Flexible discriminative learning with structured output support vector machines
A short introduction and tutorial

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Slides and code at
http://www.vlfeat.org/~vedaldi/teach.html

January 2013
Abstract

This tutorial introduces Structured Support Vector Machines (SSVMs) as a tool to effectively learn functions over arbitrary spaces. For example, one can use a SSVM to rank a set of items by decreasing relevance, to localise an object such as a cat in an image, or to estimate the pose of a human in a video. The tutorial reviews the standard notion of SVM and shows how this can be extended to arbitrary output spaces, introducing the corresponding learning formulations. It then gives a complete example on how to design and learn a SSVM with off-the-shelf solvers in MATLAB. The last part discusses how such solvers can be implemented, focusing in particular on the cutting plane and BMRM algorithms.
Classification

- sea horse
- pigeon
- scissor
- wild cat

Caltech-101 (101 classes, 3k images)

E.g. [Weber et al., 2000, Csurka et al., 2004, Fei-Fei et al., 2004, Sivic and Zisserman, 2004]
Classification on a large scale

ImageNet (80k classes, 3.2M images)

E.g. [Deng et al., 2009, Sánchez and Perronnin, 2011, Mensink et al., 2012]
Classification with an SVM

is there a cat?

x
Classification with an SVM

is there a cat?

x

![Cat images](https://via.placeholder.com/150)
Classification with an SVM

is there a cat?

x
Classification with an SVM

is there a cat?
Classification with an SVM

is there a cat?

\[ F(x; w) = \langle w, x \rangle \]
Support vector machines can do classification.

What about ...
Object category detection

Find objects of a given type (e.g. bicycle) in an image.

E.g. [Leibe and Schiele, 2004, Felzenszwalb et al., 2008, Vedaldi et al., 2009]
Pose estimation

E.g. [Ramanan et al., 2005, Ramanan, 2006, Ferrari et al., 2008]
Relative attributes

(a) Smiling
(b) ?
(c) Not smiling
(d) Natural
(e) ?
(f) Manmade

Sometimes it is less ambiguous to rank rather than to classify objects. [Parikh and Grauman, 2011]
Segmentation

E.g. [Taskar et al., 2003] (image [Lempitsky et al., 2011])
Algorithms that can “understand” images, videos, etc. are too complex to be designed entirely manually.

**Machine learning** (ML) automatises part of the design based on empirical evidence:

\[
\text{algorithmic class} + \text{example data} + \text{optimisation} \xrightarrow{\text{learning}} \text{algorithm}.
\]
There are countless ML methods:

- Nearest neighbors, perceptron, bagging, boosting, AdaBoost, logistic regression, Support Vector Machines (SVMs), random forests, metric learning, ...
- Markov random fields, Bayesian networks, Gaussian Processes, ...
- E.g. [Schölkopf and Smola, 2002b, Hastie et al., 2001]

We will focus on **SVMs and their generalisations**.

1. Good accuracy (when applicable).
2. Clean formulation.
3. Large scale.

**Structured output SVMs**

Extending SVMs to handle arbitrary output spaces, particularly ones with non-trivial structure (e.g. space of poses, textual translations, sentences in a grammar, etc.).
Outline

Support vector classification

Beyond classification: structured output SVMs

Learning formulations

Optimisation

A complete example

Further insights on optimisation
Outline

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Further insights on optimisation
The “machine” part of an SVM is a simple **classification rule** that test the sign of the score:

\[ \hat{y}(x; w) = \text{sign}\langle x, w \rangle \]

E.g. [Schölkopf and Smola, 2002a].
Feature maps

In the SVM \( \langle x, w \rangle \) the **input** \( x \) is a *vectorial representation* of a datum.

Alternatively, one can introduce a **feature map**:

\[
\Phi : \mathcal{X} \rightarrow \mathbb{R}^d, \quad x \mapsto \Phi(x).
\]

The classification rule becomes

\[
\hat{y}(x; w) = \text{sign}(\langle \Phi(x), w \rangle).
\]

With a feature map, the nature of the input \( x \in \mathcal{X} \) is irrelevant (image, video, audio, ...).
Learning formulation

- The other defining aspect of an SVM is the **objective function** used to learn it.
- Given **example pairs** \((x_1, y_1), \ldots, (x_n, y_n)\), the objective function is

\[
E(w) = \frac{\lambda}{2} \|w\|^2 + \frac{1}{n} \sum_{i=1}^{n} \max\{0, 1 - y_i \langle x_i, w \rangle\}.
\]

- Learning the SVM amounts to minimising \(E(w)\) to obtain the optimal parameter \(w^*\).
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An aside: support vectors

One can show that the minimiser has a sparse decomposition

\[
w^* = \beta_1 x_1 + \cdots + \beta_n x_n
\]

where only a few of the \(\beta_i \neq 0\). The corresponding \(x_i\) are the **support vectors**.
Hinge loss

\[ E(w) = \frac{\lambda}{2} \|w\|^2 + \frac{1}{n} \sum_{i=1}^{n} \max\{0, 1 - y_i \langle x_i, w \rangle\} \]

Intuition
When the hinge loss is small, then the scoring function fits the example data well, with a “safety margin”.
Hinge loss

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\[ L_i(w) = \max\{0, 1 - y_i \langle x_i, w \rangle\}. \]
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**Hinge loss**

$$L_i(w) = \max\{0, 1 - y_i \langle x_i, w \rangle\}.$$  

**Margin condition**

$$L_i(w) = 0 \quad \Rightarrow \quad \begin{align*}
\mathcal{L} & \quad \Rightarrow \quad y_i \langle x_i, w \rangle \geq 1 \\
\Rightarrow \quad \text{sign} \langle x_i, w \rangle &= y_i.
\end{align*}$$
Hinge loss

\[ E(w) = \frac{\lambda}{2} \|w\|^2 + \frac{1}{n} \sum_{i=1}^{n} \max\{0, 1 - y_i \langle x_i, w \rangle\} \]

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\[ \Rightarrow \quad \text{sign} \langle x_i, w \rangle = y_i. \]

**Convexity**

The hinge loss is a **convex** function!
The regulariser

\[ E(w) = \frac{\lambda}{2} \|w\|^2 + \frac{1}{n} \sum_{i=1}^{n} \max\{0, 1 - y_i \langle x_i, w \rangle \} \]

**Intuition**

If the **regulariser** \( \|w\|^2 \) is small, then the scoring function \( \langle w, x \rangle \) varies slowly.
The regulariser

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If the **regulariser** \(\|w\|^2\) is small, then the scoring function \(\langle w, x \rangle\) varies slowly.

