

Differentiable dynamic programming for structured prediction and attention

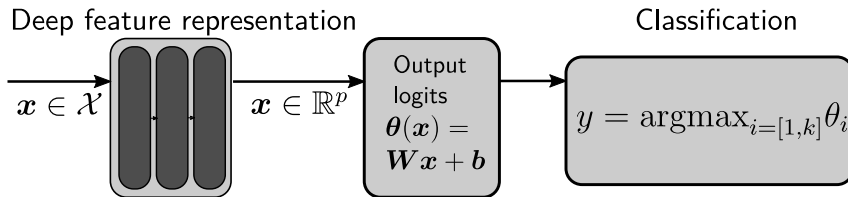
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July 12, 2018

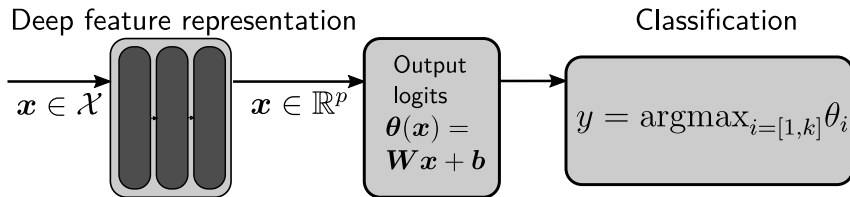
Predictive models: parametrized functions + linear programs

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



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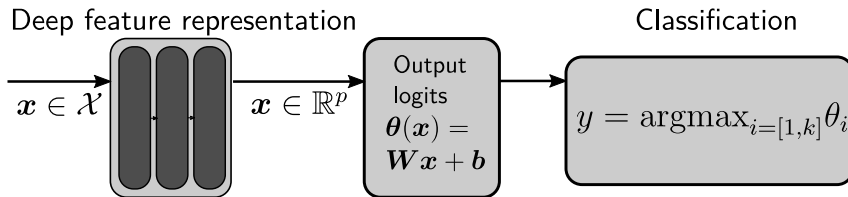
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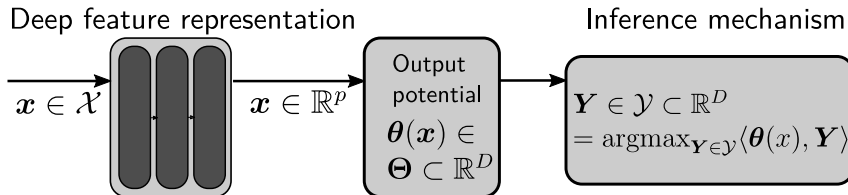
Structured output ? $\mathcal{Y} \subset \mathbb{R}^D$ (edges of a polytope), e. g. a tag sequence

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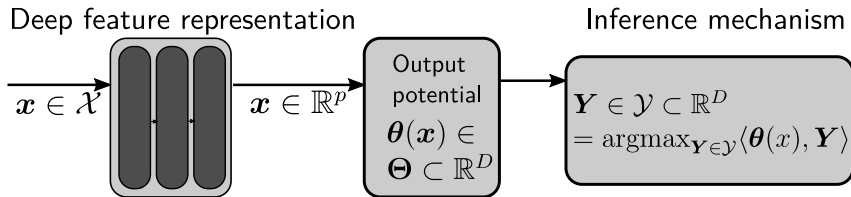
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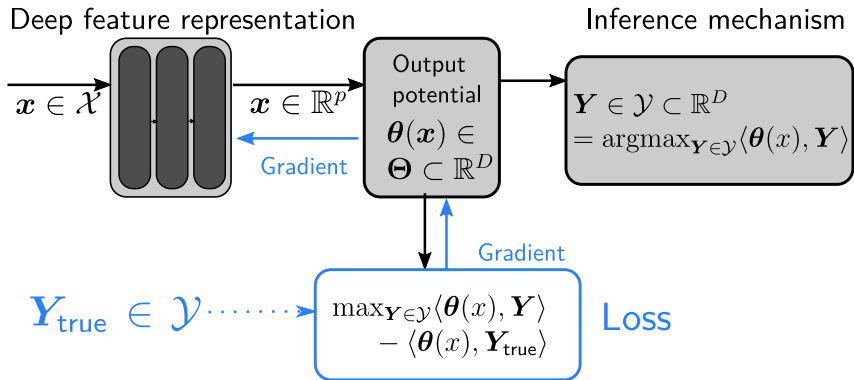


