Machine Learning 2

2. (Advanced) Support Vector Machines (SVMs)

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Outline

1. Stochastic (Sub)gradient Descent
2. Dual Coordinate Descent
3. The Adaptive Multi Hyperplane Machine

Outline

SVM Optimization Problem / Slack Variables

$$\begin{aligned}
\text{minimize } & \frac{1}{2}||\beta||^2 + \gamma \sum_{n=1}^{N} \xi_n \\
\text{w.r.t. } & y_i(\beta_0 + \beta^T x_n) \geq 1 - \xi_n, \quad n = 1, \ldots, N \\
& \xi \geq 0 \\
& \beta \in \mathbb{R}^p, \quad \beta_0 \in \mathbb{R}
\end{aligned}$$

SVM Optimization Problem / Slack Variables

$$\begin{aligned}\text{minimize } & \frac{1}{2}||\beta||^2 + \gamma \sum_{n=1}^{N} \xi_n \\ \text{w.r.t. } & y_i(\beta_0 + \beta^T x_n) \geq 1 - \xi_n, \quad n = 1, \ldots, N \\ & \xi \geq 0 \\ & \beta \in \mathbb{R}^p, \quad \beta_0 \in \mathbb{R}\end{aligned}$$

can be rewritten:

$$\begin{aligned}\text{minimize } f(\beta) :=& \frac{1}{2}||\beta||^2 + \gamma \sum_{n=1}^{N} \max(0, 1 - y_n(\beta_0 + \beta^T x_n)) \\ \propto& \frac{1}{N} \sum_{n=1}^{N} \max(0, 1 - y_n(\beta_0 + \beta^T x_n)) + \frac{1}{2}\lambda||\beta||^2, \quad \lambda := \frac{\gamma}{N}\end{aligned}$$

SVM Optimization Problem / Hinge Loss

can be rewritten (ctd.):

$$\begin{aligned}\text{minimize } f(\beta) :=& \frac{1}{2}||\beta||^2 + \gamma \sum_{n=1}^{N} \max(0, 1 - y_n(\beta_0 + \beta^T x_n)) \\ \propto& \frac{1}{N} \sum_{n=1}^{N} \max(0, 1 - y_n(\beta_0 + \beta^T x_n)) + \frac{1}{2}\lambda||\beta||^2, \quad \lambda := \frac{\gamma}{N} \\ =& \frac{1}{N} \sum_{n=1}^{N} \ell_{\text{hinge}}(y_n, \beta_0 + \beta^T x_n) + \frac{1}{2}\lambda||\beta||^2\end{aligned}$$

with

$$\ell_{\text{hinge}}(y, \hat{y}) := \max(0, 1 - y\hat{y})$$

(Sub)gradients

$$f(\beta) := \frac{1}{N} \sum_{n=1}^{N} \max(0, 1 - y_n(\beta_0 + \beta^T x_n)) + \frac{1}{2}\lambda||\beta||^2$$

$$= \frac{1}{N} \sum_{\substack{n=1 \\ y_n(\beta_0+\beta^T x_n)<1}}^{N} 1 - y_n(\beta_0 + \beta^T x_n) + \frac{1}{2}\lambda||\beta||^2$$

(Sub)gradients

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subgradients:

$$\frac{\partial f}{\partial \beta} = \frac{1}{N} \sum_{\substack{n=1 \\ y_n(\beta_0+\beta^T x_n)<1}}^{N} -y_n x_n + \lambda\beta$$

(Sub)gradients

$$f(\beta) := \frac{1}{N} \sum_{n=1}^{N} \max(0, 1 - y_n(\beta_0 + \beta^T x_n)) + \frac{1}{2}\lambda||\beta||^2$$

$$= \frac{1}{N} \sum_{\substack{n=1 \\ y_n(\beta_0+\beta^T x_n)<1}}^{N} 1 - y_n(\beta_0 + \beta^T x_n) + \frac{1}{2}\lambda||\beta||^2$$

subgradients:

$$\frac{\partial f}{\partial \beta} = \frac{1}{N} \sum_{\substack{n=1 \\ y_n(\beta_0+\beta^T x_n)<1}}^{N} -y_n x_n + \lambda\beta$$

stochastic subgradients:

$$\frac{\partial f}{\partial \beta}|_{\mathcal{D}^{(t)}} = \frac{1}{|\mathcal{D}^{(t)}|} \sum_{\substack{(x,y)\in\mathcal{D}^{(t)} \\ y(\beta_0+\beta^T x)<1}}^{N} -yx + \lambda\beta, \quad \mathcal{D}^{(t)} \subseteq \mathcal{D}^{\text{train}}, \text{iteration } t$$

