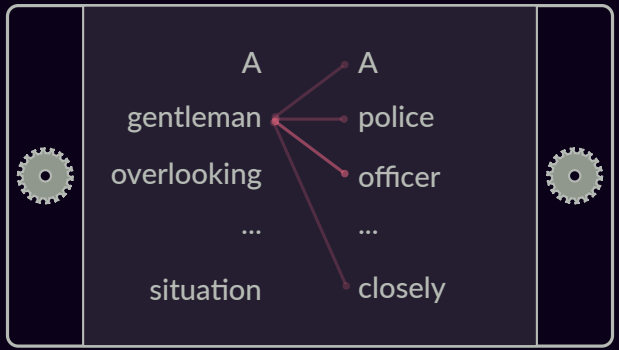

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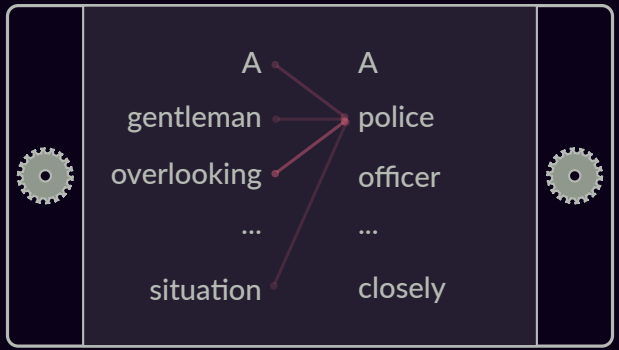

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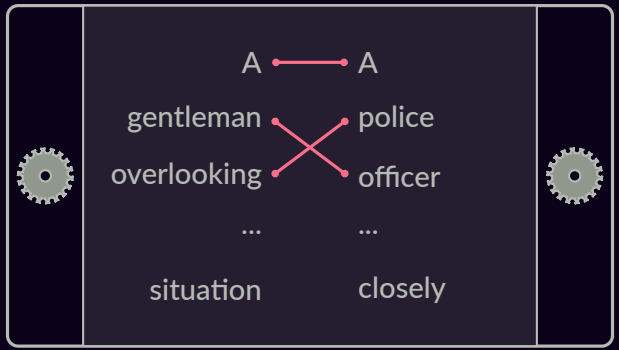

output

(Proposed model: global matching)

In code:

```
# Xp: (n_prem x k)
# Xh: (n_hypo x k)

Z = Xp @ Xh.t()

Up = softmax(Z, dim=1)
Uh = softmax(Z, dim=0)

Xp = cat([Xp, Up     @ Xh])
Xh = cat([Xh, Uh.t() @ Xp])

# ...
```

In code:

```
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Up = softmax(Z, dim=1)
Uh = softmax(Z, dim=0)

Xp = cat([Xp, Up     @ Xh])
Xh = cat([Xh, Uh.t() @ Xp])

# ...
```
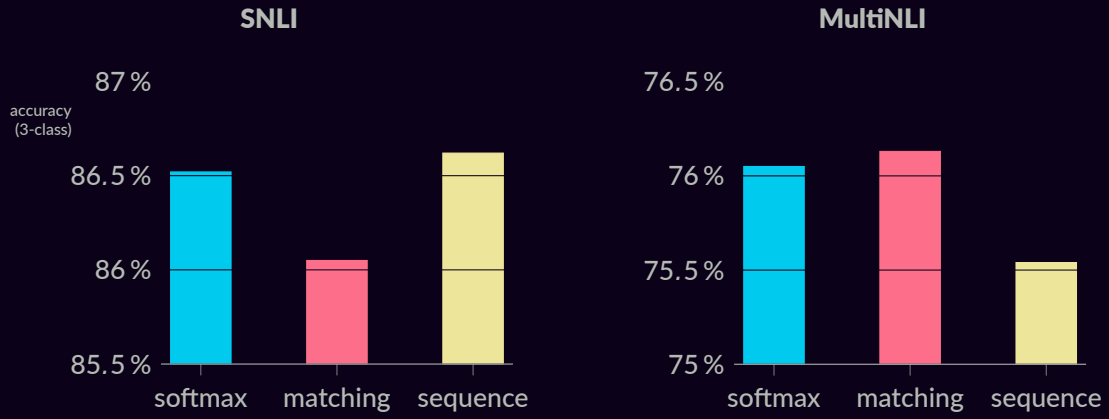
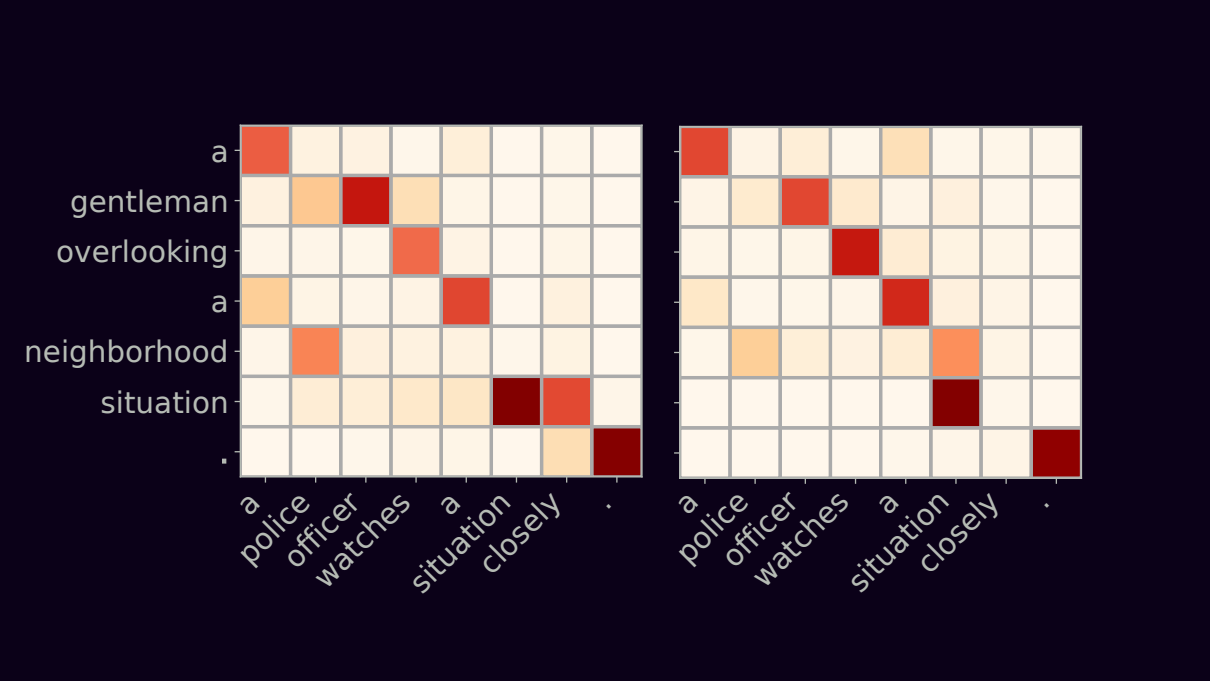

```
# Xp: (n_prem x k)
# Xh: (n_hypo x k)

Z = Xp @ Xh.t()

U = sparsemap_matching(Z)

Xp = cat([Xp, U     @ Xh])
Xh = cat([Xh, U.t() @ Xp])

# ...
```


