$\tilde{O}$ 

### marginalize over sparse distributions when training latent variable models

vlad niculae Itl uva

work with: gonçalo m. correia, wilker aziz, andré martins, mathieu blondel

🖸 github.com/deep-spin/sparse-marginalization-lvm 🛛 🏠 https://vene.ro

## helpful discrete labels

#### input

x="red tape holds up bridge"



#### output



classifier: Pr(y|x)

# helpful discrete labels

#### input

x="red tape holds up bridge"

what if we knew the newspaper category?







#### output



### helpful structure

#### input

x="squad help dog bite victim"

syntactic analysis



or is it





#### output



 $\Pr(y|x, z).$ 

### deep nets $\delta$ hope for the best



# pipeline approach



### this talk: latent variables



$$\Pr(y|x) = \sum_{z \in \mathcal{Z}} \Pr(z \mid x) \Pr(y \mid x, z).$$

### bird's eye view



### how to learn this

explicit marginalization



$$\Pr(\mathbf{y}|\mathbf{x}) = \sum_{z \in \mathcal{Z}} \Pr(z|\mathbf{x}) \Pr(\mathbf{y}|\mathbf{x}, z)$$

exact, but always slow

### how to learn this

sampling



$$\Pr(\mathbf{y}|\mathbf{x}) = \sum_{z \in \mathcal{Z}} \Pr(z|\mathbf{x}) \Pr(\mathbf{y}|\mathbf{x}, z)$$

exact, but always slow

 $\Pr(\mathbf{y}|\mathbf{x}) = \mathbb{E}_{\mathbf{z}} \Pr(\mathbf{y}|\mathbf{x}, \mathbf{z})$ 

 $\approx \Pr(y|z^+, x)$ 

always fast, but inexact, noisy

# how to learn this

#### explicit marginalization



$$\Pr(\mathbf{y}|\mathbf{x}) = \sum_{z \in \mathcal{Z}} \Pr(z|\mathbf{x}) \Pr(\mathbf{y}|\mathbf{x}, z)$$

exact, but always slow



# this talk: sparse marginalization



exact and fast, adaptive acceleration!

 $\Pr(y|x) = \mathbb{E}_z \Pr(y|x, z)$  $\approx \Pr(y|z^+, x)$ 

always fast, but inexact, noisy

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

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### second-guessing softmax

the "standard" way to map scores to probabilities (softmax / gibbs / boltzmann / ... distribution)

$$\Pr(h|x) = \frac{\exp s_i}{\sum_j \exp s_j} > 0$$

# second-guessing softmax

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$$\Pr(h|x) = \frac{\exp s_i}{\sum_j \exp s_j} > 0$$

is secretly entropy regularization:

$$\underset{\boldsymbol{p} \in \Delta}{\arg\max \boldsymbol{s}^{\mathsf{T}} \boldsymbol{p}} - \underbrace{\sum_{j} p_{j} \log p_{j}}_{\boldsymbol{H}(\boldsymbol{p})}$$



softmax

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why not try the euclidean norm?



we have  $\sim \sim \sim$  sparsity! algorithms! cool name!



sparsemax (Martins and Astudillo, 2016)

sparsemax(
$$\boldsymbol{s}$$
) = arg max  $\boldsymbol{p}^{\top}\boldsymbol{s} - \frac{1}{2} \|\boldsymbol{p}\|_{2}^{2}$   
 $\boldsymbol{p} \in \Delta$   
= arg min  $\|\boldsymbol{p} - \boldsymbol{s}\|_{2}^{2}$   
 $\boldsymbol{p} \in \Delta$ 

sparsemax(
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computation:

 $\boldsymbol{p}^{\star} = [\boldsymbol{s} - \tau \boldsymbol{1}]_{+}$  $s_{i} > s_{j} \Rightarrow p_{i} \ge p_{j}$ expected O(d) via selection

