Efficient SVM Optimization without an Optimizer

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Outline

1. Introduction
2. Core Vector Machine
3. Ball Vector Machine
4. Experiments
5. Conclusion
Supervised learning: classification / regression

- e.g., text classification
- e.g., face detection (video surveillance, digital camera)

standard digital camera: 10M pixels

Kernel method: Support vector machines (SVM) / support vector regression
Support Vector Machines (SVM)

Classification problem:

- training set \( \{(x_i, y_i)\}_{i=1}^{m}, x_i \in \mathbb{R}^d, y_i \in \{\pm 1\} \) (labels)

Large-margin method: Maximize the margin separating opposite classes
Maximizing the Margin

Let the (linear) classifier be $w'x + b$

$$\begin{align*}
\min & \quad \frac{1}{2} \|w\|^2 \quad \text{(primal)} \\
\text{s.t.} & \quad w'x_i + b \geq 1, \quad \text{if } y_i = 1, \\
& \quad w'x_i + b \leq -1, \quad \text{if } y_i = -1 \\
\max & \quad \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j x'_i x_j \\
\text{s.t.} & \quad \sum_{i=1}^{m} \alpha_i y_i = 0, \quad \alpha_i \geq 0 \quad \text{(dual)}
\end{align*}$$

($\alpha_i$ : Lagrange multiplier)

Quadratic programming (QP) problem (globally optimal solution)
Support vectors: patterns with $\alpha_i > 0$
Kernel Trick

Classifier: linear → nonlinear

- map the data from input space to feature space $\mathcal{F}$ using $\varphi$

Only inner products in $\mathcal{F}$ are needed: $\varphi(x_i)'\varphi(x_j) \rightarrow k(x_i, x_j)$
SVM Optimization

Needs a QP solver

Problem 1
Needs $O(m^2)$ memory just to write down $m \times m$ kernel matrix

$$= [k(x_i, x_j)]_{i,j=1}^m \quad (m \text{ training examples})$$

- 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 $\rightarrow O(m^3)$ time

Key observation
Near-optimal approximate solutions are often good enough in practical applications
Core Vector Machine (CVM) [Tsang, Kwok, Cheung 2005]

1. Formulate kernel methods as minimum enclosing ball problems
2. Obtain approximately optimal solutions efficiently with the use of core-sets

Classification
- one/two-class CVM [Tsang, Kwok & Cheung, (JMLR) 2005]
- one-class classification with Bregman divergence [Nock & Nielsen, (ECML) 2005]
- cluster based CVM [Asharaf, Murty & Shevade, (ICDM) 2006]
- multiclass CVM [Asharaf, Murty & Shevade, (ICML) 2007]

Regression
- core vector regression [Tsang, Kwok & Lai, (ICML) 2005]

Semi-supervised learning
- sparsified LapCVM [Tsang & Kwok, (NIPS) 2006]

Others
- coreset learning [Har-Peled, Roth & Zimak, (IJCAI) 2007]
- feature extraction [Tsang, Kocsor & Kwok, (KDD) 2006]
Minimum Enclosing Ball (MEB) ⇔ SVM

A problem in Computational Geometry

Given $\mathcal{S} = \{\mathbf{x}_1, \ldots, \mathbf{x}_m\}$, minimum enclosing ball of $\mathcal{S}$ (MEB($\mathcal{S}$)):

- the smallest ball $B(\mathbf{c}, R)$ that contains all $\mathbf{x}$'s in $\mathcal{S}$

(primal) \quad \min_{R, \mathbf{c}} \quad R^2

\quad \text{s.t.} \quad \|\mathbf{c} - \varphi(\mathbf{x}_i)\|^2 \leq R^2, \quad i = 1, \ldots, m

(dual) \quad \max_{\alpha} \quad \alpha' \text{diag}(\mathbf{K}) - \alpha' \mathbf{K} \alpha

