Statistical Machine Learning https://cvml.ist.ac.at/courses/SML_W18

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# Institute of Science and Technology 

Winter Semester 2018/2019
Lecture 11
(lots of material courtesy of S. Nowozin, http://www.nowozin.net)

## Overview (tentative)

| Date |  | no. | Topic |
| :--- | :---: | :---: | :--- |
| Oct 08 | Mon | 1 | A Hands-On Introduction |
| Oct 10 | Wed | - | self-study (Christoph traveling) <br> Bayesian Decision Theory |
| Oct 15 | Mon | 2 | Generative Probabilistic Models <br> Oct 17 |
| Wed | 3 | Discriminative Probabilistic Models <br> Maximum Margin Classifiers |  |
| Oct 22 | Mon | 4 | Generalized Linear Classifiers, Optimization <br> Oct 24 Wed |
| Oct 29 | Mon | Evaluating Predictors; Model Selection |  |
| Self-study (Christoph traveling) |  |  |  |
| Oct 31 | Wed | 6 | Overfitting/Underfitting, Regularization |
| Nov 05 | Mon | 7 | Learning Theory I: classical/Rademacher bounds |
| Nov 07 | Wed | 8 | Learning Theory II: miscellaneous |
| Nov 12 | Mon | 9 | Probabilistic Graphical Models I |
| Nov 14 | Wed | 10 | Probabilistic Graphical Models II |
| Nov 19 | Mon | 11 | Probabilistic Graphical Models III |
| Nov 21 | Wed | 12 | Probabilistic Graphical Models IV <br> final project |
| until Nov 25 |  |  |  |

# Structured Loss Functions 

$$
\Delta(\bar{y}, y)
$$

## Loss function

## How to judge if a (structured) prediction is good?

- Define a loss function

$$
\Delta: \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}^{+}
$$

$\Delta(\bar{y}, y)$ measures the loss incurred by predicting $y$ when $\bar{y}$ is correct.

- The loss function is application dependent



## Example 1: 0/1 loss

Loss is 0 for perfect prediction, 1 otherwise:

$$
\Delta_{0 / 1}(\bar{y}, y)=\llbracket \bar{y} \neq y \rrbracket= \begin{cases}0 & \text { if } \bar{y}=y \\ 1 & \text { otherwise }\end{cases}
$$

Every mistake is equally bad. Usually not very useful in structured prediction.

## Example 2: Hamming loss

Count the number of mislabeled variables:

$$
\Delta_{H}(\bar{y}, y)=\frac{1}{|V|} \sum_{i \in V} \llbracket \bar{y}_{i} \neq y_{i} \rrbracket
$$



Used, e.g., for graph labeling tasks

## Example 3: Squared error

If we can add elements in $\mathcal{Y}_{i}$
(pixel intensities, optical flow vectors, etc.).
Sum of squared errors

$$
\Delta_{Q}(\bar{y}, y)=\frac{1}{|V|} \sum_{i \in V}\left\|\bar{y}_{i}-y_{i}\right\|^{2}
$$



Used, e.g., in stereo reconstruction, part-based object detection.

## Example 4: Task specific losses

Object detection

- bounding boxes, or
- arbitrarily shaped regions


Intersection-over-union loss:

$$
\Delta_{\text {loU }}(\text { bary }, y)=1-\frac{\operatorname{area}(\bar{y} \cap y)}{\operatorname{area}(\bar{y} \cup y)}
$$



Used, e.g., in PASCAL VOC challenges for object detection, because its scale-invariance (no bias for or against big objects).

## Making Bayes-optimal Predictions

Given a distribution $p(y \mid x)$, what is the best way to predict $f: \mathcal{X} \rightarrow \mathcal{Y}$ ?
Bayesian decision theory: pick $f(x)$ that causes minimal expected loss:

$$
\begin{aligned}
f(x) & =\underset{y \in \mathcal{Y}}{\operatorname{argmin}} \mathcal{R}_{\Delta}(y) \\
\text { for } \quad \mathcal{R}_{\Delta}(y) & =\underset{\bar{y} \sim p(y \mid x)}{\mathbb{E}}\{\Delta(\bar{y}, y)\}=\sum_{\bar{y} \in \mathcal{Y}} \Delta(\bar{y}, y) p(\bar{y} \mid x)
\end{aligned}
$$