SNLI
87 %
accuracy
(3-class)
86.5 %
86 %
85.5 %
softmax
matching
sequence
MultiNLI
76.5 %
76 %
75.5 %
75 %
softmax
matching
sequence


a
gentleman
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situation
.
a
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situation
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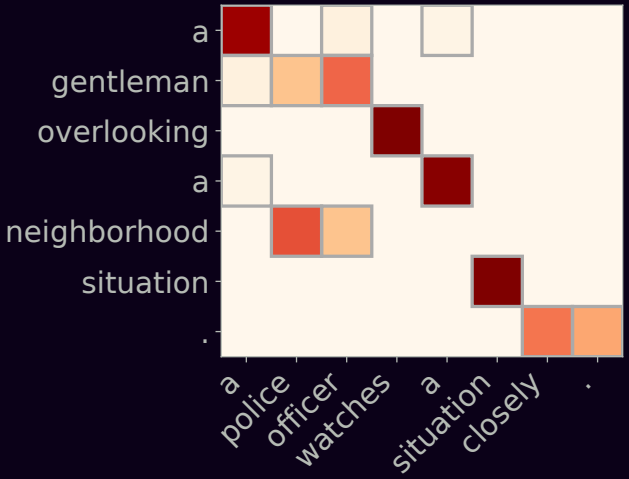
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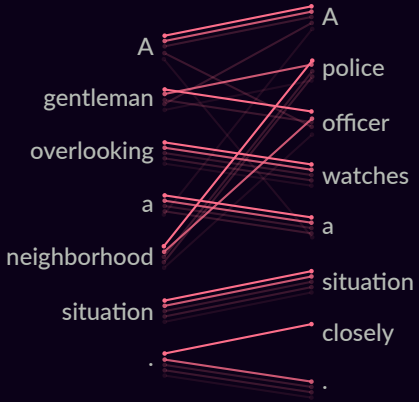
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.
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closely
.

Dynamically inferring the computation graph

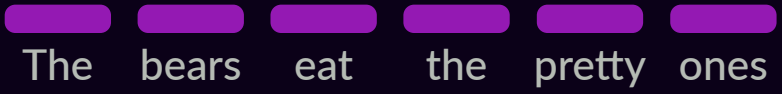
So far: a structured hidden layer

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

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

Dependency TreeLSTM

(Tai et al., 2015)



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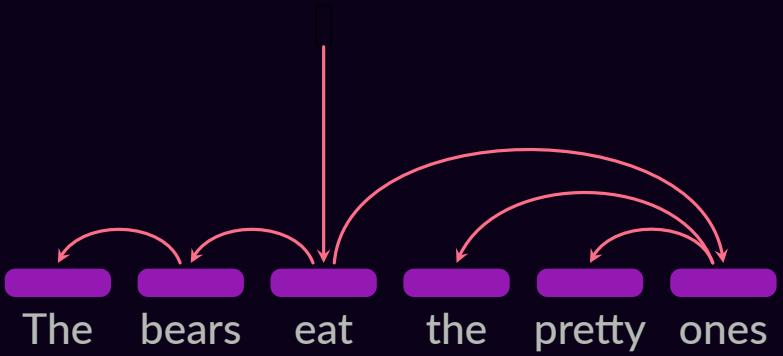

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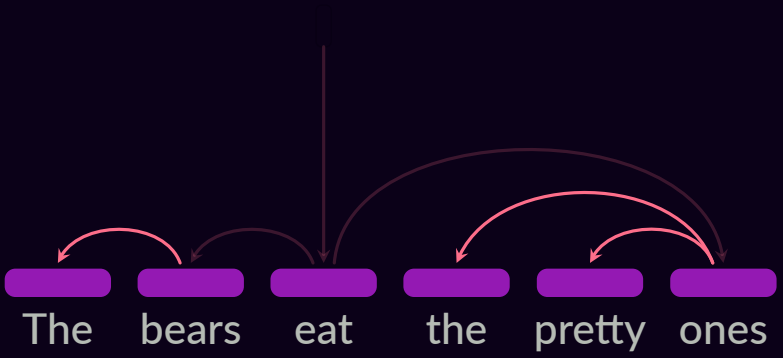