To see this:

1. The regulariser is the norm of the derivative of the scoring function:

\[
\|\nabla_x \langle x, w \rangle\|^2 = \|w\|^2.
\]
The regulariser

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   \[
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   \]

2. Using the Cauchy-Schwarz inequality:
   \[
   (\langle x, w \rangle - \langle x', w \rangle)^2 \leq \|x - x'\|^2 \|w\|^2.
   \]
The feature map

- The feature map encodes a notion of similarity:

$\left( \langle \Phi(x), w \rangle - \langle \Phi(x'), w \rangle \right)^2 \leq \|\Phi(x) - \Phi(x')\|^2 \times \|w\|^2$.

**Intuition**

Inputs with similar features receive similar scores.
The feature map

- The feature map encodes a notion of similarity:

\[ (\langle \Phi(x), w \rangle - \langle \Phi(x'), w \rangle)^2 \leq \| \Phi(x) - \Phi(x') \|^2 \times \| w \|^2. \]

**Intuition**

Inputs with similar features receive similar scores.

**Note:** in all cases, points whose difference \( \Phi(x) - \Phi(x') \) is orthogonal to \( w \) receive the same score. This is a \( d - 1 \) dimensional subspace of irrelevant variations!
The goal is to find a scoring function $\langle \mathbf{w}, \Phi(\mathbf{x}) \rangle$ that:

**Fits the data by a margin**

The scoring function $\langle \mathbf{w}, \Phi(\mathbf{x}) \rangle$ should fit the data by a margin:

- If $y_i > 0$ then $\langle \Phi(x_i), \mathbf{w} \rangle \geq 1$
- If $y_i < 0$ then $\langle \Phi(x_i), \mathbf{w} \rangle \leq -1$
SVM summary

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**Is regular**

A small variation of the feature $\Phi(x)$ should not change the score $\langle w, \Phi(x) \rangle$ too much. The regulariser $\|w\|^2$ is a bound on this variation.
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**Reflects prior information**

Whether a variation of the input \( \mathbf{x} \) is considered to be small or large depends on the choice of the feature map \( \Phi(\mathbf{x}) \). This establishes *a-priori* which inputs should receive similar scores.
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Beyond classification: structured output SVMs

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A complete example

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Beyond classification

Consider now the general problem of learning a function

$$f : \mathcal{X} \to \mathcal{Y}, \quad x \mapsto y,$$

where both the input and output spaces are general. Examples:
Beyond classification

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Ranking.
- given a set of objects \((o_1, \ldots, o_k)\) as input \(x\),
- return a order as output \(y\).
Beyond classification

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- given a set of objects \((o_1, \ldots, o_k)\) as input \(x\),
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**Pose estimation.**
- given an image of a human as input \(x\),
- return the parameters \((p_1, \ldots, p_k)\) of his/her pose as output \(y\).
Beyond classification

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**Pose estimation.**
- given an image of a human as input \(x\),
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**Image segmentation.**
- given an image from Flikr as input \(x\),
- return a mask highlighting the “foreground object” as output \(y\).
A real function $\mathbb{R}^d \to \mathbb{R}$ can be approximated directly by the SVM score:

$$f(x) \approx \langle w, \Phi(x) \rangle.$$ 

Think of the feature map $\Phi(x)$ as a collection of basis functions. For instance, if $x \in \mathbb{R}$, one can use the basis of second order polynomials:

$$\Phi(x) = [1 \ x \ x^2]^T \quad \Rightarrow \quad \langle w, \Phi(x) \rangle = w_1 + w_2 x + 2_3 x^2.$$
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$$\Phi(x) = [1 \ x \ x^2]^\top \implies \langle w, \Phi(x) \rangle = w_1 + w_2 x + 2 w_3 x^2.$$  

- The goal is to find $w$ (e.g. polynomial coefficients) such that the score fits the example data

$$\langle w, \Phi(x_i) \rangle \approx y_i$$

by minimising the $L^1$ error

$$L_i(w) = |y_i - \langle w, \Phi(x_i) \rangle|.$$
SVR is just a variant of regularised regressions:

<table>
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<tr>
<th>method</th>
<th>loss</th>
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Limitation: only real functions!
Support Vector Regression /2

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An aside: $\epsilon$-insensitive $L^1$ loss

Actually, SVR makes use of a slightly more general loss

$$L_i(\mathbf{w}) = \max\{0, |y_i - \langle \mathbf{w}, \mathbf{x}_i \rangle| - \epsilon\}$$

which is insensitive to error below a threshold $\epsilon$. One can set $\epsilon = 0$ though [Smola and Scholkopf, 2004].
A general approach: learning the graph

Use a binary SVM to classify which pairs \((x, y) \in \mathcal{X} \times \mathcal{Y}\) belongs to the graph of the function (treat the output as an input!):\

\[
y = f(x) \iff \langle w, \Psi(x, y) \rangle > 0.
\]

Joint feature map

In order to classify pairs \((x, y)\), these must be encoded as vectors. To this end, we need a joint feature map:

\[
\Phi : (x, y) \rightarrow \Phi(x, y) \in \mathbb{R}^d
\]

As long as this feature can be designed, the nature of \(x\) and \(y\) is irrelevant.
Example: learning the graph of a real function

![Graph of learned function and scoring function]

**Algorithm:**

1. Start from the true pairs \((x_i, y_i)\) (green squares) where the graph should pass.
2. Add many false pairs \((x_i, y_i)\) (red dots) where the graph should *not* pass.
Example: learning the graph of a real function

**Algorithm:**

1. Start from the true pairs \((x_i, y_i)\) (green squares) where the graph should pass.
2. Add many false pairs \((x_i, y_i)\) (red dots) where the graph should not pass.
3. Learn a scoring function \(\langle \mathbf{w}, \Psi(x, y) \rangle\) to fit these points.
4. Define the learned function graph to be the collection of points such that \(\langle \mathbf{w}, \Psi(x, y) \rangle > 0\) (green areas).
Example: learning the graph of a real function /2

In this example the joint feature map is a Fourier basis (note the ringing!)

\[
\Psi(x, y) = \begin{bmatrix}
\cos(f_{1x}x + f_{1y}y + \phi_1) \\
\cos(f_{2x}x + f_{2y}y + \phi_2) \\
\vdots \\
\cos(f_{dx}x + f_{dy}y + \phi_d)
\end{bmatrix}, \quad \text{for appropriate } (f_{1i}, f_{2i}, \phi_i).
\]
The good and the bad

The good: **works for any type of inputs and outputs!** (Not just real functions.)
The good and the bad

The good: **works for any type of inputs and outputs!** (Not just real functions.)

