Differentiable dynamic programming for structured prediction and attention

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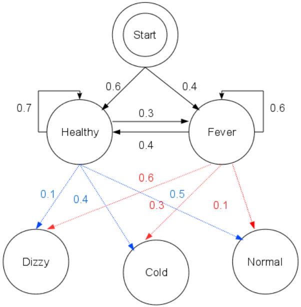
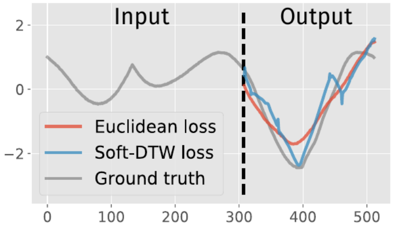
Dynamic programming in machine learning



(Fig: Wikipedia)

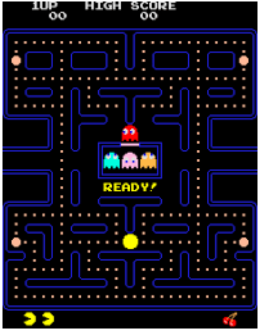
Belief propagation

Viterbi algorithm



(Fig: Cuturi & Blondel)

Dynamic time warping



Value iteration

New layers for deep predictive modelling

Dynamic programming

- Function evaluation on a big space
- From evaluation on smaller space (divide and conquer)

Modern machine learning

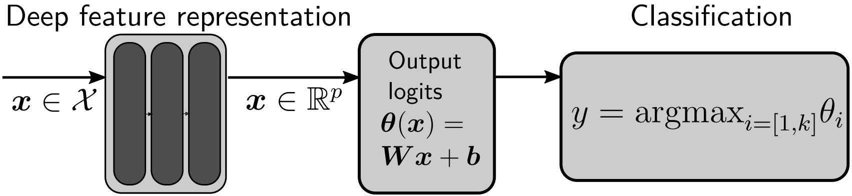
- Modular models, trainable with gradient descent

This talk: Principled differentiable dynamic programming layers

- Application to complex predictive models (e.g. attention mechanisms)
- Sparse output probabilities in structured setting

Modular structured prediction: potentials + linear programming

Classification: $\mathcal{Y} = [1, k]$



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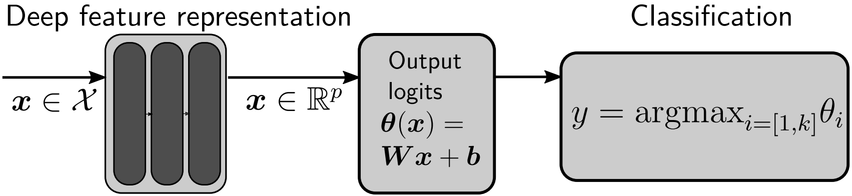

Structured output ? $\mathcal{Y} \subset \mathbb{R}^D$ (edges of a polytope), *e.g.* a tag sequence

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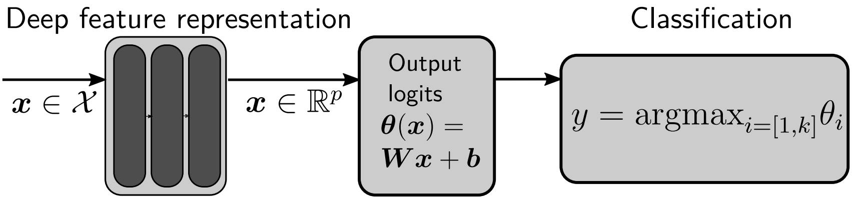

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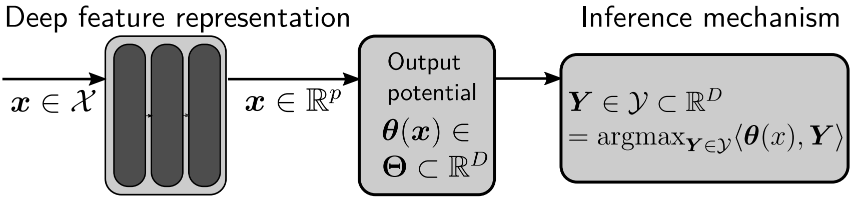
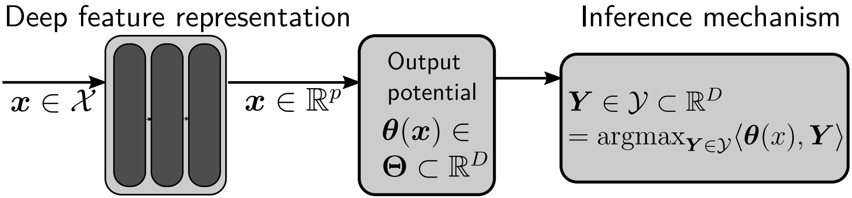
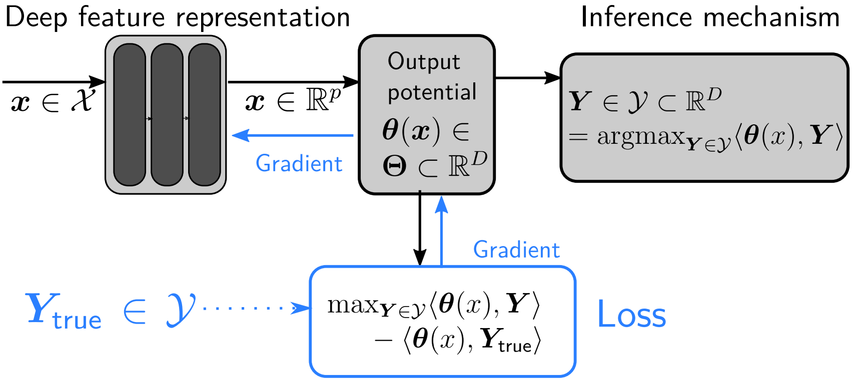


Structure prediction:



Training

Structure prediction: *Structured perceptron loss*



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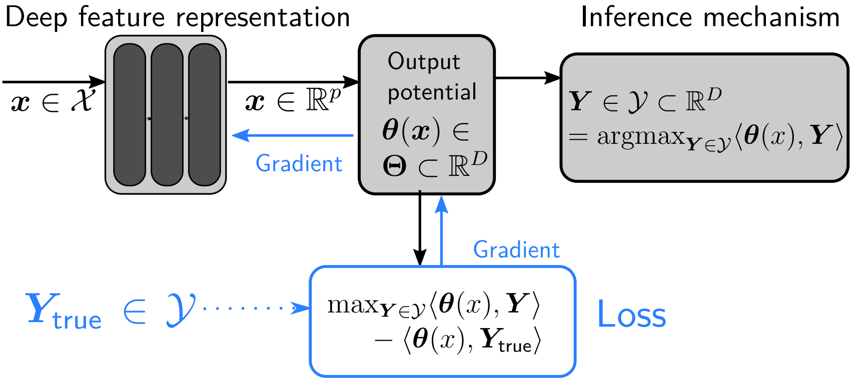

Backprop through the max operator.