For many loss functions not tractable, but some exceptions:

- $\mathcal{R}_{\Delta_{0 / 1}}(y)=1-p(y \mid x)$, so $f(x)=\operatorname{argmax}_{y} p(y \mid x)$
- $\mathcal{R}_{\Delta_{H}}(y)=1-\sum_{i \in V} p\left(y_{i} \mid x\right)$, so $f(x)=\left(y_{1}, \ldots, y_{n}\right)$ for $y_{i}=\operatorname{argmax}_{k \in \mathcal{Y}_{i}} p\left(y_{i}=k \mid x\right)$


## Structured Support Vector Machines

$$
\min _{f} \mathbb{E}_{(x, y)} \Delta(y, f(x))
$$

## Loss-Minimizing Parameter Learning

- $\mathcal{D}=\left\{\left(x_{1}, y_{1}\right), \ldots,\left(x_{n}, y_{n}\right)\right\}$ i.i.d. training set
- $\phi: \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}^{D}$ be a feature function, like for CRF
- $\Delta: \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$ be a loss function.
- Find a weight vector $w^{*}$ that minimizes the expected loss

$$
\underset{(x, y)}{\mathbb{E}} \Delta(y, f(x))
$$

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

## Loss-Minimizing Parameter Learning

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\underset{(x, y)}{\mathbb{E}} \Delta(y, f(x))
$$

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

- We directly optimize for the quantity of interest: expected loss.
- No expensive-to-compute partition function $Z$ will show up.

Disadvantage:

- We need to know the loss function already at training time.
- We can't use probabilistic reasoning to find $w^{*}$.


## Inspiration: multi-class SVM

- $\mathcal{X}$ anything, $\mathcal{Y}=\{1,2, \ldots, K\}$,
- feature $\operatorname{map} \phi: \mathcal{X} \rightarrow \mathcal{H}$ (explicit or implicit via kernel)
- training data $\left\{\left(x_{1}, y_{1}\right), \ldots,\left(x_{n}, y_{n}\right)\right\}$
- goal: learn functions $g_{k}(x)=\left\langle w_{k}, \phi(x)\right\rangle$ for $k=1, \ldots, K$.

Prediction: $\quad f(x)=\underset{k=1, \ldots}{\operatorname{argmax}} g_{k}(x)=\underset{k=1, \ldots, K}{\operatorname{argmax}}\left\langle w_{k}, \phi(x)\right\rangle$

Enforce a margin between the correct and all incorrect labels:

$$
\min _{w_{1}, \ldots, w_{K}, \xi} \frac{1}{2} \sum_{k=1}^{K}\left\|w_{k}\right\|^{2}+\frac{C}{n} \sum_{i=1}^{n} \xi_{i}
$$

subject to, for $i=1, \ldots, n$,

$$
\left\langle w_{y^{i}}, \phi\left(x^{i}\right)\right\rangle \geq 1+\left\langle w_{k}, \phi\left(x^{i}\right)\right\rangle-\xi^{i}, \quad \text { for all } k \neq y_{i} .
$$

Crammer-Singer Multiclass SVM

## Equivalent parameterization:

- $\mathcal{X}$ anything, $\mathcal{Y}=\{1,2, \ldots, K\}$,
- feature map $\psi: \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}^{D}$ (explicit or implicit via kernel)
- $\psi(x, y)=(\llbracket y=1 \rrbracket \phi(x), \llbracket y=2 \rrbracket \phi(x), \ldots, \llbracket y=K \rrbracket$
- $w=\left(w_{1}, \ldots, w_{K}\right) \in \mathbb{R}^{K D}$
- goal: learn a function $g(x, y)=\langle w, \psi(x, y)\rangle$

Prediction: $\quad f(x)=\underset{k=1, \ldots, M}{\operatorname{argmax}}\langle w, \psi(x, y)\rangle$

Enforce a margin of 1 between the correct and any incorrect label:

$$
\min _{w, \boldsymbol{\xi}} \frac{1}{2}\|w\|^{2}+\frac{C}{n} \sum_{i=1}^{n} \xi^{i}
$$

subject to, for $i=1, \ldots, n$,

$$
\left\langle w, \psi\left(x_{i}, y_{i}\right)\right\rangle \geq 1+\left\langle w, \psi\left(x_{i}, \bar{y}\right)\right\rangle-\xi_{i}, \quad \text { for all } \bar{y} \neq y_{i} .
$$