The Bad:

- **Not one-to-one.** For each $x$, there are *multiple outputs* $y$ with positive score.
- **Not complete.** There are $x$ for which all the outputs have negative score.
- **Very large negative example set.**
Structured output SVMs

**Structured output SVM.** Issues 1 and 2 can be fixed by choosing the highest scoring output for each input:

\[
\hat{y}(x; w) = \arg\max_{y \in \mathcal{Y}} \langle w, \Psi(x, y) \rangle
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**Intuition**

The scoring function

\[
\langle w, \Psi(x, y) \rangle
\]

is somewhat analogous to a posterior probability density function

\[
P(y|x)
\]

but it does not have any probabilistic meaning.
Example: real function

\[ f(x) = y \] that maximises the score along column \( x \).

\( f(x) \) is now uniquely and completely defined.

**Note:** only the relative values of the score along a column really matter (see rescaled version on the right).
Inference problem

- **Inference problem.** Evaluating a structured SVM requires solving the problem

\[
\arg\max_{y \in \mathcal{Y}} \langle \mathbf{w}, \Psi(x, y) \rangle.
\]

- The efficiency of using a structured SVM (after learning) depends on how quickly the inference problem can be solved.
Example: binary linear SVM

Standard SVMs can be easily interpreted as a structured SVMs:

- **Output space:**
  \[ y \in \mathcal{Y} = \{-1, +1\}. \]

- **Feature map:**
  \[ \Psi(x, y) = \frac{y}{2} x. \]

- **Inference:**
  \[ \hat{y}(x; w) = \arg\max_{y \in \{-1, +1\}} \frac{y}{2} \langle w, x \rangle = \text{sign} \langle w, x \rangle. \]
Example: object localisation

Let $x$ be an image and $y \in \mathcal{Y} \subset \mathbb{R}^4$ a rectangular window. The goal is to find the window containing a given object.

Let $x|_y$ denote an image window (crop).
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**Standard SVM:** score one window:

$$\Phi(x|_y) = \text{“histogram of SIFT features”},$$

$$\langle w, \Phi(x|_y) \rangle = \text{“window score”}.$$
Example: object localisation

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$$(\mathbf{x}, \mathbf{y}) \quad \text{restriction} \quad \mathbf{x}|_y \quad \text{visual features} \quad \Psi(\mathbf{x}, \mathbf{y}) \in \mathbb{R}^d$$

- Let $\mathbf{x}|_y$ denote an image window (crop).
- **Standard SVM**: score one window:
  \[ \Phi(\mathbf{x}|_y) = \text{“histogram of SIFT features”}, \]
  \[ \langle \mathbf{w}, \Phi(\mathbf{x}|_y) \rangle = \text{“window score”}. \]

- **Structured SVM**: try all windows and pick the best one:
  \[ \hat{y}(\mathbf{x}; \mathbf{w}) = \arg\max_{\mathbf{y} \in \mathcal{Y}} \langle \mathbf{w}, \Psi(\mathbf{x}, \mathbf{y}) \rangle = \arg\max_{\mathbf{y} \in \mathcal{Y}} \langle \mathbf{w}, \Phi(\mathbf{x}|_y) \rangle. \]
Example: pose estimation

Let \( \mathbf{x} \) be an image and \( \mathbf{y} = (\mathbf{p}_1, \mathbf{p}_2, \mathbf{p}_3, \mathbf{p}_4, \mathbf{p}_5) \) the pose of a human, expressed as the 2D location of five parts.

\[
\psi(x, y) = \begin{bmatrix}
\Phi(x|p_1) \\
\Phi(x|p_2) \\
\Phi(p_1, p_2) \\
\Phi(x|p_3) \\
\Phi(x|p_5) \\
\Phi(p_1, p_2) \\
\Phi(p_5, p_6)
\end{bmatrix}
\]

**Intuition**

The score \( \langle \mathbf{w}, \psi(x, y) \rangle \) reflects how well the five image parts match their appearance models and whether the deformation is reasonable or not.
Consider the problem of ranking a list of objects \( \mathbf{x} = (o_1, \ldots, o_n) \) (input).

The output \( \mathbf{y} \) is a ranking (total order). This can be represented as a matrix \( \mathbf{y} \) such that

\[
\begin{align*}
y_{ij} &= +1, & o_i \text{ has higher rank than } o_j, \\
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\]

A joint feature map for ranking

\[
\Psi(x, y) = \sum_{ij} y_{ij} \langle \Phi(o_i) - \Phi(o_j), w \rangle.
\]
This structured SVM ranks the objects by decreasing score $\langle \Phi(o_i), w \rangle$:

$$\hat{y}_{ij}(x; w) = \text{sign} \left( \langle \Phi(o_i), w \rangle - \langle \Phi(o_j), w \rangle \right).$$

In fact the score of this output

$$\langle w, \psi(x, \hat{y}(x; w)) \rangle = \sum_{ij} y_{ij} \langle \Phi(o_i) - \Phi(o_j), w \rangle$$

$$= \sum_{ij} \text{sign} \langle \Phi(o_i) - \Phi(o_j), w \rangle \langle \Phi(o_i) - \Phi(o_j), w \rangle$$

$$= \sum_{ij} |\langle \Phi(o_i) - \Phi(o_j), w \rangle|$$

is maximum.
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Further insights on optimisation
Input-output relation

The SVM defines an input-output relation based on maximising the joint score:

$$\hat{y}(x; w) = \arg\max_{y \in Y} \langle w, \psi(x, y) \rangle.$$ 

Next: how to fit the input-output relation to data.
Given $n$ example input-output pairs

$$\mathbf{(x_1, y_1), \ldots, (x_n, y_n)},$$

find $\mathbf{w}$ such that the structured SVM \textit{approximately} fit them

$$\hat{y}(x_i; \mathbf{w}) \approx y_i, \quad i = 1, \ldots, n,$$

while \textit{controlling the complexity} of the estimated function.
Learning formulation /1

Given \( n \) example input-output pairs

\[
(x_1, y_1), \ldots, (x_n, y_n),
\]

find \( w \) such that the structured SVM approximately fit them

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\hat{y}(x_i; w) \approx y_i, \quad i = 1, \ldots, n,
\]

while controlling the complexity of the estimated function.