Structure prediction:



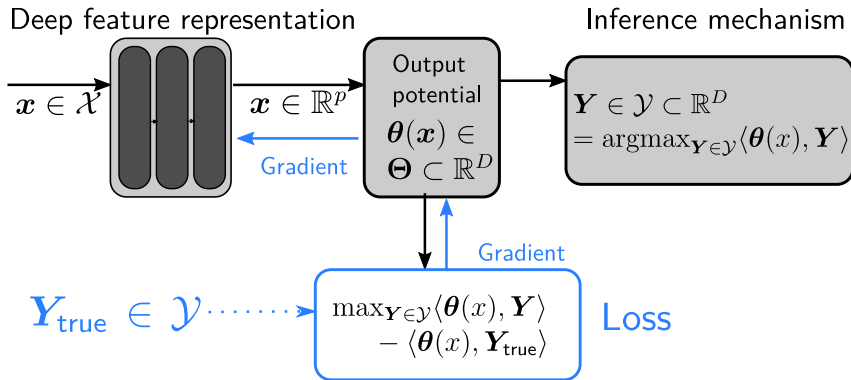
Training

Structure prediction: *Structured perceptron loss*



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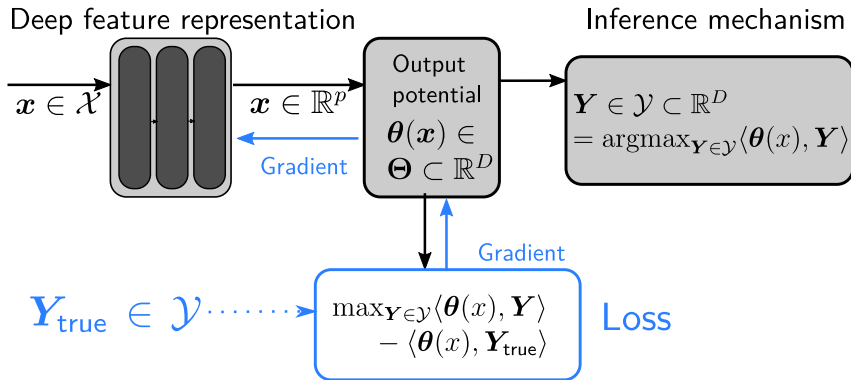
Structure prediction: *Structured perceptron loss*



Backpropagate through the max.

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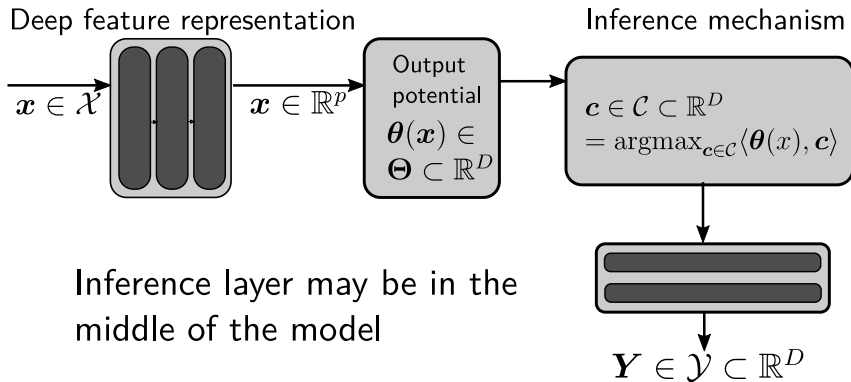
Structure prediction: *Structured perceptron loss*



Backpropagate through the max. Not differentiable everywhere !