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

sparsemax(
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) = arg max  $\mathbf{p}^{\top}\mathbf{s} - \frac{1}{2} \|\mathbf{p}\|_{2}^{2}$   
= arg min  $\|\mathbf{p} - \mathbf{s}\|_{2}^{2}$   
mputation:  
 $\mathbf{p} \in \Delta$   
backward pass:  
 $\mathbf{f} = [\mathbf{s} - \tau \mathbf{1}]_{+}$   
 $\mathbf{s}_{s} \Rightarrow \mathbf{p}_{i} > \mathbf{p}_{i}$   
where  $S = \{i : \mathbf{p}^{*} > 0\}$ 

$$p^{\star} = [s - \tau \mathbf{1}]_+$$
  
 $s_i > s_j \Rightarrow p_i \ge p_j$   
expected  $O(d)$  via selection

со

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

$$\begin{aligned} \mathbf{J}_{\text{sparsemax}} &= \text{diag}(\mathbf{s}) - \frac{1}{|\mathcal{S}|} \mathbf{s} \mathbf{s}^{\top} \\ \text{where } \mathcal{S} &= \{j : p_{j}^{\star} > 0\}, \\ s_{j} &= [\![j \in \mathcal{S}]\!] \end{aligned}$$

(Martins and Astudillo, 2016)

sparsemax(
$$s$$
) = arg max  $p^{T}s - 1/2 ||p||_{2}^{2}$   
= arg min  $||p - s||_{2}^{2}$   
computation: backward pass:  
 $p^{\star} = [s - s_{i} > s_{j} \Rightarrow s_{j} \Rightarrow s_{i} > s_{j} \Rightarrow s_{i} > s_{i} > s_{j} \Rightarrow s_{i} > s_{i} > s_{j} \Rightarrow s_{i} > s_{i} > s_{i} > s_{j} \Rightarrow s_{i} = arg min differentiation (Colson et al., 2007; Gould et al., 2016)
see also (Amos and Kolter, 2017)  $|is| \in S$$ 

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

(Martins and Astudillo, 2016)

## some applications:

sparse attention

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

sparse losses (& seq2seq)



$$d \rightarrow r \rightarrow a \rightarrow w \xrightarrow{66.4\%} e \rightarrow d \rightarrow$$

$$32.2\%$$

$$32.2\%$$

$$n \rightarrow$$

$$1.4\%$$

$$$$

### sparsemax enables fast marginalization!



#### saves us from computing Pr(y|x, z) for many $z \in \mathbb{Z}$ !

### emergent communication

$$\sum_{z \in \mathcal{Z}} \Pr(z|x) \Pr(x|z, \mathcal{V})$$

- game between two players.
- sender takes x from imagenet, and summarizes it in a message z (here: one symbol).
- receiver sees the symbol, and a group of images  $\mathcal{V} \ni x$ , and must pick the intended image.

### emergent communication



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#### (Lazaridou et al., 2017; Correia, Niculae, Aziz, et al., 2020) **emergent communication** . but make it harder: $|\mathcal{Z}| = 256$ , $|\mathcal{V}| = 16$

Method	success (%)	Dec. calls
monte carlo		
sfe	33.05 ±2.84	1
sfe+	$44.32 \pm 2.72$	2
nvil	$37.04 \pm 1.61$	1
gumbel	23.51 ±16.19	1
st-gumbel	$27.42 \pm 13.36$	1

marginalization

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marginalization		
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sparsemax	93.35 ±0.50	$3.13_{\pm 0.48}$

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$$\sum_{z\in\mathcal{Z}}\Pr\left(z|x\right)\ell(x,z)$$

- semi-supervised vae on mnist: *z* is one of 10 categories
- train with 10% labeled data



- semi-supervised vae on mnist: z is one of 10 categories
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- semi-supervised vae on mnist: z is one of 10 categories
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method	accuracy (%)	dec. calls
monte carlo sfe sfe+ nvil gumbel	$\begin{array}{c} 94.75 \scriptstyle \pm .002 \\ 96.53 \scriptstyle \pm .001 \\ 96.01 \scriptstyle \pm .002 \\ 95.46 \scriptstyle \pm .001 \end{array}$	1 2 1 1
marginalizatio softmax sparsemax	on 96.93±.001 96.87±.001	10 1.01±0.01



# limitations

- mostly (and eventually) very sparse. worst case: fully dense
- $\rightarrow$  sparsemax can't handle structured z

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today's solution: top-k sparsemax k-sparsemax $(s) = \underset{p \in \Delta, ||p||_0 \le k}{\text{arg min}} ||p - s||_2^2$ 