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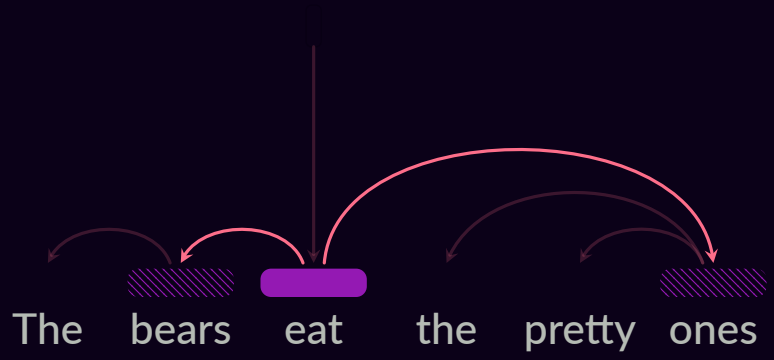

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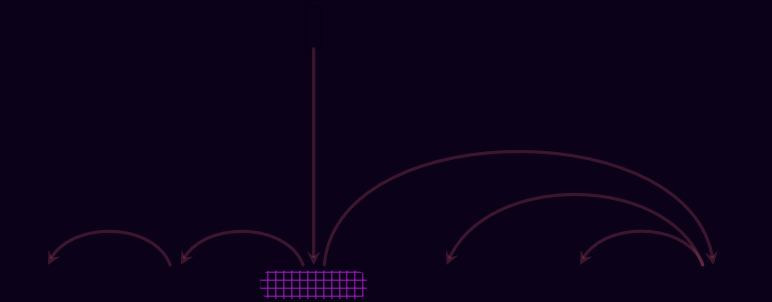
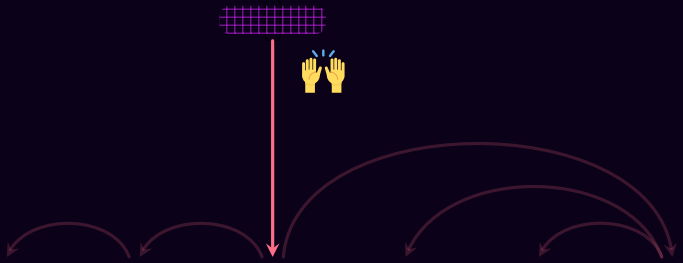


Dependency TreeLSTM

(Tai et al., 2015)



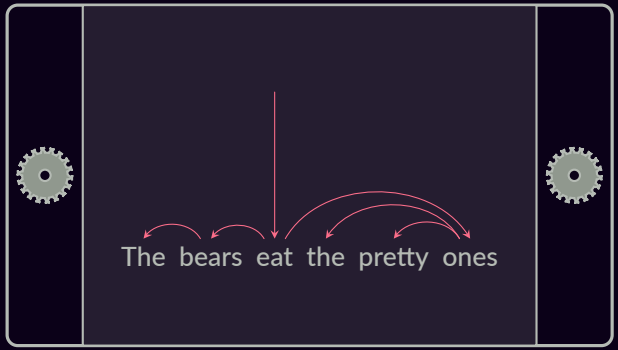
The bears eat the pretty ones

Latent Dependency TreeLSTM

(Niculae, Martins, and Cardie, 2018)

input

x



output

y

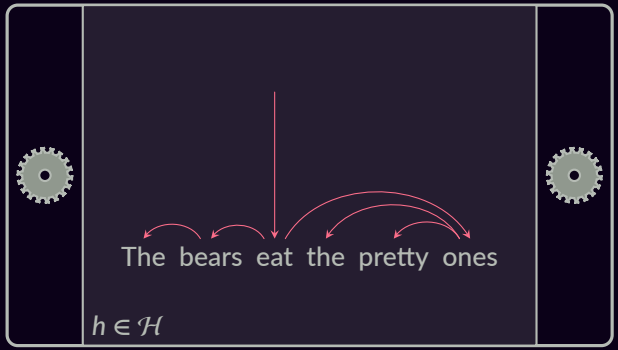
Latent Dependency TreeLSTM

(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

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

Structured Latent Variable Models

e.g., a TreeLSTM defined by h

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

Structured Latent Variable Models

sum over
all possible trees

e.g., a TreeLSTM defined by h

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Exponentially large sum!

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

idea 1
idea 2
idea 3

Structured Latent Variable Models

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

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

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idea 1 $p_{\boldsymbol{\pi}}(h \mid x) = 1$ if $h = h^\star$ else 0 argmax $\sum_{h \in \mathcal{H}}$ 😋 $\frac{\partial p(y \mid x)}{\partial \boldsymbol{\pi}}$ 😟

idea 2

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😋 😟

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

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

idea 3

Structured Latent Variable Models

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e.g., a TreeLSTM defined by h

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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	😋	😟
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idea 3				

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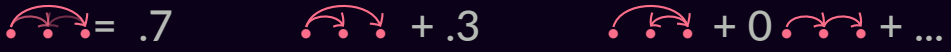
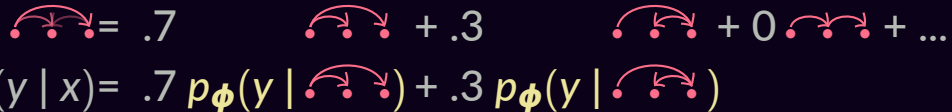
idea 1	$p_{\boldsymbol{\pi}}(h \mid x) = 1$ if $h = h^\star$ else 0	argmax	😊	😟
idea 2	$p_{\boldsymbol{\pi}}(h \mid x) \propto \exp\big(\text{score}_{\boldsymbol{\pi}}(h; x)\big)$	softmax	😱	😍
idea 3		SparseMAP	😊	😊