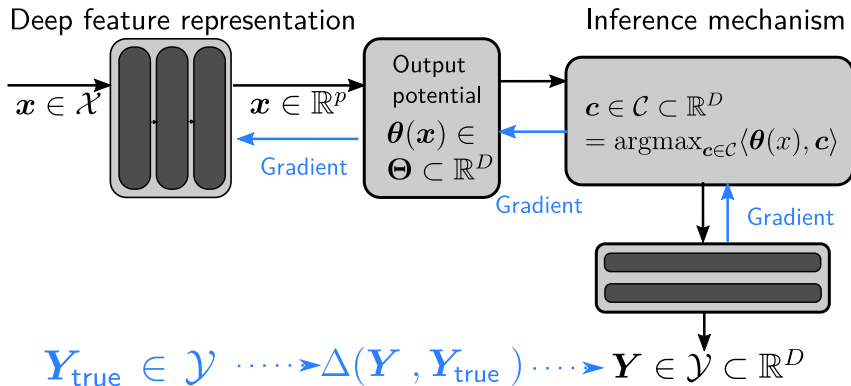
Structured prediction as an inner layer

Example: Attention mechanisms, where c are the attention weights.



Structured prediction as an inner layer

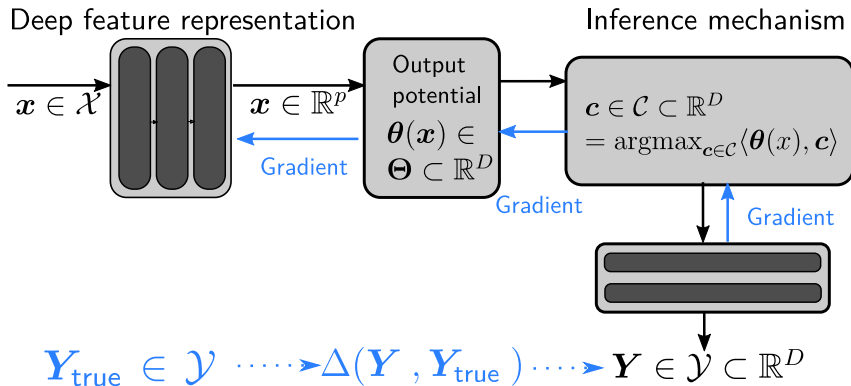
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We need to backpropagate through the argmax.

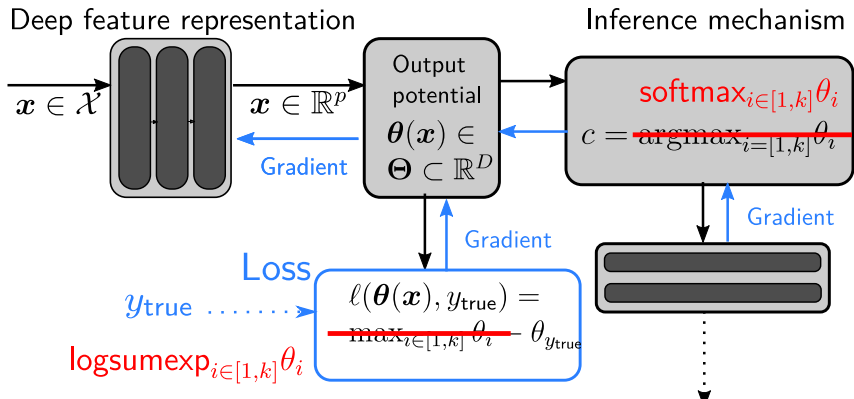
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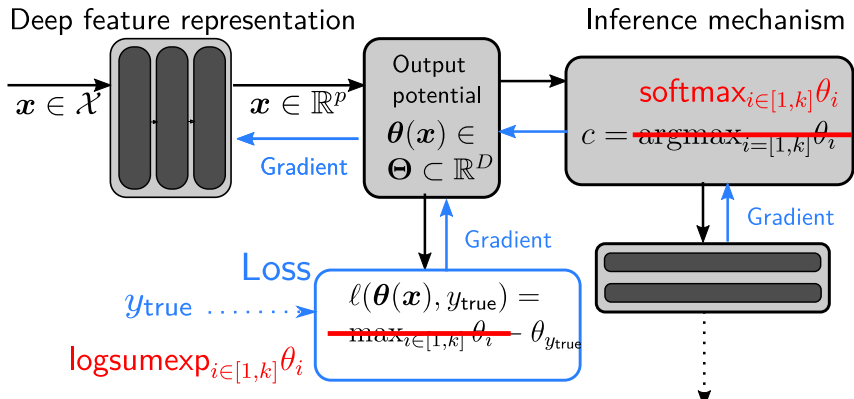


