



# Combinatorial Optimization in Computer Vision (IN2245)

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Winter Semester 2015/2016

## 23. Loss minimizing parameter learning

Parameter learning   Probabilistic parameter learning   Loss-minimizing parameter learning

### Parameter learning

### Parameter learning

*Learning graphical models* (from training data) is a way to find among a large class of possible models a single one that is *best* in some sense for the task at hand.

We assume a fixed underlying graphical model with **parameterized conditional probability distribution**

$$p(y | x, w) = \frac{1}{Z(x, w)} \exp(-E(x, y, w)) = \frac{1}{Z(x, w)} \exp(-\langle w, \varphi(x, y) \rangle),$$

where  $Z(x, w) = \sum_{y \in \mathcal{Y}} \exp(-\langle w, \varphi(x, y) \rangle)$ . The only unknown quantity is the **parameter vector  $w$** , on which the energy  $E(x, y, w)$  depends linearly.

Parameter learning   Probabilistic parameter learning   Loss-minimizing parameter learning

### Learning tasks

Let  $d(y | x)$  be the (*unknown*) conditional distribution of labels for a problem to be solved. For a parameterized conditional distribution  $p(y | x, w)$  with parameters  $w \in \mathbb{R}^D$ , **probabilistic parameter learning** is the task of finding a point estimate of the parameter  $w^*$  that minimizes the **expected dissimilarity** of  $p(y | x, w^*)$  and  $d(y | x)$ :

$$\text{KL}_{\text{tot}}(p \| d) = \sum_{x \in \mathcal{X}} d(x) \sum_{y \in \mathcal{Y}} d(y | x) \log \frac{d(y | x)}{p(y | x, w)}.$$

Let  $d(x, y)$  be the unknown distribution of data in labels, and let  $\Delta : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}_+$  be a loss function. **Loss minimizing parameter learning** is the task of finding a parameter value  $w^*$  such that the *expected prediction loss*

$$\mathbb{E}_{(x,y) \sim d(x,y)} [\Delta(y, f_p(x))]$$

is as small as possible, where  $f_p(x) = \text{argmax}_{y \in \mathcal{Y}} p(y | x, w^*)$ .

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### Probabilistic parameter learning

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### Regularized Maximum Conditional Likelihood Training

Let  $p(y | x, w) = \frac{1}{Z(x, w)} \exp(-\langle w, \varphi(x, y) \rangle)$  be a **probability distribution** parameterized by  $w \in \mathbb{R}^D$ , and let  $\mathcal{D} = \{(x^n, y^n)\}_{n=1, \dots, N}$  be a set of *i.i.d. training examples*. For any  $\lambda > 0$ , **regularized maximum conditional likelihood** training chooses the parameter as

$$w = \underset{w \in \mathbb{R}^D}{\operatorname{argmin}} L(w) = \underset{w \in \mathbb{R}^D}{\operatorname{argmin}} \lambda \|w\|^2 + \sum_{n=1}^N \langle w, \varphi(x^n, y^n) \rangle + \sum_{n=1}^N \log Z(x^n, w).$$

For  $\lambda = 0$  the simplified rule is given by

$$w = \underset{w \in \mathbb{R}^D}{\operatorname{argmin}} \sum_{n=1}^N \langle w, \varphi(x^n, y^n) \rangle + \sum_{n=1}^N \log Z(x^n, w).$$

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### Numerical solution

$$\nabla_w L(w) = 2\lambda w + \sum_{n=1}^N (\varphi(x^n, y^n) - \mathbb{E}_{y \sim p(y|x^n, w)} [\varphi(x^n, y)]).$$

In a naive way, the complexity of the gradient computation is  $\mathcal{O}(K^M ND)$ .

$$\lambda \|w\|^2 + \sum_{n=1}^N \langle w, \varphi(x^n, y^n) \rangle + \sum_{n=1}^N \log Z(x^n, w).$$

In a naive way, the complexity of a line search is  $\mathcal{O}(K^M ND)$  (for each evaluation of  $L$ ), where

- $N$  is the number of samples,
- $D$  is the dimension of weight vector,
- $M = |\mathcal{V}|$  is number of output nodes, and
- $K = \max_{i \in \mathcal{V}} |\mathcal{Y}_i|$  is (maximal) number of possible labels of each output nodes.

