



Boosting 25 Years

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Ensemble learning (集成学习)

"Ensemble methods" is a machine learning paradigm where multiple (homogenous/heterogeneous) individual learners are trained for the same problem e.g. neural network ensemble, decision tree ensemble, etc.



The more **accurate** and **diverse** the component learners, the better the ensemble



- □ KDDCup'07: 1st place for "... Decision Forests and ..."
- KDDCup'08: 1st place of Challenge1 for a method using Bagging; 1st place of Challenge2 for "... Using an Ensemble Method "
- KDDCup'09: 1st place of Fast Track for "Ensemble ... "; 2nd place of Fast Track for "... bagging ... boosting tree models ...", 1st place of Slow Track for "Boosting ... "; 2nd place of Slow Track for "Stochastic Gradient Boosting"
- □ KDDCup'10: 1st place for "… Classifier ensembling"; 2nd place for "… Gradient Boosting machines … "



- KDDCup'11: 1st place of Track 1 for "A Linear Ensemble ... "; 2nd place of Track 1 for "Collaborative filtering Ensemble", 1st place of Track 2 for "Ensemble ..."; 2nd place of Track 2 for "Linear combination of ..."
- KDDCup'12: 1st place of Track 1 for "Combining... Additive Forest..."; 1st place of Track 2 for "A Two-stage Ensemble of..."
- KDDCup'13: 1st place of Track 1 for "Weighted Average Ensemble"; 2nd place of Track 1 for "Gradient Boosting Machine"; 1st place of Track 2 for "Ensemble the Predictions"



KDDCup'14: 1st place for "ensemble of GBM, ExtraTrees, Random Forest..." and "the weighted average"; 2nd place for "use both R and Python GBMs"; 3rd place for "gradient boosting machines... random forests" and "the weighted average of..."

□ Netflix Prize:

- ✓ 2007 Progress Prize Winner: Ensemble
- ✓ 2008 Progress Prize Winner: Ensemble
- ✓ 2009 \$1 Million Grand Prize Winner:

Ensemble !!



More about ensemble methods

Chapman & Hall/CBC

Machine Learning & Pattern Recognition Series **Ensemble Methods** Foundations and Algorithms Zhi-Hua Zhou

Z.-H. Zhou. <u>Ensemble Methods:</u> <u>Foundations and Algorithms</u>, Boca Raton, FL: Chapman & Hall/CRC, Jun. 2012. (ISBN 978-1-439-830031)

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- Sequential methods
 - AdaBoost
- [Freund & Schapire, JCSS97]
- Arc-x4 [Breiman, AnnStat98]
- LPBoost [Demiriz, Bennett, Shawe-Taylor, MLJ06]

- Parallel methods
 - Bagging
 - Random Subspace
 - Random Forests

[Breiman, MLJ96] [Ho, TPAMI98] [Breiman, MLJ01]



Significant advantageous:

- Very accurate prediction
- Very simple ("just 10 lines of code" as Schapire said)
- Wide and successful applications
- Sound theoretical foundation

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Gödel Prize (2003)

Freund & Schapire, A decision theoretic generalization of on-line learning and an application to Boosting. Journal of Computer and System Sciences, 1997, 55: 119-139.



An open problem [Kearns & Valiant, STOC'89]: "weakly learnable" ?= "strongly learnable"

a problem is *learnable* or *strongly learnable* if there exists an algorithm that outputs a learner *h* in polynomial time such that for all $0 < \delta$, $\epsilon \le 0.5$, $P(\mathbb{E}_{x \sim \mathcal{D}}[\mathbb{I}[h(x) \neq f(x)]] < \epsilon) \ge 1 - \delta$

a problem is *weakly learnable* if there exists an algorithm that outputs a learner with error 0.5-1/p where p is a polynomial in problem size and other parameters

In other words, whether a "weak" learning algorithm that works just slightly better than random guess can be "boosted" into an arbitrarily accurate "strong" learning algorithm

- Amazingly, in 1990 Schapire proves that the answer is "yes". More importantly, the proof is a construction! This is the first Boosting algorithm
- In 1993, Freund presents a scheme of combining weak learners by majority voting in Phd thesis at UC Santa Cruz

However, these algorithms are not practical

Later, at AT&T Bell Labs, Freund & Schapire published the 1997 journal paper (the work was reported in EuroCOLT'95), which proposed the AdaBoost algorithm, a practical algorithm