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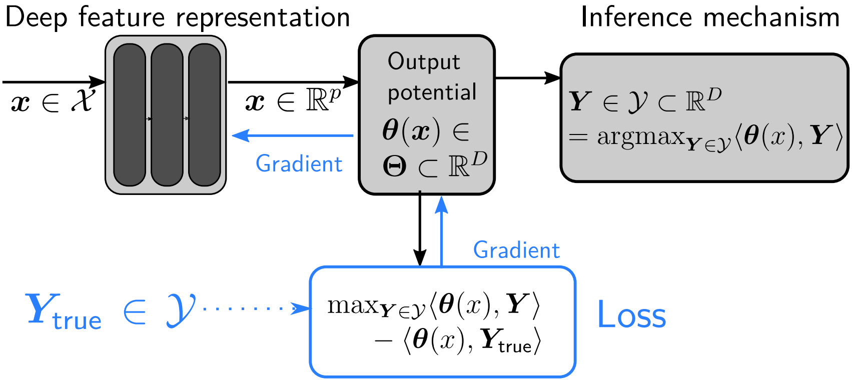
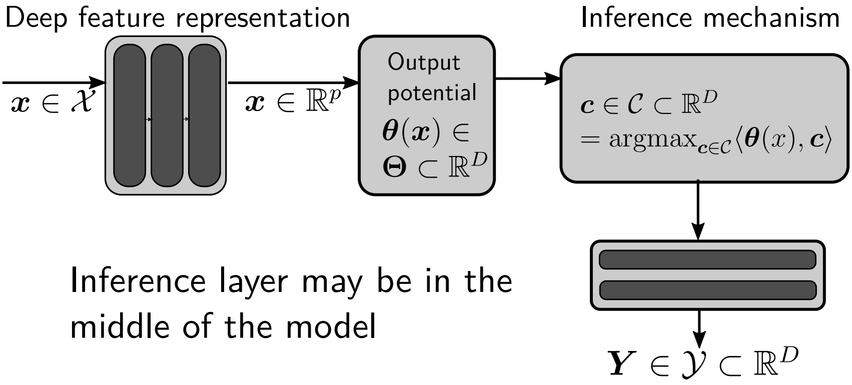


Backprop through the max operator. Not differentiable everywhere.

Structured prediction as an inner layer

Example: Attention mechanisms,[1] where $\boldsymbol{c}$ are the attention weights.



Inference layer may be in the middle of the model

[1] Dzmitry Bahdanau et al. (2015). "Neural Machine Translation by Jointly Learning to Align and Translate". In: *Proc. of ICLR*.

Structured prediction as an inner layer

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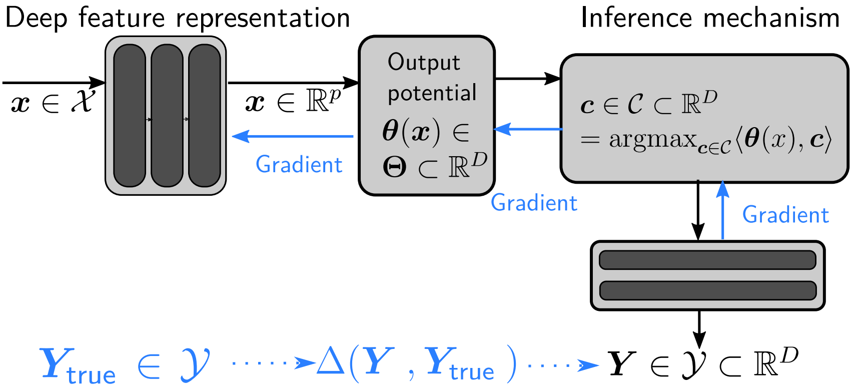

We need to backpropagate through the argmax.

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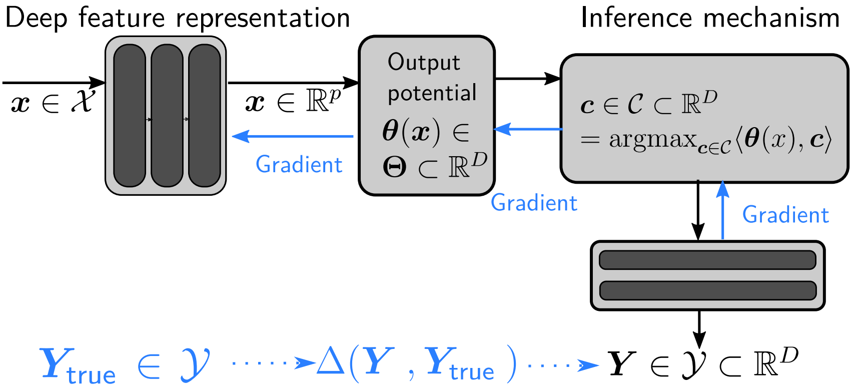

We need to backpropagate through the argmax. Zero gradient.

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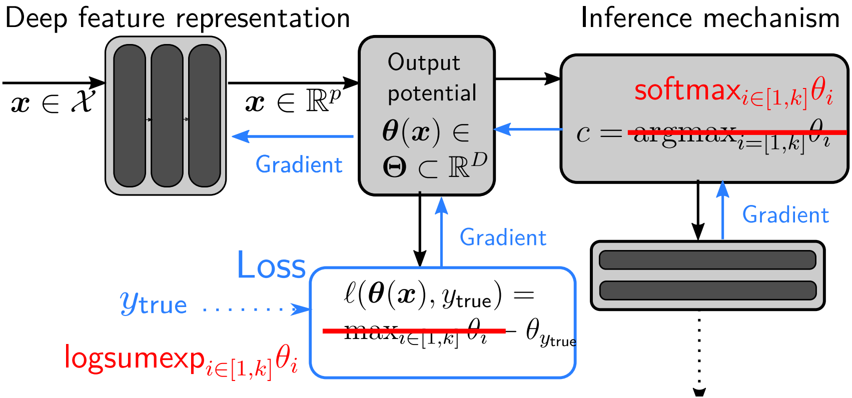
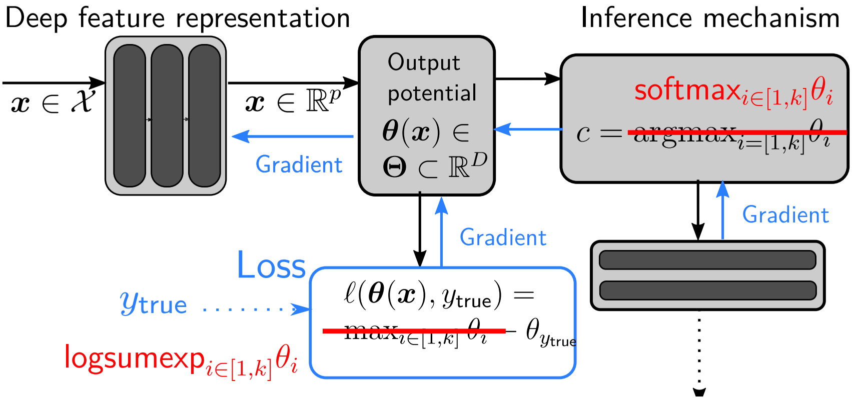
Gradient from regularization: from max to softmax