Objective function (non-convex)

\[
E_1(w) = \frac{\lambda}{2} \|w\|^2 + \frac{1}{n} \sum_{i=1}^{n} \Delta(y_i, \hat{y}(x_i; w))
\]

Notation reminder: \( \Delta \) is the loss function, \( \hat{y} \) the output estimated by the SVM, \( y_i \) the ground truth output, and \( x_i \) the ground truth input.
Loss function

The **loss function** measures the fit quality:

\[ \Delta(y, \hat{y}) \]

such that \( \Delta(y, \hat{y}) \geq 0 \) and \( \Delta(y, \hat{y}) = 0 \) if, and only if, \( y = \hat{y} \).

**Examples:**

- For a **binary SVM** the loss is

\[
\Delta(y, \hat{y}) = \begin{cases} 
1, & y \neq \hat{y}, \\
0, & \text{otherwise.}
\end{cases}
\]
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  1, & y \neq \hat{y}, \\
  0, & \text{otherwise}. 
  \end{cases}
  \]

- In **object localisation** the loss could be one minus the ratio of the areas of the intersection and union of the rectangles \( y \) and \( \hat{y} \):
  \[
  \Delta(y, \hat{y}) = 1 - \frac{|y \cap \hat{y}|}{|y \cup \hat{y}|}.
  \]
The **loss function** measures the fit quality:

\[ \Delta(y, \hat{y}) \]

such that \( \Delta(y, \hat{y}) \geq 0 \) and \( \Delta(y, \hat{y}) = 0 \) if, and only if, \( y = \hat{y} \).

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  \[ \Delta(y, \hat{y}) = 1 - \frac{|y \cap \hat{y}|}{|y \cup \hat{y}|}. \]

- In **ranking** ...
Example: a ranking loss

In ranking, suitable losses include the ROC-AUC, the precision-recall AUC, precision @ \(k\), ...

- The ROC curve plots the true positive rate against the true negative rate.

- Given the “true” ranking \(y\) and the estimated \(\hat{y}\), we can define

\[
\Delta(y, \hat{y}) = 1 - \text{ROCAUC}(y, \hat{y})
\]

- One can show that this is simply the number of incorrectly ranked pairs, i.e.

\[
\Delta(y, \hat{y}) = \frac{1}{n^2} \sum_{i,j=1}^{n} [y_{ij} \neq \hat{y}_{ij}]
\]
The goal of learning is to find the minimiser $\mathbf{w}^*$ of:

$$E_1(\mathbf{w}) = \frac{\lambda}{2}\|\mathbf{w}\|^2 + \frac{1}{n} \sum_{i=1}^{n} \Delta(y_i, \hat{y}(x_i; \mathbf{w})), \quad \text{where } \hat{y}(x_i; \mathbf{w}) = \arg\max_{y \in Y} \langle \mathbf{w}, \Phi(x_i, y) \rangle.$$  

The dependency of the loss on $\mathbf{w}$ is very complex: $\Delta$ is non-convex and is composed with argmax!
The goal of learning is to find the minimiser $w^*$ of:

$$E_1(w) = \frac{\lambda}{2} \|w\|^2 + \frac{1}{n} \sum_{i=1}^{n} \Delta(y_i, \hat{y}(x_i; w)),$$

where $\hat{y}(x_i; w) = \arg\max_{y \in Y} \langle w, \Phi(x_i, y) \rangle$.

The dependency of the loss on $w$ is very complex: $\Delta$ is non-convex and is composed with argmax!

**Objective function (convex)**

Given a **convex surrogate loss** $L_i(w) \approx \Delta(y_i, \hat{y}(x_i; w))$ we consider the objective

$$E(w) = \frac{\lambda}{2} \|w\|^2 + \frac{1}{n} \sum_{i=1}^{n} L_i(w).$$
The surrogate loss

- The key in the success of the structured SVMs is the existence of good surrogates. There are standard constructions that work well in a variety of cases (but not always!).
The surrogate loss

- The key in the success of the structured SVMs is the existence of good surrogates. There are standard constructions that work well in a variety of cases (but not always!).
- The aim is to make minimising $L_i(w)$ have the same effect as minimising $\Delta(y_i, \hat{y}(x_i; w))$.
- **Bounding property:**
  \[
  \Delta(y_i, \hat{y}(x_i; w)) \leq L_i(w).
  \]
The surrogate loss

- The key in the success of the structured SVMs is the existence of good surrogates. There are standard constructions that work well in a variety of cases (but not always!).
- The aim is to make minimising $L_i(w)$ have the same effect as minimising $\Delta(y_i, \hat{y}(x_i; w))$.
- Bounding property:

$$\Delta(y_i, \hat{y}(x_i; w)) \leq L_i(w).$$

Tightness

- If we can find $w^*$ s.t. $L_i(w^*) = 0$, then $\Delta(y_i, y(x_i; w^*)) = 0$.
- But can we?
- Not always! Consider setting $L_i(w) = “$very large constant$”$.
- We need a tight bound. E.g.:

$$\Delta(y_i, y(x_i; w^*)) = 0 \implies L_i(w^*) = 0.$$
Margin rescaling surrogate

- **Margin rescaling** is the first *standard surrogate construction*:

\[
L_i(w) = \sup_{y \in \mathcal{Y}} \Delta(y_i, y) + \langle \Psi(x_i, y), w \rangle - \langle \Psi(x_i, y_i), w \rangle.
\]
Margin rescaling surrogate

