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Efficient SVM Optimization without an Optimizer

James Kwok

Department of Computer Science and Engineering Hong Kong University of Science and Technology Hong Kong

Joint work with Ivor Tsang, Andras Kocsor

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Supervised learning: classification / regression

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



standard digital camera: 10M pixels

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



Classification problem:

• training set $\{(\mathbf{x}_i, y_i)\}_{i=1}^m, \mathbf{x}_i \in \mathbb{R}^d, y_i \in \{\pm 1\}$ (labels)



Large-margin method: Maximize the margin separating opposite classes

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Maxim	izing the	Margin			

Let the (linear) classifier be $\mathbf{w}'\mathbf{x} + b$

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



 $(\alpha_i : \text{Lagrange multiplier})$ Quadratic programming (QP) problem (globally optimal solution) Support vectors: patterns with $\alpha_i > 0$

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Kernel	Trick				

$Classifier: \ linear \rightarrow \ nonlinear$

 $\bullet\,$ map the data from input space to feature space ${\mathcal F}$ using φ





Only inner products in \mathcal{F} are needed: $\varphi(\mathbf{x}_i)'\varphi(\mathbf{x}_j) \rightarrow \underbrace{k(\mathbf{x}_i, \mathbf{x}_j)}_{\text{kernel}}$

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SVM (Optimizati	on			

Needs a QP solver

Problem 1

Needs $O(m^2)$ memory just to write down $m \times m$ kernel matrix $= [k(\mathbf{x}_i, \mathbf{x}_j)]_{i,j=1}^m$ (*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 $\rightarrow O(m^3)$ time

Key observation

Near-optimal approximate solutions are often good enough in practical applications

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- I Formulate kernel methods as minimum enclosing ball problems
- 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]

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 Minimum
 Enclosing
 Ball
 (MER)
 →
 SV/M

Minimum Enclosing Ball (MEB) \Leftrightarrow SVM

A problem in Computational Geometry

Given $S = {x_1, ..., x_m}$, minimum enclosing ball of S (MEB(S)):

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

(primal) min R^2



$$\begin{array}{ll} \text{(prival)} & \stackrel{R, \mathbf{c}}{\underset{R, \mathbf{c}}{\text{s.t.}}} & \|\mathbf{c} - \varphi(\mathbf{x}_i)\|^2 \leq R^2, & i = 1, \dots, m \\ \text{(dual)} & \max_{\boldsymbol{\alpha}} \ \boldsymbol{\alpha}' \text{diag}(\mathbf{K}) - \boldsymbol{\alpha}' \mathbf{K} \boldsymbol{\alpha} \\ & \text{s.t.} \quad \boldsymbol{\alpha}' \mathbf{1} = 1, \ \boldsymbol{\alpha} \geq \mathbf{0} \end{array}$$

α = [α_i,...,α_m]': Lagrange multipliers
 K_{m×m} = [k(x_i, x_j)]: kernel matrix
 0 = [0,...,0]', 1 = [1,...,1]'

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MEB	⇔ SVM				

Assume
$$k(\mathbf{x}, \mathbf{x}) = \kappa$$
, a constant (1)

Holds for

1 isotropic kernel
$$k(\mathbf{x}, \mathbf{y}) = K(||\mathbf{x} - \mathbf{y}||)$$
 (e.g., Gaussian)

Outproduct kernel k(x, y) = K(x'y) (e.g., polynomial) with normalized inputs

3 any normalized kernel
$$k(\mathbf{x}, \mathbf{y}) = \frac{K(\mathbf{x}, \mathbf{y})}{\sqrt{K(\mathbf{x}, \mathbf{x})}\sqrt{K(\mathbf{y}, \mathbf{y})}}$$

Combine with ${m lpha}' {m 1} = 1$, we have ${m lpha}' {
m diag}({m K}) = \kappa$

$$\max_{\alpha} - \alpha' \mathbf{K} \alpha \quad : \quad \alpha \ge \mathbf{0}, \quad \alpha' \mathbf{1} = 1$$
 (2)