# limitations

- mostly (and eventually) very sparse. worst case: fully dense
- $\rightarrow$  sparsemax can't handle structured z

today's solution: top-k sparsemax k-sparsemax $(s) = \underset{p \in \Delta, ||p||_0 \le k}{\text{arg min}} ||p - s||_2^2$ 

- 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 z gets Pr(z|x) = 0, k-sparsemax = sparsemax! starts with bias, sheds the bias along the way

#### bit-vector variational autoencoder

 $\sum q(z|x) \ell(x,z)$  $z \in \{0,1\}^D$ 

# bit-vector variational autoencoder

for elbo: 
$$\ell(x, z) = -\log \frac{\Pr(x, z)}{q(z|x)}$$

$$\sum_{z \in \{0,1\}^D} q(z|x) \ell(x, \tilde{z})$$

posterior approx / inference network

• vae where z is a collection of D bits

# bit-vector variational autoencoder for elbo: $l(x, z) = -\log \frac{\Pr(x, z)}{q(z|x)}$ exponentially large sum $\sum_{z \in \{0,1\}^D} q(z|x) \ell(x, \tilde{z})$ posterior approx / inference network

• vae where z is a collection of D bits

<b>test nll</b> (bits/dim), lower is better								
method	D = 32	D = 128						
monte carlo								
sfe	3.74	3.77						
sfe+	3.61	3.59						
nvil	3.65	3.60						
gumbel	3.57	3.49						
marginalization softmax/sparsemax		_						
top-k sparsemax	3.62	3.61						

D = 128

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Rate (nats)

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marginalize over sparse distributions when training latent variable models

🜍 github.com/deep-spin/sparse-marginalization-lvm 🏤 vene.ro

marginalize over sparse distributions when training latent variable models

discrete and structured

0.2 0.6 0.1 0.4 0.4 0.5 0.5 0.3

🜍 github.com/deep-spin/sparse-marginalization-lvm 🏻 🆀 vene.ro

marginalize over sparse distributions when training latent variable models



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# **Extra slides**

## Acknowledgements



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

finally

is essentially a (very high-dimensional) argmax



#### is essentially a (very high-dimensional) argmax



is essentially a (very high-dimensional) argmax



on wheels dog  $\star$ 

















∗→dog	1	0	0		.1	I
on→dog	0	1	1		.2	I
wheels→dog	0	0	0		1	
*→on	0	1	1		.3	
<b>A</b> = dog→on	1	0	0	 <b>η</b> =	.8	
wheels→on	0	0	0		.1	
★→wheels	0	0	0		3	
dog→wheels	0	1	0		.2	
on→wheels	1	0	1		1	



	dog-hond	[ 1	0	0		.1
	dog—op	0	1	1		.2
	dog—wielen	0	0	0		1
	on-hond	0	0	0		.3
<b>A</b> =	on—op	1	 0	0	<b>η</b> =	.8
	on-wielen	0	1	1		.1
wł	eels-hond	0	1	0		3
wł	neels—op	0	0	0		.2
wł	neels-wielen	1	0	1		1











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





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$$= \left\{ \boldsymbol{A}\boldsymbol{p} : \boldsymbol{p} \in \Delta \right\}$$
$$= \left\{ \mathbb{E}_{H \sim \boldsymbol{p}} \boldsymbol{a}_{H} : \boldsymbol{p} \in \Delta \right\}$$






















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





• **argmax** arg max  $p^T s$  $p \in \Delta$ 



#### • softmax $\arg \max p^{\top} s + H(p)$ $p \in \Delta$





- **argmax**  $\arg \max p^T s$  $p \in \Delta$
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- **argmax** arg max  $p^{\top}s$  $p \in \Delta$
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 $\mathbf{MAP} \underset{\boldsymbol{\mu} \in \mathcal{M}}{\operatorname{arg\,max}} \boldsymbol{\mu}^{\mathsf{T}} \boldsymbol{\eta} \qquad \bullet$ marginals  $\operatorname{arg\,max} \boldsymbol{\mu}^{\mathsf{T}} \boldsymbol{\eta} + \widetilde{\mathsf{H}}(\boldsymbol{\mu}) \qquad \bullet$  $\boldsymbol{\mu} \in \mathcal{M}$ 

#### *e.g.* sequence labeling $\rightarrow$ forward-backward

(Rabiner, 1989)