## Observation:

- for structure outputs, not all "incorrect" labels are equally bad $\rightarrow$ margin between $y_{i}$ and $\bar{y}$ should depend on $\Delta\left(y_{i}, \bar{y}\right)$


## Structured (Output) Support Vector Machine

Goal: learn a function $g(x, y)=\langle w, \psi(x, y)\rangle$
Prediction: $\quad f(x)=\underset{k=1, \ldots, M}{\operatorname{argmax}}\langle w, \psi(x, y)\rangle$

Enforce a margin $\Delta\left(y_{i}, y\right)$ between the correct and any incorrect label:

$$
\min _{w, \boldsymbol{\xi}} \quad \frac{1}{2}\|w\|^{2}+\frac{C}{n} \sum_{i=1}^{n} \xi_{i}
$$

subject to, for $i=1, \ldots, n$,

$$
\left\langle w, \psi\left(x_{i}, y_{i}\right)\right\rangle \geq \Delta\left(y_{i}, \bar{y}\right)+\left\langle w, \psi\left(x_{i}, \bar{y}\right)\right\rangle-\xi_{i}, \quad \text { for all } \bar{y} \in \mathcal{Y} .
$$

## Structured Output Support Vector Machine

Equivalent unconstrained formulation (solve for optimal $\xi_{1}, \ldots, \xi_{n}$ ):

$$
\min _{w} \frac{\lambda}{2}\|w\|^{2}+\frac{1}{n} \sum_{i=1}^{n} \max _{\bar{y} \in \mathcal{Y}}\left[\Delta\left(y_{i}, \bar{y}\right)+\left\langle w, \psi\left(x_{i}, \bar{y}\right)\right\rangle-\left\langle w, \psi\left(x_{i}, y_{i}\right)\right\rangle\right]
$$

## Conditional Random Field

Regularized conditional log-likelihood:

$$
\min _{w} \frac{\lambda}{2}\|w\|^{2}+\frac{1}{n} \sum_{i=1}^{n} \log \sum_{\bar{y} \in \mathcal{Y}} \exp \left(\left\langle w, \psi\left(x_{i}, \bar{y}\right)\right\rangle-\left\langle w, \phi\left(x_{i}, y_{i}\right)\right\rangle\right)
$$

CRFs and SSVMs have more in common than usually assumed.

- $\log \sum_{y} \exp (\cdot)$ can be interpreted as a soft-max (differentiable)
- SSVM training takes loss function into account
- CRF is trained without specific loss, loss enters at prediction time


## Structured Output Support Vector Machine

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CRFs and SSVMs have more in common than usually assumed.

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## Example: RNA Secondary Structure Prediction De Bona et al., 2007]

## AAAAACCCCCCCCAGAGGAGAUUG

 GAGAUCAAAGGUGGUUCGGAUGUC $\rightarrow$ GAAGUGUACCGAACCCGGGGG

- $\mathcal{X}=\Sigma^{*}$ for $\Sigma=\{\mathrm{A}, \mathrm{C}, \mathrm{G}, \mathrm{U}\}$ (nucleotide sequence)
- $\mathcal{Y}=\{(i, j): i, j \in \mathbb{N}, i<j\} \quad(i, j)$ mean " $x_{i}$ binds with $x_{j}$ "
- $\psi(x, y)$ domain-specific features: binding energy of $x_{i} \leftrightarrow x_{j}$, prefered patterns (motifs), loop properties, ...
- $\Delta(\bar{y}, y)$ : number of wrong/missing bindings (Hamming loss)
$\min _{w} \frac{\lambda}{2}\|w\|^{2}+\frac{1}{n} \sum_{i=1}^{n} \max _{\bar{y} \in \mathcal{Y}}\left[\Delta\left(y_{i}, \bar{y}\right)+\left\langle w, \psi\left(x_{i}, \bar{y}\right)\right\rangle-\left\langle w, \psi\left(x_{i}, y_{i}\right)\right\rangle\right]$


