Kernel Methods in Machine Learning

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2. When Kernels Meet Balls: Core Vector Machines (CVM)
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   - Minimum Enclosing Ball (MEB)
   - Transforming Kernel Methods as MEB Problems
   - Extension: Generalized CVM
3. When Kernels Meet Bags
   - Multi-Instance Learning
   - Constrained Concave-Convex Procedure
   - Loss Function
   - Optimization Problem
   - Experiments
4. Conclusion
Popularity of Kernel Methods

**Supervised learning**
- Classification: Support vector machines (SVM)
- Regression: Support vector regression

**Unsupervised learning**
- Novelty detection: One-class SVM / Support vector domain description
- Clustering: Kernel clustering
- Principal component analysis: Kernel PCA

**Other learning scenarios**
- Semi-supervised learning, transductive learning, etc.

**Applications**
- Text classification, speaker adaptation, image fusion, texture classification ...
Basic Idea in Kernel Methods

Map the data from input space to feature space $\mathcal{F}$ using $\varphi$. Apply a linear procedure in $\mathcal{F}$

- hyperplane classifier, linear regression, PCA, etc.

Only inner products in $\mathcal{F}$ are needed

- **Kernel trick**: $\varphi(x)\varphi(y) = k(x, y)$
Support Vector Machines

Classification problem: \( \{(x_i, y_i)\}_{i=1}^{N}, x_i \in \mathbb{R}^m, y_i \in \{\pm 1\} \)

\[
\begin{align*}
\text{min} & \quad \frac{1}{2} \|w\|^2 \quad \text{(primal)} \\
\text{s.t.} & \quad y_i (w' \varphi(x_i) + b) \geq 1
\end{align*}
\]

\[
\begin{align*}
\text{max} & \quad \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{N} \alpha_i \alpha_j y_i y_j \varphi(x_i)' \varphi(x_j) \\
\text{s.t.} & \quad \sum_{i=1}^{N} \alpha_i y_i = 0, \quad \alpha_i \geq 0 \quad \text{(dual)}
\end{align*}
\]

Quadratic programming (QP) problem
Scale-up Problem

Problem 1
Need $O(m^2)$ memory just to write down $K$ ($m$ training examples)
- If $m = 20,000$ and it takes 4 bytes to represent a kernel entry, we would need 1.6Gbytes to store the kernel matrix.

Problem 2
Involves inverting the kernel matrix $K_{m \times m} = [k(x_i, x_j)]_{i,j=1}^m$
- Requires $O(m^3)$ time

Existing methods
- sampling, low-rank approximations, decomposition methods
- in practice, time complexities $O(m) - O(m^{2.3})$
- empirical observations and not theoretical guarantees
Observation

SVM implementations only approximate the optimal solution by an iterative strategy:

1. Pick a subset of Lagrange multipliers
2. Optimize the reduced optimization problem
3. Repeat until all the Lagrange multipliers are “accurate enough” (loose KKT condition)

These near-optimal solutions are often good enough in practical applications.
Approximation Algorithm

Approximation algorithms have been extensively used theoretical computer science

- E.g., for NP-complete problems such as vertex-cover problem, traveling-salesman problem, set-covering problem, ...

Denote

- $C^*$: cost of the optimal solution
- $C$: cost of the solution returned by approximation algorithm

Performance guarantee: Approximation ratio $\rho(n)$ for input size $n$

$$\max \left( \frac{C}{C^*}, \frac{C^*}{C} \right) \leq \rho(n)$$

- large $\rho(n)$: solution is much worse than the optimal solution
- small $\rho(n)$: solution is more or less optimal

If the ratio does not depend on $n$, we may just write $\rho$ and call the algorithm an $\rho$-approximation algorithm
The Minimum Enclosing Ball Problem

Problem in Computational Geometry
Given: \( S = \{x_1, \ldots, x_m\} \), where each \( x_i \in \mathbb{R}^d \)
Minimum enclosing ball of \( S \) (MEB(S)): the smallest ball that contains all the points in \( S \)