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

Any QP of the form in (??) \leftrightarrow a MEB problem



$$\max_{\boldsymbol{\alpha}} - \boldsymbol{\alpha}' \mathbf{K} \boldsymbol{\alpha} \quad : \quad \boldsymbol{\alpha}' \mathbf{1} = 1, \ \boldsymbol{\alpha} \geq \mathbf{0}$$

$$\{\mathbf{z}_i = (\mathbf{x}_i, y_i)\}_{i=1}^m$$



(primal)
$$\min_{\mathbf{w},b,\rho,\xi_{i}} \|\mathbf{w}\|^{2} + b^{2} - 2\rho + C \sum_{i=1}^{m} \xi_{i}^{2} : y_{i}(\mathbf{w}'\varphi(\mathbf{x}_{i}) + b) \geq \rho - \xi_{i}$$

(dual)
$$\max_{\boldsymbol{\alpha}} -\boldsymbol{\alpha}' \left(\mathbf{K} \odot \mathbf{y}\mathbf{y}' + \mathbf{y}\mathbf{y}' + \frac{1}{C}\mathbf{I}\right)\boldsymbol{\alpha} : \boldsymbol{\alpha} \geq \mathbf{0}, \quad \boldsymbol{\alpha}'\mathbf{1} = 1$$
$$\mathbf{\tilde{K}} = \left[y_{i}y_{j}k(\mathbf{x}_{i},\mathbf{x}_{j}) + y_{i}y_{j} + \frac{\delta_{ij}}{C}\right], \quad \text{with} \quad \tilde{k}(\mathbf{z},\mathbf{z}) = \kappa + 1 + \frac{1}{C} \quad (\text{constant})$$

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Appro	ximate M	IEB 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]

- At the *t*th iteration, the current estimate B(c_t, r_t) is expanded incrementally by including the furthest point outside the (1 + ε)-ball B(c_t, (1 + ε)r_t)
 - we relax it to any point outside $B(\mathbf{c}_t, (1+\epsilon)r_t)$
- ② Repeat until all the points in ${\cal S}$ are covered by $B({f c}_t,(1+\epsilon)r_t)$

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Exam	ple				







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Numer	ical Opti	mization			

CVM algorithm

- 1: Initialize $\mathbf{c}_0 = \varphi(\mathbf{z}_0)$, $R_0 = 0$ and $\mathcal{S}_0 = \{\varphi(\mathbf{z}_0)\}$.
- 2: Terminate if no $\varphi(\mathbf{z})$ falls outside $B(\mathbf{c}_t, (1 + \epsilon)R_t)$. Otherwise, let $\varphi(\mathbf{z}_t)$ be such a point. Set $S_{t+1} = S_t \cup \{\varphi(\mathbf{z}_t)\}$
- 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 ⇒ internal optimization can be expensive

Question

Can we have a simpler algorithm without using any numerical solver?

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Enclos	ing Ball (E	EB) Problem			

 $\mathsf{CVM} \leftrightarrow \textbf{minimum} \text{ enclosing ball}$

Minimum Enclosing Ball (MEB) Problem

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

• some optimization appears inevitable

Enclosing Ball (EB) Problem

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

•
$$\|\mathbf{c} - \varphi(\mathbf{z}_i)\|^2 \le r^2$$
 for all $\varphi(\mathbf{z}_i)$'s in \mathcal{S}

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Ball V	ector Ma	chine (BVM)			

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

- 1: Initialize $\mathbf{c}_0 = \varphi(\mathbf{z}_0)$
- 2: Terminate if no $\varphi(\mathbf{z})$ falls outside $B(\mathbf{c}_t, (1 + \epsilon)r)$. Otherwise, let $\varphi(\mathbf{z}_t)$ be such a point
- Find the smallest update to the center such that B(c_{t+1}, r) touches φ(z_t)
- 4: Increment t by 1 and go back to step 2

CVM algorithm

- 1: Initialize $\mathbf{c}_0 = \varphi(\mathbf{z}_0)$, $R_0 = 0$ and $\mathcal{S}_0 = \{\varphi(\mathbf{z}_0)\}$.
- 2: Terminate if no $\varphi(\mathbf{z})$ falls outside $B(\mathbf{c}_t, (1 + \epsilon)R_t)$. Otherwise, let $\varphi(\mathbf{z}_t)$ be such a point. Set $S_{t+1} = S_t \cup \{\varphi(\mathbf{z}_t)\}$
- 3: Find $MEB(S_{t+1})$
- 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

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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 $\varphi(\mathbf{z}_t)$

$$\min_{\mathbf{c}} \|\mathbf{c} - \mathbf{c}_t\|^2 : r^2 \ge \|\mathbf{c} - \varphi(\mathbf{z}_t)\|^2$$

The new center can be obtained analytically as

$$\mathbf{c}_{t+1} = \varphi(\mathbf{z}_t) + \beta_t(\mathbf{c}_t - \varphi(\mathbf{z}_t))$$

•
$$\beta_t = r/\|\mathbf{c}_t - \varphi(\mathbf{z}_t)\|$$

• no numerical optimization solver is needed!