## Example: Sentence Parsing [Taskar et al., 2004]

The screen was a sea of red. $\rightarrow$


- $\mathcal{X}=\{$ English sentences $\}$
- $\mathcal{Y}=\{$ parse tree $\}$
- $\psi(x, y)$ domain-specific features:
- word properties, e.g. ". starts with capital letter", ". ends in ing"
- grammatical rules: $N P \rightarrow D T+N N$
- $\Delta(\bar{y}, y)$ : number of wrong assignments


## Solving S-SVM Training in Practice

$$
\min _{w} \frac{\lambda}{2}\|w\|^{2}+\frac{1}{n} \sum_{i=1}^{n} \max _{\bar{y} \in \mathcal{Y}}\left[\Delta\left(y_{i}, \bar{y}\right)+\left\langle w, \psi\left(x_{i}, \bar{y}\right)\right\rangle-\left\langle w, \psi\left(x_{i}, y_{i}\right)\right\rangle\right]
$$

- continuous
- unconstrained
- convex
- non-differentiable


## Solving S-SVM Training Numerically - Subgradient Method

## Computing a subgradient:

$$
\min _{w} \frac{\lambda}{2}\|w\|^{2}+\frac{1}{n} \sum_{i=1}^{n} \ell\left(x_{i}, y_{i}, w\right)
$$

with $\ell\left(x_{i}, y_{i}, w\right)=\max _{y} \ell_{y}\left(x_{i}, y_{i}, w\right)$, and

$$
\ell_{y}\left(x_{i}, y_{i}, w\right):=\Delta\left(y_{i}, y\right)+\left\langle w, \psi\left(x_{i}, y\right)\right\rangle-\left\langle w, \psi\left(x_{i}, y_{i}\right)\right\rangle
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## Solving S-SVM Training Numerically - Subgradient Method

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$$



For each $y \in \mathcal{Y}, \quad \ell_{y}(w)$ is a linear function of $w$.

## Solving S-SVM Training Numerically - Subgradient Method

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$$


max over finite $\mathcal{Y}$ : piece-wise linear

## Solving S-SVM Training Numerically - Subgradient Method

Computing a subgradient:

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Subgradient of $\ell$ at $w_{0}$ :

## Solving S-SVM Training Numerically - Subgradient Method

Computing a subgradient:

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Subgradient of $\ell$ at $w_{0}$ : find maximal (active) $y$.

## Solving S-SVM Training Numerically - Subgradient Method

Computing a subgradient:

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\min _{w} \frac{\lambda}{2}\|w\|^{2}+\frac{1}{n} \sum_{i=1}^{n} \ell\left(x_{i}, y_{i}, w\right)
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$$



Subgradient of $\ell$ at $w_{0}$ : find maximal (active) $y$, use $v=\nabla \ell_{y}\left(w_{0}\right)$.

## Solving S-SVM Training Numerically - Subgradient Method

## Computing a subgradient:

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$$



Not necessarily unique, but $v=\nabla \ell_{y}\left(w_{0}\right)$ works for any maximal $y$

## Solving S-SVM Training Numerically - Subgradient Method

## Subgradient Method S-SVM Training

input training pairs $\left\{\left(x^{1}, y^{1}\right), \ldots,\left(x^{n}, y^{n}\right)\right\} \subset \mathcal{X} \times \mathcal{Y}$, input feature map $\phi(x, y)$, loss function $\Delta\left(y, y^{\prime}\right)$, regularizer $\lambda$, input number of iterations $T$, stepsizes $\eta_{t}$ for $t=1, \ldots, T$

1: $w \leftarrow \overrightarrow{0}$
2: for $t=1, \ldots, T$ do
3: $\quad$ for $\mathrm{i}=1, \ldots, \mathrm{n}$ do
4: $\quad \hat{y} \leftarrow \operatorname{argmax}_{y \in \mathcal{Y}} \quad \Delta\left(y^{n}, y\right)+\left\langle w, \phi\left(x^{n}, y\right)\right\rangle-\left\langle w, \phi\left(x^{n}, y^{n}\right)\right\rangle$
5: $\quad v^{n} \leftarrow \phi\left(x^{n}, \hat{y}\right)-\phi\left(x^{n}, y^{n}\right)$
6: end for
7: $\quad w \leftarrow w-\eta_{t}\left(\lambda w-\frac{1}{N} \sum_{n} v^{n}\right)$
8: end for
output prediction function $f(x)=\operatorname{argmax}_{y \in \mathcal{Y}}\langle w, \phi(x, y)\rangle$.
Obs: each update of $w$ needs $N$ argmax-prediction (one per example). Obs: computing the argmax is (loss augmented) energy minimizatio $\eta_{34}$

