### MDI341 Structured Data

2 - Energy-based approaches for structured prediction

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**Structured output prediction** 

with energy-based methods

## Statistical framework of structured prediction

Let P(x,y) be the unknown true distribution of the data Let  $\mathcal{S} = \{(x_i,y_i), i=1,\ldots,n\}$  be iid sample from P. Let  $\Delta: \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$  a loss function

- Find g that minimizes the expected loss  $\mathbb{E}_{(x,y)}[\Delta(y,f(x))]$
- With  $f(x) = \arg \max_{y \in \mathcal{Y}} g(x, y, \mathbf{w})$

## **Energy-based learning**

- Choose the space of functions g
- Define an appropriate loss  $\Delta(y, y')$ ,
- $\bullet$  Define a surrogate loss  $\ell$  and solve an optimization problem to learn  ${\it g}$  ,

## **Energy-based learning: score functions**

- $g(x,y) = w^T \phi(x,y)$ :struct perceptron, struct-SVM
- $g(x,y) = \sum_r g_r(x,y_r)$  with  $g_r(x,y_r) = NN_r(x,y)$  and r index subsets of components: deep structured prediction (Chen et al., 2015), structured prediction neural networks (Bellanger and Mc Callum, 2016)
- $g(x,y) = \hat{P}(Y = y|x)$ : logistic regression, CRF, graphical probabilistic models

## Losses for multiple classes

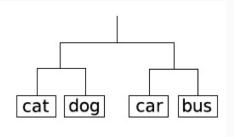
Without a hierarchy among classes

$$\Delta(y, y') = 1$$
, if  $y \neq y'$ , 0 otherwise

Loss for a hierarchy of classes

$$\Delta(y, y') = \frac{1}{2} D_{tree}(y, y')$$

For the shown hierarchy:  $\Delta(cat, cat) = 0, \Delta(cat, dog) = 1$ ,  $\Delta(cat, bus) = 2$ ; . . .



4

## Loss for localization of an object in an image

Object detection: find a bounding box and a class



Credit Blaschko & Lampert, ECCV2008.

## Localization of an object in an image: choice of loss function

Blatschko and Lampert (2008) propose to solve it as a a structured prediction problem.

$$\mathcal{X} = \{images\}$$
 and  $\mathcal{Y} = \{bounding\ boxes\ in\ images\}$   
More precisely,  $\mathcal{Y} = \{(\omega,t,l,b,r)|\omega\in\{+1,-1\},(t,l,b,r)\in\mathbb{R}^4\}$   
For  $\omega=-1$ , the vector  $(t,l,b,r)$  is ignored.

#### Loss function

$$\Delta(y, y_i) = \Delta_i(y) = 1 - \frac{Area(y_i \cap y)}{area(y_i \cup y)}$$
 if  $y_{i\omega} = y_\omega = 1$ ,  $1 - (\frac{1}{2}(y_{i\omega}y_\omega + 1))$  otherwise.

Learning with Max margin

**Approaches** 

### Structured SVM

$$\ell(x, y_i, \mathbf{w}) = [\max_{\mathbf{v}} (\Delta(y_i, y) + \mathbf{w}^T \phi_i(y) - \mathbf{w}^T \phi_i(y_i))]_+$$

 $\ell$  is an upper bound of  $\Delta$ , continuous and convex. Regularized Empirical Risk Minimization :

$$\min_{\mathbf{w}} \frac{1}{2} \|\mathbf{w}\|^2 + \frac{C}{n} \sum_{i} \max(0, \max_{y} [\Delta(y_i, y) + \mathbf{w}^T \phi_i(y) - \mathbf{w}^T \phi_i(y_i)])$$

## Max Margin Approaches: pb in the primal

#### Margin maximization with slack variables

$$\min_{\mathbf{w}} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_i \xi_i$$

s.t. :

$$\forall i, \forall y \neq y_i, \mathbf{w}^T \phi_i(y_i) + \xi_i \geq \mathbf{w}^T \phi_i(y) + \Delta_i(y)$$

$$\forall i, \xi_i \geq 0$$

 $\Delta_i(y) = \Delta(y_i,y)$  reflects the loss between y and  $y_i$ 

#### Pb in the dual

We note: 
$$\delta\phi(x_i, y_i, y) = \phi(x_i, y_i) - \phi(x_i, y) = \phi_i(y_i) - \phi_i(y)$$
  
**Dual Struct-SVM pb**  
 $\max_{\alpha} \sum_{iy} \alpha_{iy} \Delta_i(y) - \frac{1}{2} \sum_{i,j,y,y'} \alpha_{iy} \alpha_{jy'} < \delta\phi(x_i, y_i, y), \delta\phi(x_j, y_j, y') >$   
s.t. :  
 $\forall i = 1, \dots, n, \sum_{y \in \mathcal{Y}} \alpha_{i,y} \leq \frac{C}{N}$ 