Finding exact MEBs is inefficient for large \( d \)
Given an $\epsilon > 0$, a ball $B(c, (1 + \epsilon)R)$ is an $(1 + \epsilon)$-approximation of $\text{MEB}(S)$ if $R \leq r_{\text{MEB}(S)}$ and $S \subset B(c, (1 + \epsilon)R)$.
Approximate MEB Algorithm

Proposed by Bădoiu and Clarkson (2002)

A simple iterative scheme:

- At the $t$th iteration, the current estimate $B(c_t, r_t)$ is expanded incrementally by including the furthest point outside the $(1 + \epsilon)$-ball $B(c_t, (1 + \epsilon)r_t)$
- Repeat until all the points in $S$ are covered by $B(c_t, (1 + \epsilon)r_t)$

Surprising property

- Number of iterations (and hence the size of the final core-set) depends only on $\epsilon$ but not on $d$ or $m$
MEB Problems and Kernel Methods

What is **obvious**

- MEB is equivalent to the hard-margin support vector data description (SVDD)
- The MEB problem can also be used to find the radius component of the radius-margin bound
  \[ \Rightarrow \text{SVM parameter tuning} \]

What is **not so obvious**

- Other kernel-related problems can also be viewed as MEB problems
- soft-margin one-class SVM, multi-class SVM, ranking SVM, SVR, Laplacian SVM, etc.
Hard-Margin SVDD

Denote:

- Kernel $k$; feature map $\varphi$  
- MEB in the feature space: $B(c, R)$

\[
\begin{align*}
\text{(primal)}: \min_{R,c} R^2 & : \|c - \varphi(x_i)\|^2 \leq R^2, \ i = 1, \ldots, m \\
\text{(dual)}: \max_{\alpha} \alpha' \text{diag}(K) - \alpha'K\alpha & : \alpha \geq 0, \ \alpha'1 = 1
\end{align*}
\]

- $\alpha = [\alpha_1, \ldots, \alpha_m]'$: Lagrange multipliers  
- $K_{m \times m} = [k(x_i, x_j)]$: kernel matrix  
- $0 = [0, \ldots, 0]'$, $1 = [1, \ldots, 1]'$
Kernel Methods as MEB Problems

Assume \( k(x, x) = \kappa \), a constant

\[ k(x, x) = \kappa \]

Holds for

1. isotropic kernel \( k(x, y) = K(||x - y||) \) (e.g., Gaussian)
2. dot product kernel \( k(x, y) = K(x'y) \) (e.g., polynomial) with normalized inputs
3. any normalized kernel \( k(x, y) = \frac{K(x,y)}{\sqrt{K(x,x)} \sqrt{K(y,y)}} \)

Combine with \( \alpha'1 = 1 \), we have \( \alpha' \text{diag}(K) = \kappa \)

\[ \max_{\alpha} -\alpha'K\alpha \quad : \quad \alpha \geq 0, \quad \alpha'1 = 1 \]  

Conversely, whenever the kernel \( k \) satisfies (1),

Any QP of the form in (2) \( \leftrightarrow \) a MEB problem
Two-Class SVM

\[ \{z_i = (x_i, y_i)\}_{i=1}^m \text{ with } y_i \in \{-1, 1\} \]

(primal) \[ \min_{w, b, \rho, \xi_i} \|w\|^2 + b^2 - 2\rho + C \sum_{i=1}^m \xi_i^2 : y_i(w' \varphi(x_i) + b) \geq \rho - \xi_i \]

(dual) \[ \max_\alpha -\alpha' \left( K \odot yy' + yy' + \frac{1}{C}I \right) \alpha : \alpha \geq 0, \; \alpha' 1 = 1 \]

\[ \tilde{K} = \left[ y_i y_j k(x_i, x_j) + y_i y_j + \frac{\delta_{ij}}{C} \right], \text{ with } \tilde{k}(z, z) = \kappa + 1 + \frac{1}{C} \text{ (constant)} \]
Core Vector Machine (CVM)

At the $t$th iteration, denote

- $S_t$: core-set; $c_t$: ball’s center; $R_t$: ball’s radius

Given an $\epsilon > 0$

1. **Initialize** $S_0$, $c_0$ and $R_0$

2. **Terminate** if there is no training point $z$ such that $\tilde{\phi}(z)$ falls outside the $(1 + \epsilon)$-ball $B(c_t, (1 + \epsilon)R_t)$