We need to backpropagate through the **argmax**. Zero derivative !

From max to softmax



From max to softmax



Multinomial loss, softmax attention: **differentiable**

Questions and contributions

- 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?

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

Questions and contributions

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Inference mechanisms often rely on a **dynamic programming** algorithm

Contribution: differentiable dynamic programming

- Smooth **max** layers to design new structured losses
- Differentiable **argmax** layers for inner inference mechanisms

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: [LeCun et al., 2006, Lample et al., 2016, Kim et al., 2017, Cuturi and Blondel, 2017], etc.

Dynamic programming

Dynamic programming solve the structure prediction problem

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

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

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

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

$$\underset{\mathbf{Y} \in \mathcal{Y}}{\text{argmax}} \langle \boldsymbol{\theta}, \mathbf{Y} \rangle$$

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$$\operatorname{argmax}_{\mathbf{Y} \in \mathcal{Y}} \langle \boldsymbol{\theta}, \mathbf{Y} \rangle$$

Examples:

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

Generic (max, +) DP is best path finding

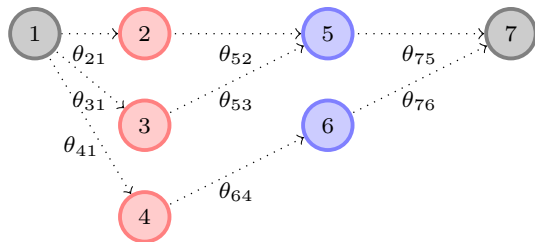
Directed acyclic graph

- $G = (\mathcal{N}, \mathcal{E})$, 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. $\theta \in \mathbb{R}^{n \times n}$ incidence matrix
- Path $\mathbf{Y} \in \mathcal{Y} \subset \{0, 1\}^{N \times N}$: $y_{i,j} = 1$ iff (i, j) is taken

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

Highest score among all paths

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



Maximum value computation (finding the max)

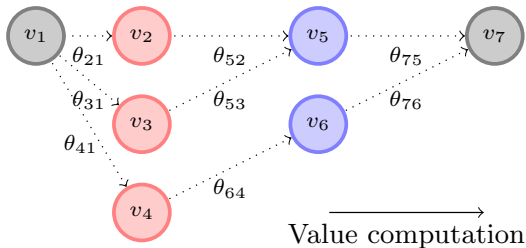
- Max value from 1 to i

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

- One pass over the graph

$$(v_1 = 0, v_2, \dots, v_n \triangleq \text{DP}(\theta))$$

= Bellman equation



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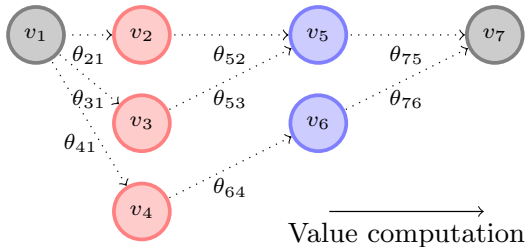
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The DP recursion solves the linear problem [Bellman, 1958]

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



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The argmax is computable using backpropagation = backtracking

Danskin theorem [Danskin, 1966]

$$\partial \text{DP}(\theta) = \partial_{\theta}(\theta \rightarrow \max_{\mathbf{Y} \in \mathcal{Y}} \langle \mathbf{Y}, \theta \rangle) = \text{conv}(\text{argmax}_{\mathbf{Y} \in \mathcal{Y}} \langle \mathbf{Y}, \theta \rangle)$$