\quad \text{s.t.} \quad \alpha' \mathbf{1} = 1, \quad \alpha \geq 0

- $\alpha = [\alpha_1, \ldots, \alpha_m]'$: Lagrange multipliers
- $\mathbf{K}_{m \times m} = [k(\mathbf{x}_i, \mathbf{x}_j)]$: kernel matrix
- $\mathbf{0} = [0, \ldots, 0]'$, $\mathbf{1} = [1, \ldots, 1]'$
Assume \( k(x, x) = \kappa \), a constant \( \quad (1) \)

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 \( \alpha'\text{diag}(K) = \kappa \)

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

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

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

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

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

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

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

• Finding **exact** MEBs is **inefficient** for large $d$

  - $(1 + \epsilon)$-approximation
  - the $(1 + \epsilon)$-expansion of the blue ball contains all the points
  - the blue ball is the MEB of the red points (**coreset**)

Approximate MEB algorithm [Bădoiu & Clarkson, 2002]

1. 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 $B(c_t, (1 + \epsilon)r_t)$
   - we relax it to any point outside $B(c_t, (1 + \epsilon)r_t)$
2. Repeat until all the points in $S$ are covered by $B(c_t, (1 + \epsilon)r_t)$
Example
Example
Example
Example
Example
Core Vector Machine (CVM)
Numerical Optimization

CVM algorithm

1. Initialize $c_0 = \varphi(z_0)$, $R_0 = 0$ and $S_0 = \{\varphi(z_0)\}$.
2. Terminate if no $\varphi(z)$ falls outside $B(c_t, (1 + \epsilon)R_t)$. Otherwise, let $\varphi(z_t)$ be such a point. Set $S_{t+1} = S_t \cup \{\varphi(z_t)\}$.
3. **Find MEB($S_{t+1}$)**
4. Increment $t$ by 1 and go back to step 2

**Numerical solver** is still required in finding MEB($S_t$)
- QP subproblem
- Requires the use of a sophisticated numerical solver for an efficient implementation
  - LIBSVM
- For complicated/very large data sets $\Rightarrow$ internal optimization can be expensive

**Question**

Can we have a simpler algorithm without using any numerical solver?
Enclosing Ball (EB) Problem

CVM $\leftrightarrow$ minimum enclosing ball

Minimum Enclosing Ball (MEB) Problem

Find the smallest ball $B(c, r)$ that encloses all the points in $S$

- some optimization appears inevitable

Enclosing Ball (EB) Problem

Given the radius $r \geq R^*$, find a ball $B(c, r)$ that encloses all the points in $S$

- $\|c - \varphi(z_i)\|^2 \leq r^2$ for all $\varphi(z)$'s in $S$
Ball Vector Machine (BVM)

$(1 + \epsilon)$-approximation algorithm for $\text{EB}(S, r)$

1. Initialize $c_0 = \varphi(z_0)$
2. Terminate if no $\varphi(z)$ falls outside $B(c_t, (1 + \epsilon)r)$. Otherwise, let $\varphi(z_t)$ be such a point
3. Find the smallest update to the center such that $B(c_{t+1}, r)$ touches $\varphi(z_t)$
4. Increment $t$ by 1 and go back to step 2

CVM algorithm

1. Initialize $c_0 = \varphi(z_0)$, $R_0 = 0$ and $S_0 = \{\varphi(z_0)\}$.
2. Terminate if no $\varphi(z)$ falls outside $B(c_t, (1 + \epsilon)R_t)$. Otherwise, let $\varphi(z_t)$ be such a point. Set $S_{t+1} = S_t \cup \{\varphi(z_t)\}$
3. Find $\text{MEB}(S_{t+1})$
4. Increment $t$ by 1 and go back to step 2

BVM is similar to CVM except that the update of the ball's center is different
Example
Efficient Update of the Ball’s Center

At the $t$th iteration, the ball’s center is updated such that the new ball just touches $\varphi(z_t)$

$$\min_c \| c - c_t \|^2 : r^2 \geq \| c - \varphi(z_t) \|^2$$

The new center can be obtained analytically as

$$c_{t+1} = \varphi(z_t) + \beta_t (c_t - \varphi(z_t))$$

- $\beta_t = r / \| c_t - \varphi(z_t) \|$
- no numerical optimization solver is needed!