If the training set  $\mathcal{D}$  is too large, one can create a random subset  $\mathcal{D}' \subset \mathcal{D}$  and estimate the gradient  $\nabla_w L(w)$  on  $\mathcal{D}'$ . In an extreme case, one may randomly select only **one** sample and calculate the gradient

$$\tilde{\nabla}_w^{(x^n, y^n)} L(w) = 2\lambda w + \varphi(x^n, y^n) - \mathbb{E}_{y \sim p(y|x^n, w)} [\varphi(x^n, y)].$$

This approach is called **stochastic gradient descent** (SGD). Note that line search is not possible, therefore, we need for an extra parameter, referred to as step-size  $\eta_t$  for each iteration.

## Using of the output structure

Assume the set of factors  $\mathcal{F}$  in a graphical model representation, such that  $\varphi(x, y)$  decomposes as  $\varphi(x, y) = [\varphi_F(x_F, y_F)]_{F \in \mathcal{F}}$ . Thus

$$\begin{aligned} \mathbb{E}_{y \sim p(y|x, w)} [\varphi(x, y)] &= [\mathbb{E}_{y \sim p(y|x, w)} [\varphi_F(x_F, y_F)]]_{F \in \mathcal{F}} \\ &= [\mathbb{E}_{y_F \sim p(y_F|x_F, w)} [\varphi_F(x_F, y_F)]]_{F \in \mathcal{F}}, \end{aligned}$$

where

$$\mathbb{E}_{y_F \sim p(y_F|x_F, w)} [\varphi_F(x_F, y_F)] = \sum_{y_F \in \mathcal{Y}_F} p(y_F | x_F, w) \varphi_F(x_F, y_F).$$

Factor marginals  $\mu_F = p(y_F | x_F, w)$  are generally (much) easier to calculate than the complete joint distribution  $p(y | x, w)$ .

They can be either computed exactly (e.g., by applying Belief propagation yielding  $\mathcal{O}(K^2 MND)$ ) or approximated. In general, the approximation yields  $\mathcal{O}(K^{|F_{\max}|} MND)$ , where  $|F_{\max}|$  is the maximal factor size.

## Basic sampling

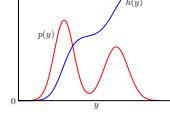
Let  $Z$  be a uniformly distributed random variable on the interval  $[0, 1]$  and  $h(y)$  be a continuous and strictly monotonic cumulative distribution function. Then

$$Y = h^{-1}(Z)$$

is a random variable with cumulative distribution function (cdf.)  $h(y)$ , where  $h^{-1}(y)$  is the inverse of  $h(y)$ .

The cdf. of the uniformly distributed  $Z$  is given by

$$F(z) = \begin{cases} 0, & \text{if } z \leq 0 \\ z, & \text{if } 0 < z \leq 1 \\ 1, & \text{if } 1 < z \end{cases}$$



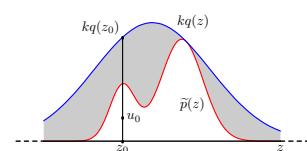
Therefore, the cdf. of  $Y$  is given by

$$P(Y < y) = P(h^{-1}(Z) < y) = P(Z < h(y)) = F(h(y)) = h(y).$$

## Rejection sampling \*

- Generate a sample  $z_0$  from the distribution  $q(z)$ .
- Generate a sample  $u_0 \sim \mathcal{U}(0, kq(z_0))$ .

This pair of random samples has uniform distribution under the curve of the function  $kq(z)$ .



If  $u_0 > \tilde{p}(z_0)$  then the sample is *rejected*, otherwise  $u_0$  is retained. Note that the remaining pairs then have uniform distribution under the curve of  $\tilde{p}(z)$ .

The values of  $z$  are generated from  $q(z)$ , and these samples are accepted with probability  $\tilde{p}(z)/kq(z)$ , therefore

$$p(\text{accept}) = \int \frac{\tilde{p}(z)}{kq(z)} q(z) dz = \frac{1}{k} \int \tilde{p}(z) dz.$$

**Input:** Step-sizes  $\eta_1, \dots, \eta_T$  for all the  $T$  iterations.

**Output:** The learned weight vector  $w \in \mathbb{R}^D$ .

```

1:  $w \leftarrow 0$ 
2: for  $t = 1, \dots, T$  do
3:    $(x^n, y^n) \leftarrow$  randomly chosen training example pair
4:    $d \leftarrow -\tilde{\nabla}_w^{(x^n, y^n)} L(w)$ 
5:    $w \leftarrow w + \eta_t d$ 
6: end for
7: return  $w$ 
```

If the step-size is chosen correctly (e.g.,  $\eta_t = \frac{1}{t}$ ), then SGD converges to  $\arg\min_{w \in \mathbb{R}^D} L(w)$ . However, it needs more iterations, but each one is much faster.