Bound on Parameter Norm

The optimal parameters are bound from above:

$$||\beta^*|| \leq \frac{1}{\sqrt{\lambda}}$$

Trivially,

$$\frac{1}{2}\lambda||\beta^*||^2 \leq f(\beta^*) \leq f(0) = 1$$

$$\rightsquigarrow ||\beta^*|| \leq \frac{\sqrt{2}}{\sqrt{\lambda}}$$

[SSSS07] have a more complex proof to show the tighter bound (p. 4, end of proof of theorem 1).

Primal Estimated Subgradient Solver for SVMs (Pegasos)

- use **stochastic (sub)gradient descent**

$$\tilde{\beta}^{(t+1)} := \beta^{(t)} - \eta^{(t)} \frac{\partial f}{\partial \beta}|_{\mathcal{D}^{(t)}}$$

  - use gradient sample size K
    - though no empirical evidence that $K > 1$ has any benefits

- after each SGD step, **reproject/rescale** β:

$$\beta^{(t+1)} := \tilde{\beta}^{(t+1)} \frac{1}{\min(\sqrt{\lambda}, ||\tilde{\beta}^{(t+1)}||)}$$

- use **fixed hyperbola schedule as learning rate**:

$$\eta^{(t)} := \frac{1}{\lambda t}$$

- see [SSSS07]

Performance Comparison

Table 1. Training time in CPU-seconds

	Pegasos	SVM-Perf	SVM-Light
CCAT	2	77	20,075
Covertype	6	85	25,514
astro-ph	2	5	80

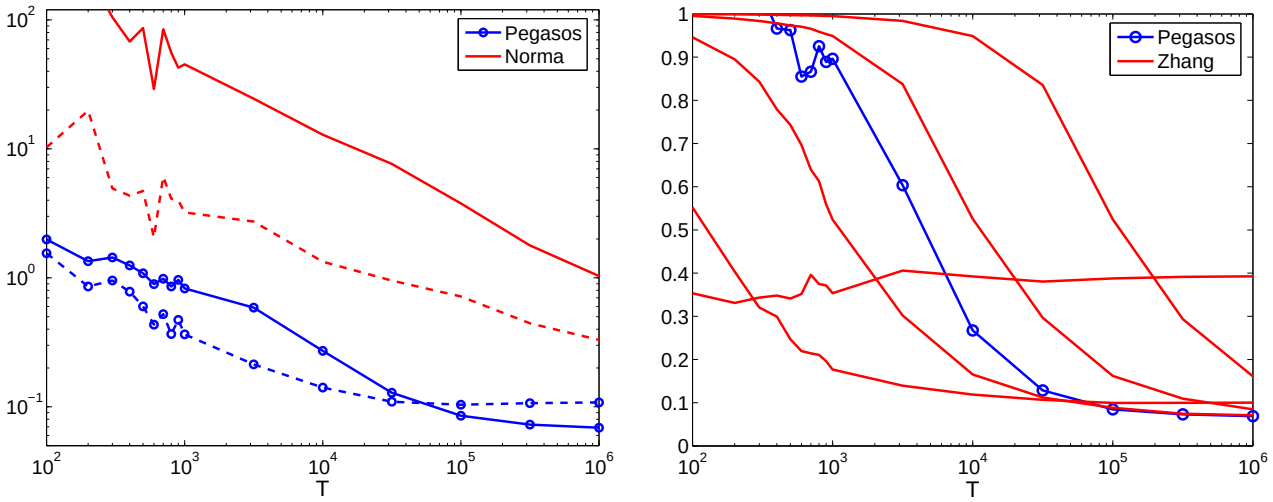

Figure 2. Comparisons of Pegasos to Norma (left) and Pegasos to stochastic gradient descent with a fixed learning rate (right) on the Astro-Physics datset. In the left plot, the solid lines designate the objective value and the dashed lines depict the loss on the test set.