Gradient from regularization: from max to softmax



Multinomial loss, softmax attention: **differentiable layers**

Questions and goal

- From **max** to **softmax**: Where does this comes from and can we use different smoothing techniques ?

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- How to smooth a wide class of **structured prediction** LP problems?

$$\max_{\boldsymbol{Y} \in \mathcal{Y}} \langle \boldsymbol{\theta}(x), \boldsymbol{Y} \rangle \qquad \boldsymbol{Y} \in \mathcal{Y} \subset \mathbb{R}^D = \operatorname*{argmax}_{\boldsymbol{Y} \in \mathcal{Y}} \langle \boldsymbol{\theta}(x), \boldsymbol{Y} \rangle$$

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Focus on inference mechanisms that relies on **dynamic programming**

- Smooth **max** layers for new structured losses
- Differentiable **argmax** layers for test and inner inference mechanisms

Contributions

Generic framework for differentiable structured prediction:

- Regularizing the max operators with strongly convex penalties.
- May output **sparse** continuous outputs

Applications:

- End-to-end audio to score alignment
- Named entity recognition with sparse predictions
- Block sparse attention mechanisms

Extends and ground in theory[2,3,4,5]

[2] Yann LeCun et al. (2006). "A tutorial on energy-based learning". In: *Predicting structured data* 1.0.

[3] Guillaume Lample et al. (2016). "Neural Architectures for Named Entity Recognition". In: *Proc. of NAACL*, pp. 260–270.

[4] Yoon Kim et al. (2017). "Structured Attention Networks". In: *Proc. of ICLR*.

[5] Marco Cuturi and Mathieu Blondel (2017). "Soft-DTW: a Differentiable Loss Function for Time-Series". In: *Proc. of ICML*, pp. 894–903.

Dynamic programming

Dynamic programming solve the structure prediction problem

$$\mathrm{LP}(\boldsymbol{\theta}) \triangleq \max_{\boldsymbol{Y} \in \mathcal{Y}} \langle \boldsymbol{\theta}, \boldsymbol{Y} \rangle$$

by splitting the combinatorial set $\mathcal{Y} \subset \mathbb{R}^D$ into **sets of smaller dimensions**

- Compute $\mathrm{LP}(\boldsymbol{\theta})$ in linear time $\mathcal{O}(D)$ vs exponential naive resolution

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Also provide the **argmax** in $\mathcal{O}(D)$:

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Examples:

- Viterbi algorithm for infering tag sequences
- Dynamic time warping algorithm for infering alignment matrices

Dynamic programming as best path in a DAG

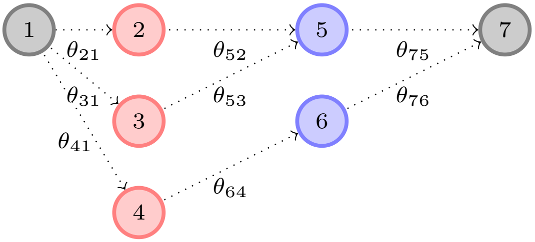
Directed acyclic graph

- $G = (\mathcal{N}, \mathcal{E})$, with 1 root and 1 leaf, nodes numbered in topo. order $[1, N]$
- Edge (i, j) has weight $\theta_{i,j}$ — j parent, i child. $\boldsymbol{\theta} \in \mathbb{R}^{n \times n}$ incidence matrix
- Path $\boldsymbol{Y} \in \mathcal{Y} \subset \{0, 1\}^{N \times N}$: $y_{i,j} = 1$ iff (i, j) is taken

Single path value: $\langle \boldsymbol{Y}, \boldsymbol{\theta} \rangle$

Highest score among all paths

$$\mathrm{LP}(\boldsymbol{\theta}) = \max_{\boldsymbol{Y} \in \mathcal{Y}} \langle \boldsymbol{Y}, \boldsymbol{\theta} \rangle$$



Maximum value computation (finding the max)

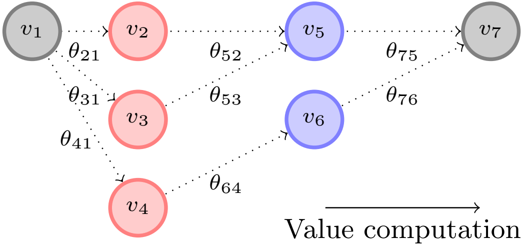
- **Max value from 1 to i**

$$v_i(\boldsymbol{\theta}) = \max_{j \in \mathcal{P}_i} \theta_{i,j} + v_j(\boldsymbol{\theta})$$

- One pass over the graph

$$(v_1 = 0, v_2, \ldots, v_n \triangleq \mathrm{DP}(\boldsymbol{\theta}))$$

= **Bellman equation**



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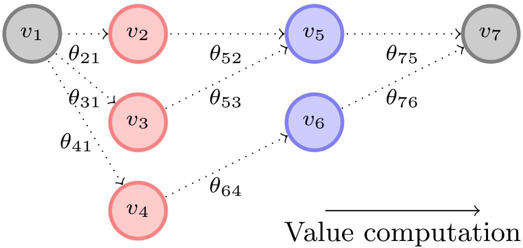

The DP recursion solves the linear problem (Bellman, 1958)

$$\mathrm{DP}(\boldsymbol{\theta}) = \mathrm{LP}(\boldsymbol{\theta}) = \max_{\boldsymbol{Y} \in \mathcal{Y}} \langle \boldsymbol{Y}, \boldsymbol{\theta} \rangle$$