As attention: (Kim et al., 2017)





• **argmax** arg max  $p^T s$  $p \in \Delta$ 

softmax  $\arg \max p^{\top}s + H(p)$  $p \in \Delta$ 

$$\mathbf{MAP} \operatorname{arg\,max} \boldsymbol{\mu}^{\mathsf{T}} \boldsymbol{\eta} \qquad \bullet \\ \boldsymbol{\mu} \in \mathcal{M} \qquad \bullet \\ \mathbf{marginals} \operatorname{arg\,max} \boldsymbol{\mu}^{\mathsf{T}} \boldsymbol{\eta} + \widetilde{\mathsf{H}}(\boldsymbol{\mu}) \qquad \bullet \\ \boldsymbol{\mu} \in \mathcal{M} \qquad \bullet \\ \mathbf{\mu} \in \mathcal{M} \qquad$$

#### e.g. dependency parsing $\rightarrow$ 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)







softmax  $\arg \max p^{\top}s + H(p)$  $p \in \Delta$   $\mathbf{MAP} \operatorname{arg\,max}_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^{\mathsf{T}} \boldsymbol{\eta} \qquad \bullet$ marginals  $\operatorname{arg\,max}_{\boldsymbol{\mu} \in \mathcal{M}} \boldsymbol{\mu}^{\mathsf{T}} \boldsymbol{\eta} + \widetilde{\mathsf{H}}(\boldsymbol{\mu}) \qquad \bullet$ 



• softmax  $\arg \max \mathbf{p}^{\mathsf{T}}\mathbf{s} + \mathsf{H}(\mathbf{p})$  $\mathbf{p} \in \Delta$ 

• sparsemax  $\arg \max p^{\top} s - \frac{1}{2} ||p||^2$  $p \in \Delta$ 

$$\mathbf{MAP} \operatorname{arg\,max} \boldsymbol{\mu}^{\mathsf{T}} \boldsymbol{\eta} \qquad \bullet \\ \boldsymbol{\mu} \in \mathcal{M} \qquad \bullet \\ \mathbf{marginals} \operatorname{arg\,max} \boldsymbol{\mu}^{\mathsf{T}} \boldsymbol{\eta} + \widetilde{\mathsf{H}}(\boldsymbol{\mu}) \qquad \bullet \\ \boldsymbol{\mu} \in \mathcal{M} \qquad \bullet \\ \mathbf{\mu} \in \mathcal{M} \qquad$$





• **argmax**  $\arg \max p^T s$  $p \in \Delta$ 

• softmax  $\arg \max p^T s + H(p)$  $p \in \Delta$ 

• sparsemax  $\arg \max p^{T}s - \frac{1}{2} \|p\|^{2}$  $p \in \Delta$  (Niculae, Martins, Blondel, and Cardie, 2018) **MAP** arg max $\mu^{T}\eta$  •  $\mu \in \mathcal{M}$  **marginals** arg max $\mu^{T}\eta + \widetilde{H}(\mu)$  •  $\mu \in \mathcal{M}$  **SparseMAP** arg max $\mu^{T}\eta - 1/2||\mu||^{2}$  •  $\mu \in \mathcal{M}$ 





# **Algorithms for SparseMAP**

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

Algorithms for SparseMAP  

$$\mu^{\star} = \arg \max \mu^{\top} \eta - 1/2 \|\mu\|^{2}$$
Inter constraints  
(alas, exponentially many!) (alas, exponentially many!) (blue) (blue) (classified of the second second



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

Algorithms for SparseMAP  

$$\mu^{\star} = \arg \max \mu^{\top} \eta - 1/2 \|\mu\|^{2}$$
(alas, exponentially many!)  

$$\mu \in \mathcal{M}$$
(alas, exponentially many!)