- **Margin rescaling** is the first standard surrogate construction:

$$L_i(w) = \sup_{y \in \mathcal{Y}} \Delta(y_i, y) + \langle \Psi(x_i, y), w \rangle - \langle \Psi(x_i, y_i), w \rangle.$$ 

- This surrogate **bounds** the loss:

$$\Delta(y_i, \hat{y}(x_i; w)) \leq \Delta(y_i, \hat{y}(x_i; w)) + \langle \Psi(x_i, \hat{y}(x_i; w)), w \rangle - \langle \Psi(x_i, y_i), w \rangle$$

$$\leq \sup_{y \in \mathcal{Y}} \Delta(y_i, y) + \langle \Psi(x_i, y), w \rangle - \langle \Psi(x_i, y_i), w \rangle$$

$$= L_i(w)$$

\(\geq 0\) because \(\hat{y}(x_i; w)\) maximises the score by definition.
Margin condition

- Is margin rescaling a tight approximation?
- The following margin condition holds

\[ L_i(w^*) = 0 \iff \forall y \in Y : \langle \Psi(x_i, y), w \rangle \geq \langle \Psi(x_i, y), w \rangle + \Delta(y_i, y) \]
Margin condition

- Is margin rescaling a *tight* approximation?
- The following **margin condition** holds

\[
L_i(w^*) = 0 \iff \forall y \in Y : \langle \Psi(x_i, y_i), w \rangle \geq \langle \Psi(x_i, y), w \rangle + \Delta(y_i, y)
\]

Tightness

- The surrogate is **not** tight in the sense above:

\[
\Delta(y_i, y(x_i; w^*)) = 0 \not\Rightarrow L_i(w^*) = 0.
\]

- In order to minimise the surrogate, the more stringent margin condition has to be satisfied!
- But this is usually good enough, and in fact beneficial (implies robustness).
Slack rescaling surrogate

- **Slack rescaling** is the second standard surrogate construction:

\[
L_i(w) = \sup_{y \in \mathcal{Y}} \Delta(y_i, y) \left[ 1 + \langle \Psi(x_i, y), w \rangle - \langle \Psi(x_i, y_i), w \rangle \right].
\]

- May give better results than marging rescaling.
- However, it is often significantly harder to treat in calculations.
- The margin condition is

\[
L_i(w^*) = 0 \iff \forall y \neq y_i : \langle \Psi(x_i, y), w \rangle \geq \langle \Psi(x_i, y_i), w \rangle + 1
\]
Augmented inference

- Evaluating the objective $E(w)$ requires computing the supremum in the augment loss

$$\sup_{y \in Y} \Delta(y_i, y) + \langle \Psi(x_i, y), w \rangle - \langle \Psi(x_i, y_i), w \rangle.$$

- Maximising this quantity is the **augmented inference** problem due to its similarity with the inference problem

$$\max_{y \in Y} \langle \Psi(x_i, y), w \rangle$$

- Augmented inference can be significantly harder than inference, especially for slack rescaling.
Recall that for a binary linear SVM:

\[ \mathcal{Y} = \{-1, +1\}, \quad \psi(x, y) = \frac{y}{2} x, \quad \Delta(y_i, \hat{y}) = [y_i \neq y]. \]
Example: binary linear SVM

- Recall that for a binary linear SVM:
  \[ \mathcal{Y} = \{-1, +1\}, \quad \Psi(x, y) = \frac{y}{2}x, \quad \Delta(y_i, \hat{y}) = [y_i \neq y]. \]

- Then in the margin rescaling construction, solving the augmented inference problem yields
  \[
  L_i(w) = \sup_{y \in \{-1, 1\}} [y_i \neq y] + \frac{y}{2} \langle x_i, w \rangle - \frac{y_i}{2} \langle x_i, w \rangle
  \]
  \[
  = \max_{y \in \{-y_i, y_i\}} [y_i \neq y] + \frac{y - y_i}{2} \langle x_i, w \rangle
  \]
  \[
  = \max\{0, 1 - y_i \langle x_i, w \rangle\},
  \]
  i.e. the same loss of a standard SVM.

- In this case, slack rescaling yields the same result.
The good and the bad of convex surrogates

Good:

- Convex surrogates separate the ground truth outputs $y_i$ from other outputs $y$ by a margin modulated by the loss.

Bad:

- Despite their construction, they can be poor approximations of the original loss.
- They are unimodal, and therefore cannot model situations in which different outputs are equally acceptable.
- If the ground truth $y_i$ is not separable, they may be incapable of identifying which is the best output that can actually be achieved instead – no graceful fallback.
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Input-output relation

The SVM defines an input-output relation based on maximising the joint score:

\[ \hat{y}(x; w) = \arg\max_{y \in \mathcal{Y}} \langle w, \psi(x, y) \rangle. \]

Convex surrogate objective

The joint score can be designed to fit the data \((x_1, y_1), \ldots, (x_n, y_n)\) by optimising

\[ E(w) = \frac{\lambda}{2} \|w\|^2_2 + \frac{1}{n} \sum_{i=1}^{n} L_i(w). \]

Next: how to solve this optimisation problem.
A (naive) direct approach

Learning a structured SVM requires solving an optimisation problem of the type:

\[
E(w) = \frac{\lambda}{2} \|w\|_2^2 + \frac{1}{n} \sum_{i=1}^{n} L_i(w),
\]

\[
L_i(w) = \sup_{y \in Y} \Delta(y_i, y) + \langle \psi(x_i, y), w \rangle - \langle \psi(x_i, y_i), w \rangle.
\]
A (naive) direct approach

- Learning a structured SVM requires solving an optimisation problem of the type:

\[ E(w) = \frac{\lambda}{2} \|w\|_2^2 + \frac{1}{n} \sum_{i=1}^{n} L_i(w), \]

\[ L_i(w) = \sup_{y \in Y} \Delta(y_i, y) + \langle \psi(x_i, y), w \rangle - \langle \psi(x_i, y_i), w \rangle. \]

- More in general, this can be rewritten as

\[ E(w) = \frac{\lambda}{2} \|w\|_2^2 + \frac{1}{n} \sum_{i=1}^{n} L_i(w), \quad L_i(w) = \sup_{y \in Y} b_{iy} - \langle a_{iy}, w \rangle. \]
A (naive) direct approach /2