3. Find (core vector) $z$ such that $\tilde{\phi}(z)$ is furthest away from $c_t$. Set $S_{t+1} = S_t \cup \{z\}$

4. Find the new $\text{MEB}(S_{t+1})$ and set $c_{t+1} = c_{\text{MEB}(S_{t+1})}$ and $R_{t+1} = r_{\text{MEB}(S_{t+1})}$

5. Increment $t$ by 1 and go back to Step 2
Convergence to (Approximate) Optimality

When $\epsilon = 0$
- CVM outputs the exact solution of the kernel problem

When $\epsilon > 0$

CVM is an $(1 + \epsilon)^2$-approximation algorithm
Time Complexity

CVM converges in at most $2/\epsilon$ iterations [Bădoiu and Clarkson, 2002]

No probabilistic speedup:

- Overall time for $\tau = O(1/\epsilon)$ iterations: $O\left(\frac{m}{\epsilon^2} + \frac{1}{\epsilon^4}\right)$
- linear in $m$ for a fixed $\epsilon$

With probabilistic speedup:

- Overall time: $O\left(\frac{1}{\epsilon^4}\right)$
- independent of $m$ for a fixed $\epsilon$
Space Complexity

Space complexity for the whole procedure: $O(1/\epsilon^2)$

- independent of $m$ for a fixed $\epsilon$
Forest Cover Type Data (522,911 patterns)
**Extended MIT Face Data**

<table>
<thead>
<tr>
<th>training set</th>
<th># faces</th>
<th># nonfaces</th>
<th>total</th>
</tr>
</thead>
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<tr>
<td>original</td>
<td>2,429</td>
<td>4,548</td>
<td>6,977</td>
</tr>
<tr>
<td>set A</td>
<td>2,429</td>
<td>481,914</td>
<td>484,343</td>
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<tr>
<td>set B</td>
<td>19,432 (blur+flip)</td>
<td>481,914</td>
<td>501,346</td>
</tr>
<tr>
<td>set C</td>
<td>408,072 (rotate)</td>
<td>481,914</td>
<td>889,986</td>
</tr>
</tbody>
</table>

![Graphs showing CPU time, number of support vectors, AUC, and balanced loss for different training sets and kernel methods.](image-url)
KDDCUP-99 Intrusion Detection (4,898,431 patterns)

Used in KDD-99’s Knowledge Discovery and Data Mining Tools Competition: Separate normal connections from attacks

<table>
<thead>
<tr>
<th>method</th>
<th># train patns input to SVM</th>
<th># test errors</th>
<th>SVM training time (in sec)</th>
<th>other proc time (in sec)</th>
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<tbody>
<tr>
<td>random sampling</td>
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<td></td>
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<tr>
<td>0.001%</td>
<td>47</td>
<td>25,713</td>
<td>0.000991</td>
<td>500.02</td>
</tr>
<tr>
<td>0.01%</td>
<td>515</td>
<td>25,030</td>
<td>0.120689</td>
<td>502.59</td>
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<tr>
<td>0.1%</td>
<td>4,917</td>
<td>25,531</td>
<td>6.944</td>
<td>504.54</td>
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<tr>
<td>1%</td>
<td>49,204</td>
<td>25,700</td>
<td>604.54</td>
<td>509.19</td>
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<tr>
<td>5%</td>
<td>245,364</td>
<td>25,587</td>
<td>15827.3</td>
<td>524.31</td>
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<td>active learning</td>
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<td>747</td>
<td>21,634</td>
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<td>94192.213</td>
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<tr>
<td>CB-SVM (KDD’03)</td>
<td>4,090</td>
<td>20,938</td>
<td>7.639</td>
<td>4745.483</td>
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<tr>
<td>CVM</td>
<td>4,898,431</td>
<td>19,513</td>
<td></td>
<td>1.4</td>
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<table>
<thead>
<tr>
<th>AUC</th>
<th>$\ell_{bal}$</th>
<th># core vectors</th>
<th># support vectors</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.977</td>
<td>0.042</td>
<td>55</td>
<td>20</td>
</tr>
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</table>
Limitations