## Example: Image Segmenatation

- $\mathcal{X}$ images, $\mathcal{Y}=\{$ binary segmentation masks $\}$.
- Training example(s): $\left(x^{n}, y^{n}\right)=(x)$
- $\Delta(y, \bar{y})=\sum_{p} \llbracket y_{p} \neq \bar{y}_{p} \rrbracket \quad$ (Hamming loss)


## Example: Image Segmenatation

- $\mathcal{X}$ images, $\mathcal{Y}=\{$ binary segmentation masks $\}$.
- Training example(s): $\left(x^{n}, y^{n}\right)=(-x, 0)$
- $\Delta(y, \bar{y})=\sum_{p} \llbracket y_{p} \neq \bar{y}_{p} \rrbracket \quad$ (Hamming loss)

$$
t=1: w=0,
$$

$$
\begin{aligned}
\hat{y} & =\underset{y}{\operatorname{argmax}}\left[\left\langle w, \phi\left(x^{n}, y\right)\right\rangle+\Delta\left(y^{n}, y\right)\right] \\
& \stackrel{w=0}{=} \underset{y}{\operatorname{argmax}} \Delta\left(y^{n}, y\right)=\text { "the opposite of } y^{n \prime \prime}
\end{aligned}
$$

## Example: Image Segmenatation

- $\mathcal{X}$ images, $\mathcal{Y}=\{$ binary segmentation masks $\}$.
- Training example(s): $\left(x^{n}, y^{n}\right)=(x, x, 0)$
- $\Delta(y, \bar{y})=\sum_{p} \llbracket y_{p} \neq \bar{y}_{p} \rrbracket \quad$ (Hamming loss)
$t=1: \hat{y}=\quad \phi\left(y^{n}\right)-\phi(\hat{y})$ black + , white + , green - , blue - , gray -


## Example: Image Segmenatation

- $\mathcal{X}$ images, $\mathcal{Y}=\{$ binary segmentation masks $\}$.
- Training example(s): $\left(x^{n}, y^{n}\right)=(-x, m)$
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## Example: Image Segmenatation

- $\mathcal{X}$ images, $\mathcal{Y}=\{$ binary segmentation masks $\}$.
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- $\Delta(y, \bar{y})=\sum_{p} \llbracket y_{p} \neq \bar{y}_{p} \rrbracket \quad$ (Hamming loss)
$t=1: \hat{y}=\quad \phi \quad \phi\left(y^{n}\right)-\phi(\hat{y})$ : black + , white + , green - , blue - , gray -
$t=2: \hat{y}=-\phi\left(y^{n}\right)-\phi(\hat{y})$ : black + , white + , green $=$, blue $=$, gray -
$t=3: \hat{y}=\$\left(y^{n}\right)-\phi(\hat{y})$ : black $=$, white $=$, green - , blue - , gray -


## Example: Image Segmenatation

- $\mathcal{X}$ images, $\mathcal{Y}=\{$ binary segmentation masks $\}$.
- Training example(s): $\left(x^{n}, y^{n}\right)=(-x,-x, 0)$
- $\Delta(y, \bar{y})=\sum_{p} \llbracket y_{p} \neq \bar{y}_{p} \rrbracket \quad$ (Hamming loss)
$t=1: \hat{y}=$
$t=2: \hat{y}=\phi\left(y^{n}\right)-\phi(\hat{y}):$ black + , white + , green - , blue - , gray -
$t=3: \hat{y}=$
$t=4: \hat{y}=, \phi\left(y^{n}\right)-\phi(\hat{y}):$ black + , white + , green $=$, blue $=$, gray -
$t\left(y^{n}\right)-\phi(\hat{y}):$ black $=$, white $=$, green - , blue - , gray -


## Example: Image Segmenatation

- $\mathcal{X}$ images, $\mathcal{Y}=\{$ binary segmentation masks $\}$.
- Training example(s): $\left(x^{n}, y^{n}\right)=$


- $\Delta(y, \bar{y})=\sum_{p} \llbracket y_{p} \neq \bar{y}_{p} \rrbracket \quad$ (Hamming loss)