This problem can be rewritten as a constrained quadratic program in the parameters $w$ and the slack variables $\xi$:

$$E(w, \xi) = \frac{\lambda}{2} \|w\|_2^2 + \frac{1}{n} \sum_{i=1}^{n} \xi_i,$$

$$\xi_i \geq b_i y - \langle a_i y, w \rangle \quad \forall i = 1, \ldots, n, \ y \in \mathcal{Y}.$$ 

Can we use a standard quadratic solver (e.g. quadprog in MATLAB)?
A (naive) direct approach /2

This problem can be rewritten as a constrained quadratic program in the parameters \( w \) and the slack variables \( \xi \):

\[
E(w, \xi) = \frac{\lambda}{2} \|w\|_2^2 + \frac{1}{n} \sum_{i=1}^{n} \xi_i,
\]

\[
\xi_i \geq b_i y - \langle a_{iy}, w \rangle \quad \forall i = 1, \ldots, n, \; y \in Y.
\]

Can we use a standard quadratic solver (e.g. quadprog in MATLAB)?

The size of this problem

- There is one set of constraints for each data point \((x_i, y_i)\).
- Each set of constraints contains one linear constraint for each output \(y\).
- Way too large (even infinite!) to be directly fed to a quadratic solver.
Let’s look again to the original problem is a slightly different form:

\[ E(w) = \frac{\lambda}{2} \|w\|_2^2 + L(w), \]

\[ L(w) = \frac{1}{n} \sum_{i=1}^{n} \sup_{y \in Y} \Delta(y_i, y) + \langle \Psi(x_i, y), w \rangle - \langle \Psi(x_i, y_i), w \rangle. \]

\( L(w) \) is a convex, non-smooth function, with bounded Lipschitz constant (i.e., it does not vary too fast). Optimisation of such functions is extensively studied in operational research.

We are going to discuss the Bundle Method for Regularized Risk Minimization (BMRM) method, a special case of bundle method for regularised loss functions, which in turns is a stabilised variant of cutting plane.
Assumption: $L(w)$ convex, not necessarily smooth, with bounded Lipschitz constant $G$.

A subgradient of $L(w)$ at $w$ is any vector $g$ such that

$$\forall w': L(w') \geq L(w) + \langle g, w' - w \rangle.$$ 

$\|g\| \leq G$.

The subdifferential $\partial L(w)$ is the set of all subgradients and contains only the gradient $\nabla L(w)$ if the function is differentiable.
Given a point $w_0$, we approximate the convex $L(w)$ from below by a tangent plane:

$$L(w) \geq b - \langle a, w \rangle, \quad -a \in \partial L(w_0) \quad b = L(w_0) + \langle a, w_0 \rangle.$$ 

$(a, b)$ is the cutting plane at $w$.

Given the cutting planes at $w_1, \ldots, w_t$, we define the lower approximation

$$L^{(t)}(w) = \max_{i=1,\ldots,t} b_i - \langle a_i, w \rangle.$$
Cutting plane algorithm

- Goal: minimize a convex non-necessarily smooth function $L(w)$.
- Method: incrementally construct a lower approximation $L^{(t)}(w)$. At each iteration, minimise the latter to obtain $w_t$ and add a cutting plane at that point.

**Cutting plane algorithm**

Start with $w_0 = 0$ and $t = 0$. Then repeat:

1. $t \leftarrow t + 1$.
2. Get a cutting plane $(a_t, b_t)$ by computing the subgradient of $L(w)$ at $w_{t-1}$.
3. Add the plane to the current approximation $L^{(t)}(w)$.
4. Set $w_t = \text{argmin}_w L^{(t)}(w)$.
5. If $L(w_t) - L^{(t)}(w_t) < \epsilon$ stop as converged.

[Kiwiel, 1990, Lemaréchal et al., 1995, Joachims et al., 2009]
The algorithm stops when \( L(w_t) - L^{(t)}(w_t) < \epsilon \).

The true optimum \( L(w^*) \) is sandwiched:

\[
\begin{align*}
    L^{(t)}(w_t) & \leq L^{(t)}(w^*) \leq L(w^*) \leq L(w_t) \\
    L^{(t)} & \leq L
\end{align*}
\]

Hence when the algorithm converge one has the guarantee:

\[ L(w_t) \leq L(w^*) + \epsilon. \]
Optimizing the function $L(w) = w \log w$ in the interval $[0.001, 1]$. 
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Cutting plane example

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The standard cutting plane algorithm takes forever to converge (it is not the one used for SVM...) as it can take wild steps. 

*Bundle methods* try to regularise the steps but are generally difficult to tune. **BMRM** notes that one has already a regulariser in the SVM objective function:

\[
E(w) = \frac{\lambda}{2} ||w||^2 + L(w).
\]

**BMRM algorithm**

Start with \(w_0 = 0\) and \(t = 0\). Then repeat:

1. \(t \leftarrow t + 1\).
2. Get a cutting plane \((a_t, b_t)\) by computing the subgradient of \(L(w)\) at \(w_{t-1}\).
3. Add the plane to the current approximation \(L^{(t)}(w)\).
4. Set \(E_t(w) = \frac{\lambda}{2} ||w||^2 + L^{(t)}(w)\).
5. Set \(w_t = \text{argmin}_w E_t(w)\).
6. If \(E(w_t) - E_t(w_t) < \epsilon\) stop as converged.