[SSSS07]

Performance Comparison (2/2)

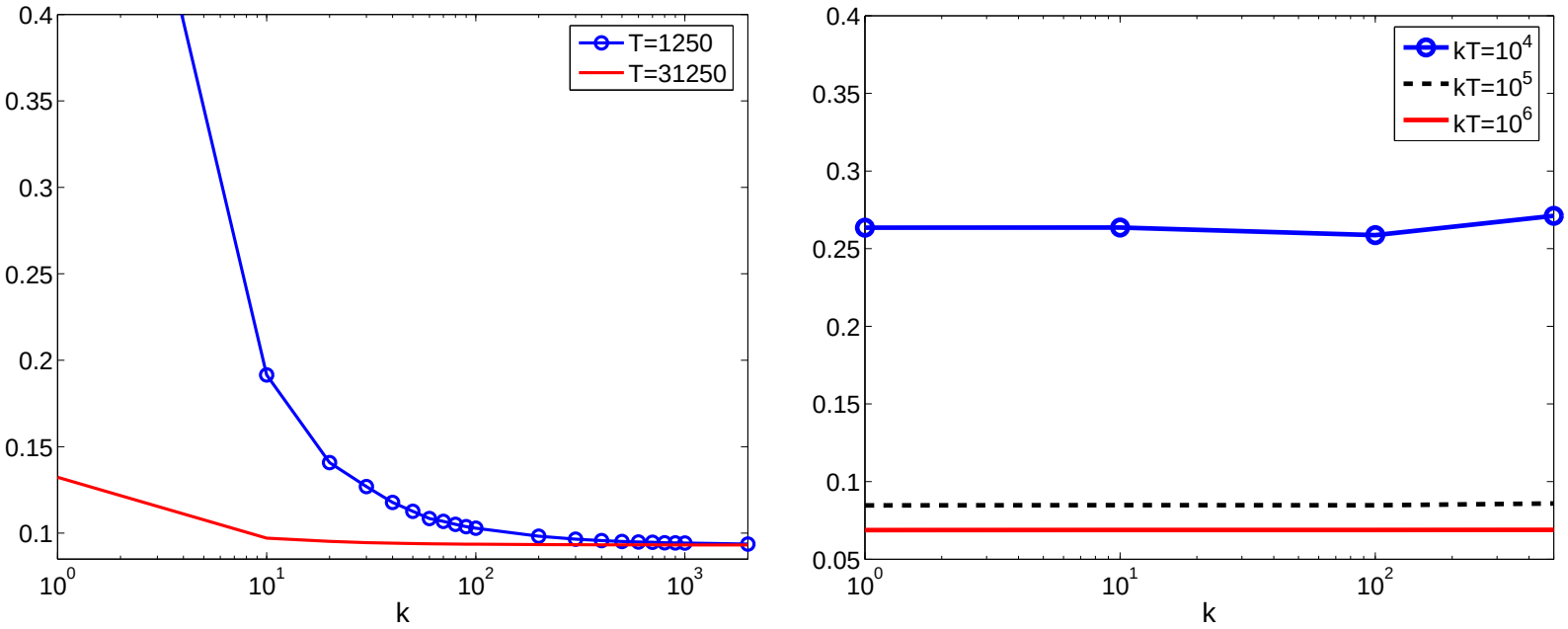

Figure 3. The effect of k on the objective value of Pegasos on the Astro-Physics dataset. Left: T is fixed. Right: kT is fixed.

[SSSS07]

(Non-Linear) Kernels

SGD in the primal first works for **linear kernels**.

Any linear model can be kernelized by **representing instances in terms of kernel features**:

original feature representation:

$$x_n \in \mathbb{R}^M, \quad n \in \{1, \ldots, N\}$$

kernel feature representation:

$$\tilde{x}_n \in \mathbb{R}^N, x_{n,m} := k(x_n, x_m), \quad m \in \{1, \ldots, N\}$$

then:

$$\hat{y}_{\text{linear}}(\tilde{x}_n; \beta) = \beta^T \tilde{x}_n = \sum_{m=1}^{N} \beta_m \tilde{x}_{n,m}$$

$$= \sum_{m=1}^{N} \alpha_m k(x_m, x_n) = \hat{y}_{\text{kernel } k}(x_n; \alpha), \quad \alpha_m := \beta_m$$