1. \( k(x, x) = \text{constant} \) for any pattern \( x \)
2. The QP problem is of the form

\[
\max -\alpha'K\alpha \quad \text{s.t.} \quad \alpha'1 = 1, \quad \alpha \geq 0
\]

Condition 1 holds for kernels, including
- Isotropic kernel (e.g., Gaussian kernel)
- Dot product kernel (e.g., polynomial kernel) with normalized input
- Any normalized kernel

Condition 2 holds for kernel methods including the one-class and two-class SVMs
- there are still some popular kernel methods that violate these conditions and so cannot be used
Motivating Example

Example (L2-support vector regression (SVR))

Training set: \( \{ z_i = (x_i, y_i) \}_{i=1}^m \) with \( x_i \in \mathbb{R}^d \) and \( y_i \in \mathbb{R} \)

Find \( f(x) = w' \varphi(x) + b \) in \( \mathcal{F} \) that minimizes \( \bar{\epsilon} \)-insensitive loss

Primal

\[
\begin{align*}
\min & \quad \|w\|^2 + b^2 + \frac{C}{\mu m} \sum_{i=1}^m (\xi_i^2 + \xi_i'^2) + 2C\bar{\epsilon} \\
\text{s.t.} & \quad y_i - (w' \varphi(x_i) + b) \leq \bar{\epsilon} + \xi_i, \quad (w' \varphi(x_i) + b) - y_i \leq \bar{\epsilon} + \xi_i'
\end{align*}
\]

Dual

\[
\begin{align*}
\max & \quad [\lambda' \lambda'^*'] \left[ \begin{array}{c} \frac{2}{C} y \\ -\frac{2}{C} y \end{array} \right] - [\lambda' \lambda'^*'] \tilde{K} \left[ \begin{array}{c} \lambda \\ \lambda^* \end{array} \right] \\
\text{s.t.} & \quad [\lambda' \lambda'^*']1 = 1, \quad \lambda, \lambda^* \geq 0
\end{align*}
\]

\( \tilde{K} = [\tilde{k}(z_i, z_j)] = \left[ \begin{array}{cc} K + 11' + \frac{\mu m}{C} I & -(K + 11') \\ -(K + 11') & K + 11' + \frac{\mu m}{C} I \end{array} \right] \)
Center-Constrained MEB Problem

Modifications to the original MEB problem:

1. Augment an extra $\Delta_i \in \mathbb{R}$ to each $\varphi(x_i) \rightarrow \begin{bmatrix} \varphi(x_i) \\ \Delta_i \end{bmatrix}$

2. Constrain the last coordinate of the ball’s center to zero $\begin{bmatrix} c \\ 0 \end{bmatrix}$

Finding the center-constrained MEB

Primal:

$$\min R^2 \text{ s.t. } \left\| \begin{bmatrix} c \\ 0 \end{bmatrix} - \begin{bmatrix} \varphi(x_i) \\ \Delta_i \end{bmatrix} \right\|^2 \leq R^2$$

where $\Delta = [\Delta_1^2, \ldots, \Delta_m^2]' \geq 0$

Dual:

$$\max \alpha'(\text{diag}(K) + \Delta) - \alpha'K\alpha \text{ s.t. } \alpha'1 = 1, \alpha \geq 0$$

Goal: Transform the dual of SVR to this form
SVR as a Center-Constrained MEB Problem

SVR’s dual:

$$\max \begin{bmatrix} \lambda' & \lambda'^* \end{bmatrix} \begin{bmatrix} 2 & y \\ -2 & -y \end{bmatrix} - [\lambda' \ \lambda'^*] \tilde{K} \begin{bmatrix} \lambda \\ \lambda'^* \end{bmatrix}$$

s.t. $[\lambda' \ \lambda'^*]1 = 1$, $\lambda, \lambda^* \geq 0$

Define $\Delta = -\text{diag}(\tilde{K}) + \eta 1 + \frac{2}{C} \begin{bmatrix} y \\ -y \end{bmatrix}$ for $\eta$ large enough such that $\Delta \geq 0$

$$\max \tilde{\alpha}'(\text{diag}(\tilde{K}) + \Delta - \eta 1) - \tilde{\alpha}'\tilde{K}\tilde{\alpha} : \tilde{\alpha}'1 = 1, \ \tilde{\alpha} \geq 0$$