The AdaBoost algorithm

Given:
$$(x_1, y_1), \ldots, (x_m, y_m)$$
 where $x_i \in X, y_i \in Y = \{-1, +1\}$
Initialize $D_1(i) = 1/m$.
For $t = 1, \ldots, T$:
• Train base learner using distribution D_t .
• Get base classifier $h_t : X \to \mathbb{R}$.
 $typically \ \alpha_t = \frac{1}{2} \ln \left(\frac{1 - \epsilon_t}{\epsilon_t}\right)$
where $\epsilon_t = \Pr_{i \sim D_t} [h_t(x_i) \neq y_i]$

- Train base learner using distribution D_t.
- Get base classifier h_t : X → ℝ.
- Choose α_t ∈ ℝ.−
- Update:

$$D_{t+1}(i) = \frac{D_t(i)\exp(-\alpha_t y_i h_t(x_i))}{Z_t}$$

where Z_t is a normalization tion).

the weights of incorrectly classified examples are increased such that the base learner is forced to focus on the "hard" examples in the training set Output the final classifier:

$$H(x) = \operatorname{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(x)\right)$$

A flowchart illustration





weighted combination

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First, it is simple yet effective

can be applied to almost all tasks where one wants to apply machine learning techniques

For example, in computer vision, the **Viola-Jones detector** AdaBoost using harr-like features in a cascade structure



in average, only 8 features needed to be evaluated per image

The Viola-Jones detector





"the first real-time face detector"

Comparable accuracy, but **15 times faster** than state-of-the-art of face detectors (at that time)





Longuet-Higgins Prize (2011)

Viola & Jones, Rapid object detection using a Boosted cascade of simple features. CVPR, 2001.



Second, it generates the Boosting Family of algorithms

A general boosting procedure

Input: Sample distribution \mathcal{D} ; Base learning algorithm \mathfrak{L} ; Number of learning rounds T.

Process:

1. $\mathcal{D}_1 = \mathcal{D}$. % Initialize distribution 2. **for** t = 1, ..., T: 3. $h_t = \mathfrak{L}(\mathcal{D}_t)$; % Train a weak learner from distribution \mathcal{D}_t 4. $\epsilon_t = P_{\boldsymbol{x} \sim D_t}(h_t(\boldsymbol{x}) \neq f(\boldsymbol{x}))$; % Evaluate the error of h_t 5. $\mathcal{D}_{t+1} = Adjust_Distribution(\mathcal{D}_t, \epsilon_t)$ 6. **end Output:** $H(\boldsymbol{x}) = Combine_Outputs(\{h_1(\boldsymbol{x}), ..., h_t(\boldsymbol{x})\})$

A lot of Boosting algorithms:

AdaBoost.M1, AdaBoost.MR, FilterBoost, GentleBoost, GradientBoost, MadaBoost, LogitBoost, LPBoost, MultiBoost, RealBoost, RobustBoost, ...



Third, there are sound theoretical results

Freund & Schapire [JCSS97] proved that the training error of AdaBoost is bounded by:

$$\epsilon = \mathbb{E}_{\boldsymbol{x} \sim \mathcal{D}} \mathbb{I}[H(\boldsymbol{x}) \neq f(\boldsymbol{x})] \leq 2^T \prod_{t=1}^T \sqrt{\epsilon_t (1 - \epsilon_t)} \leq e^{-2\sum_{t=1}^T \gamma_t^2}$$

where $\gamma_t = 0.5 - \epsilon_t$

Thus, if each base classifier is slightly better than random such that $\gamma_t \geq \gamma$ for some $\gamma > 0$, then the training error drops exponentially fast in T because the above bound is at most $e^{-2T\gamma^2}$



Freund & Schapire [JCSS97] proved that the generalization error of AdaBoost is bounded by:

$$\epsilon_{\mathcal{D}} \le \epsilon_D + \tilde{O}\left(\sqrt{\frac{dT}{m}}\right)$$

with probability at least $1-\delta$, where *d* is the **VC-dimension** of base learners, *m* is the number of training instances, *T* is the number of learning rounds and $\tilde{O}(\cdot)$ is used instead of $O(\cdot)$ to hide logarithmic terms and constant factors.