Outline

Dual Problem

Remember, the dual problem was:

$$\text{minimize } f(\alpha) := \frac{1}{2}\alpha^T Q\alpha - 1^T\alpha, \quad Q_{n,m} := y_n y_m x_n^T x_m$$

$$\text{w.r.t. } \alpha \in [0, \frac{1}{N\lambda}]$$

Dual Problem

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$$\text{w.r.t. } \alpha \in [0, \frac{1}{N\lambda}]$$

coordinate descent w.r.t. coordinate α_n:

$$f_n(\alpha_n) := f(\alpha_n; \alpha_{-n}) \propto \frac{1}{2}Q_{n,n}\alpha_n^2 + Q_{n,-n}\alpha_{-n}\alpha_n - \alpha_n$$

$$\frac{\partial f_n}{\partial \alpha_n} = Q_{n,n}\alpha_n + Q_{n,-n}\alpha_{-n} - 1 \stackrel{!}{=} 0$$

$$\rightsquigarrow \quad \alpha_n = \frac{1 - Q_{n,-n}\alpha_{-n}}{Q_{n,n}}$$

possibly clip α_n:

$$\alpha_n = \max(0, \min(\frac{1}{N\lambda}, \frac{1 - Q_{n,-n}\alpha_{-n}}{Q_{n,n}}))$$

Avoid Computing $Q_{n,-n}\alpha_{-n}$

$$\begin{aligned}
\alpha_n^{(t+1)} :=& \frac{1 - Q_{n,-n}\alpha_{-n}^{(t)}}{Q_{n,n}} \\
=& \frac{1 - Q_{n,.}\alpha^{(t)} + Q_{n,n}\alpha_n^{(t)}}{Q_{n,n}} \\
=& \alpha_n^{(t)} - \frac{Q_{n,.}\alpha^{(t)} - 1}{Q_{n,n}} \\
=& \alpha_n^{(t)} - \frac{y_n\hat{y}_n - 1}{Q_{n,n}}
\end{aligned}$$

Avoid Computing $Q_{n,-n}\alpha_{-n}$

$$\alpha_n^{(t+1)} = \alpha_n^{(t)} - \frac{y_n \hat{y}_n - 1}{Q_{n,n}}$$

with

$$\hat{y}_n = \beta^T x_n$$

and due to

$$\beta = \sum_{n=1}^{N} \alpha_n y_n x_n$$

as only α_n changes:

$$\beta^{(t+1)} := \beta^{(t)} + (\alpha_n^{(t+1)} - \alpha_n^{(t)}) y_n x_n$$

- accelerates from $O(N)$ to $O(M)$
- even $O(M_{\text{nz}})$ for sparse predictor vectors x (M_{nz} being the average number of nonzeros)

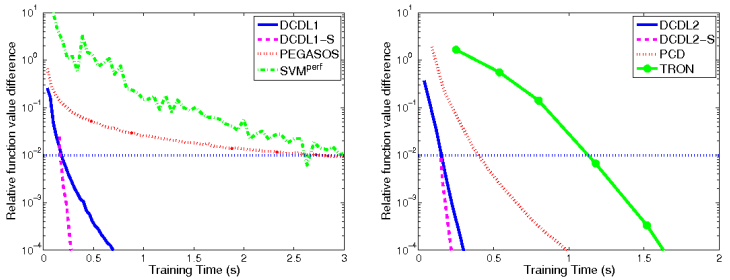
Performance Comparison

Table 2. On the right training time for a solver to reduce the primal objective value to within 1% of the optimal value; see (20). Time is in seconds. The method with the shortest running time is boldfaced. Listed on the left are the statistics of data sets: l is the number of instances and n is the number of features.

Data set	Data statistics			Linear L1-SVM			Linear L2-SVM		
	l	n	# nonzeros	DCDL1	Pegasos	SVM^{perf}	DCDL2	PCD	TRON
a9a	32,561	123	451,592	**0.2**	1.1	6.0	0.4	**0.1**	0.1
astro-physic	62,369	99,757	4,834,550	**0.2**	2.8	2.6	**0.2**	0.5	1.2
real-sim	72,309	20,958	3,709,083	**0.2**	2.4	2.4	**0.1**	0.2	0.9
news20	19,996	1,355,191	9,097,916	**0.5**	10.3	20.0	**0.2**	2.4	5.2
yahoo-japan	176,203	832,026	23,506,415	**1.1**	12.7	69.4	**1.0**	2.9	38.2
rcv1	677,399	47,236	49,556,258	**2.6**	21.9	72.0	**2.7**	5.1	18.6
yahoo-korea	460,554	3,052,939	156,436,656	**8.3**	79.7	656.8	**7.1**	18.4	286.1