Using the constraint $\alpha'1 = 1$

$$\max \tilde{\alpha}'(\text{diag}(\tilde{K}) + \Delta) - \tilde{\alpha}'\tilde{K}\tilde{\alpha} : \tilde{\alpha}'1 = 1, \ \tilde{\alpha} \geq 0$$

which is thus of the required form!
Advantages

1. Allows a more general QP formulation
2. Can be used with any linear/nonlinear kernels
   - no longer require “\(k(x, x) = \text{constant}\)” on the kernel
Friedman (200,000 Patterns)

- CPU time (in seconds)
- Number of SVs
- RMSE
- MRE

Comparison of L2-SVR (CVR), L1-SVR (LIBSVM), and L1-SVR (SVM-Light) for different sizes of training set.
Semi-Supervised Learning

**Labeled** patterns are rare, expensive and time consuming to collect

- supervised learning can have poor performance when only very few labeled patterns are available

**Unlabeled** data are abundant and readily available without any cost

- e.g., unlabeled webpages on the internet
- often has a manifold structure
Laplacian SVM

Incorporate a manifold regularizer [Belkin et al 2005]:

\[
\begin{align*}
\min & \quad \frac{1}{\ell} \sum_{i=1}^{\ell} \xi_i + \frac{\lambda}{2} \|f\|_{\mathcal{H}_k}^2 + \frac{\lambda G}{2} \|\nabla G f\|^2 \\
y_i f(x_i) & \geq 1 - \xi_i, \quad \xi_i \geq 0
\end{align*}
\]

Sparse Laplacian SVM

\[
\begin{align*}
\min & \quad \|w\|^2 + b^2 + \frac{C}{\ell \mu} \sum_{i=1}^{\ell} \xi_i^2 + 2C\epsilon + \frac{C\theta}{u\mu} \sum_{e \in \mathcal{E}} (\zeta_e^2 + \zeta_e'^2) \\
s.t. & \quad y_i (w^\prime \varphi(x_i) + b) \geq 1 - \epsilon - \xi_i, \\
& \quad -w^\prime \psi_e \leq \epsilon + \zeta_e, \quad w^\prime \psi_e \leq \epsilon + \zeta_e', \quad e \in \mathcal{E}.
\end{align*}
\]

Dual: center-constrained MEB problem
Two Moons ($\ell = 2; u = 1,000,000$)
Extended USPS: 0-vs-1 ($\ell = 2; u = 266,077$)
Extended MIT Face ($\ell = 10; u = 100,000$)
Multi-Instance Learning: Motivating Example

Content-based image retrieval: Classify/retrieve images based on content

- each image is a **bag** and each local image patch an **instance**
- an image is labeled positive when **at least one** of its segments is positive

**Weak** label information of the training data

- **only** the bags (but **not** the individual instances) have known labels
Kernel-Based MI Learning Methods

Design **MI kernels** that operate on **bags**

- the underlying quadratic programming (QP) problem only involves variables corresponding to the **bags**, but not instances

(More direct approach) Associate the variables with **instances**, but not with bags

- bag label information still used implicitly
- bag $B_i$: instances $\{x_{ij}\}_{j=1}^{n_i}$

\[
f(B_i) = \max_{j=1,\ldots,n_i} f(x_{ij})
\]
**Problems**

**Mixed integer problem**

- MI-SVM uses a simple optimization heuristic
- convergence properties unclear

Only the **sign** is important in classification

$$\text{sign}(f(B_i)) = \text{sign}(\max_{j=1,\ldots,n_i} f(x_{ij}))$$

$$f(B_i) = \max_{j=1,\ldots,n_i} f(x_{ij})$$ may be too restrictive

Cannot utilize **both** the bag and instance information simultaneously

- MI kernels: variables correspond only to the **bags**, but not instances
- MI-SVM: variables correspond only to the **instances**, but not bags
Proposed Approach