[Teo et al., 2009] but also [Kiwiel, 1990, Lemaréchal et al., 1995, Joachims et al., 2009]
Optimizing the function $E(w) = \frac{w^2}{2} + w \log w$ in the interval $[0.001, 1]$. 
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Optimizing the function $E(w) = \frac{w^2}{2} + w \log w$ in the interval $[0.001, 1]$. 
Application of BMRM to structured SVMs

- In this case:

$$L(w) = \frac{1}{n} \sum_{i=1}^{n} \sup_{y \in Y} \Delta(y_i, y) + \langle \psi(x_i, y), w \rangle - \langle \psi(x_i, y_i), w \rangle.$$  

- $\partial L(w)$ is just the average of the subgradients of the terms.
- The subgradient $g_i$ at $w$ of a term is computed by determining the maximally violated output

$$\bar{y}_i = \arg\max_{y \in Y} \Delta(y_i, y) + \langle \psi(x_i, y), w \rangle - \langle \psi(x_i, y_i), w \rangle,$$
Application of BMRM to structured SVMs

- In this case:
  \[
  L(w) = \frac{1}{n} \sum_{i=1}^{n} \sup_{y \in \mathcal{Y}} \Delta(y_i, y) + \langle \psi(x_i, y), w \rangle - \langle \psi(x_i, y_i), w \rangle.
  \]

- \( \partial L(w) \) is just the average of the subgradients of the terms.
- The subgradient \( g_i \) at \( w \) of a term is computed by determining the maximally violated output
  \[
  \bar{y}_i = \arg\max_{y \in \mathcal{Y}} \Delta(y_i, y) + \langle \psi(x_i, y), w \rangle - \langle \psi(x_i, y_i), w \rangle,
  \]

- **Remark 1.** This is the augmented inference problem.
- **Remark 2.** Once \( \bar{y}_i \) is obtained, the subgradient is given by
  \[
  g_i = \psi(x_i, \bar{y}_i) - \psi(x_i, y_i).
  \]

Thus BMRM can be applied provided that the augmented inference problem can be solved (even when \( \mathcal{Y} \) is infinite!).
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Structured SVM: fitting a real function

Consider the problem of learning a real function $f : \mathbb{R} \rightarrow [-1, 1]$ by fitting points $(x_1, y_1), \ldots, (x_n, y_n)$.

**Loss**

$$\Delta(y, \hat{y}) = |\hat{y} - y|.$$ 

**Joint feature map**

$$\Psi(x, y) = \begin{bmatrix} y \\ yx \\ yx^2 \\ yx^3 \\ -\frac{1}{2}y^2 \end{bmatrix}.$$ 

To see why this works we will look at the resulting inference problem.
First, program a callback for the loss.

```matlab
function delta = lossCB(param, y, ybar)
    delta = abs(ybar - y);
end
```
MATLAB implementation

First, program a callback for the loss.

```matlab
function delta = lossCB(param, y, ybar)
    delta = abs(ybar - y);
end
```

Then a callback for the feature map.

```matlab
function psi = featureCB(param, x, y)
    psi = [y;
           y * x;
           y * x^2;
           y * x^3;
           - 0.5 * y^2];
    psi = sparse(psi);
end
```
The inference problem is

\[ \hat{y}(x; w) = \arg\max_{y \in [-1,1]} \langle w, \Psi(x, y) \rangle \]

\[ = \arg\max_{y \in [-1,1]} y(w_1 + w_2 x + w_3 x^2 + w_4 x^3) - \frac{1}{2} y^2 w_5. \]
The inference problem is

\[
\hat{y}(x; w) = \arg\max_{y \in [-1, 1]} \langle w, \Psi(x, y) \rangle
\]

\[
= \arg\max_{y \in [-1, 1]} y(w_1 + w_2x + w_3x^2 + w_4x^3) - \frac{1}{2}y^2w_5.
\]

Differentiate w.r.t. \(y\) and set to zero to obtain:

\[
\hat{y}(x; w) = \frac{w_1}{w_5} + \frac{w_2}{w_5}x + \frac{w_3}{w_5}x^2 + \frac{w_4}{w_5}x^3.
\]

Note: there are some other special cases due to the fact that \(y \in [-1, +1]\) and \(w_5\) may be negative.
Solving the augmented inference problem is needed to compute the value and sub-gradient of the **margin-rescaling loss**

\[
L_i(w) = \max_{\hat{y} \in [-1, 1]} \Delta(y, \hat{y}) + \langle w, \Psi(x, y) \rangle - \langle w, \Psi(x, y_i) \rangle \\
= \max_{\hat{y} \in [-1, 1]} |\hat{y} - y_i| + y(w_1 + w_2x + w_3x^2 + w_4x^3) - \frac{1}{2}y^2w_5 - \text{const.}
\]
Augmented inference

- Solving the augmented inference problem is needed to compute the value and sub-gradient of the **margin-rescaling loss**

\[
L_i(w) = \max_{\hat{y} \in [-1, 1]} \Delta(y, \hat{y}) + \langle w, \Psi(x, y) \rangle - \langle w, \Psi(x, y_i) \rangle \\
= \max_{\hat{y} \in [-1, 1]} |\hat{y} - y_i| + y(w_1 + w_2x + w_3x^2 + w_4x^3) - \frac{1}{2}y^2w_5 - \text{const.}
\]

- The maximiser is one of at most four possibilities:

\[
y \in \left\{-1, 1, \frac{z - 1}{w_5}, \frac{z + 1}{w_5}\right\} \cap [-1, 1], \quad z = y(w_1 + w_2x + w_3x^2 + w_4x^3).
\]

- Try the four cases and pick the one with larger augmented loss.
MATLAB implementation /2

Finally program the augmented inference.

```matlab
function yhat = constraintCB(param, model, x, y)
    w = model.w;
    z = w(1) + w(2) * x + w(3) * x.^2 + w(4) * x.^3;
    yhat = [];
    if w(5) > 0
        yhat = [z - 1, z + 1] / w(5);
        yhat = max(min(yhat, 1),-1);
    end
    yhat = [yhat, -1, 1];

    aloss = @(y_) abs(y_ - y) + z * y_ - 0.5 * y_.^2 * w(5);
    [drop, worse] = max(aloss(yhat));
    yhat = yhat(worse);
end
```
Once the callbacks are coded, we use an off-the-shelf-solver
(http://www.vlfeat.org/~vedaldi/code/svm-struct-matlab.html)

```matlab
% training examples
parm.patterns = {-2, -1, 0, 1, 2} ;
parm.labels = {0.5, -0.5, 0.5, -0.5, 0.5} ;

% callbacks & other parameters
parm.lossFn = @lossCB ;
parm.constraintFn = @constraintCB ;
parm.featureFn = @featureCB ;
parm.dimension = 5 ;

% call the solver and print the model
model = svm_struct_learn(’-c 10 -o 2 ’, parm) ;
model.w
```
After each cutting plane iteration the scoring function

\[ F(x, y) = \langle \psi(x, y), w \rangle \]

is updated. Remember:

- The output function is obtained by maximising the score along the columns.
- The relative scaling of the columns is irrelevant and rescaling them reveals the structure better.
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Outline

Support vector classification

Beyond classification: structured output SVMs

Learning formulations

Optimisation

A complete example

Further insights on optimisation
How fast is BMRM?