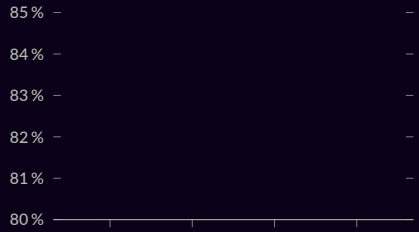
SparseMAP

SparseMAP



SparseMAP

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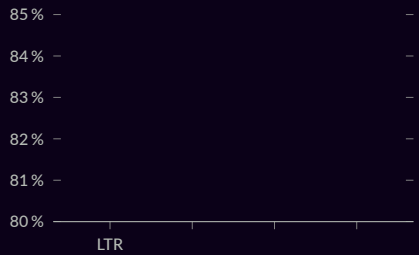
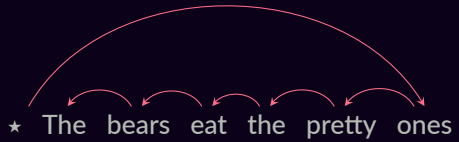
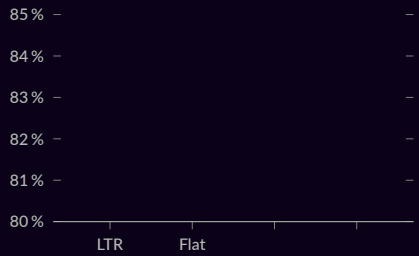
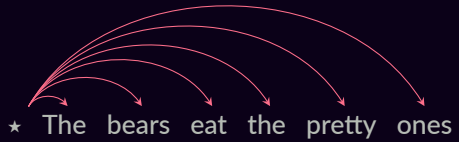


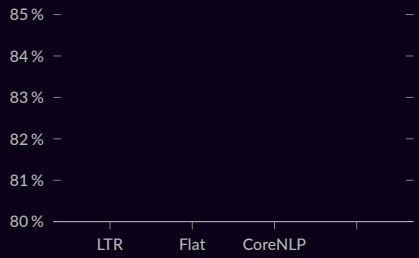


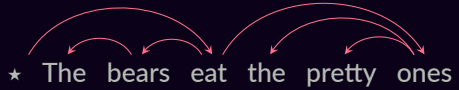
Left-to-right: regular LSTM



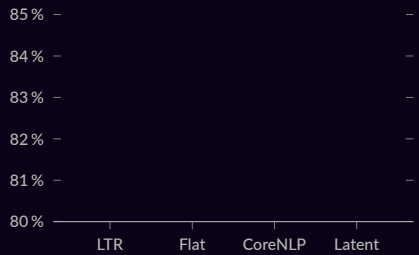


Flat: bag-of-words–like





CoreNLP: off-line parser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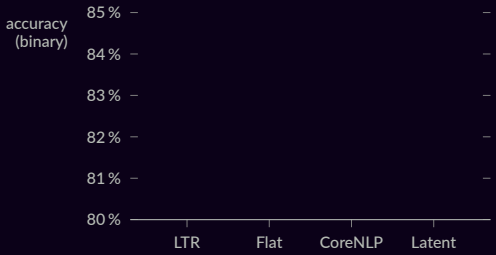
LTR
Flat
CoreNLP
Latent

Sentiment classification (SST)



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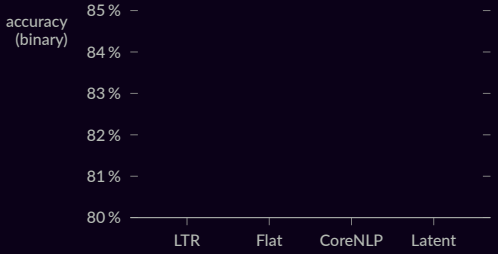
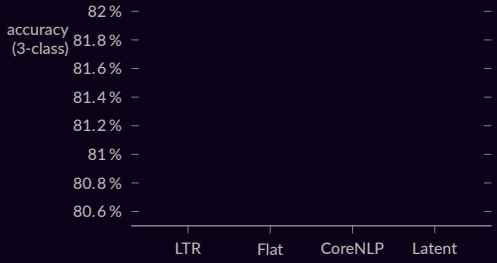


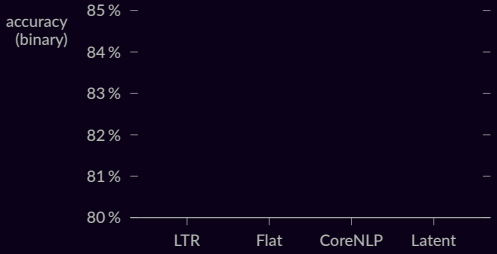
Natural Language Inference (SNLI)



Sentence pair classification (P, H)

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

Sentiment classification (SST)



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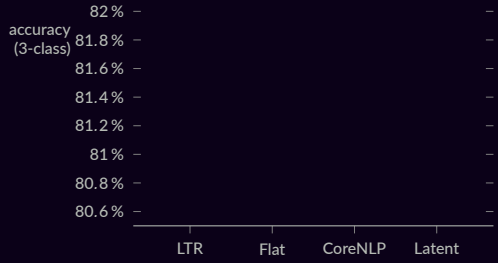
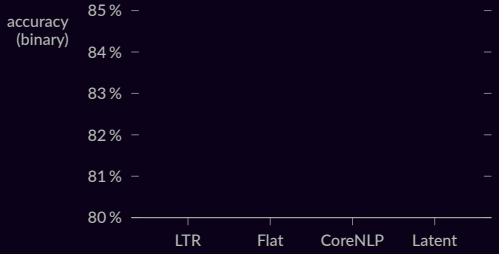