$c_{t+1}$ is a convex combination of $c_t$ and $\varphi(z_t)$

- for any $t > 0$, $c_t$ is always a linear combination of $c_0$ and $S_t = \{ \varphi(z_i) \}_{i=1}^t$
- distance between $c_{t+1}$ and any pattern $\varphi(z)$ can be computed efficiently
Quality of Prediction

Let $B(\hat{c}, (1 + \epsilon)r)$ be any $(1 + \epsilon)$-approximation of $EB(S, r)$, then

$$\frac{\|\hat{c} - c^*\|}{R^*} \leq \sqrt{\frac{(1+\epsilon)^2 r^2}{R^*^2}} - 1$$

Recall that for the L2-SVM:

$$\min_{w, b, \xi_i, \rho} \|w\|^2 + b^2 - 2\rho + C \sum_{i=1}^{n} \xi_i^2$$

s.t. $y_i(w'\varphi(x_i) + b) \geq \rho - \xi_i, \quad i = 1, \ldots, n,$

$c = [w', b, \sqrt{C}\xi_1, \ldots, \sqrt{C}\xi_n]'$

For any input $x$,

- optimal prediction function $f^*(x) = w^*'\varphi(x) + b^*$
- approximated prediction function $\hat{f}(x) = \hat{w}'\varphi(x) + \hat{b}$

$$|\hat{f}(x) - f^*(x)| = \left| (\hat{w} - w^*)'\varphi(x) + (\hat{b} - b^*) \right| \leq \sqrt{\|\hat{c} - c^*\|^2} \sqrt{k_{ii}} + 1$$

$\epsilon$ small $\Rightarrow \|\hat{c} - c^*\|^2$ small $\Rightarrow \hat{f}(x)$ close to $f^*(x)$
Theorem 1 in [Panigraphy, 2004]
When a point falling outside $B(c_t, (1 + \epsilon)r)$ is picked
- BVM algorithm obtains an $(1 + \epsilon)$-approximation of $EB(S, r)$ in $O(1/\epsilon^2)$ iterations
- overall time complexity: $O(1/\epsilon^4)$

When the furthest point is picked
- BVM algorithm obtains an $(1 + \epsilon)$-approximation of $EB(S, r)$ in $O(1/\epsilon)$ iterations
- computing such a point takes $O(m|S_t|)$
- overall time complexity: $O(m/\epsilon^2)$
  $\Rightarrow$ computationally expensive for large $m$
Multi-Scale \((1 + \epsilon)\)-Approximation Algorithm for \(EB(S, r)\)

Idea

- Instead of using a small \(\epsilon\) from the very beginning, start with a much larger \(\epsilon' = 2^{-1}\)
- After an \((1 + \epsilon')\)-approximation of \(EB(S, r)\) has been obtained, reduce \(\epsilon'\) by half and repeated until \(\epsilon' = \epsilon\)

Assume that \(2^{-1} \geq \epsilon = 2^{-M}\) for some positive integer \(M\)

1. Initialize \(c_{EB_0} = \varphi(z_0)\).
2. For \(m = 1\) to \(M\) do
3. Set \(\epsilon_m = 2^{-m}\). Find \((1 + \epsilon_m)\)-approximation of \(EB(S, r)\) using BVM Algorithm, with \(c_{EB_{m-1}}\) as warm start

In finding the EB, only requires \(\varphi(z_t)\) to be outside \(B(c_t, (1 + \epsilon)r)\)

\[\Rightarrow \text{avoid expensive distance computations}\]
Multi-Scale Approximation Algorithm...