Introduce a **loss function** between $f(B_i)$ and the associated $f(x_{ij})$'s

- allows **both** the bags and instances to directly participate in the optimization process
- the learned function is smooth over both bags and instances

Optimization technique

- MI-SVM uses an optimization heuristic
- we use **constrained concave-convex procedure**
An optimization tool for **nonlinear optimization** problems whose objective function can be expressed as a **difference of convex functions**
Constrained Concave-Convex Procedure (CCCP)

\[
\begin{align*}
\min_x & \quad f_0(x) - g_0(x) \\
\text{s.t.} & \quad f_i(x) - g_i(x) \leq c_i, \quad i = 1, \ldots, m,
\end{align*}
\]

- \(f_i, g_i \ (i = 0, \ldots, m)\) are real-valued, convex and differentiable functions on \(\mathbb{R}^n\); \(c_i \in \mathbb{R}\)

**Procedure:**

1. start with an initial \(x^{(0)}\)
2. replace \(g_i(x)\) with its first-order Taylor expansion at \(x^{(t)}\)
3. set \(x^{(t+1)}\) to the solution of the relaxed optimization problem:

\[
\begin{align*}
\min_x & \quad f_0(x) - \left[ g_0(x^{(t)}) + \nabla g_0(x^{(t)})' (x - x^{(t)}) \right] \\
\text{s.t.} & \quad f_i(x) - \left[ g_i(x^{(t)}) + \nabla g_i(x^{(t)})' (x - x^{(t)}) \right] \leq c_i
\end{align*}
\]

Converges to a local minimum solution
A set of training bags: \( \{(B_1, y_1), \ldots, (B_m, y_m)\} \)
- \( B_i = \{x_{i1}, x_{i2}, \ldots, x_{in_i}\} \): \( i \)th bag containing instances \( x_{ij} \)'s
- \( y_i \in \{\pm 1\} \)

Define a loss function that depends on both the training bags and training instances:

\[
V \left( \{B_i, y_i, f(B_i)\}_{i=1}^{m}, \{f(x_{ij})\}_{j=1}^{n_i} \right)
\]

Split the loss function \( V \) into two parts

1. between each bag label and its bag prediction
   \[
   V \left( \{B_i, y_i, f(B_i)\}_{i=1}^{m}, \{f(x_{ij})\}_{j=1}^{n_i} \right)
   \]

2. between the predictions of each bag and its constituent instances
   \[
   V \left( \{B_i, y_i, f(B_i)\}_{i=1}^{m}, \{f(x_{ij})\}_{j=1}^{n_i} \right)
   \]
Loss Function $V$: 1st Part

Between each bag label $y_i$ and its corresponding prediction $f(B_i)$

- hinge loss $(1 - y_i f(B_i))_+$ where $(z)_+ = \max(0, z)$
Loss Function V: 2nd Part

Between the predictions of each bag $f(B_i)$ and its constituent instances $\{f(x_{ij}) \mid j = 1, \ldots, n_i\}$

$$\ell(f(B_i), \max_j f(x_{ij}))$$

- $\ell(v_1, v_2) = \begin{cases} 
0 & \text{if } v_1 = v_2, \\
\infty & \text{otherwise}. 
\end{cases}$
- L1 loss: $\ell(v_1, v_2) = |v_1 - v_2|$
- L2 loss: $\ell(v_1, v_2) = (v_1 - v_2)^2$
Combining

\[ V = \frac{1}{m} \sum_{i=1}^{m} (1 - y_i f(B_i))_+ + \frac{\lambda}{m} \sum_{i=1}^{m} \ell(f(B_i), \max_j f(x_{ij})) \]

- \( \lambda \): trades off the two components

Special cases:

1. Only the first part: \( \frac{1}{m} \sum_{i=1}^{m} (1 - y_i f(B_i))_+ \)
   - the same as that with the MI kernel

2. \( \ell(v_1, v_2) = \begin{cases} 
0 & \text{if } v_1 = v_2, \\
\infty & \text{otherwise.} 
\end{cases} \)
   - same as the MI-SVM
Optimization Problem