 \mathbf{c}_{t+1} is a convex combination of \mathbf{c}_t and $\varphi(\mathbf{z}_t)$

- for any t > 0, \mathbf{c}_t is always a linear combination of \mathbf{c}_0 and $\mathcal{S}_t = \{\varphi(\mathbf{z}_i)\}_{i=1}^t$
- distance between \mathbf{c}_{t+1} and any pattern $\varphi(\mathbf{z})$ can be computed efficiently

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Quality of Prediction

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

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

n

Recall that for the L2-SVM:

$$\begin{split} \min_{\mathbf{w},b,\xi_i,\rho} & \|\mathbf{w}\|^2 + b^2 - 2\rho + C\sum_{i=1}^n \xi_i^2 \\ \text{s.t.} & y_i(\mathbf{w}'\varphi(\mathbf{x}_i) + b) \ge \rho - \xi_i, \quad i = 1,\dots,n, \\ \mathbf{c} = [\mathbf{w}', b, \sqrt{C}\xi_1, \dots, \sqrt{C}\xi_n]' \end{split}$$

For any input \mathbf{x} ,

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

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

 $\epsilon \text{ small} \Rightarrow \|\hat{\mathbf{c}} - \mathbf{c}^*\|^2 \text{ small} \Rightarrow \hat{f}(\mathbf{x}) \text{ close to } f^*(\mathbf{x})$

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Time	Complexi	ty			

Theorem 1 in [Panigraphy, 2004]

When a point falling outside $B(\mathbf{c}_t, (1+\epsilon)r)$ is picked

- BVM algorithm obtains an (1 + $\epsilon)\text{-approximation}$ 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 $O(m|\mathcal{S}_t|)$
- overall time complexity: $O(m/\epsilon^2)$ \Rightarrow computationally expensive for large m



Idea

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

Assume that $2^{-1} \ge \epsilon = 2^{-M}$ for some positive integer M

- 1: Initialize $\mathbf{c}_{\mathsf{EB}_0} = \varphi(\mathbf{z}_0)$.
- 2: For m = 1 to M do
- 3: Set ε_m = 2^{-m}. Find (1 + ε_m)-approximation of EB(S, r) using BVM Algorithm, with c_{EB_{m-1}} as warm start
 In finding the EB, only requires φ(z_t) to be outside B(c_t, (1 + ε)r)
 - \Rightarrow avoid expensive distance computations

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Multi	-Scale An	proximation A	loorithm		

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

 $r = R^*$

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

 $r \to R^*$

- \bullet the $1/\epsilon^2$ term becomes negligible
- number of iteration is close to $O(1/\epsilon)$
- cf. CVM takes ${\it O}(1/\epsilon^8)$ time and ${\it O}(1/\epsilon^2)$ space

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 How to Set r in the SVM Setting?



primal
min
$$\|\mathbf{w}\|^2 + b^2 - 2\rho + C \sum_{i=1}^m \xi_i^2$$

s.t. $y_i(\mathbf{w}'\varphi(\mathbf{x}_i) + b) \ge \rho - \xi_i$
dual
max $-\alpha' \left(\mathbf{K} \odot \mathbf{y}\mathbf{y}' + \mathbf{y}\mathbf{y}' + \frac{1}{C}\mathbf{I}\right) \alpha$
s.t. $\alpha \ge \mathbf{0}, \ \alpha'\mathbf{1} = 1$
 $\tilde{k}_{ij} = y_i y_j k(\mathbf{x}_i, \mathbf{x}_j) + y_i y_j + \frac{\delta_{ij}}{C}$

•
$$\tilde{k}_{ii} = k_{ii} + rac{1}{C} \equiv \tilde{\kappa}$$
. Set $r = \sqrt{\tilde{\kappa}}$