It implies that AdaBoost will **overfit** if T is large

Overfit (过拟合): The trained model fits the training data too much such that it can exaggerate minor fluctuations in the training data, leading to poor generalization performance



However, AdaBoost often does not overfit in real practice



Seems contradict with the **Occam's Razor**

Knowing the reason may inspire new methodology for algorithm design

Understanding why AdaBoost seems resistant to overfitting is the most fascinating fundamental theoretical issue



□ Margin Theory

Started from [Schapire, Freund, Bartlett & Lee, Boosting the margin: A new explanation for the effectiveness of voting methods. Annals of Statistics, 26(5):1651–1686, 1998]

□ Statistical View

Started from [Friedman, Hastie & Tibshirani. Additive logistic regression: A statistical view of boosting (with discussions). Annals of Statistics, 28(2):337–407, 2000]



In binary classification, we want to optimize the 0/1-loss

Because it is non-smooth, non-convex, ..., in statistical learning usually we instead optimize a **surrogate loss**



The key step of the AdaBoost algorithm seems closely related to the exponential loss:

$$D_{t+1}(i) = \frac{D_t(i)}{Z_t} e^{-\alpha_t y_i h_t(\boldsymbol{x}_i)} \qquad \alpha_t = \frac{1}{2} \ln\left(\frac{1-\epsilon_t}{\epsilon_t}\right)$$

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Friedman, Hastie & Tibshirani [Ann. Stat. 2000] showed that if we consider the **additive model** $H(\mathbf{x}) = \sum_{t=1}^{T} \alpha_t h_t(\mathbf{x}_t)$, take a logistic function and estimate probability via

$$P(f(\boldsymbol{x}) = 1 \mid \boldsymbol{x}) = \frac{e^{H(\boldsymbol{x})}}{e^{H(\boldsymbol{x})} + e^{-H(\boldsymbol{x})}}$$

then AdaBoost algorithm is a Newton-like procedure optimizing the exponential loss function and the log loss function (negative log-likelihood)

$$\ell_{log}(h \mid \mathcal{D}) = \mathbb{E}_{\boldsymbol{x} \sim \mathcal{D}} \left[\ln \left(1 + e^{-2f(\boldsymbol{x})h(\boldsymbol{x})} \right) \right]$$

That is, AdaBoost can be viewed as a stage-wise estimation procedure for fitting an additive logistic regression model



As alternatives, one can fit the additive logistic regression model by optimizing the log loss function via other procedures, leading to many variants

e.g., LogitBoost [Friedman, Hastie & Tibshirani, Ann. Stat. 2000] LPBoost [Demiriz, Bennett & Shawe-Taylor, MLJ 2002] L2Boost [Bühlmann & Yu, JASA 2003] RegBoost [Lugosi & Vayatis, Ann. Stat. 2004], etc.

The statistical view also encouraged the study of some specific statistical properties of AdaBoost

e.g., for **consistency**: Boosting with early stopping is consistent [Zhang & Yu, Ann. Stat. 2004], Exponential and logistic loss is consistent [Zhang, Ann. Stat. 2004, Bartlett, Jordana & McAuliffea, JASA 2006], etc.



However, many aspects of the statistical view have been questioned by empirical results

e.g., in a famous article [Mease & Wyner. Evidence contrary to the statistical view of boosting (with discussions). JMLR, 9:131–201, 2008] it was disclosed that:

Larger-size trees will lead to overfitting because of higherlevel interaction [Friedman, Hastie & Tibshirani, Ann. Stat. 2000]

But in practice ...



Concerns about the statistical view (con't)



LogitBoost is better than AdaBoost for noisy data [Hastie, Tibshirani & Friedman, "The Elements of Statistical Learning", Springer 2001]

But in practice ...

Early stopping can be used to prevent overfitting [Zhang & Yu, Ann. Stat. 2004]

But in practice ...