## Gradient approximation via sampling

$$\nabla_w L(w) = 2\lambda w + \sum_{n=1}^N (\varphi(x^n, y^n) - \mathbb{E}_{y \sim p(y|x^n, w)} [\varphi(x^n, y)]).$$

We have seen that the computationally demanding part in the gradient computation has the form of the expectation of  $\varphi(x, y)$  with respect to the distribution  $p(y | x, w)$ .

If we have a method to obtain *i.i.d* samples  $\{y^{(1)}, \dots, y^{(S)}\}$  from this distribution, we can form an estimator

$$\mathbb{E}_{y \sim p(y|x^n, w)} [\varphi(x^n, y)] \approx \frac{1}{S} \sum_{i=1}^S \varphi(x^n, y^{(i)}).$$

Inserting this into  $\nabla_w L$ , the law of large numbers guarantees convergence of the approximation to the exact gradient. Consequently, any procedure to sample from  $p(y | x^n, w)$  for  $n = 1, \dots, N$  provides us with a tool for estimating  $\nabla_w L$ .

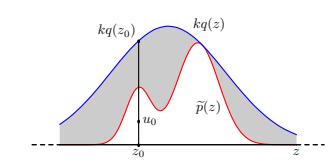
## Rejection sampling \*

Suppose we wish to sample from a distribution  $p(z)$  that can be a relatively complex distributions, and that sampling directly from  $p(z)$  is *difficult*.

Furthermore suppose that we are easily able to evaluate  $p(z)$  for any given value of  $z$ , up to some normalizing constant  $Z_p$ , so that

$$p(z) = \frac{1}{Z_p} \tilde{p}(z),$$

where  $\tilde{p}(z)$  can readily be evaluated, but  $Z_p$  is unknown.



We need some simpler distribution  $q(z)$ , called a **proposal distribution**, from which we can readily draw samples. Let  $k$  a constant such that  $kq(z) \geq \tilde{p}(z)$  for all values of  $z$ .

## Metropolis-Hastings algorithm \*

**Input:**  $\tilde{p}(y | x, w) \propto p(y | x, w)$ , unnormalized target distribution and  $q(y' | y)$ , proposal distribution

**Output:**  $y^{(t)}$ , sequence of samples with approximately  $y^{(t)} \sim p(y | x, w)$

```

1:  $y^0 \leftarrow$  arbitrary in  $\mathcal{Y}$ 
2: for  $t = 1, \dots, T$  do
3:    $y^{(t)} \sim q(y' | y^{(t-1)})$  ▷ Generate candidate
4:    $\sigma \leftarrow \min \left( 1, \frac{\tilde{p}(y'|x,w)q(y^{(t-1)}|y')}{\tilde{p}(y^{(t-1)}|x,w)q(y'|y^{(t-1)})} \right)$  ▷ Compute accept. prob.
5:    $y^{(t)} \leftarrow \begin{cases} y' & \text{with probability } \sigma \text{ (accept)} \\ y^{(t-1)} & \text{otherwise (reject)} \end{cases}$  ▷ Update
6:   output  $y^{(t)}$ 
7: end for
```

## Loss-minimizing parameter learning

Let  $\mathcal{D} = \{(x^1, y^1), \dots, (x^N, y^N)\}$  be i.i.d. samples from the (unknown) *true data distribution*  $d(x, y)$  and  $\Delta : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}_+$  be a *loss function*. The task is to find a weight vector  $w$  that leads to **minimal expected loss**

$$\mathbb{E}_{(x,y) \sim d(x,y)} [\Delta(y, f(x))]$$

for a *prediction function*  $f(x) = \operatorname{argmax}_{y \in \mathcal{Y}} g(x, y; w)$ , where  $g : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}$  is an auxiliary function that is parameterized by  $w \in \mathbb{R}^D$ .