Introduce

- $\xi = [\xi_1, \ldots, \xi_m]'$: slack variables for the errors on bags
- $\gamma, \lambda$: tradeoff parameters

$$
\min_{f \in \mathcal{H}, \xi} \frac{1}{2} ||f||_\mathcal{H}^2 + \frac{\gamma}{m} \xi'1 + \frac{\gamma \lambda}{m} \sum_{i=1}^{m} \ell(f(B_i), \max_{j=1,\ldots,n_i} f(x_{ij}))
$$

s.t. $y_i f(B_i) \geq 1 - \xi_i,$

$$\xi \geq 0$$

Representer Theorem

$$f(x) = \sum_{i=1}^{m} \left( \alpha_{i0} k(x, B_i) + \sum_{j=1}^{n_i} \alpha_{ij} k(x, x_{ij}) \right), \quad \alpha_{i0}, \alpha_{ij} \in \mathbb{R}$$

- $\alpha$: vector for all the $\alpha_{i0}$'s and $\alpha_{ij}$'s
Using the L1 Loss for $\ell(\cdot, \cdot)$

- **$K$:** kernel matrix; **$k_i$:** $i$th column of $K$

\[
\begin{align*}
\min_{\alpha, \xi, \delta, b} & \quad \frac{1}{2} \alpha' K \alpha + \frac{\gamma}{m} \xi' 1 + \frac{\gamma \lambda}{m} \delta' 1 \\
\text{s.t.} & \quad y_i (k'_I(B_i) \alpha + b) \geq 1 - \xi_i, \\
& \quad \xi \geq 0, \\
& \quad k'_I(x_{ij}) \alpha - \delta_i \leq k'_I(B_i) \alpha, \\
& \quad k'_I(B_i) \alpha - \max_{j=1,...,n_i} (k'_I(x_{ij}) \alpha) \leq \delta_i
\end{align*}
\]

**Objective:** quadratic; First three constraints: linear
Last constraint: nonlinear, but is a *difference of two convex functions*
Optimization using CCCP

Iterative procedure:
1. obtain $\alpha$ from this QP
2. use this as $\alpha^{(t+1)}$ and iterate

- $\alpha^{(t)}$: estimate of $\alpha$ at the $t$th iteration
- $\beta_{ij}^{(t)}$: estimate of $\beta_{ij}$

\[
\min_{\alpha, \xi, \delta, b} \frac{1}{2} \alpha' K \alpha + \frac{\gamma}{m} \xi' 1 + \frac{\gamma \lambda}{m} \delta' 1
\]

\[
\text{s.t. } y_i (k'_I(B_i) \alpha + b) \geq 1 - \xi_i,
\]

$\xi \geq 0$,

$k'_I(x_{ij}) \alpha - \delta_i \leq k'_I(B_i) \alpha$,

$k'_I(B_i) \alpha - \sum_{j=1}^{n_i} \beta_{ij}^{(t)} k'_I(x_{ij}) \alpha \leq \delta_i$
Using the Loss Function in MI-SVM

With a particular choice of the subgradient

- identical to the optimization heuristic in MI-SVM
- MI-SVM: no convergence proof
- CCCP: guaranteed convergence
Classification: Image Categorization on Corel Images

Data set

- Used in Chen and Wang (JMLR 2004)
- 10 classes (beach, flowers, horses, etc.), with each class containing 100 images
- Each image: bag; Image segments: instance

Procedure

- Same as in (Chen and Wang)
- Randomly divided into a training and test set, each containing 50 images of each category
- Repeated 5 times, and report the average accuracy
- Model parameters selected by a validation set
## Results

<table>
<thead>
<tr>
<th>Method</th>
<th>Accuracy (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>DD-SVM (Chen and Wang 2004)</td>
<td>81.5 ± 3.0</td>
</tr>
<tr>
<td>Hist-SVM (Chapelle et al. 1999)</td>
<td>66.7 ± 2.2</td>
</tr>
<tr>
<td>MI-SVM (Andrews et al. 2003)</td>
<td>74.7 ± 0.6</td>
</tr>
<tr>
<td>SVM (MI kernel) (Gärtnер et al. 2002)</td>
<td>84.1 ± 0.90</td>
</tr>
<tr>
<td><strong>Our method</strong></td>
<td><strong>84.4 ± 1.38</strong></td>
</tr>
</tbody>
</table>