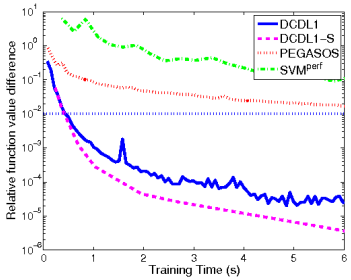
[HCL+08]

Performance Comparison (2/2)

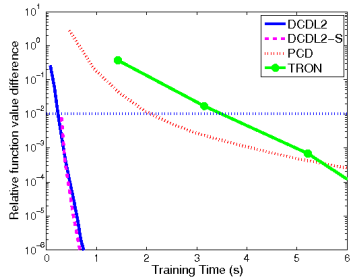


(a) L1-SVM: astro-physic

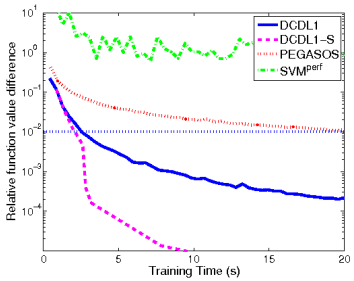
(b) L2-SVM: astro-physic



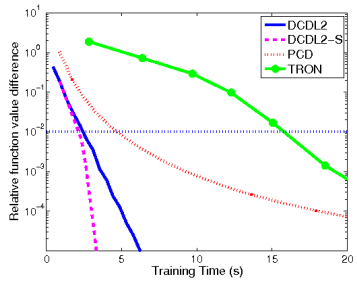
(c) L1-SVM: news20



(d) L2-SVM: news20

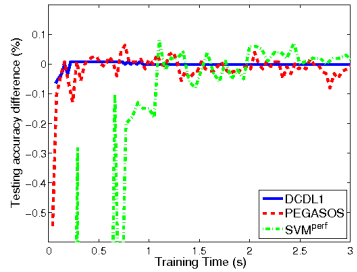


(e) L1-SVM: rcv1

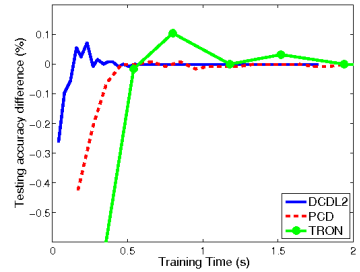


(f) L2-SVM: rcv1

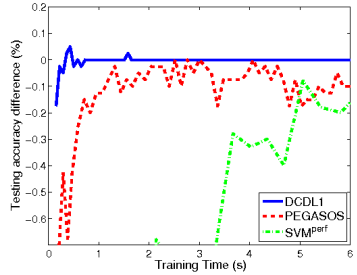
Figure 1. Time versus the relative error (20). DCDL1-S, DCDL2-S are DCDL1, DCDL2 with shrinking. The dotted line indicates the relative error 0.01. Time is in seconds.



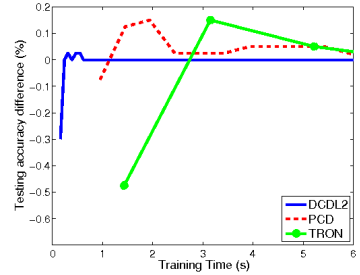
(a) L1-SVM: astro-physic



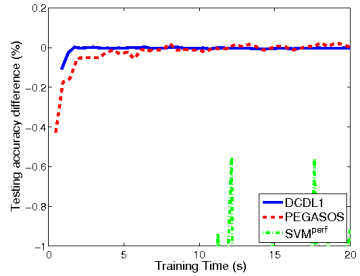
(b) L2-SVM: astro-physic



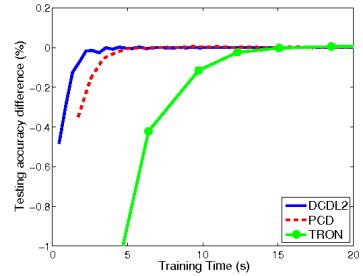
(c) L1-SVM: news20



(d) L2-SVM: news20



(e) L1-SVM: rcv1



(f) L2-SVM: rcv1

Figure 2. Time versus the difference of testing accuracy between the current model and the reference model (obtained using strict stopping conditions). Time is in seconds.