Pros:

- We directly optimize for the *quantity of interest*, i.e. the expected loss.
- We do not need to compute the *partition function*  $Z$ .

Cons:

- There is no probabilistic reasoning to find  $w$ .
- We need to know the *loss function* already at training time.

## Regularized loss minimization

Let us define the auxiliary function  $g(x, y; w) := -\langle w, \varphi(x, y) \rangle$ . We aim to find the parameter  $w^*$  that minimizes

$$\mathbb{E}_{(x,y) \sim d(x,y)} [\Delta(y, \operatorname{argmax}_{y \in \mathcal{Y}} g(x, y; w))].$$

However,  $d(x, y)$  is unknown, hence we apply *approximation*:

$$\mathbb{E}_{(x,y) \sim d(x,y)} [\Delta(y, \operatorname{argmax}_{y \in \mathcal{Y}} g(x, y; w))] \approx \frac{1}{N} \sum_{n=1}^N \Delta(y^n, \operatorname{argmax}_{y \in \mathcal{Y}} g(x^n, y^n; w)).$$

Moreover, we add the **regularizer**  $\lambda \|w\|^2$  in order to avoid *overfitting*.

Therefore, we get a new objective, that is

$$w^* \in \operatorname{argmin}_{w \in \mathbb{R}^D} \lambda \|w\|^2 + \frac{1}{N} \sum_{n=1}^N \Delta(y^n, \operatorname{argmax}_{y \in \mathcal{Y}} g(x^n, y^n; w)).$$

## Hinge loss

The **hinge loss** is defined as

$$\begin{aligned} \ell(x^n, y^n, w) &\stackrel{\Delta}{=} \max_{y \in \mathcal{Y}} (\Delta(y^n, y) + g(x^n, y; w) - g(x^n, y^n; w)) \\ &= \max_{y \in \mathcal{Y}} (\Delta(y^n, y) + \langle w, \varphi(x^n, y) \rangle - \langle w, \varphi(x^n, y^n) \rangle). \end{aligned}$$

$\ell$  is continuous and convex, since it is a maximum over linear functions.

The **hinge loss**  $\ell$  provides an upper bound for the *loss function*  $\Delta$ . To see this, let  $\bar{y} = \operatorname{argmax}_{y \in \mathcal{Y}} g(x^n, y; w)$ , then

$$\begin{aligned} \Delta(x^n, \bar{y}) &\leq \Delta(x^n, \bar{y}) + g(x^n, \bar{y}; w) - g(x^n, y^n; w) \\ &\leq \max_{y \in \mathcal{Y}} (\Delta(x^n, y) + g(x^n, y; w) - g(x^n, y^n; w)) \\ &= \ell(x^n, y^n, w). \end{aligned}$$

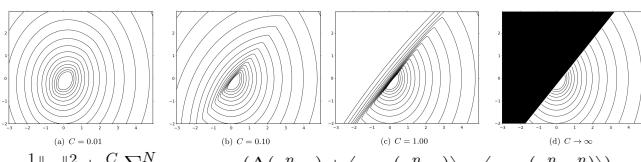
## S-SVM: Toy example \*

Consider a simple CRF model with a single variable, where  $\mathcal{Y} = \{-1, +1\}$ . We define the energy function as

$$E(x, y, w) = w_1 \varphi_1(x, y) + w_2 \varphi_2(x, y).$$

Assuming a training set  $\mathcal{D} = \{(-10, +1), (-4, +1), (6, -1), (5, -1)\}$  with

$$\varphi_1(x, y) = \begin{cases} 0, & \text{if } y = -1 \\ x, & \text{if } y = +1 \end{cases} \quad \text{and} \quad \varphi_2(x, y) = \begin{cases} x, & \text{if } y = -1 \\ 0, & \text{if } y = +1 \end{cases}.$$



## Structured Support Vector Machine

Let  $g(x, y; w) = \langle w, \varphi(x, y) \rangle$  be an auxiliary function parameterized by  $w \in \mathbb{R}^D$ . For any  $C > 0$ , **structured support vector machine** (S-SVM) training chooses the parameter

$$w^* \in \operatorname{argmin}_{w \in \mathbb{R}^D} \frac{1}{2} \|w\|^2 + \frac{C}{N} \sum_{n=1}^N \ell(x^n, y^n, w)$$

with

$$\ell(x^n, y^n, w) = \max_{y \in \mathcal{Y}} (\Delta(y^n, y) + \langle w, \varphi(x^n, y) \rangle - \langle w, \varphi(x^n, y^n) \rangle).$$