[Mease & Wyner, JMLR 2008]

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Margin Theory

Started from [Schapire, Freund, Bartlett & Lee, Boosting the margin: A new explanation for the effectiveness of voting methods. Annals of Statistics, 26(5):1651–1686, 1998]

□ Statistical View

Started from [Friedman, Hastie & Tibshirani. Additive logistic regression: A statistical view of boosting (with discussions). Annals of

Stati

The biggest issue: The statistical view did not explain why AdaBoost is resistant to overfitting



Binary classification can be viewed as the task of separating classes in a feature space



The bigger the margin, the higher the predictive confidence

For binary classification, the ground-truth $f(\boldsymbol{x}) \in \{-1, +1\}$

The margin of a single classifier h: $f(\mathbf{x})h(\mathbf{x})$

For
$$H(\boldsymbol{x}) = \sum_{t=1}^{T} \alpha_t h_t(\boldsymbol{x}_t)$$

the margin is
 $f(\boldsymbol{x})H(\boldsymbol{x}) = \sum_{t=1}^{T} \alpha_t f(\boldsymbol{x})h_t(\boldsymbol{x})$

and the normalized margin:

$$\frac{\sum_{t=1}^{T} \alpha_t f(\boldsymbol{x}) h_t(\boldsymbol{x})}{\sum_{t=1}^{T} \alpha_t}$$



Based on the concept of margin, Schapire et al. [1998] proved that, given any threshold $\theta > 0$ of margin over the training data D, with probability at least $1 - \delta$, the generalization error of the ensemble $\epsilon_{\mathcal{D}} = P_{\boldsymbol{x}\sim\mathcal{D}}(f(\boldsymbol{x}) \neq$ $H(\boldsymbol{x}))$ is bounded by

$$\epsilon_{\mathcal{D}} \leq P_{\boldsymbol{x}\sim D}(f(\boldsymbol{x})H(\boldsymbol{x}) \leq \theta) + \tilde{O}\left(\sqrt{\frac{d}{m\theta^2} + \ln\frac{1}{\delta}}\right)$$
$$\leq 2^T \prod_{t=1}^T \sqrt{\epsilon_t^{1-\theta}(1-\epsilon_t)^{1+\theta}} + \tilde{O}\left(\sqrt{\frac{d}{m\theta^2} + \ln\frac{1}{\delta}}\right)$$

This bound implies that, when other variables are fixed, the larger the margin over the training data, the smaller the generalization error



Why AdaBoost tends to be resistant to overfitting?

the margin theory answers: Because it is able to increase the ensemble margin even after the training error reaches zero



This explanation is quite intuitive

It receives good support in empirical study



Schapire et al.'s bound depends heavily on the smallest margin, because $P_{x\sim D}(f(x)H(x) \le \theta)$ will be small if the smallest margin is large

Thus, by considering the minimum margin:

 $\varrho = \min_{\boldsymbol{x} \in D} \ f(\boldsymbol{x}) H(\boldsymbol{x})$

Breiman [Neural Comp. 1999] proved a generalization bound, which is tighter than Schapire et al.'s bound



The two generalization bounds

Theorem 1. (Schapire et al., 1998) For any $\delta > 0$ and $\theta > 0$, with probability at least $1 - \delta$ over the random choice of sample S with size m, every voting classifier $f \in C(\mathcal{H})$ satisfies the following bound:

$$\Pr_{D}[yf(x) < 0] \le \Pr_{S}[yf(x) \le \theta] + O\left(\frac{1}{\sqrt{m}}\left(\frac{\ln m \ln |\mathcal{H}|}{\theta^{2}} + \ln \frac{1}{\delta}\right)^{1/2}\right).$$

Theorem 2. (Breiman, 1999) If

$$\theta = \hat{y}_1 f(\hat{x}_1) > 4\sqrt{\frac{2}{|\mathcal{H}|}} \text{ and } R = \frac{32\ln 2|\mathcal{H}|}{m\theta^2} \le 2m,$$

then, for any $\delta > 0$, with probability at least $1 - \delta$ over the random choice of sample S with size m, every voting classifier $f \in C(\mathcal{H})$ satisfies the following bound:

$$\Pr_{D}[yf(x) < 0] \le \underline{R\left(\ln(2m) + \ln\frac{1}{R} + 1\right) + \frac{1}{m}\ln\frac{|\mathcal{H}|}{\delta}}{O(\log m/m)}$$

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 $O(\sqrt{\log m}/m)$



Breiman [Neural Comp. 1999] designed a variant of AdaBoost, the arc-gv algorithm, which directly maximizes the minimum margin

the margin theory would appear to predict that arc-gv should perform better than AdaBoost

However, experiments show that, comparing with AdaBoost:

- arc-gv does produce uniformly larger minimum margin
- the test error increases drastically in almost every case

Thus, Breiman convincingly concluded that **the margin theory was in serious doubt**. This almost sentenced the margin theory to death