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

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

Algorithms for SparseMAP  

$$\mu^{\star} = \arg \max \mu^{\top} \eta - 1/2 \|\mu\|^{2}$$
Inter constraints  
(alas, exponentially many!) (under a constraints) (under a constraints)

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

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

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

Algorithms for SparseMAP  

$$\mu^{\star} = \arg \max \mu^{\top} \eta - 1/2 \|\mu\|^{2}$$
Inter constraints  
(alas, exponentially many!) (under a constraints) (under a constraints)

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

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

Algorithms for SparseMAP  

$$\mu^{*} = \arg \max \mu^{\top} \eta - 1/2 \|\mu\|^{2}$$
Inter constraints  
(alas, exponentially many!)
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(black)

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

- select a new corner of  ${\cal M}$
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  - Quadratic objective: Active Set (Nocedal and Wright, 1999, Ch. 16.4 & 16.5) (Wolfe, 1976; Vinyes and Obozinski, 2017)

# Algorithms for SparseMAP $\mu^{\star} = \arg \max \mu^{\top} \eta - 1/2 \|\mu\|^{2}$ Inter constraints (alas, exponentially many!) (alas, exponentially many!) (black)

Active Set achieves

#### **Conditional Gradient**

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

- select a new corne
- update the (sparse
  - Update rules: var pairwise **finite** & **linear** convergence!
  - Quadratic objecti

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

Algorithms for SparseMAP  

$$\mu^{\star} = \arg \max \mu^{\top} \eta - 1/2 \|\mu\|^{2}$$
Inter constraints  
(alas, exponentially many!) (ultrace) (ultra

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

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**Backward pass** 

Algorithms for SparseMAP  

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(alas, exponentially many!)

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Backward pass

$$\frac{\partial \boldsymbol{\mu}}{\partial \boldsymbol{\eta}} \text{ is sparse} \\ \text{computing } \left(\frac{\partial \boldsymbol{\mu}}{\partial \boldsymbol{\eta}}\right)^{\mathsf{T}} \boldsymbol{d} y \\ \text{cakes } O(\dim(\boldsymbol{\mu}) \operatorname{nnz}(\boldsymbol{p}^*)) \end{cases}$$



(Wolfe, 1976; Vinyes and Obozinski, 2017)













(Tai et al., 2015)



#### The bears eat the pretty ones

### Latent Dependency TreeLSTM

(Niculae, Martins, and Cardie, 2018)



output

y

\_X

input

# Latent Dependency TreeLSTM

(Niculae, Martins, and Cardie, 2018)

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



output y

input

X

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

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

e.g., a TreeLSTM defined by h  $p(y \mid x) = \sum p'_{\phi}(y \mid h, x) p_{\pi}(h \mid x)$ h∈H

e.g., a TreeLSTM defined by h  $p(y \mid x) = \sum_{h \in \mathcal{H}} p_{\phi}'(y \mid h, x) p_{\pi}(h \mid x)$ latent classifier



#### Exponentially large sum!



idea 1

idea 2

idea 3



idea 3



idea 3














# **SparseMAP**



# **SparseMAP**

## $\bullet \bullet \bullet \bullet = .7 \qquad \bullet \bullet \bullet \bullet + .3 \qquad \bullet \bullet \bullet \bullet \bullet \bullet \bullet + ...$

# **SparseMAP**

# $f(y \mid x) = .7 \quad f(y \mid e^{-y}) + .3 \quad e^{-y} + 0 \quad e^{-y} + ...$ $p(y \mid x) = .7 \quad p_{\phi}(y \mid e^{-y}) + .3 \quad p_{\phi}(y \mid e^{-y})$

















## Sentiment classification (SST)





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



**Reverse dictionary lookup** 

given word description, predict word embedding (Hill et al., 2016) instead of p(y | x), we model  $\mathbb{E}_{p_m} g(x) = \sum_{h \in \mathcal{H}} g(x; h) p_m(h | x)$ 

#### Sentiment classification (SST) Natural Language Inference (SNLI) 82% accuracy accuracy 81.8% -(binarv) (3-class) 81.6% -83% -81.4% -81.2% -82% -81% -80.8% -80.6% -80 % Flat CoreNLP Latent LTR Flat CoreNLP Latent **Reverse dictionary lookup** (definitions) (concepts) 38 % accuracy@10 accuracy@10 38% -32% -32% -30 % LTR Flat Latent Flat Latent

## **Sentiment classification** (SST)



## Natural Language Inference (SNLI)



**Reverse dictionary lookup** 

## (definitions)



(concepts)



# Syntax vs. Composition Order



# Syntax vs. Composition Order

p = 22.6%



CoreNLP parse, p = 21.4%



# Syntax vs. Composition Order

\*

\*

p = 15.33%