- Provably convergent to a desired approximation $\epsilon$.
- The convergence rates with respect to the accuracy $\epsilon$ are not bad:

<table>
<thead>
<tr>
<th>loss $L(w)$</th>
<th>number of iterations accounting for $\lambda$</th>
</tr>
</thead>
<tbody>
<tr>
<td>non-smooth</td>
<td>$O\left(\frac{1}{\epsilon}\right)$, $O\left(\frac{1}{\lambda\epsilon}\right)$</td>
</tr>
<tr>
<td>smooth</td>
<td>$O\left(\log\left(\frac{1}{\epsilon}\right)\right)$, $O\left(\frac{1}{\lambda\log\left(\frac{1}{\epsilon}\right)}\right)$</td>
</tr>
</tbody>
</table>

- Note: the convergence rate depends also on the amount of regularisation $\lambda$.
- Difficult learning problems (e.g. object detection) typically have
  - large $n$,
  - small $\lambda$,
  - small $\epsilon$.

so fast convergence is not so obvious.
BMRM for structured SVMs: problem size

- BMRM *decouples* the data from the approximation of $L(w)$.
- The number of data points $n$ affects the cost of evaluating $L(w)$ and its subgradient.
- However, the cost of optimising $L(t)(w)$ depends only on the iteration number $t$!
- In practice $t$ is small and $L(t)(w)$ may be *minimised very efficiently in the dual*. 
BMRM subproblem in the primal

The problem

\[
\min_w \frac{\lambda}{2} \|w\|^2 + L(t)(w), \quad L(t)(w) = \max_{i=1,...,n} b_i - \langle a_i, w \rangle
\]

reduces to the constrained quadratic program

\[
\min_{w,\xi} \frac{\lambda}{2} \|w\|^2 + \xi,
\]

\[
\xi \geq b_i - \langle a_i, w \rangle, \quad i = 1, \ldots, t.
\]

Note that there is a single (scalar) slack variable. This is known as one-slack formulation.
BMRM subproblem in the dual

Let $\mathbf{b}^\top = [b_1, \ldots, b_t]$, $A = [\mathbf{a}_1, \ldots, \mathbf{a}_t]$ and $K = A^\top A/\lambda$. The corresponding dual problem is

$$
\max_{\alpha \geq 0} \langle \alpha, \mathbf{b} \rangle - \frac{1}{2} \alpha^\top K \alpha, \quad \mathbf{1}^\top \alpha \leq 1.
$$

where at optimum $\mathbf{w}^* = \frac{1}{\lambda} A \alpha^*$. 

### Intuition: why it is efficient

- The original infinite constraints are approximated by just $t$ constraints in $L^{(t)}(\mathbf{w})$.
- This is possible because:
  1. The approximation needs to be good only around the optimum.
  2. The effective dimensionality and redundancy of the data are exploited.
- Solving the corresponding quadratic problem is easy because $t$ is small.

**Remark.** BMRM is a primal solver. Switching to the dual for the subproblems is convenient but completely optional.
Implementation

- An attractive aspect is the ease of implementation.

```java
1 A = [];  
2 B = [];  
3 minimum = -inf;  
4 while getObjective(w) - minimum > epsilon  
5     [a,b] = getCuttingPlane(w);  
6     A = [A, a];  
7     B = [B, b];  
8     [w, minimum] = quadraticSolver(lambda, A, B);  
9 end
```

- A simple quadratic solver may do as the problem is small (e.g. MATLAB quadprog).

- `getCuttingPlane` computes an average of subgradients, in turn obtained by solving the augmented inference problems.
For each novel $w_t$ a new constraint per example is generated by running augmented inference.

The overall loss is an average of per-example losses:

$$L(w) = \frac{1}{n} \sum_{i=1}^{n} L_i(w)$$

And so for each cutting plane:

$$a_t = \frac{1}{n} \sum_{i=1}^{n} a_{it}(w), \quad b_t = \frac{1}{n} \sum_{i=1}^{n} b_{it}(w),$$
Caching recombines constraints generated so far to obtain a novel cutting plane without running augmented inference (expensive) [Joachims, 2006, Felzenszwalb et al., 2008].

1. For each example $i = 1, \ldots, n$ pick the most violated constraint in the cache:

   $t_i^* = \arg \max_{t=1,\ldots,t} b_{it} - \langle a_{it}, w \rangle.$

2. Now form a novel cutting plane by recombining the existing constraints:

   $a_{t+\delta t} = \frac{1}{n} \sum_{i=1}^{n} a_{it_i^*}(w), \quad b_{t+\delta t} = \frac{1}{n} \sum_{i=1}^{n} b_{it_i^*}(w).$
Caching is very important for problems like object detection in which inference is very expensive (seconds or minutes per image).

Consider for example [Felzenszwalb et al., 2008] object detector. With 5000 training images and five seconds/image for inference it requires an hour for one round of augmented inference!

Thus the solver should be iterated until examples in the cache are correctly separated. It is pointless to fetch more before the solution has stabilised due to the huge cost.

Preventive caching. During a round of inference it is also possible to return and store in the cache a small set of “highly violated” constraints. They may become “most violated” at a later iteration.
Tricks of the trade: incremental training

- Another speedup is to train the model gradually, by adding progressively more training samples.
- The intuition is that a lot of samples are only needed to refine the model.
Structured output SVMs extend standard SVMs to arbitrary output spaces.

“New” optimisation techniques allow to learn models on a large scale (e.g. BMRM).

Benefits
- Apply well understood convex formulations and optimisation techniques to a variety problems, from ranking to image segmentation and pose estimation.
- Good solvers + explicit feature maps = large scale non-linear models.
- Can incorporate latent variables (not discussed).

Caveats
- Surrogate losses have many limitations.
- Inference and augmented inference must be solved ad hoc for every new design.
- All the limitations of discriminative learning.