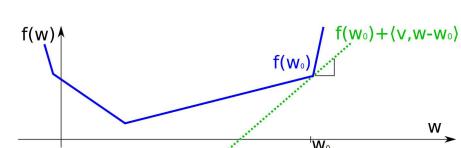
Both CRF and S-SVM do *regularized risk minimization*. For CRF models, the *regularized conditional log-likelihood function* can be written as:

$$w^* \in \operatorname{argmin}_{w \in \mathbb{R}^D} \frac{\|w\|^2}{2\sigma^2} + \sum_{n=1}^N \log \sum_{y \in \mathcal{Y}} \exp (\langle w, \varphi(x^n, y) \rangle - \langle w, \varphi(x^n, y^n) \rangle).$$

## Subgradient

Let  $f : \mathbb{R}^D \rightarrow \mathbb{R}$  be a convex, not necessarily differentiable, function. A vector  $v \in \mathbb{R}^D$  is called a **subgradient** of  $f$  at  $w_0$ , if

$$f(w) \geq f(w_0) + \langle v, w - w_0 \rangle \quad \text{for all } w.$$



Note that for differentiable  $f$ , the gradient  $v = \nabla f(w_0)$  is the **only** subgradient.

Subgradient descent methods work basically like gradient descent ones.

**Input:** Tolerance  $\epsilon > 0$  and step-sizes  $\eta_t$ .

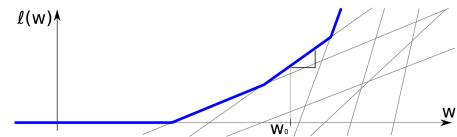
**Output:** The minimizer  $w$  of  $F$ .

- 1:  $w \leftarrow \mathbf{0}$
- 2: **repeat**
- 3:    $v \in \nabla_w^{\text{sub}} F(w)$
- 4:    $w \leftarrow w - \eta_t v$
- 5: **until**  $F$  changed less than  $\epsilon$
- 6: **return**  $w$

Converges to global minimum, but rather inefficient if the objective function  $F$  is non-differentiable.

$$\underset{w \in \mathbb{R}^D}{\operatorname{argmin}} \frac{1}{2} \|w\|^2 + \frac{C}{N} \sum_{n=1}^N \max_{y \in \mathcal{Y}} (\Delta(y^n, y) + \langle w, \varphi(x^n, y) \rangle - \langle w, \varphi(x^n, y^n) \rangle).$$

As we have discussed, this function is non-differentiable. Therefore, we cannot use gradient descent directly, so we have to use subgradients.



For each  $y \in \mathcal{Y}$ ,  $\ell$  is a linear function, since it is the maximum over all  $y \in \mathcal{Y}$ . In order to calculate the subgradient at  $w_0$ , one may find the maximal (active)  $y$ , and then use  $v = \nabla \ell(w_0)$ .

## Calculating the subgradient

$$\underset{w \in \mathbb{R}^D}{\operatorname{argmin}} \frac{1}{2} \|w\|^2 + \frac{C}{N} \sum_{n=1}^N \max_{y \in \mathcal{Y}} (\Delta(y^n, y) + \langle w, \varphi(x^n, y) \rangle - \langle w, \varphi(x^n, y^n) \rangle).$$

Let  $\hat{y} \in \operatorname{argmax}_{y \in \mathcal{Y}} \Delta(y^n, y) + \langle w, \varphi(x^n, y) \rangle$ .