Best path computation (finding the argmax)

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The argmax is computable using backpropagation = backtracking

Danskin theorem (Danskin, 1966)

$$\partial \mathrm{DP}(\boldsymbol{\theta}) = \partial_{\boldsymbol{\theta}}(\boldsymbol{\theta} \to \max_{\boldsymbol{Y} \in \mathcal{Y}} \langle \boldsymbol{Y}, \boldsymbol{\theta} \rangle)) = \mathrm{conv}(\operatorname*{argmax}_{\boldsymbol{Y} \in \mathcal{Y}} \langle \boldsymbol{Y}, \boldsymbol{\theta} \rangle)$$

- When the argmax is unique: $\partial_{\boldsymbol{\theta}} \mathrm{DP}(\boldsymbol{\theta}) = \mathrm{argmax}_{\boldsymbol{Y} \in \mathcal{Y}} \langle \boldsymbol{Y}, \boldsymbol{\theta} \rangle$

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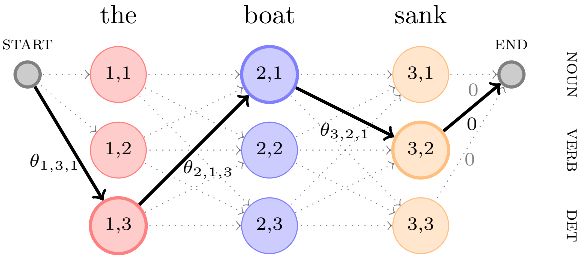
Dynamic programming layers

- **Max** layer: $\boldsymbol{\theta} \to \mathrm{DP}(\boldsymbol{\theta}) = \max_{\boldsymbol{Y}} \langle \boldsymbol{Y}, \boldsymbol{\theta} \rangle$
- **Argmax** layer: $\boldsymbol{\theta} \to \partial_{\boldsymbol{\theta}} \mathrm{DP}(\boldsymbol{\theta}) \sim \operatorname{argmax}_{\boldsymbol{Y}} \langle \boldsymbol{Y}, \boldsymbol{\theta} \rangle$

Example: Linear conditional random field

$(\boldsymbol{x}_1, \dots, \boldsymbol{x}_T)$ observation, $(y_1, \dots, y_T) \in [S]^T$ states. $\boldsymbol{Y} \in \mathcal{Y} \in \{0, 1\}^{S \times S \times T}$

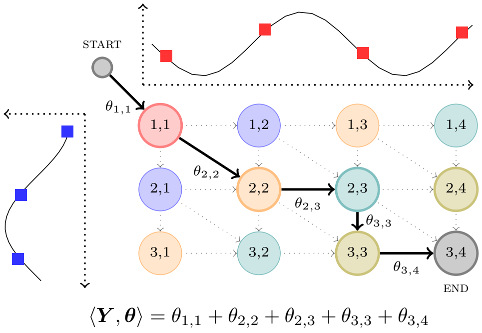
$$\boldsymbol{y} = \operatorname*{argmax}_{\boldsymbol{y} \in \mathcal{Y}} \sum_{t=1}^{T} \theta_t(y_t, y_{t-1}, \boldsymbol{x}_t) = \operatorname*{argmax}_{\boldsymbol{Y} \in \mathcal{Y}} \langle \boldsymbol{\theta}, \boldsymbol{Y} \rangle$$



$$\langle \boldsymbol{Y}, \boldsymbol{\theta} \rangle = \theta_{1,3,1} + \theta_{2,1,3} + \theta_{3,2,1}$$

$\boldsymbol{Y}$ computed with dynamic programming = **Viterbi algorithm.**

Example: Dynamic time warping



Elastic matching

- Two time-series $\boldsymbol{A}$, $\boldsymbol{B}$
- Distance matrix: $\boldsymbol{\theta}_{i,j} = \|a_i - b_i\|_2^2$

Alignment matrices

- $(1,1) \to (N_A, N_B)$
- $\downarrow, \rightarrow, \searrow$ moves

Best alignment: $\boldsymbol{Y}(\boldsymbol{A}, \boldsymbol{B}) = \underset{\boldsymbol{Y} \in \mathcal{Y}}{\operatorname{argmax}} \langle \boldsymbol{Y}, \boldsymbol{\theta} \rangle$

DTW distance: $d(\boldsymbol{A}, \boldsymbol{B}) = \max_{\boldsymbol{Y} \in \mathcal{Y}} \langle \boldsymbol{Y}, \boldsymbol{\theta} \rangle$

Computable by dynamic programming

- $\mathcal{Y}$ set of alignment matrices
- $\boldsymbol{\theta}$ distance matrix

Regularizing dynamic programming

Obstacles to end-to-end training

- Max layer $\boldsymbol{\theta} \to \mathrm{DP}(\boldsymbol{\theta})$ is not differentiable everywhere
- Argmax layer $\boldsymbol{\theta} \to \partial\mathrm{DP}(\boldsymbol{\theta})$ is piecewise constant / not defined

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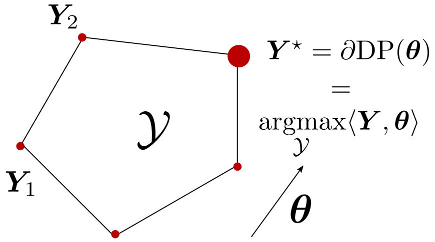
Culprit is the Bellman recursion

$$\boldsymbol{x} \in \mathbb{R}^d \to \max(\boldsymbol{x}) \in \mathbb{R}$$

- Not differentiable everywhere
- Piecewise linear (null Hessian)



Hard geometry

Regularizing dynamic programming

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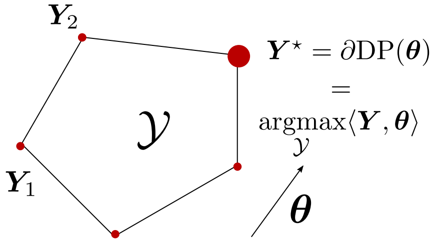

Hard geometry

Solution: smooth the maximum operator

Max smoothing

$\Omega : \mathbb{R} \to \mathbb{R}$ strongly-convex function. $\boldsymbol{x} \in \mathbb{R}^d$. Δ^d: d-dim simplex.