• Prediction function:

$$f(x) = \arg\max_{y} \left( \sum_{iy'} \alpha_{iy'} (\phi_i(y') - \phi_i(y_i)) \right)^T \phi(x, y)$$

Le Cun et al. Energy-based models (2006)

## Solving the optimization pb

- Solving the problem in the dual
- However there are many constraints (size  $|\mathcal{Y}|$  n)
- Working set training (active constraints)
- Eventually: easy to kernelize (we'll see that later)

## **Algorithm**

### Working set S-SVM - Learning Algorithm

- 1. input:  $(x_1, y_1), (x_n, y_n), C, \epsilon$
- 2.  $S \leftarrow 0$
- 3. repeat
  - for  $i=1,\ldots,n$ 
    - solution to the quadratic pb with constraints from the working set S
       (subspace ascent)
    - Define:  $H(y) = \Delta(y, y_i) \mathbf{w}^T \phi_i(y_i) + \mathbf{w}^T \phi_i(y)$
    - with  $\mathbf{w} := \sum_{i} \sum_{y' \in S_i} \alpha_{jy'} (\phi(x_j, y_j) \phi(x_j, y'))$
    - Compute  $\hat{y} = \arg\max_{y \in \mathcal{Y}} H(y)$
    - Compute  $\xi_i = \max(0, \max_{y \in S_i} H(y))$
    - If  $H(\hat{y}) > \xi_i + \epsilon$  then
      - $S \leftarrow S \cup \{(i, \hat{y})\}$  add the most violated constraint
  - End for
- 4. until S has not significantly changed.

## More efficient: subgradient algorithm

For the penalized unconstrained formulation :

$$\min_{\mathbf{w}} \frac{1}{2} \|\mathbf{w}\|^2 + \frac{C}{n} \sum_{i} \max(0, \max_{y} [\Delta(y_i, y) + \mathbf{w}^T \phi_i(y) - \mathbf{w}^T \phi_i(y_i)])$$

Convex, non-differentiable loss:

We can use sub-gradient method instead of gradient decent algorithm.

## Subgradient Descent algorithm for Struct-SVM

### Algo

- w = 0
- for t=1,..., *T* 
  - for  $i=1,\ldots,n$
  - $\hat{y} := \arg \max_{y \in \mathcal{Y}} \Delta(y, y_i) + \langle \mathbf{w}, \phi(x_i, y) \rangle$  (loss augmented step)
  - $v_i := \phi(x_i, \hat{y}) \phi(x_i, y_i)$
  - endfor
- $\mathbf{w} := \mathbf{w} \eta_t (\mathbf{w} \frac{c}{n} \sum_i v_i)$
- endfor

N.B.: Stochastic updates are usually chosen

## Subgradient

Want to minimize:  $\min_{\mathbf{w}} \frac{1}{2} \|\mathbf{w}\|^2 + \frac{C}{n} \ell_i(\mathbf{w})$  with

$$\ell_i^{y}(\mathbf{w}) = \Delta(y_i, y) + \mathbf{w}^{T} \phi_i(y) - \mathbf{w}^{T} \phi_i(y_i)$$
  
$$\ell_i(\mathbf{w}) = \sum_{i} \max(0, \max_{y} \ell_i^{y}(\mathbf{w}))$$

The subgradient of  $\ell_i(\mathbf{w})$  for  $\mathbf{w} = \mathbf{w}_0$  is the vector v defined as follows:

$$\hat{y} = \arg \max \ell_i(\mathbf{w}_0)$$
 $v = \nabla \ell_i^{\hat{y}}(\mathbf{w}_0)$ 

## More efficient Struct SVM learning

- Distributedly training structured support vector machines based on a distributed block-coordinate descent method: Lee, Chang, Upaydin and Roth, NIPS 2016
- Alternating DirectionMethod of Multipliers (ADMM) for structural SVM: Balamurugan et al; SDM 2011, and SIAM 2016.

## To go further: Kernelization

#### Ref: Blatchko and Lampert 2008.

- A joint kernel function  $k:(\mathcal{X} \times \mathcal{Y}) \times (\mathcal{X} \times \mathcal{Y}) \to \mathbb{R}$ 
  - $k((x,y),(x',y')) = <\phi(x,y),\phi(x',y')>$
  - k measures how the two pairs (x,y) and (x',y') are similar
- We can show that

$$<\delta\phi(x_i, y_i, y), \delta\phi(x_j, y_j, y')>=k((x_i, y), (x_j, y_j)) - k((x_i, y_i), (x_j, y')) - k((x_i, y), (x_j, y_j)) + k((x_i, y), (x_j, y'))$$