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

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Dynamic programming layers

We define:

- **Max** layer: $\theta \rightarrow \text{DP}(\theta) = \max_Y \langle Y, \theta \rangle$
- **Argmax** layer: $\theta \rightarrow \partial_{\theta} \text{DP}(\theta) \sim \text{argmax}_Y \langle Y, \theta \rangle$

Operator regularization

Obstacles to end-to-end training

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

Operator regularization

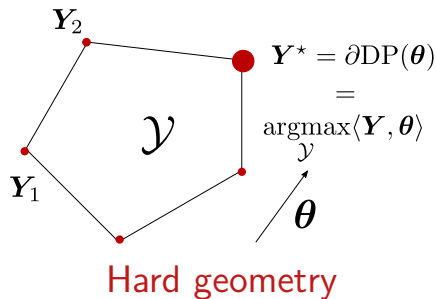
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Culprit is the Bellman recursion

$$\mathbf{x} \in \mathbb{R}^d \rightarrow \max(\mathbf{x}) \in \mathbb{R}$$

- Not differentiable everywhere
- Piecewise linear (null Hessian)



Operator regularization

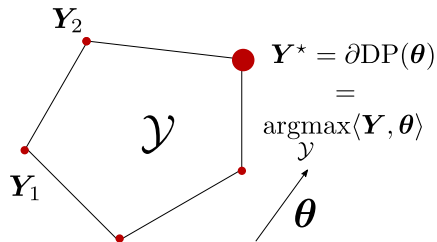
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Hard geometry

Solution: smooth the maximum operator

Max smoothing

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

Smoothed max operator [Moreau, 1965, Nesterov, 2005]

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

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Properties:

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

Dynamic programming regularization

What we have at hand

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

Dynamic programming regularization

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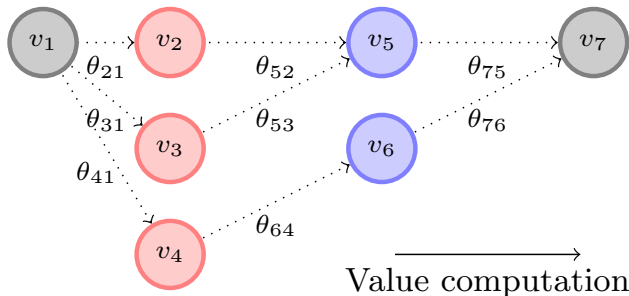
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Bottom-up construction

For all $i \in [N]$:

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

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



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

From max to smoothed max:

$$Y(\theta) = \partial \text{DP}(\theta) \implies Y_\Omega(\theta) \triangleq \nabla \text{DP}_\Omega(\theta)$$

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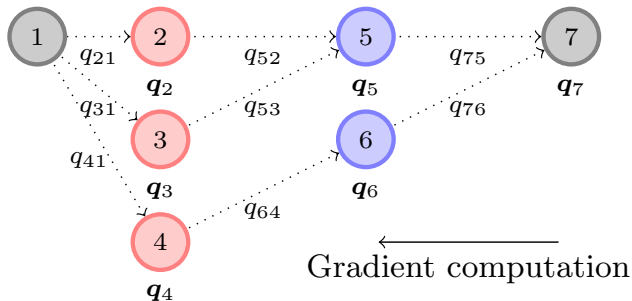
From max to smoothed max:

$$Y(\theta) = \partial \text{DP}(\theta) \implies Y_\Omega(\theta) \triangleq \nabla \text{DP}_\Omega(\theta)$$

Computed with
backpropagation

Requirements: Gradients
of Bellman equations

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



Entropy and sparsity-inducing ℓ_2^2 regularization

Entropy: $\Omega(x) = \gamma x \log(x) \longrightarrow \textit{Softmax}$ operator

$$\max_{\Omega}(\mathbf{x}) = \log(Z), \text{ where } Z = \sum_j \exp(x_j/\gamma)$$