Smoothed max operator (Moreau, 1965; Nesterov, 2005)

$$\max_\Omega(\boldsymbol{x}) = \max_{\boldsymbol{y} \in \Delta^d} \langle \boldsymbol{x}, \boldsymbol{y} \rangle - \sum_{i=1}^d \Omega(y_i)$$

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Properties:

- Consistent smoothing: $\max_0(\boldsymbol{x}) = \max(\boldsymbol{x})$
- Twice differentiable almost everywhere with non-zero Hessian

Examples of regularization

Shannon entropy: $\Omega(x) = x \log(x) \longrightarrow$ *Softmax* operator

$$\max_\Omega(\boldsymbol{x}) = \log(Z), \; \text{where } Z = \sum_j \exp(x_j)$$

$$\nabla \max_\Omega(\boldsymbol{x}) = (\exp(x_i)/Z)_{i \in \mathbb{R}^d}$$

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ℓ_2^2 **norm:** $\Omega(x) = x^2 \longrightarrow$ *Sparsemax* (Martins and Astudillo, 2016)

$\nabla \max_\Omega(\boldsymbol{x}) = \operatorname{argmin}_{p \in \triangle^d} \|\boldsymbol{x} - \boldsymbol{p}\|_2^2$ Sparse: eucl. projection on simplex

Dynamic programming regularization

What we have at hand

1. **Smooth max:** $\max_\Omega(\boldsymbol{x}) = \max_{\boldsymbol{y} \in \Delta^d} \langle \boldsymbol{x}, \boldsymbol{y} \rangle - \sum_{i=1}^d \Omega(y_i)$
2. **Bellman recursion:** $v_i = \max_{j \in \mathcal{P}_i} \theta_{i,j} + v_j, \quad \mathrm{DP}(\boldsymbol{\Theta}) \triangleq v_N$

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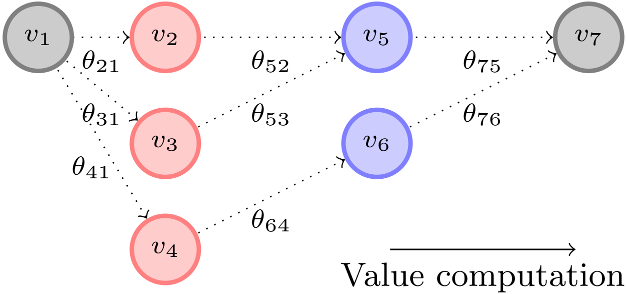
2. **Bellman recursion:** $v_i = \max_{j \in \mathcal{P}_i} \theta_{i,j} + v_j, \quad \mathrm{DP}(\boldsymbol{\Theta}) \triangleq v_N$

Bottom-up construction

For all $i \in [N]$:

$$v_i(\boldsymbol{\theta}) = \max_\Omega(\theta_{i,j} + v_j)_{j \in \mathcal{P}_i}$$

$$\mathrm{DP}_\Omega(\boldsymbol{\theta}) \triangleq v_N(\boldsymbol{\theta})$$



Regularized best-path: $\nabla \mathrm{DP}_\Omega(\boldsymbol{\theta})$

From max to smoothed max:

$$\boldsymbol{Y}(\boldsymbol{\theta}) = \partial \mathrm{DP}(\boldsymbol{\theta}) \Longrightarrow \boldsymbol{Y}_\Omega(\boldsymbol{\theta}) \triangleq \nabla \mathrm{DP}_\Omega(\boldsymbol{\theta})$$

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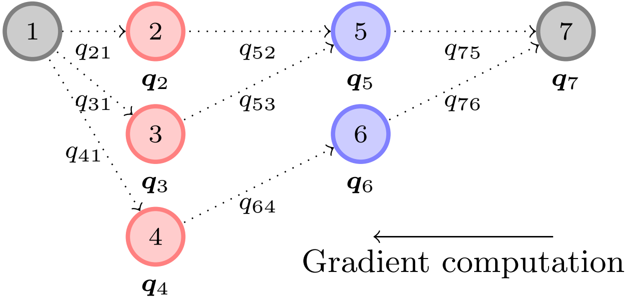
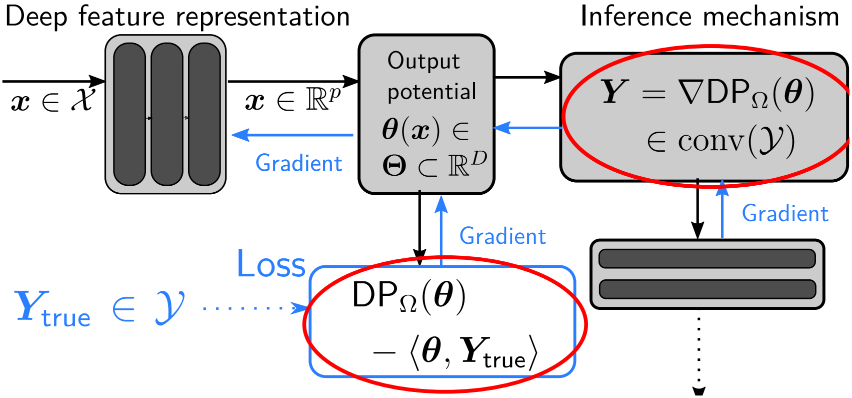
Computed with backpropagation

Requirements: Gradients of Bellman equations

$$\boldsymbol{q}_i = \nabla \max{}_\Omega(\theta_{i,j} + v_j)_{j \in \mathcal{P}_i}$$



Differentiable dynamic programming layers



Differentiable DP properties

Usable for loss design: $\boldsymbol{\theta} \to \mathrm{DP}_\Omega(\boldsymbol{\theta})$ is convex, bounds $\mathrm{DP}(\boldsymbol{\theta})$

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Is local regularization equivalent to global regularization ?

$$\mathrm{LP}_\Omega(\boldsymbol{\theta}) \triangleq \max\nolimits_\Omega \left(\langle \boldsymbol{Y}, \boldsymbol{\theta}\rangle\right)_{\boldsymbol{Y}\in\mathcal{Y}} = \max\nolimits_{\boldsymbol{p}\in\triangle^D} \left\langle \boldsymbol{p}, (\langle \boldsymbol{Y}, \boldsymbol{\theta}\rangle)_{\boldsymbol{y}\in\mathcal{Y}} \right\rangle - \Omega(\boldsymbol{p})$$

Theorem:

- $\mathrm{DP}_\Omega(\boldsymbol{\theta}) = \mathrm{LP}_\Omega(\boldsymbol{\theta})$ **if and only if** $\Omega(p) = -\gamma \sum_i p_i \log p_i$
- $\mathrm{DP}_\Omega(\boldsymbol{\theta})$ is the CRF (Lafferty et al., 2001) log-partition

$$\mathrm{DP}_\Omega(\boldsymbol{\theta}) = \log\Big(\sum_{\boldsymbol{Y}\in\mathcal{Y}} \exp(\langle \boldsymbol{\theta}, \boldsymbol{Y}\rangle)\Big)$$

New motivation for Shannon reg. But ℓ_2^2 has other interesting properties.