• Let us denote  $<\delta\phi(x_i,y_i,y),\delta\phi(x_j,y_j,y')>=k_{ijyy'}$ 

#### Pb in the dual

### **Dual Struct-SVM pb**

$$\max_{\alpha} \sum_{i,y} \alpha_{iy} \Delta_i(y) - \frac{1}{2} \sum_{i,j,y,y'} \alpha_{iy} \alpha_{jy'} k_{ijyy'}$$
 s.t. :

$$\forall i = 1, \dots n, \sum_{y \in \mathcal{Y}} \alpha_{i,y} \leq \frac{C}{N}$$

• Prediction function:

$$f(x) = \arg\max_{y \in \mathcal{Y}} \sum_{iy'} \alpha_{iy'} [k((x_i, y'), (x, y)) - k((x_i, y_i), (x, y))]$$

## **Examples of joint kernels**

Both x and y decompose into components

$$k((x,y),(x',y')) = \sum_{p} k_{p}((x_{p},y_{p}),(x'_{p},y'_{p}))$$

## Kernel for localization of an object in an image

Now the kernel used here is defined by

$$k_{restr}((x, y), (x', y')) = k(x_{|y}, x_{|y'})$$

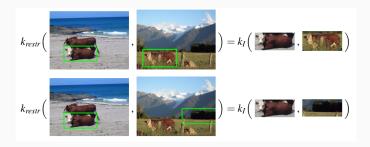


Figure from Blaschko and Lampert (http://www.robots.ox.ac.uk/~vgg/research/joint\_kernel\_detection/)

#### Restriction kernel

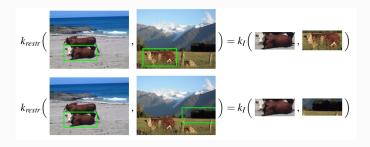


Figure from Blaschko and Lampert (http://www.robots.ox.ac.uk/~vgg/research/joint\_kernel\_detection/)

## **Prediction phase**

- During training computation of  $\xi_i$
- Prediction function:

$$f(x) = \arg\max_{y} (\sum_{iy'} \alpha_{iy'} (\phi_i(y') - \phi_i(y_i)))^T \phi(x, y)$$

Very expensive, need to be done for each possible window (or a sample of them) in the image:

#### **Alternative**

Branch and Bound algorithm to search  $\mathcal{Y}$ .

## Branch and bound algorithm

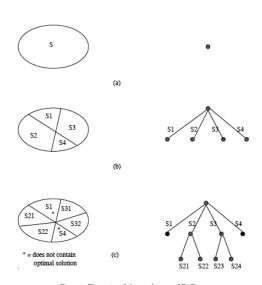


Figure 1: Illustration of the search space of B&B.

## Results on VOC 2006 (Lampert, Blaschko 2006)

Visual Object Recognition Challenge 2006. Area under the Precision Recall curve (Pr = TP/P, Rec = TP)

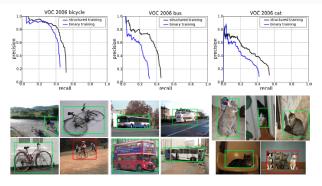


Fig. 5. Precision—recall curves and example detections for the PASCAL VOC bicycle, bus and cat category (from left to right). Structured training improves both, precision and recall. Red boxes are counted as mistakes by the VOC evaluation routine, because they are too large or contain more than one object.

**Software libraries** 

#### **SVM**<sup>struct</sup>

▶ SVM-struct

```
Author: Thorsten Joachims

Cornelll University

Language: in C but Python interface exists

https:

//www.cs.cornell.edu/people/tj/svm_light/svm_struct.html
```

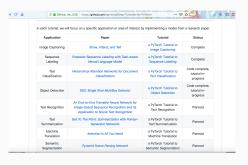
## **PyStruct**

Authors: Andreas C. Mueller, Sven Behnke University of Bonn
Structured Output Prediction
https://pystruct.github.io/ PyStruct

## **PyTorch** (2016)

Authors: Adam Paszke, Sam Gross, Soumith Chintala, Gregory Chanan https://pytorch.org/ PyTorch Based on Torch: Ronan Collobert, Koray Kavukcuoglu, Clement Farabet.

Many Deep Structured prediction tools are written in PyTorch



**Conclusion and References** 

### Conclusion

#### Structured Output Prediction

- Enlarges considerably the scope of supervised learning
- Refers to a large set of problems
- Prediction in the original output space is an issue (usually expensive)
- Learning can be implemented either by learning a score or a surrogate problem
- No restriction to a specific model (MLP, CNN, SVM, trees)
- End-to-end learning refers to approaches in which the decoding problem is rather simple
- Theoretical framework for structured output learning: PAC-Bayes for SOP, Calibration theory

## New challenges

- Bridge the gap between approaches that work for millions of data (deep learning) but still very computationally demanding, with nearly no theory and surrogate loss approaches
- Combination of deep architectures with margin losses, or with a kernel-based last layer
- Learning surrogate loss it self is one of the next challenge

## References

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## To go further: References for this lecture

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