## Solving S-SVM Training Numerically - Subgradient Method

Same trick as for CRFs: stochastic updates:

## Stochastic Subgradient Method S-SVM Training

 input training pairs $\left\{\left(x^{1}, y^{1}\right), \ldots,\left(x^{n}, y^{n}\right)\right\} \subset \mathcal{X} \times \mathcal{Y}$, input feature map $\phi(x, y)$, loss function $\Delta\left(y, y^{\prime}\right)$, regularizer $\lambda$, input number of iterations $T$, stepsizes $\eta_{t}$ for $t=1, \ldots, T$1: $w \leftarrow \overrightarrow{0}$
2: for $t=1, \ldots, T$ do
3: $\quad\left(x^{n}, y^{n}\right) \leftarrow$ randomly chosen training example pair
4: $\quad \hat{y} \leftarrow \operatorname{argmax}_{y \in \mathcal{Y}} \Delta\left(y^{n}, y\right)+\left\langle w, \phi\left(x^{n}, y\right)\right\rangle-\left\langle w, \phi\left(x^{n}, y^{n}\right)\right\rangle$
5: $\quad w \leftarrow w-\eta_{t}\left(\lambda w-\frac{1}{N}\left[\phi\left(x^{n}, \hat{y}\right)-\phi\left(x^{n}, y^{n}\right)\right]\right)$
6: end for
output prediction function $f(x)=\operatorname{argmax}_{y \in \mathcal{Y}}\langle w, \phi(x, y)\rangle$.
Observation: each update of $w$ needs only 1 argmax-prediction (but we'll need many iterations until convergence)

## Solving S-SVM Training Numerically

## Structured Support Vector Machine:

$\left.\min _{w} \frac{\lambda}{2}\|w\|^{2}+\frac{1}{N} \sum_{n=1}^{N} \max _{y \in \mathcal{Y}}\left[\Delta\left(y^{n}, y\right)+\left\langle w, \phi\left(x^{n}, y\right)\right\rangle-\left\langle w, \phi\left(x^{n}, y^{n}\right)\right\rangle\right)\right]$

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## Subgradient method converges slowly. Can we do better?

We can use inequalities and slack variables to reformulate the optimization.

## Solving S-SVM Training Numerically

## Structured SVM (equivalent formulation):

Idea: slack variables

$$
\min _{w, \xi} \quad \frac{\lambda}{2}\|w\|^{2}+\frac{1}{N} \sum_{n=1}^{N} \xi^{n}
$$

subject to, for $n=1, \ldots, N$,

$$
\max _{y \in \mathcal{Y}}\left[\Delta\left(y^{n}, y\right)+\left\langle w, \phi\left(x^{n}, y\right)\right\rangle-\left\langle w, \phi\left(x^{n}, y^{n}\right)\right\rangle\right] \leq \xi^{n}
$$

Note: $\xi^{n} \geq 0$ automatic, because left hand side is non-negative.

Differentiable objective, convex, $N$ non-linear contraints,

## Solving S-SVM Training Numerically

## Structured SVM (also equivalent formulation):

Idea: expand max term into individual constraints

$$
\min _{w, \xi} \quad \frac{\lambda}{2}\|w\|^{2}+\frac{1}{N} \sum_{n=1}^{N} \xi^{n}
$$

subject to, for $n=1, \ldots, N$,

$$
\Delta\left(y^{n}, y\right)+\left\langle w, \phi\left(x^{n}, y\right)\right\rangle-\left\langle w, \phi\left(x^{n}, y^{n}\right)\right\rangle \leq \xi^{n}, \quad \text { for all } y \in \mathcal{Y}
$$

Differentiable objective, convex, $N|\mathcal{Y}|$ linear constraints

## Solving S-SVM Training Numerically

## Solve an S-SVM like a linear Support Vector Machine:

$$
\min _{w \in \mathbb{R}^{D}, \xi \in \mathbb{R}^{n}} \frac{\lambda}{2}\|w\|^{2}+\frac{1}{N} \sum_{n=1}^{N} \xi^{n}
$$

subject to, for $i=1, \ldots n$,

$$
\left\langle w, \phi\left(x^{n}, y^{n}\right)\right\rangle-\left\langle w, \phi\left(x^{n}, y\right)\right\rangle \geq \Delta\left(y^{n}, y\right)-\xi^{n}, \quad \text { for all } y \in \mathcal{Y} .
$$

Introduce feature vectors $\delta \phi\left(x^{n}, y^{n}, y\right):=\phi\left(x^{n}, y^{n}\right)-\phi\left(x^{n}, y\right)$.