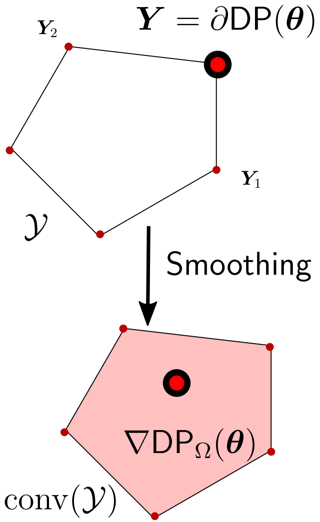
Relaxed gradient properties

Probabilistic interpretation

Backprop defines a distribution $\mathcal{D}_\Omega$ on the set of paths $\mathcal{Y}$

$$\nabla \mathrm{DP}_\Omega(\boldsymbol{\theta}) = \mathbb{E}_{\mathcal{D}_\Omega}[\boldsymbol{Y}] \in \mathrm{conv}(\mathcal{Y})$$

$\Rightarrow$ Probability of path $\boldsymbol{Y}$: $p_{\boldsymbol{\theta},\Omega}(\boldsymbol{Y})$



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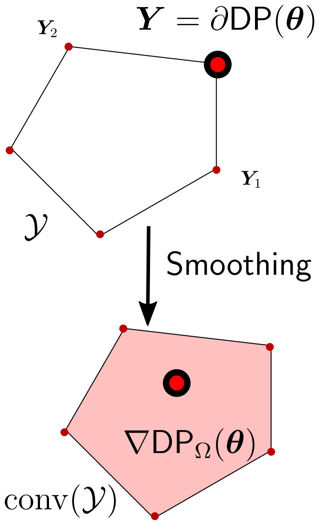
$$\nabla \mathrm{DP}_\Omega(\boldsymbol{\theta}) = \mathbb{E}_{\mathcal{D}_\Omega}[\boldsymbol{Y}] \in \mathrm{conv}(\mathcal{Y})$$

$\Rightarrow$ Probability of path $\boldsymbol{Y}$: $p_{\boldsymbol{\theta},\Omega}(\boldsymbol{Y})$

- **Shannon:** Gibbs distribution: $p_{\boldsymbol{\theta},\Omega}(\boldsymbol{Y}) \propto \langle \boldsymbol{Y}, \boldsymbol{\theta} \rangle$
- ℓ_2^2: $\mathcal{D}_\Omega$ has a small support $\to \nabla \mathrm{DP}_\Omega(\boldsymbol{\theta})$ is **sparse**



Backpropagating through $\nabla \mathrm{DP}_\Omega(\boldsymbol{\Theta})$

Regularized best-path layer: $\boldsymbol{\theta} \in \mathbb{R}^{N \times N} \to \nabla \mathrm{DP}_\Omega(\boldsymbol{\theta})$

Jacobian ? $\nabla \nabla \mathrm{DP}_\Omega(\boldsymbol{\Theta}) = \nabla^2 \mathrm{DP}_\Omega(\boldsymbol{\Theta}) = \text{Hessian}$

Hessian vector-product

$$\nabla(\nabla \mathrm{DP}_\Omega(\boldsymbol{\Theta}))\boldsymbol{Z} = \nabla^2 \mathrm{DP}_\Omega(\boldsymbol{\Theta})\boldsymbol{Z}, \qquad \boldsymbol{Z} \in \mathbb{R}^{n \times n} \quad \text{direction}$$

Computable in $\mathcal{O}(|\mathcal{E}|)$: reverse-on-forward differentiation

Differentiable dynamic programming layers

Highest-score layer, forward-pass

$$\boldsymbol{\theta} \in \mathbb{R}^{N \times N} \to \mathrm{DP}_\Omega(\boldsymbol{\theta})$$

Highest score layer, backward pass
Best path layer, forward-pass

$$\boldsymbol{\theta} \in \mathbb{R}^{N \times N} \to \nabla \mathrm{DP}_\Omega(\boldsymbol{\theta})$$

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Highest-score layer, forward-pass

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Best-path layer: backward pass

$$\boldsymbol{\theta}, Z \in \mathbb{R}^{N \times N} \times \mathbb{R}^{N \times N} \to \nabla^2 \mathrm{DP}_\Omega(\boldsymbol{\theta}) Z$$

Differentiable dynamic programming layers

Highest-score layer, forward-pass

$$\boldsymbol{\theta} \in \mathbb{R}^{N \times N} \to \mathrm{DP}_\Omega(\boldsymbol{\theta})$$

Highest score layer, backward pass
Best path layer, forward-pass

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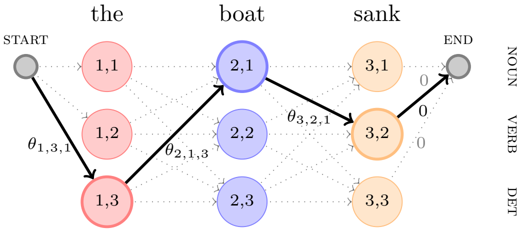
Best-path layer: backward pass

$$\boldsymbol{\theta}, \boldsymbol{Z} \in \mathbb{R}^{N \times N} \times \mathbb{R}^{N \times N} \to \nabla^2 \mathrm{DP}_\Omega(\boldsymbol{\theta}) \boldsymbol{Z}$$

- Sparse/dense output with ℓ_2/entropy regularization
- Total computational cost: $\mathcal{O}(|\mathcal{E}|)$

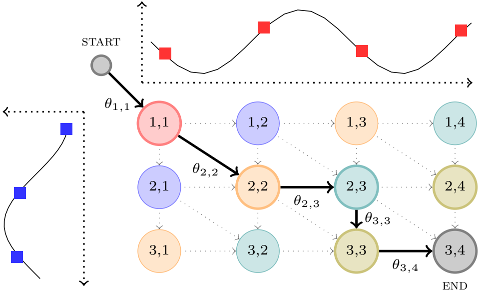
Applications

Viterbi



$$\langle \boldsymbol{Y}, \boldsymbol{\theta} \rangle = \theta_{1,3,1} + \theta_{2,1,3} + \theta_{3,2,1}$$