Reverse dictionary lookup

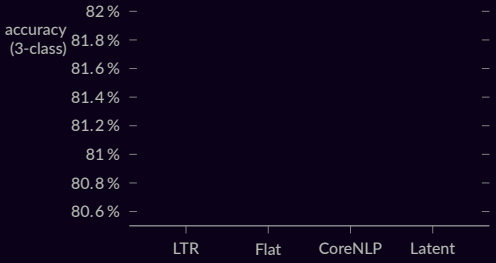
given word description, predict word embedding (Hill et al., 2016)

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

Sentiment classification (SST)

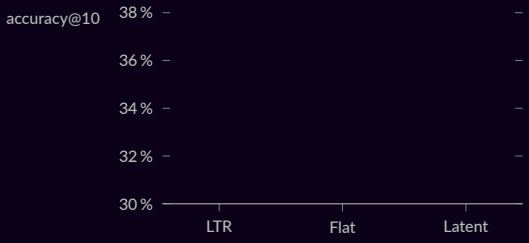


Natural Language Inference (SNLI)

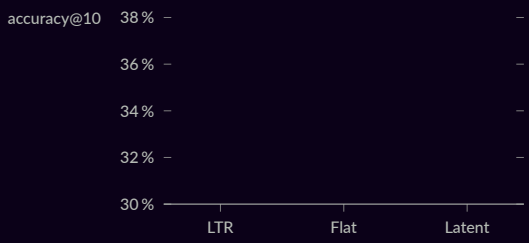


Reverse dictionary lookup

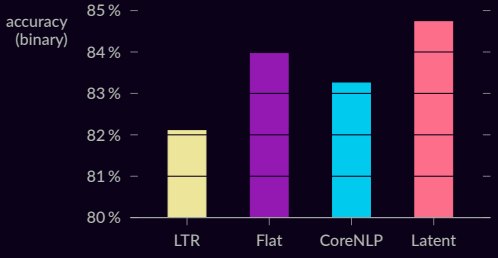
(definitions)



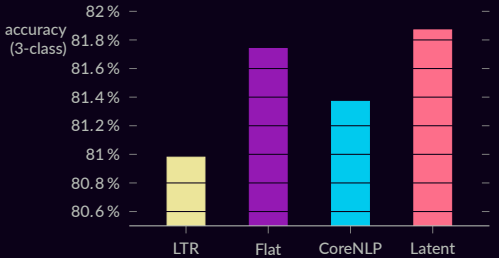
(concepts)



Sentiment classification (SST)



Natural Language Inference (SNLI)



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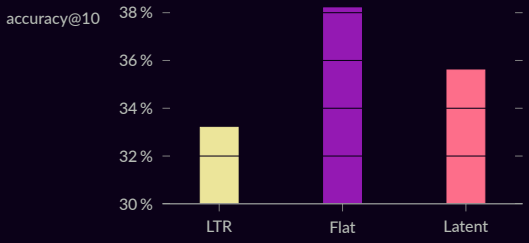

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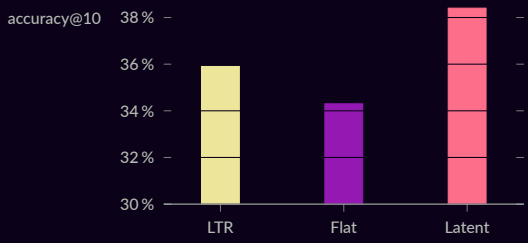
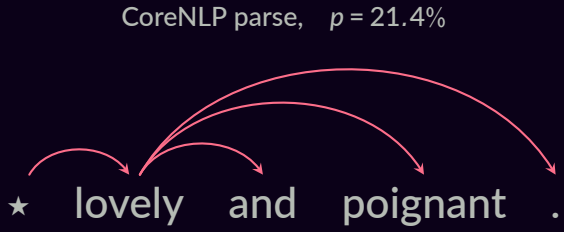
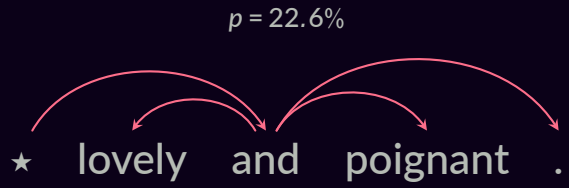


Syntax vs. Composition Order



Syntax vs. Composition Order



Syntax vs. Composition Order

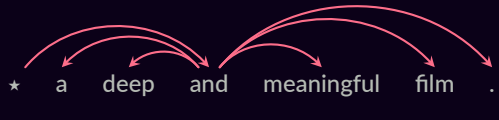
$p = 22.6\%$

CoreNLP parse, $p = 21.4\%$

. . .

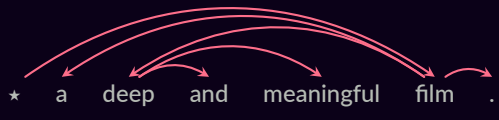
$p = 15.33\%$

$p = 15.27\%$



. . .

CoreNLP parse, $p = 0\%$



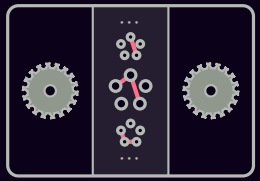
Conclusions

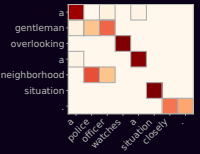
Differentiable & sparse structured inference

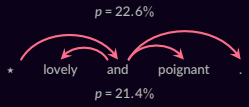
Generic, extensible algorithms

Interpretable structured attention

Dynamically-inferred computation graphs







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github.com/vene/sparsemap
@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.

(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.