- Results on DD-SVM, Hist-SVM and MI-SVM are from (Chen and Wang 2004).
- MI kernel used: normalized set kernel
  \[
  k(B_1, B_2) = \frac{k_{set}(B_1, B_2)}{\sqrt{k_{set}(B_1, B_1)} \sqrt{k_{set}(B_2, B_2)}}
  \]
  \[
  k_{set}(B_1, B_2) = \sum_{x \in B_1, z \in B_2} k(x, z), \quad k: \text{Gaussian kernel}
  \]
- Our method: use the L1 loss
  - significant at the 0.01 level of significance

Our method is shown to be competitive with existing methods and demonstrates good performance.
Regression: Synthetic Musk Molecules

Predict the real-valued binding energies of musk molecules

Synthetic data sets generated by Dooly et al. (JMLR 2002)

- based on using an affinity model between the musk molecules and receptors
- LJ-16.30.2, LJ-80.166.1 and LJ-160.166.1
- LJ-16.30.2: # relevant features: 16; total # features: 30; # scale factors: 2

Make it more challenging

- created three more data sets (LJ-16-50-2, LJ-80-206-1 and LJ-160-566-1) by adding irrelevant features
- e.g., LJ-16-50-2 is generated by adding 20 more irrelevant features to LJ-16-30-2 while keeping its real-valued outputs intact
Results

<table>
<thead>
<tr>
<th>data set</th>
<th>DD</th>
<th>citation-kNN</th>
<th>SVM (MI kernel)</th>
<th>our method</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>%err</td>
<td>MSE</td>
<td>%err</td>
<td>MSE</td>
</tr>
<tr>
<td>LJ-16.30.2</td>
<td>6.7</td>
<td>0.0240</td>
<td>16.7</td>
<td>0.0260</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>LJ-80.166.1</td>
<td>(not available)</td>
<td>8.6</td>
<td>0.0109</td>
<td>8.7</td>
</tr>
<tr>
<td>LJ-160.166.1</td>
<td>23.9</td>
<td>0.0852</td>
<td>4.3</td>
<td>0.0014</td>
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<tr>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>LJ-16-50-2</td>
<td>-</td>
<td>-</td>
<td>53.3</td>
<td>0.0916</td>
</tr>
<tr>
<td></td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>LJ-80-206-1</td>
<td>-</td>
<td>-</td>
<td>30.4</td>
<td>0.0463</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>LJ-160-566-1</td>
<td>-</td>
<td>-</td>
<td>34.8</td>
<td>0.0566</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

- Results of DD, citation-kNN on the first three data sets are from (Dooly et al. 2002)
- DD: does not perform well
- **Easier** data sets: ours has comparable/better performance
- **More challenging** data sets
  - nearest neighbor-based and DD algorithms degrade with more irrelevant features
  - our SVM-based approach is consistently the best
Kernel methods can now be used on **massive** data sets:
- novelty detection (unsupervised learning)
- classification/regression (supervised learning)
- manifold regularization (semi-supervised learning)
- maximum margin discriminant analysis (feature extraction)

Kernel methods can also be used for multi-instance learning in a disciplined manner:
- allows a **loss function** between the outputs of a bag and its associated instances
- both bags and instances can now directly participate in the optimization process
- by using **CCCP**, no need to use optimization **heuristics**
- how to design MI kernels? → **marginalized kernel**
Recent Research

Kernel methods

- feature extraction
  - KDD 2006
- large datasets
  - JMLR 2005
  - ICML 2005
- multi-instance learning
  - ICML 2006a
  - IJCAI 2007a
- ensemble learning
  - IJCAI 2007b
- kernel learning
  - ICML 2003
  - IJCAI 2003
  - ICML 2004
  - MLJ 2006
  - TNN 2006b
- semi-supervised learning
  - NIPS 2006a
- applications
  - NIPS 2003
  - TSAP 2005
  - TASLP 2006
  - TNN 2004
- speech recognition
  - IJCAI 2005
  - TKDE 2006
  - GLOBECOM 2005
- image / vision
- pervasive computing

James Kwok

Kernel Methods in Machine Learning
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