## Solving S-SVM Training Numerically

Solve

$$
\min _{w \in \mathbb{R}^{D}, \xi \in \mathbb{R}_{+}^{n}} \frac{\lambda}{2}\|w\|^{2}+\frac{1}{N} \sum_{n=1}^{N} \xi^{n}
$$

subject to, for $i=1, \ldots n$, for all $y \in \mathcal{Y}$,

$$
\left\langle w, \delta \phi\left(x^{n}, y^{n}, y\right)\right\rangle \geq \Delta\left(y^{n}, y\right)-\xi^{n} .
$$

Same structure as an ordinary SVM!

- quadratic objective ©
- linear constraints ©


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Same structure as an ordinary SVM!

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Question: Can we use an ordinary SVM/QP solver?

## Solving S-SVM Training Numerically

Solve

$$
\min _{w \in \mathbb{R}^{D}, \xi \in \mathbb{R}_{+}^{n}} \frac{\lambda}{2}\|w\|^{2}+\frac{1}{N} \sum_{n=1}^{N} \xi^{n}
$$

subject to, for $i=1, \ldots n$, for all $y \in \mathcal{Y}$,

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$$

Same structure as an ordinary SVM!

- quadratic objective ©
- linear constraints $\odot$

Question: Can we use an ordinary SVM/QP solver?

Answer: Almost! We could, if there weren't $N|\mathcal{Y}|$ constraints.

- E.g. 100 binary $16 \times 16$ images: $10^{79}$ constraints


## Solving S-SVM Training Numerically - Working Set

Solution: working set training

- It's enough if we enforce the active constraints. The others will be fulfilled automatically.
- We don't know which ones are active for the optimal solution.
- But it's likely to be only a small number $\leftarrow$ can of course be formalized.

Keep a set of potentially active constraints and update it iteratively:

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## Solving S-SVM Training Numerically - Working Set

- Start with working set $S=\emptyset \quad$ (no contraints)
- Repeat until convergence:
- Solve S-SVM training problem with constraints from $S$
- Check, if solution violates any of the full constraint set
- if no: we found the optimal solution, terminate.
- if yes: add most violated constraints to $S$, iterate.


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- if yes: add most violated constraints to $S$, iterate.

Good practical performance and theoretic guarantees:

- polynomial time convergence $\epsilon$-close to the global optimum


## Working Set S-SVM Training

input training pairs $\left\{\left(x^{1}, y^{1}\right), \ldots,\left(x^{n}, y^{n}\right)\right\} \subset \mathcal{X} \times \mathcal{Y}$,
input feature map $\phi(x, y)$, loss function $\Delta\left(y, y^{\prime}\right)$, regularizer $\lambda$
1: $w \leftarrow 0, S \leftarrow \emptyset$
2: repeat
3: $\quad(w, \xi) \leftarrow$ solution to QP only with constraints from $S$
4: $\quad$ for $\mathrm{i}=1, \ldots, \mathrm{n}$ do
5: $\quad \hat{y} \leftarrow \operatorname{argmax}_{y \in \mathcal{Y}} \quad \Delta\left(y^{n}, y\right)+\left\langle w, \phi\left(x^{n}, y\right)\right\rangle$
6: $\quad$ if $\hat{y} \neq y^{n}$ then
7: $\quad S \leftarrow S \cup\left\{\left(x^{n}, \hat{y}\right)\right\}$
8: $\quad$ end if
9: end for
10: until $S$ doesn't change anymore.
output prediction function $f(x)=\operatorname{argmax}_{y \in \mathcal{Y}}\langle w, \phi(x, y)\rangle$.
Obs: each update of $w$ needs $N$ argmax-predictions (one per example), but we solve globally for next $w$, not by local steps.