Dynamic time warping



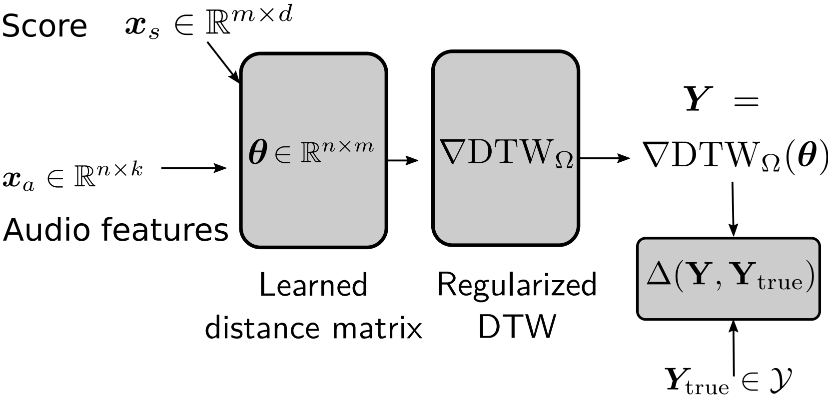
$$\langle \boldsymbol{Y}, \boldsymbol{\theta} \rangle = \theta_{1,1} + \theta_{2,2} + \theta_{2,3} + \theta_{3,3} + \theta_{3,4}$$

$$\nabla \mathrm{Vit}_\Omega : \mathbb{R}^{T \times S \times S} \to \mathbb{R}^{T \times S \times S}$$

$$\nabla \mathrm{DTW}_\Omega : \mathbb{R}^{m \times n} \to \mathbb{R}^{m \times n}$$

Audio-to-score alignment

- **Input data:** audio sequence $\boldsymbol{x}_a \in \mathbb{R}^{n \times k}$, one-hot key sequence $\boldsymbol{x}_s \in \mathbb{R}^{m \times d}$
- **Labels:** Alignment $\boldsymbol{Y}_{\text{true}} \in \mathcal{Y} \subset \mathbb{R}^{n \times m}$



Metric learning experiment

Learn the distance matrix:

- Baseline: multinomial classification, audio-frame to score key
- Our model: end-to-end training of a linear model with final soft-DTW layer

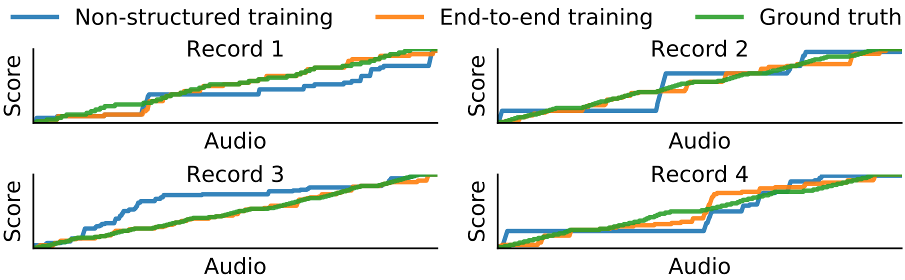
Data: Supervised dataset: 10 annotated Bach quatuors (**Bach10**)

Validation:

- Leave-one-out prediction
- At test time: Hard DTW on the learned distance matrix
- RMSE between predicted onsets

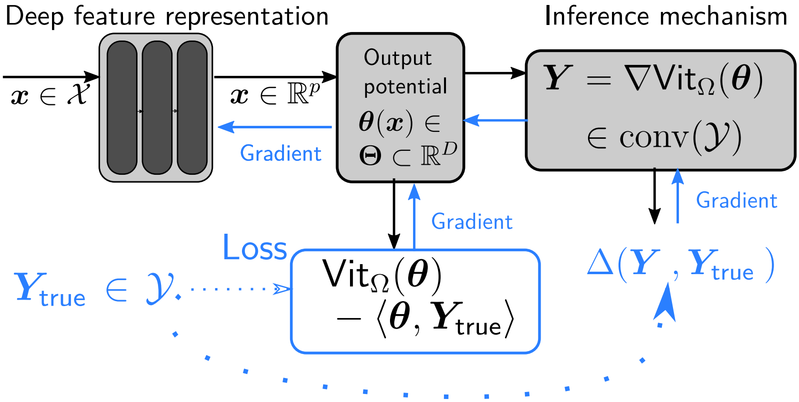
Results

RMSE	Test set	Train set
End-to-end training	$\mathbf{1.26 \pm 0.64}$	$\mathbf{0.17 \pm 0.01}$
Non-structure training	3.70 ± 2.85	1.80 ± 0.14
Random	14.64 ± 2.63	14.64 ± 0.29



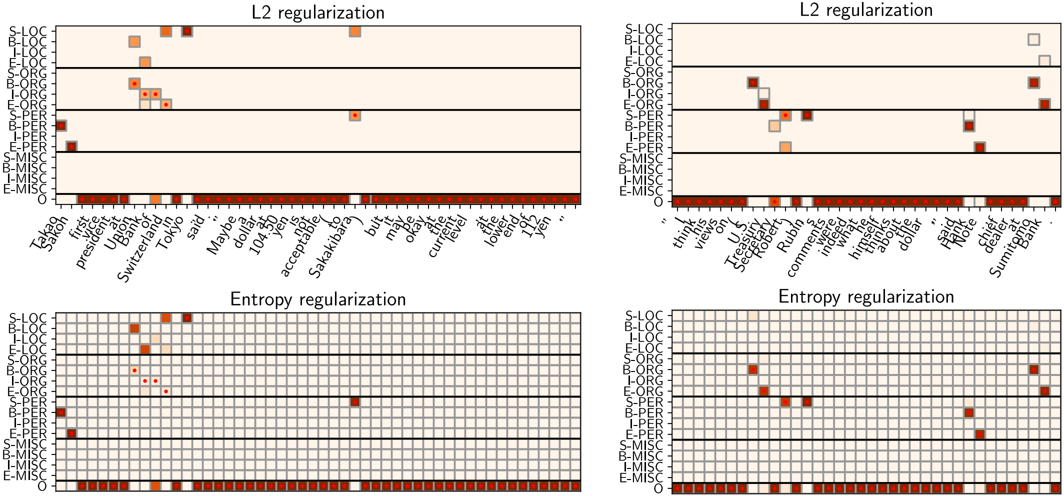
Named entity recognition

- **Input data:** Sentences $\boldsymbol{x}$ of length T
- **Labels** $\boldsymbol{Y}$**:** {Begin/Inside/Outside}{Person/Org./Loc./Misc.}



K-best set predictions in named entity recognition

$\Omega = \ell_2^2$: $\nabla \mathrm{DP}_\Omega(\boldsymbol{\theta}(x))$ k-best subset of $\boldsymbol{Y}$ such that $p_{\boldsymbol{\theta},\Omega}(\boldsymbol{Y}) \neq 0$



Quantitative comparison of losses

- **Potential-convex loss:** $\ell_\Omega(\boldsymbol{\theta}, \boldsymbol{Y}) = \mathrm{DP}_\Omega(\boldsymbol{\theta}) - \langle \boldsymbol{Y}, \boldsymbol{\theta} \rangle$
- **Cost-sensitive loss:** $\ell_\Omega(\boldsymbol{\theta}, \boldsymbol{Y}) = \Delta(\nabla \mathrm{DP}_\Omega(\boldsymbol{\theta}), \boldsymbol{Y}\rangle$.