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

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ℓ_2^2 **penalty:** $\Omega(x) = \gamma x^2$ *Sparsemax* [Martins and Astudillo, 2016]

$$\nabla \max_{\Omega}(\mathbf{x}) = \mathbf{P}_{\Delta^d}(\mathbf{x}/\gamma) \quad \text{Sparse: } \ell_2 \text{ projection on simplex}$$

Differentiable DP properties

$DP_{\Omega}(\theta)$ properties

- $\theta \rightarrow DP_{\Omega}(\theta)$ is convex.
- $DP_{\Omega}(\theta) = LP_{\Omega}(\theta)$ **if and only if** $\Omega = -\gamma H(\theta)$

$$LP_{\Omega}(\theta) \triangleq \max_{\Omega} (\langle \mathbf{Y}, \theta \rangle)_{\mathbf{Y} \in \mathcal{Y}} = \max_{\mathbf{p} \in \Delta^D} \langle \mathbf{p}, (\langle \mathbf{Y}, \theta \rangle)_{\mathbf{Y} \in \mathcal{Y}} \rangle - \Omega(\mathbf{p})$$

In this (only) case:

- Local Bellman regularization = full LP regularization

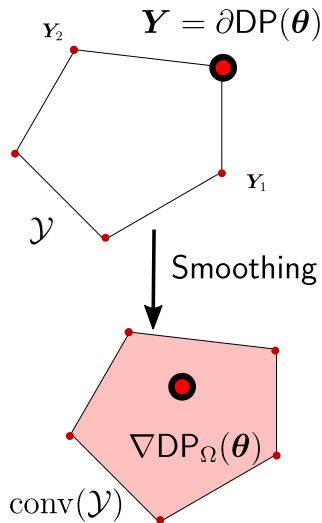
Relaxed gradient properties

Probabilistic interpretation

We can define a distribution \mathcal{D}_Ω on the set of paths \mathcal{Y} such that

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

Predicted path probabilities: $p_{\theta,\Omega}(\mathbf{Y})$



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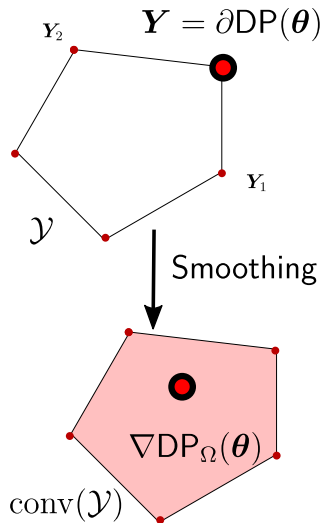
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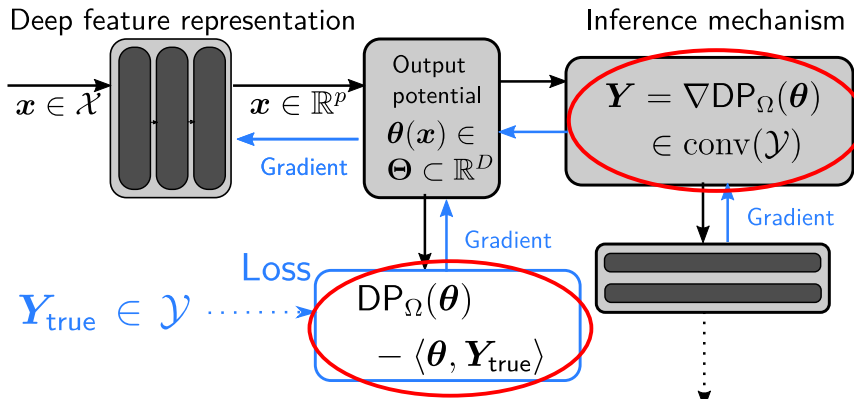
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- **Negentropy:** Gibbs distribution: $p_{\theta, \Omega}(\mathbf{Y}) \propto \langle \mathbf{Y}, \theta \rangle$
- ℓ_2^2 : \mathcal{D}_Ω has a small support $\rightarrow \nabla \text{DP}_\Omega(\theta)$ is sparse