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

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

- *ϵ* is small and *r* ≃ *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





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



- training time and number of support vectors are stable for $\epsilon \leq 10^{-4}$
- BVM training is faster than CVM



BVM has almost the same accuracies as LIBSVM

• training time and number of support vectors obtained by BVM (with $\epsilon \ge 10^{-4}$) are comparable with those of LIBSVM



 Both BVM and CVM have comparable accuracies as the other implementations

10⁴

training set size

10⁵

10²

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Differ	ent Kerne	els ("usps")			

		normaliz	ed polynom	ial kernel	Gaussian	Laplacian
		<i>d</i> = 2	d = 3	d = 4	kernel	kernel
	BVM	99.39	99.54	99.63	99.51	99.36
accur.	CVM	99.48	99.54	99.64	99.46	99.46
(%)	LIBSVM	99.42	99.60	99.64	99.53	99.52
	LASVM	99.43	99.62	99.64	99.54	99.53
	BVM	51.26	52.67	66.16	124.57	224.74
CPU	CVM	47.12	94.42	214.40	26.47	143.61
time	LIBSVM	1,808.28	2,506.49	3,642.42	2,404.75	4,964.87
	LASVM	1,424.28	1,156.23	1,770.63	1,167.86	2,473.22
	BVM	665	691	793	1,105	1,538
#SV	CVM	453	783	1,353	560	1,522
	LIBSVM	1,428	2,326	3,544	2,050	4,462
	LASVM	933	1,899	3,187	1,624	4,059

Both BVM and CVM are fast and have good performance

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Data S	ets				

data sets	#class	dim	#train patns.	#test patns
optdigits	10	64	3,823	1,797
satimage	6	36	4,435	2,000
w3a	2	300	4,912	44,837
pendigits	10	16	7,494	3,498
reuters	2	8,315	7,770	3,299
letter	26	16	15,000	5,000
web	2	300	49,749	14,951
ijcnn1	2	22	49,990	91,701
extended usps	2	676	266,079	75,383
intrusion	2	127	4,898,431	311,029

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Testing	g Accura	cies (in %)			

data	BVM	CVM	LIBSVM	LASVM	SimpleSVM
optdigits	96.38	96.38	96.77	N/A	96.88
satimage	89.35	89.55	89.55	N/A	89.65
w3a	97.89	97.80	97.70	97.72	97.42
pendigits	97.97	97.85	97.91	N/A	97.97
reuters	96.75	96.96	97.15	97.09	_
letter	94.47	94.12	94.25	N/A	94.23
web	99.13	99.09	99.01	98.93	_
ijcnn1	97.58	98.67	98.19	98.42	94.10
usps	99.42	99.52	99.53	99.53	_
intrusion	91.97	92.44	-	—	_

- 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)

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CPU	Time (in s	sec) used in S	VM Training		

data	BVM	CVM	LIBSVM	LASVM	SimpleSVM
optdigits	1.65	24.86	1.79	N/A	81.15
satimage	1.82	14.81	1.06	N/A	221.01
w3a	0.85	13.82	1.46	1.54	1384.34
pendigits	1.31	12.10	0.82	N/A	41.22
reuters	6.32	63.51	9.76	13.81	_
letter	19.87	215.73	10.85	N/A	1290.55
web	32.59	54.46	168.84	178.73	_
ijcnn1	99.95	62.78	57.96	140.25	2201.35
usps	150.46	288.96	1578.27	753.09	_
intrusion	0.73	0.70	_	_	—

• BVM is usually faster than CVM, and is faster/comparable with the other implementations

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Number of Support Vectors

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

- 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

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MNIS	T 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

	BVM	LASVM
accuracy (%)	98.66	99.33
CPU time (s)	8 hours	(8 days)

Using 1/3 of the training patterns

	BVM	LIBSVM	LASVM
#misclassified patterns	2	3	2
accuracy (in %)	99.91	99.86	99.91
CPU time (s)	238.33	7981.48	1797.43
#support vectors	1,605	2,183	1,618

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Conclu	ision				

Enclosing Ball (EB) problem is simpler than Minimum Enclosing Ball (MEB) problem

- update of \mathbf{c}_t does not require any numerical solver
- multi-scale $(1 + \epsilon)$ -approximation algorithm for faster convergence
- \Rightarrow easy to implement
- \Rightarrow 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