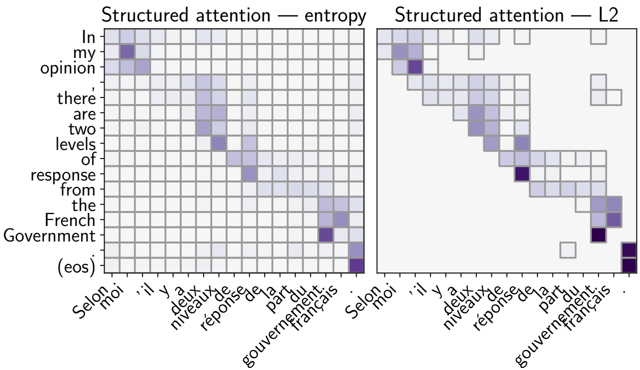
Ω	Loss	English	Spanish	German	Dutch
Negentropy	Convex loss	90.80	**86.68**	77.35	**87.56**
	Cost-sensitive	90.47	86.20	**77.56**	87.37
ℓ_2^2	Convex loss	**90.86**	85.51	76.01	86.58
	Cost-sensitive	89.49	84.07	76.91	85.90
Lample et al., 2016[6]		*90.96*	*85.75*	*78.76*	*81.74*

- ℓ_2^2 reg. achieves comparable accuracy with more interpretable predictions
- Training directly from potential-derived losses is slightly better

[6] Guillaume Lample et al. (2016). "Neural Architectures for Named Entity Recognition". In: *Proc. of NAACL*, pp. 260–270.

Structured attention — Neural machine transation

- Compute an attention vector $\boldsymbol{c}$: 2 state linear-chain CRF
- $\boldsymbol{c} = \mathbb{E}[\boldsymbol{z}]$, $z_i = 1$ if attention, $z_i = 0$ if no-attention
- Use Vit_Ω, with sparse marginal computation $\Omega = \ell_2^2$.



Similar BLEU scores WMT14 1M

Attention model	fr→en	en→fr
Softmax	**27.96**	**28.08**
CRF + entropy	**27.96**	27.98
CRF + ℓ_2^2 reg.	27.21	27.28

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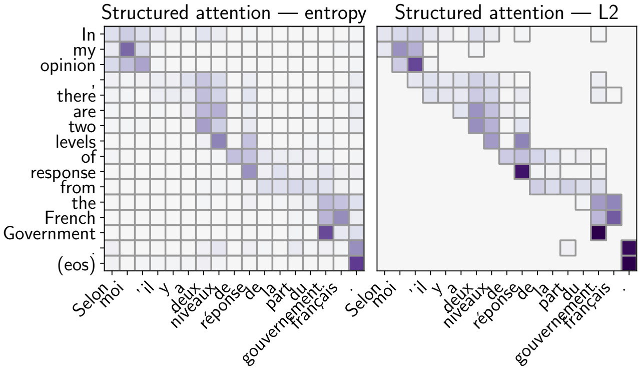

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Block sparse attention

Conclusion

General framework to use DP algorithms in arbitrary networks

- Efficient and stable algorithms
- Flexibility of regularization (sparse output)

Experiments: ℓ_2/entropy have similar performance

- ℓ_2^2: More interpretable outputs / k-best sets with sparsity

PyTorch package *didyprog* available (fast custom Viterbi and DTW layer)

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Related work at Google: Framwork formalizes differentiable beam search (Goyal et al., 2017), similar effor in reinforcement learning (Haarnoja et al., 2018)

Bibliography I

Bahdanau, Dzmitry, Kyunghyun Cho, and Yoshua Bengio (2015). "Neural Machine Translation by Jointly Learning to Align and Translate". In: *Proc. of ICLR*.

Bellman, Richard (1958). "On a routing problem". In: *Quarterly of applied mathematics* 16.1, pp. 87–90.

Cuturi, Marco and Mathieu Blondel (2017). "Soft-DTW: a Differentiable Loss Function for Time-Series". In: *Proc. of ICML*, pp. 894–903.

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

Goyal, Kartik et al. (July 2017). "A Continuous Relaxation of Beam Search for End-to-End Training of Neural Sequence Models". In: *arXiv:1708.00111 [cs]*. arXiv: `1708.00111 [cs]`.

Bibliography II

Haarnoja, Tuomas et al. (2018). "Off-Policy Maximum Entropy Deep Reinforcement Learning with a Stochastic Actor". en. In: *Proceedings of the International Conference on Machine Learning*, p. 10.

Kim, Yoon et al. (2017). "Structured Attention Networks". In: *Proc. of ICLR*.

Lafferty, John, Andrew McCallum, and Fernando CN Pereira (2001). "Conditional random fields: Probabilistic models for segmenting and labeling sequence data". In: *Proc. of ICML*, pp. 282–289.

Lample, Guillaume et al. (2016). "Neural Architectures for Named Entity Recognition". In: *Proc. of NAACL*, pp. 260–270.

LeCun, Yann et al. (2006). "A tutorial on energy-based learning". In: *Predicting structured data* 1.0.

Bibliography III

Martins, André F.T. and Ramón Fernandez Astudillo (2016). "From softmax to sparsemax: A sparse model of attention and multi-label classification". In: *Proc. of ICML*, pp. 1614–1623.

Mensch, Arthur and Mathieu Blondel (2018). "Differentiable Dynamic Programming for Structured Prediction and Attention". In: *Proceedings of the International Conference on Machine Learning*.

Moreau, Jean-Jacques (1965). "Proximité et dualité dans un espace hilbertien". In: *Bullet de la Société Mathémathique de France* 93.2, pp. 273–299.

Nesterov, Yurii (2005). "Smooth minimization of non-smooth functions". In: *Mathematical Programming* 103.1, pp. 127–152.