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

Example: maximum of a vector

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

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Example: maximum of a vector

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

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

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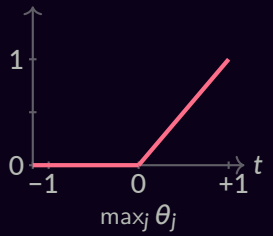
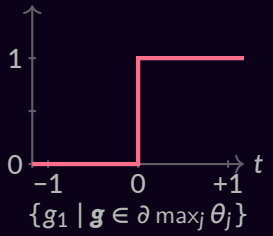
&= \operatorname{conv}\{\nabla_{\boldsymbol{\theta}} \phi(\boldsymbol{p}^\star, \boldsymbol{\theta})\} \\
&= \operatorname{conv}\{\boldsymbol{p}^\star\}
\end{aligned}$$

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

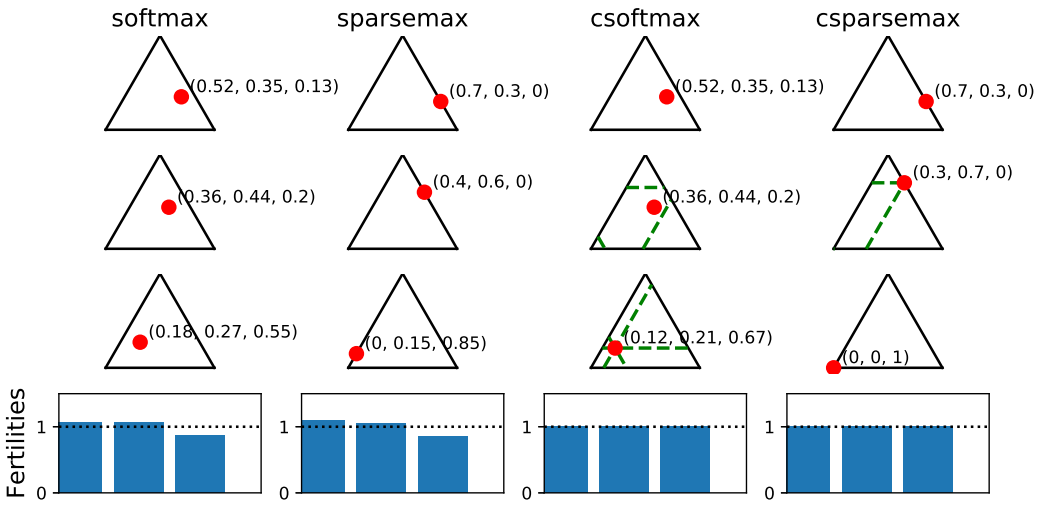


$\max_j \theta_j$

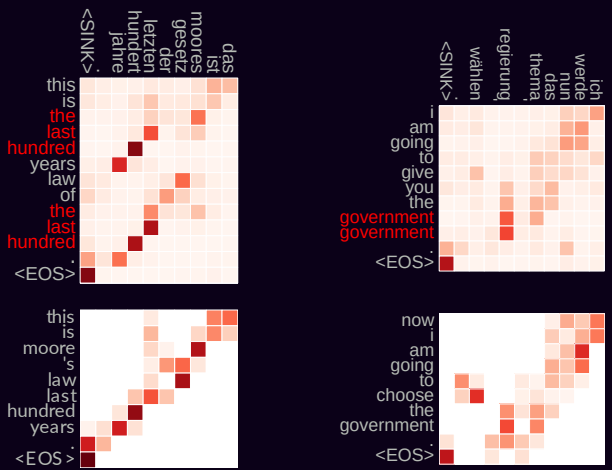


$\{g_1 \mid \boldsymbol{g} \in \partial \max_j \theta_j\}$

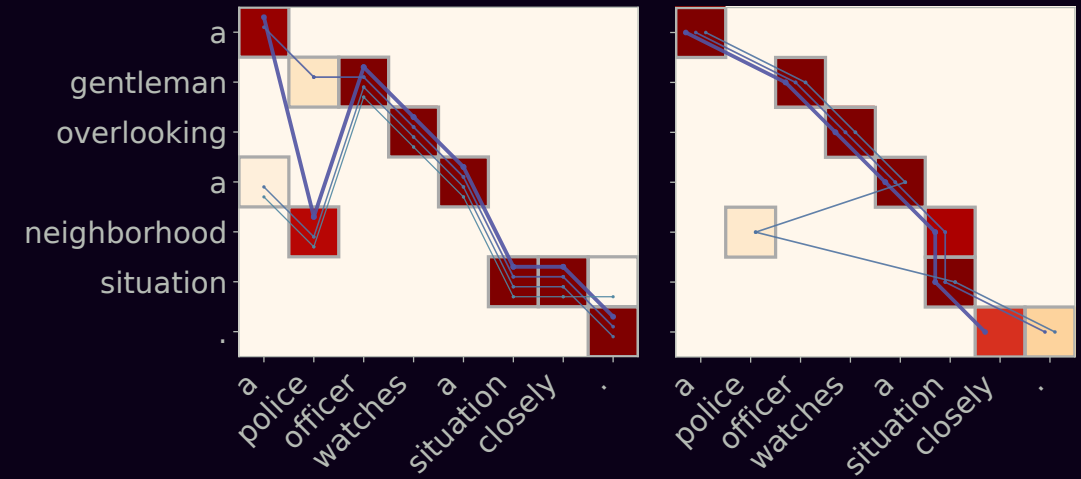
Example: Source Sentence with Three Words



e.g., fertility constraints for NMT



constrained softmax: (Martins and Kreutzer, 2017) constrained sparsemax: (Malaviya et al., 2018)