Converges in at most $3 \log_2 \frac{1}{\epsilon} + \left(1 - \frac{R^*}{r^2}\right) \frac{1}{\epsilon^2} + \frac{6}{\epsilon}$ iterations

$r = R^*$
- number of iteration is $O(1/\epsilon)$
- time complexity $O(1/\epsilon^2)$
- space complexity $O(1/\epsilon)$

$r \rightarrow R^*$
- the $1/\epsilon^2$ term becomes negligible
- number of iteration is close to $O(1/\epsilon)$

cf. CVM takes $O(1/\epsilon^8)$ time and $O(1/\epsilon^2)$ space
How to Set $r$ in the SVM Setting?

Primal:
\[
\min \|w\|^2 + b^2 - 2\rho + C \sum_{i=1}^{m} \xi_i^2 \\
\text{s.t. } y_i(w'\varphi(x_i) + b) \geq \rho - \xi_i
\]

Dual:
\[
\max -\alpha' (K \odot yy' + yy' + \frac{1}{C} I) \alpha \\
\text{s.t. } \alpha \geq 0, \; \alpha'1 = 1
\]

\[
\tilde{k}_{ij} = y_iy_jk(x_i, x_j) + y_iy_j + \frac{\delta_{ij}}{C}
\]

\[\tilde{k}_{ii} = k_{ii} + \frac{1}{C} \equiv \tilde{\kappa}. \text{ Set } r = \sqrt{\tilde{\kappa}}\]

$\sqrt{\kappa} \geq R^*$, where $R^*$ is the radius of the MEB

Often, $r = \sqrt{\tilde{\kappa}} \simeq R^*$

- $\epsilon$ is small and $r \simeq R^*$, center of this EB problem is close to the center of MEB
- ball’s center $\leftrightarrow$ SVM’s weight and bias
- the obtained BVM is also close to the desired SVM solution
Varying $\epsilon$ ("letter", "usps")

- BVM and CVM have high accuracies for $\epsilon \in [10^{-8}: 10^{-3}]$
- performance deteriorates when $\epsilon$ is further increased

- training time and number of support vectors are stable for $\epsilon \leq 10^{-4}$
- BVM training is faster than CVM
Varying $C$ ("reuters", "usps")

- BVM has almost the same accuracies as LIBSVM
- training time and number of support vectors obtained by BVM (with $\epsilon \geq 10^{-4}$) are comparable with those of LIBSVM
Both BVM and CVM have comparable accuracies as the other implementations.
## Different Kernels (‘‘usps’’)

<table>
<thead>
<tr>
<th></th>
<th>normalized polynomial kernel</th>
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<th>Gaussian kernel</th>
<th>Laplacian kernel</th>
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<td>99.54</td>
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<td></td>
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<td>99.60</td>
<td><strong>99.64</strong></td>
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<td></td>
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<td>LASVM</td>
<td>933</td>
<td>1,899</td>
<td>3,187</td>
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Both BVM and CVM are fast and have good performance
## Data Sets

<table>
<thead>
<tr>
<th>data sets</th>
<th>#class</th>
<th>dim</th>
<th>#train patns.</th>
<th>#test patns</th>
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## Testing Accuracies (in %)

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<th>BVM</th>
<th>CVM</th>
<th>LIBSVM</th>
<th>LASVM</th>
<th>SimpleSVM</th>
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<td>94.23</td>
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<td>intrusion</td>
<td>91.97</td>
<td><strong>92.44</strong></td>
<td>–</td>
<td>–</td>
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</tr>
</tbody>
</table>

- BVM and CVM have accuracies comparable with the other SVM implementations
- Only BVM and CVM (but neither LIBSVM nor LASVM) can work on “intrusion” (with around 5 million training examples)
### CPU Time (in sec) used in SVM Training

<table>
<thead>
<tr>
<th>data</th>
<th>BVM</th>
<th>CVM</th>
<th>LIBSVM</th>
<th>LASVM</th>
<th>SimpleSVM</th>
</tr>
</thead>
<tbody>
<tr>
<td>optdigits</td>
<td><strong>1.65</strong></td>
<td>24.86</td>
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<tr>
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<td><strong>0.70</strong></td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
</tbody>
</table>