[HCL+08]

Outline

Multi-Class SVM

multi-class SVM:

$$\hat{y}(x) := \arg\max_{y \in \mathcal{Y}} s_y(x)$$

$$s_y(x; \beta) := \beta_y^T x, \quad \beta_y \in \mathbb{R}^M \quad \forall y \in \mathcal{Y} = \{y_1, \ldots, y_L\}$$

$$f(\beta) := \frac{1}{N} \sum_{n=1}^{N} \ell(y_n, x_n) + \frac{\lambda}{2} ||\beta||^2, \quad \beta := (\beta_{y_1}, \beta_{y_2}, \ldots, \beta_{y_L})$$

margin-based loss:

$$\ell(y, x; \beta) := \max(0, \quad 1 + \max_{y' \in \mathcal{Y}, y' \neq y} s_{y'}(x) - s_y(x))$$

Multi-Hyperplane Machine

multi-hyperplane score function:

$$s_y(x; \beta) := \max_{k=1,\ldots,K} \beta_{y,k}^T x, \quad \beta_{y,k} \in \mathbb{R}^M, k \in \{1, \ldots, K\}$$

margin-based loss:

$$\ell(y, x; \beta) := \max(0, \quad 1 + \max_{y' \in \mathcal{Y}, y' \neq y} s_{y'}(x) - s_y(x))$$

relaxation / convex upper bound:

$$\ell(y_n, x_n; \beta, z_n) := \max(0, \quad 1 + \max_{y' \in \mathcal{Y}, y' \neq y_n} s_{y'}(x_n) - \beta_{y_n, z_n}^T x_n)$$

- block coordinate descent / EM type training (β, z)
- use SGD to train β.

SGD for Training the Multi-Hyperplane Machine

relaxation / convex upper bound:

$$\ell(y_n, x_n; \beta, z_n) := \max(0, \quad 1 + \max_{y' \in \mathcal{Y}, y' \neq y_n} s_{y'}(x_n) - \beta_{y_n, z_n}^T x_n)$$

gradient:

$$\frac{\partial \ell}{\partial \beta_{y,k}}(y_n, x_n; z_n) = \begin{cases} x_n, & \text{if } (y,k) = \arg\max_{\substack{y' \in \mathcal{Y}, y' \neq y_n \\ k' = 1, \ldots, K}} \beta_{y',k'}^T x_n \\ -x_n, & \text{if } (y,k) = (y_n, z_n) \\ 0, & \text{otherwise} \end{cases}$$

Adaptive Multi-Hyperplane Machine:

- initialize $\beta \equiv 0$.
- if all $\beta_{y',k'}^T x < 0^T x = 0$, create a new hyperplane $K+1$ with $\beta_{y,K+1} = 0$.
  (conceptually infinite number of hyperplanes)

Performance Comparison

Table 3: Error rate and training time comparison with large-scale algorithms (RBF SVM is solved by LibSVM unless specified otherwise. Poly2 and LibSVM results are from [5]).

Datasets	Error rate (%)					Training time (seconds)[1]				
	AMM *batch*	AMM *online*	Linear (Pegasos)	Poly2 SVM	RBF SVM	AMM *batch*	AMM *online*	Linear (Pegasos)	Poly2 SVM	RBF SVM
a9a	15.03±0.11	16.44±0.23	15.04±0.07	14.94	14.97	2	0.2	1	2	99
ijcnn	2.40±0.11	3.02±0.14	7.76±0.19	2.16	1.31	2	0.1	1	11	27
webspam	4.50±0.24	6.14±1.08	7.28±0.09	1.56	0.80	80	4	12	3,228	15,571
mnist_bin	0.53±0.05	0.54±0.03	2.03±0.04	NA	0.43[2]	3084	300	277	NA	2 days[2]
mnist_mc	3.20±0.16	3.36±0.20	8.41±0.11	NA	0.67[3]	13864	1200	1180	NA	8 days[3]
rcv1_bin	2.20±0.01	2.21±0.02	2.29±0.01	NA	NA	1100	80	25	NA	NA
url	1.34±0.21	2.87±1.49	1.50±0.39	NA	NA	400	24	100	NA	NA

[1] excludes data loading time.
[2] achieved by parallel training P-packSVMs on 512 processors; results from [28].
[3] achieved by LaSVM; results from [12].

[WDCV11]

Outlook

See [DLVW13] for

- two further scalable learning algorithms for non-linear SVMs,
- an implementation, and
- an evaluation

Further Readings

- See the cited original papers.

References

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