A subgradient  $v$  is given by

$$\begin{aligned} \nabla_w^{\text{sub}} & \left( \frac{1}{2} \|w\|^2 + \frac{C}{N} \sum_{n=1}^N \max_{y \in \mathcal{Y}} (\Delta(y^n, y) + \langle w, \varphi(x^n, y) \rangle - \langle w, \varphi(x^n, y^n) \rangle) \right) \\ & \ni \nabla_w \left( \frac{1}{2} \|w\|^2 + \frac{C}{N} \sum_{n=1}^N (\Delta(y^n, \hat{y}) + \langle w, \varphi(x^n, \hat{y}) \rangle - \langle w, \varphi(x^n, y^n) \rangle) \right) \\ & = w + \frac{C}{N} \sum_{n=1}^N \varphi(x^n, \hat{y} - \varphi(x^n, y^n)) =: v. \end{aligned}$$

## Stochastic subgradient descent S-SVM learning

**Input:** Training set  $\mathcal{D} = \{(x^1, y^1), \dots, (x^N, y^N)\}$ , energies  $\varphi(x, y)$ , loss function  $\Delta(y, y')$ , regularizer  $C$  and step-sizes  $\eta_1, \dots, \eta_T$  for all the  $T$  iterations.

**Output:** The weight vector  $w$  for the prediction function

$$f(x) = \operatorname{argmax}_{y \in \mathcal{Y}} \langle w, \varphi(x, y) \rangle.$$

- 1:  $w \leftarrow \mathbf{0}$
- 2: **for**  $t = 1, \dots, T$  **do**
- 3:    $(x^n, y^n) \leftarrow$  randomly chosen training example pair
- 4:    $\hat{y} \leftarrow \operatorname{argmax}_{y \in \mathcal{Y}} \Delta(y^n, y) + \langle w, \varphi(x^n, y) \rangle$
- 5:    $w \leftarrow w - \eta_t \left( w + \frac{C}{N} \sum_{n=1}^N (\varphi(x^n, \hat{y}) - \varphi(x^n, y^n)) \right)$
- 6: **end for**

Note that each update step of  $w$  needs only one argmax-prediction, however we will generally need **many** iterations until convergence.

## Subgradient descent S-SVM learning

**Input:** Training set  $\mathcal{D} = \{(x^1, y^1), \dots, (x^N, y^N)\}$ , energies  $\varphi(x, y)$ , loss function  $\Delta(y, y')$ , regularizer  $C$  and step-sizes  $\eta_1, \dots, \eta_T$  for all the  $T$  iterations.

**Output:** the weight vector  $w$  for the prediction function

$$f(x) = \operatorname{argmax}_{y \in \mathcal{Y}} \langle w, \varphi(x, y) \rangle.$$

- 1:  $w \leftarrow \mathbf{0}$
- 2: **for**  $t = 1, \dots, T$  **do**
- 3:   **for**  $n = 1, \dots, N$  **do**
- 4:      $\hat{y} \leftarrow \operatorname{argmax}_{y \in \mathcal{Y}} \Delta(y^n, y) + \langle w, \varphi(x^n, y) \rangle$
- 5:      $v^n \leftarrow \varphi(x^n, \hat{y}) - \varphi(x^n, y^n)$
- 6:   **end for**
- 7:    $w \leftarrow w - \eta_t \left( w + \frac{C}{N} \sum_{n=1}^N v^n \right)$
- 8: **end for**

The step-size can be chosen as  $\eta_t = \frac{1}{t}$  for all  $t = 1, \dots, T$ .

Note that each update of  $w$  needs only one argmax-prediction.

## Summary of S-SVM learning

We are given a *training set*  $\mathcal{D} = \{(x^1, y^1), \dots, (x^N, y^N)\} \subset \mathcal{X} \times \mathcal{Y}$  and a problem specific *loss function*  $\Delta : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$ .

The task is to *learn* parameter  $w$  for prediction function

$$f(x) = \operatorname{argmax}_{y \in \mathcal{Y}} \langle w, \varphi(x, y) \rangle$$

that minimizes *expected loss* on *test data*.

S-SVM solution derived by *maximum margin framework*:

$$\langle w, \varphi(x^n, y^n) \rangle \geq \Delta(y^n, y) + \langle w, \varphi(x^n, y) \rangle,$$

that is the correct output is enforced to be better than others by a margin.

We have seen that S-SVM learning ends up a convex optimization problem, but it is non-differentiable. Furthermore it requires repeated *argmax prediction*.

## Literature \*

- Sebastian Nowozin and Christoph H. Lampert. **Structured Prediction and Learning in Computer Vision**. In *Foundations and Trends in Computer Graphics and Vision*, Volume 6, Number 3-4. Note: Chapter 5, 6.
- Christopher Bishop. **Pattern Recognition and Machine Learning**. Springer, 2006. Note: Chapter 11.