- BVM is usually faster than CVM, and is faster/comparable with the other implementations.
## Number of Support Vectors

<table>
<thead>
<tr>
<th>data</th>
<th>BVM</th>
<th>CVM</th>
<th>LIBSVM</th>
<th>LASVM</th>
</tr>
</thead>
<tbody>
<tr>
<td>optdigits</td>
<td>1583</td>
<td>2154</td>
<td>1306</td>
<td>N/A</td>
</tr>
<tr>
<td>satimage</td>
<td>1956</td>
<td>2333</td>
<td>1433</td>
<td>N/A</td>
</tr>
<tr>
<td>w3a</td>
<td>694</td>
<td>1402</td>
<td>1072</td>
<td>979</td>
</tr>
<tr>
<td>pendigits</td>
<td>1990</td>
<td>2827</td>
<td>1206</td>
<td>N/A</td>
</tr>
<tr>
<td>reuters</td>
<td>925</td>
<td>1496</td>
<td>1356</td>
<td>1359</td>
</tr>
<tr>
<td>letter</td>
<td>10536</td>
<td>12440</td>
<td>8436</td>
<td>N/A</td>
</tr>
<tr>
<td>web</td>
<td>2522</td>
<td>2960</td>
<td>4674</td>
<td>5718</td>
</tr>
<tr>
<td>ijcnn1</td>
<td>4006</td>
<td>3637</td>
<td>5700</td>
<td>5525</td>
</tr>
<tr>
<td>usps</td>
<td>1524</td>
<td>2576</td>
<td>2178</td>
<td>1803</td>
</tr>
<tr>
<td>intrusion</td>
<td>99</td>
<td>51</td>
<td>–</td>
<td>–</td>
</tr>
</tbody>
</table>

- All obtain comparable numbers of support vectors
- On the large data sets (“reuters”, “web”, “ijcnn1”, “usps” and “intrusion”), CVM and, even better, BVM can have fewer support vectors
MNIST Digits Database

An extended MNIST digit database

- the original training set contains 60,000 patterns with 784 features
- Loosli, Canu & Bottou [2007] extended the training set to 8.1 million patterns by incorporating 135 transformations

Using all 8.1M patterns

<table>
<thead>
<tr>
<th></th>
<th>BVM</th>
<th>LASVM</th>
</tr>
</thead>
<tbody>
<tr>
<td>accuracy (%)</td>
<td>98.66</td>
<td>99.33</td>
</tr>
<tr>
<td>CPU time (s)</td>
<td>8 hours</td>
<td>(8 days)</td>
</tr>
</tbody>
</table>

Using 1/3 of the training patterns

<table>
<thead>
<tr>
<th></th>
<th>BVM</th>
<th>LIBSVM</th>
<th>LASVM</th>
</tr>
</thead>
<tbody>
<tr>
<td>#misclassified patterns</td>
<td>2</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>accuracy (in %)</td>
<td>99.91</td>
<td>99.86</td>
<td>99.91</td>
</tr>
<tr>
<td>CPU time (s)</td>
<td>238.33</td>
<td>7981.48</td>
<td>1797.43</td>
</tr>
<tr>
<td>#support vectors</td>
<td>1,605</td>
<td>2,183</td>
<td>1,618</td>
</tr>
</tbody>
</table>
Enclosing Ball (EB) problem is simpler than Minimum Enclosing Ball (MEB) problem

- update of $c_t$ does not require any numerical solver
- multi-scale $(1 + \epsilon)$-approximation algorithm for faster convergence

⇒ easy to implement
⇒ BVM is faster than CVM

Experimentally,

- BVM’s accuracy is comparable with the other SVM implementations
- usually faster than CVM, and is faster/comparable with others
- can handle very large data sets
- can have fewer support vectors