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

Structured Output Prediction

SparseMAP

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

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

Structured Output Prediction

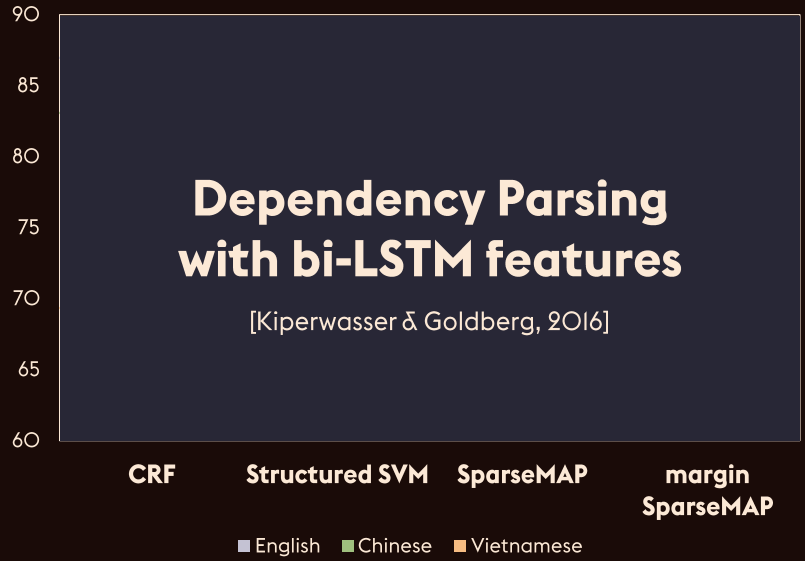
SparseMAP

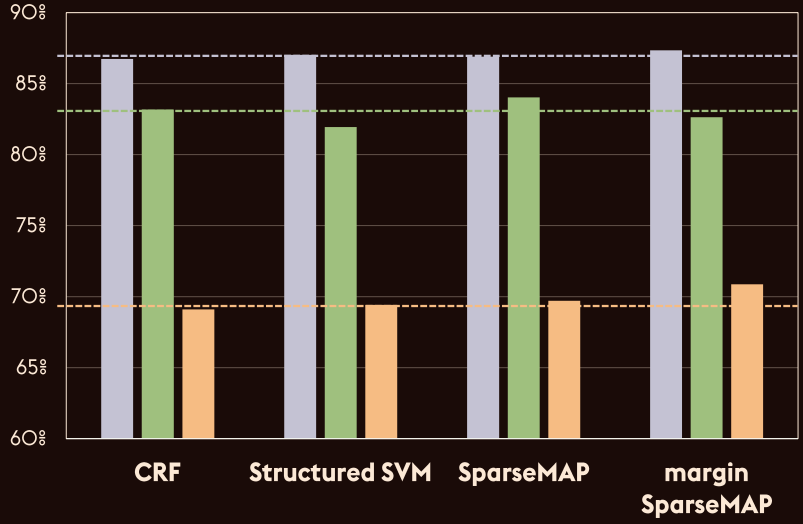
$$L_A(\boldsymbol{\eta}, \bar{\boldsymbol{\mu}}) = \max_{\boldsymbol{\mu} \in \mathcal{M}} \left\{ \boldsymbol{\eta}^\top \boldsymbol{\mu} - 1/2 \|\boldsymbol{\mu}\|^2 \right\} - \boldsymbol{\eta}^\top \bar{\boldsymbol{\mu}} + 1/2 \|\bar{\boldsymbol{\mu}}\|^2$$

cost-SparseMAP

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

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

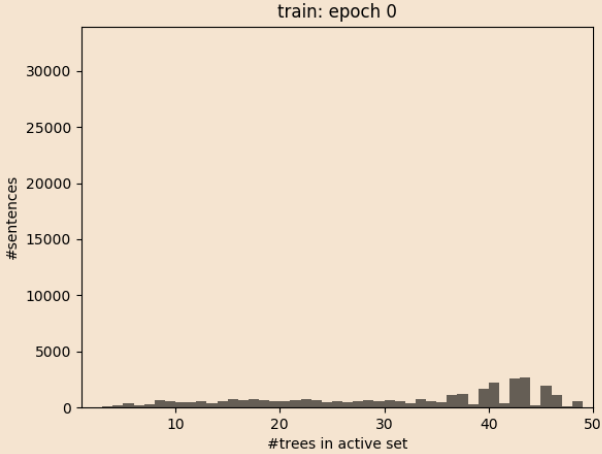

90
85
80
75
70
65
60
Dependency Parsing with bi-LSTM features
[Kiperwasser & Goldberg, 2016]
CRF
Structured SVM
SparseMAP
margin SparseMAP
English
Chinese
Vietnamese



Unlabeled Accuracy (UAS)
Universal Dependencies dataset

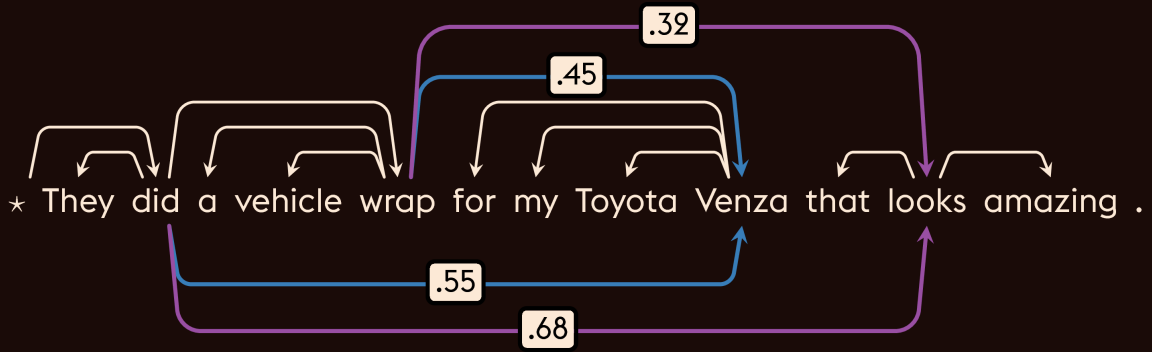
Sparse Structured Output Prediction

As models train, inference gets sparser!