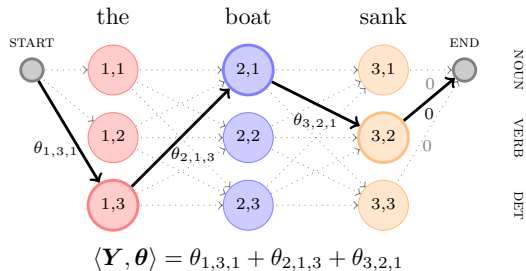


Differentiable dynamic programming layers



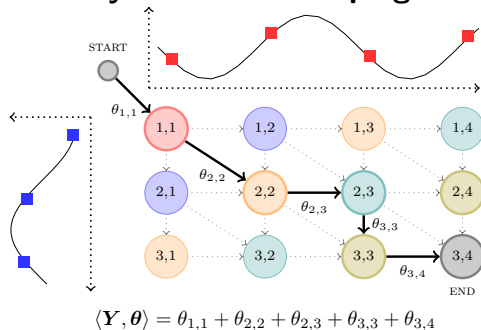
Applications

Viterbi



$$\nabla \text{Vit}_{\Omega} : \mathbb{R}^{T \times S \times S} \rightarrow \mathbb{R}^{T \times S \times S}$$

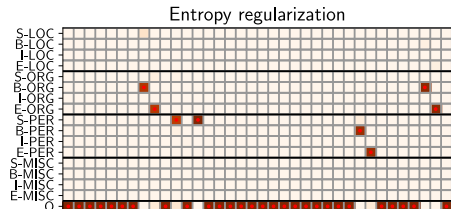
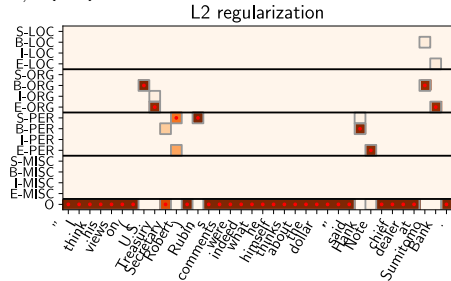
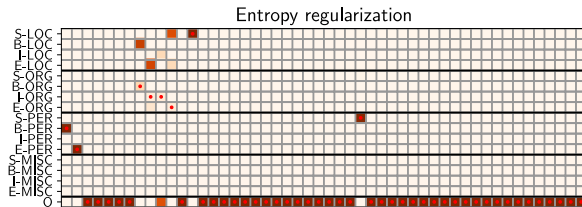
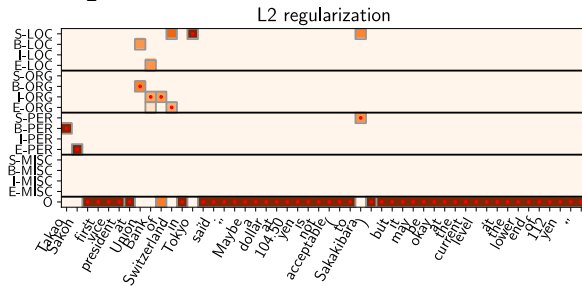
Dynamic time warping



$$\nabla \text{DTW}_{\Omega} : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}^{m \times n}$$

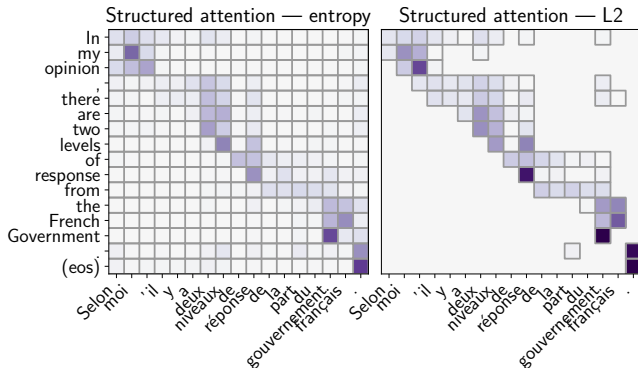
K-best set predictions in named entity recognition