## Example: Object Localization

- $\mathcal{X}$ images, $\quad \mathcal{Y}=\{$ object bounding box $\} \subset \mathbb{R}^{4}$.
- Training examples:

- Goal: $f: \mathcal{X} \rightarrow \mathcal{Y}$

- Loss function: area overlap $\Delta\left(y, y^{\prime}\right)=1-\frac{\operatorname{area}\left(y \cap y^{\prime}\right)}{\operatorname{area}\left(y \cup y^{\prime}\right)}$


## Example: Object Localization

## Structured SVM:

- $\phi(x, y):=$ "bag-of-words histogram of region $y$ in image $x^{\text {" }}$

$$
\min _{w \in \mathbb{R}^{D}, \xi \in \mathbb{R}^{n}} \frac{\lambda}{2}\|w\|^{2}+\frac{1}{N} \sum_{n=1}^{N} \xi^{n}
$$

subject to, for $i=1, \ldots n$,

$$
\left\langle w, \phi\left(x^{n}, y^{n}\right)\right\rangle-\left\langle w, \phi\left(x^{n}, y\right)\right\rangle \geq \Delta\left(y^{n}, y\right)-\xi^{n}, \quad \text { for all } y \in \mathcal{Y} .
$$

## Interpretation:

- For every image, the correct bounding box, $y^{n}$, should have a higher score than any wrong bounding box.
- Less overlap between the boxes $\rightarrow$ bigger difference in score


## Example: Object Localization

## Working set training - Step 1 :

- $w \leftarrow 0$.

For every example:

- $\hat{y} \leftarrow \operatorname{argmax}_{y \in \mathcal{Y}} \Delta\left(y^{n}, y\right)+\underbrace{\left\langle w, \phi\left(x^{n}, y\right)\right\rangle}_{=0}$
maximal $\Delta$-loss $\equiv$ minimal overlap with $y^{n} \equiv \hat{y} \cap y^{n}=\emptyset$
- add constraint

$$
\left\langle w, \phi\left(x^{n}, y^{n}\right)\right\rangle-\left\langle w, \phi\left(x^{n}, \hat{y}\right)\right\rangle \geq 1-\xi^{n}
$$

Note: similar to binary SVM training for object detection:

- positive examples: ground truth bounding boxes
- negative examples: random boxes from 'image background'


## Example: Object Localization

## Working set training - Later Steps:

For every example:

- $\hat{y} \leftarrow \operatorname{argmax}_{y \in \mathcal{Y}} \underbrace{\Delta\left(y^{n}, y\right)}_{\text {bias towards 'wrong' regions }}+\underbrace{\left\langle w, \phi\left(x^{n}, y\right)\right\rangle}_{\text {object detection score }}$
- if $\hat{y}=y^{n}$ : do nothing, else: add constraint

$$
\left\langle w, \phi\left(x^{n}, y^{n}\right)\right\rangle-\left\langle w, \phi\left(x^{n}, \hat{y}\right)\right\rangle \geq \Delta\left(y^{n}, \hat{y}\right)-\xi^{n}
$$

enforces $\hat{y}$ to have lower score after re-training.
Note: similar to hard negative mining for object detection:

- perform detection on training image
- if detected region is far from ground truth, add as negative example

Difference: S-SVM handles regions that overlap with ground truth.

## Dual S-SVM

We can also dualize the S-SVM optimization:

$$
\max _{\alpha \in \mathbb{R}^{N|\mathcal{Y}|}}-\frac{1}{2} \sum_{\substack{y, \bar{y} \in \mathcal{Y} \\ n, \bar{n}=1, \ldots, N}} \alpha_{n y} \alpha_{\bar{n} \bar{y}}\left\langle\phi\left(x^{n}, y\right), \phi\left(x^{\bar{n}}, \bar{y}\right)\right\rangle+\sum_{\substack{n=1, \ldots, N \\ y \in \mathcal{Y}}} \alpha_{n y} \Delta\left(y^{n}, y\right)
$$

subject to, for $n=1, \ldots, N$,

$$
\alpha_{n y} \geq 0, \quad \text { and } \quad \sum_{y \in \mathcal{Y}} \alpha_{n y} \leq \frac{2}{\lambda N}
$$

Quadratic (convex) objective, linear constraints, $N|\mathcal{Y}|$ unknowns

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$$

Quadratic (convex) objective, linear constraints, $N|\mathcal{Y}|$ unknowns
Recover weight vector from dual coefficients:

$$
w=\sum_{n, \alpha} \alpha_{n y} \phi\left(x^{n}, y\right)
$$

State-of-the-art: solve dual with Frank-Wolfe algorithm.