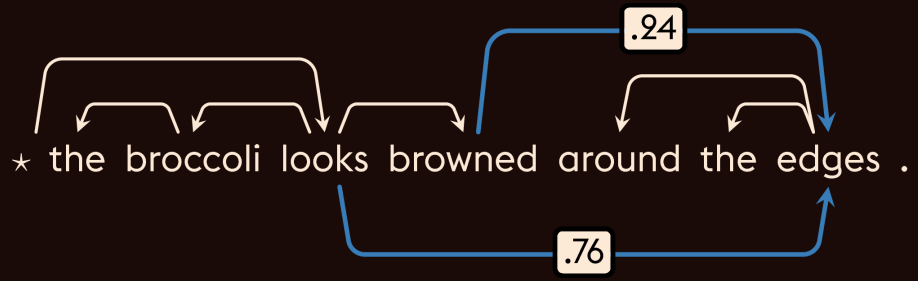
Sparse Structured Output Prediction

Inference captures linguistic ambiguity!



Sparse Structured Output Prediction

Inference captures linguistic ambiguity!



References I

Amos, Brandon and J. Zico Kolter (2017). "OptNet: Differentiable optimization as a layer in neural networks". In: *Proc. of ICML*.

Bertsekas, Dimitri P (1999). *Nonlinear Programming*. Athena Scientific Belmont.

Blondel, Mathieu, André FT Martins, and Vlad Niculae (2019). "Learning with Fenchel-Young Losses". In: *preprint arXiv:1901.02324*.

Brucker, Peter (1984). "An $O(n)$ algorithm for quadratic knapsack problems". In: *Operations Research Letters* 3.3, pp. 163–166.

Chen, Qian et al. (2017). "Enhanced LSTM for natural language inference". In: *Proc. of ACL*.

Condat, Laurent (2016). "Fast projection onto the simplex and the ℓ_1 ball". In: *Mathematical Programming* 158.1-2, pp. 575–585.

Danskin, John M (1966). "The theory of max-min, with applications". In: *SIAM Journal on Applied Mathematics* 14.4, pp. 641–664.

Dantzig, George B, Alex Orden, and Philip Wolfe (1955). "The generalized simplex method for minimizing a linear form under linear inequality restraints". In: *Pacific Journal of Mathematics* 5.2, pp. 183–195.

References II

Frank, Marguerite and Philip Wolfe (1956). “An algorithm for quadratic programming”. In: *Nav. Res. Log.* 3.1-2, pp. 95–110.

Gould, Stephen et al. (2016). “On differentiating parameterized argmin and argmax problems with application to bi-level optimization”. In: *preprint arXiv:1607.05447*.

Held, Michael, Philip Wolfe, and Harlan P Crowder (1974). “Validation of subgradient optimization”. In: *Mathematical Programming* 6.1, pp. 62–88.

Hill, Felix et al. (2016). “Learning to understand phrases by embedding the dictionary”. In: *TACL* 4.1, pp. 17–30.

Kim, Yoon et al. (2017). “Structured attention networks”. In: *Proc. of ICLR*.

Koo, Terry et al. (2007). “Structured prediction models via the matrix-tree theorem”. In: *Proc. of EMNLP*.

Lacoste-Julien, Simon and Martin Jaggi (2015). “On the global linear convergence of Frank-Wolfe optimization variants”. In: *Proc. of NeurIPS*.

References III

Liu, Yang and Mirella Lapata (2018). “Learning structured text representations”. In: *TACL 6*, pp. 63–75.

Malaviya, Chaitanya, Pedro Ferreira, and André F. T. Martins (2018). “Sparse and constrained attention for neural machine translation”. In: *Proc. of ACL*.

Martins, André FT and Ramón Fernandez Astudillo (2016). “From softmax to sparsemax: A sparse model of attention and multi-label classification”. In: *Proc. of ICML*.

Martins, André FT and Julia Kreutzer (2017). “Learning What’s Easy: Fully Differentiable Neural Easy-First Taggers”. In: *Proc. of EMNLP*, pp. 349–362.

McDonald, Ryan T and Giorgio Satta (2007). “On the complexity of non-projective data-driven dependency parsing”. In: *Proc. of ICPT*.

Niculae, Vlad and Mathieu Blondel (2017). “A regularized framework for sparse and structured neural attention”. In: *Proc. of NeurIPS*.

Niculae, Vlad, André FT Martins, Mathieu Blondel, et al. (2018). “SparseMAP: Differentiable sparse structured inference”. In: *Proc. of ICML*.

References IV

Niculae, Vlad, André FT Martins, and Claire Cardie (2018). “Towards dynamic computation graphs via sparse latent structure”. In: *Proc. of EMNLP*.

Nocedal, Jorge and Stephen Wright (1999). *Numerical Optimization*. Springer New York.

Rabiner, Lawrence R. (1989). “A tutorial on Hidden Markov Models and selected applications in speech recognition”. In: *P. IEEE* 77.2, pp. 257–286.

Smith, David A and Noah A Smith (2007). “Probabilistic models of nonprojective dependency trees”. In: *Proc. of EMNLP*.

Tai, Kai Sheng, Richard Socher, and Christopher D Manning (2015). “Improved semantic representations from tree-structured Long Short-Term Memory networks”. In: *Proc. of ACL-IJCNLP*.

Taskar, Ben (2004). “Learning structured prediction models: A large margin approach”. PhD thesis. Stanford University.

Tibshirani, Robert et al. (2005). “Sparsity and smoothness via the fused lasso”. In: *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 67.1, pp. 91–108.

References V

Valiant, Leslie G (1979). “The complexity of computing the permanent”. In: *Theor. Comput. Sci.* 8.2, pp. 189–201.

Vinyes, Marina and Guillaume Obozinski (2017). “ Fast column generation for atomic norm regularization”. In: *Proc. of AISTATS*.

Wolfe, Philip (1976). “Finding the nearest point in a polytope”. In: *Mathematical Programming* 11.1, pp. 128–149.