$\Omega = \ell_2^2$: output k-best subset of \mathcal{Y} such that $p_{\theta, \Omega}(\mathcal{Y}) \neq 0$



Structured attention — Neural machine translation

- Compute the attention vector c by marginalizing a 2 state linear-chain CRF.
- Use Vit_Ω , with sparse marginal computation $\Omega = \ell_2^2$.
- Versus simple softmax in original version



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 |

Conclusion

General framework to put dynamic programming algorithms into arbitrary networks

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

Experiments

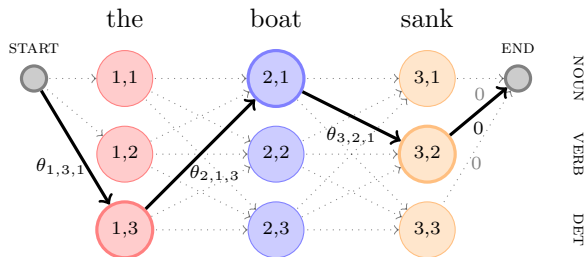
- ℓ_2 /entropy have similar performance
- More interpretable outputs / k-best sets with sparsity
- *PyTorch* package *didyprog* available (fast custom Viterbi and DTW layer)
- Other applications, instantiated algorithms, backprop through $\nabla \text{DP}_\Omega(\theta)$

Poster #48

Example: Linear conditional random field

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

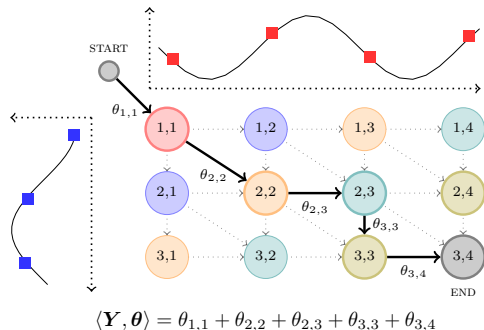
$$\mathbf{y} = \operatorname{argmax}_{\mathbf{y} \in \mathcal{Y}} \sum_{t=1}^T \theta_t(y_t, y_{t-1}, \mathbf{x}_t) = \operatorname{argmax}_{\mathbf{Y} \in \mathcal{Y}} \langle \boldsymbol{\theta}, \mathbf{Y} \rangle$$



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

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

Example: Dynamic time warping



Elastic matching

- Two time-series A, B
- Distance matrix: e.g.,
 $\theta_{i,j} = \|a_i - b_j\|_2^2$

Alignment matrices

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

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

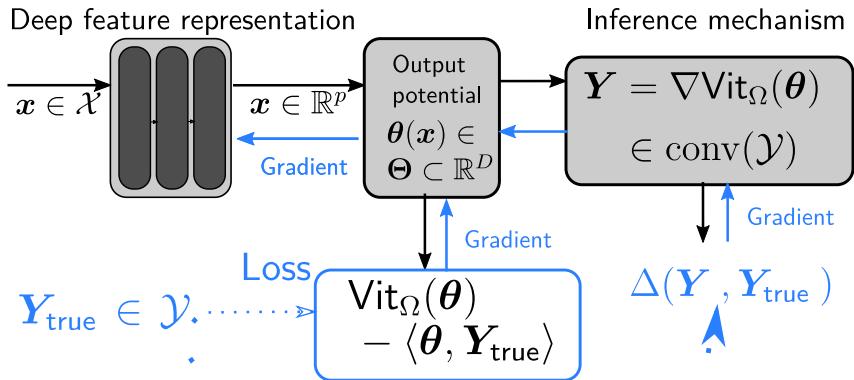
DTW distance: $d(A, B) = \max_{Y \in \mathcal{Y}} \langle Y, \theta \rangle$

Computable by dynamic programming

- \mathcal{Y} set of alignment matrices
- θ distance matrix

Named entity recognition

- **Input data:** Sentences x of length T
- **Labels Y :** $\{\text{Begin/Inside/Outside}\} \{\text{Person/Org./Loc./Misc.}\}$
- **Model:** Char + Word LSTM + **smooth inference mechanism**



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