Reyzin & Schapire [ICML'06 best paper] found that, amazingly, Breiman had not controlled model complexity well in exps

Breiman controlled the model complexity by using decision trees with a fixed number of leaves

Reyzin & Schapire found that, the trees of arc-gv are generally "deeper" than the trees of AdaBoost

Reyzin & Schapire repeated Brieman's exps using decision stumps with two leaves: arc-gv is with larger minimum margin, but worse margin distribution

R&S claimed that the minimum margin is not crucial, and the *average* or *median margin* is crucial

Experimental results



Tree depth using fixed number of leaves

Margin distribution using decision stumps



FIGURE 2.8: (a) Tree depth and (b) margin distribution of AdaBoost against arc-gv on the UCI *clean1* data set.



Not necessarily ... Breiman's minimum margin bound is tighter

To claim margin distribution is more crucial, we need a margin distribution bound which is even tighter



Equilibrium margin (Emargin) bound

Theorem 3. (Wang et al., 2011) If $8 < |\mathcal{H}| < \infty$, then for any $\delta > 0$, with probability at least $1 - \delta$ over the random choice of the training set S of size m > 1, every voting classifier $f \in C(\mathcal{H})$ such that

$$q_0 = \Pr_S \left[yf(x) \le \sqrt{8/|\mathcal{H}|} \right] < 1 \tag{3}$$

satisfies the following bound:

$$\begin{split} & \Pr_{D}[yf(x) < 0] \leq \frac{\ln |\mathcal{H}|}{m} + \inf_{\substack{q \in \{q_0, q_0 + \frac{1}{m}, \cdots, 1\}}} KL^{-1}(q; u[\hat{\theta}(q)]), \\ & \text{Proved to be tighter} \\ & \text{where} \\ & u[\hat{\theta}(q)] = \frac{1}{m} \Big(\frac{8 \ln |\mathcal{H}|}{\hat{\theta}^2(q)} \ln \frac{2m^2}{\ln |\mathcal{H}|} + \ln |\mathcal{H}| + \ln \frac{m}{\delta} \Big) \\ & \text{and } \hat{\theta}(q) = \sup \left\{ \theta \in (\sqrt{8/|\mathcal{H}|}, 1] : \Pr_S[yf(x) \leq \theta] \leq q \right\}. \text{ Also, the Emargin} \\ & \text{is given by } \theta^* \in \arg \inf_{q \in \{q_0, q_0 + \frac{1}{m}, \cdots, 1\}} KL^{-1}(q; u[\hat{\theta}(q)]). \end{split}$$

- Considered factors different from Schapire et al. and Breiman's bounds
- No intuition to optimize

First presented in [Wang, Sugiyama, Yang, Zhou, Feng, COLT'08] http://cs.nju.edu.cn/zhouzh/



Given a sample S of size m, we define the kth margin as the kth smallest margin over sample S, i.e., the kth smallest value in $\{y_i f(x_i), i \in [m]\}$

Theorem 4. For any $\delta > 0$ and $k \in [m]$, if $\theta = \hat{y}_k f(\hat{x}_k) > \sqrt{8/|\mathcal{H}|}$, then with probability at least $1 - \delta$ over the random choice of sample with size m, every voting classifier $f \in C(\mathcal{H})$ satisfies the following bound:

$$\Pr_{D}[yf(x) < 0] \le \frac{\ln |\mathcal{H}|}{m} + KL^{-1}\left(\frac{k-1}{m}; \frac{q}{m}\right),\tag{4}$$

where

$$q = \frac{8\ln(2|\mathcal{H}|)}{\theta^2}\ln\frac{2m^2}{\ln|\mathcal{H}|} + \ln|\mathcal{H}| + \ln\frac{m}{\delta}.$$

The minimum margin bound and Emargin bound are special cases of the kth margin bound, both are single-margin bound (not margin distribution bound)

[Gao & Zhou, AIJ 2013]

Theorem 8. For any $\delta > 0$, with probability at least $1 - \delta$ over the random choice of sample S with size $m \ge 5$, every voting classifier $f \in C(\mathcal{H})$ satisfies the following bound:

$$\begin{split} \Pr_{D}[yf(x) < 0] &\leq \frac{2}{m} + \inf_{\theta \in (0,1]} \left[\Pr_{S}[yf(x) < \theta] + \frac{7\mu + 3\sqrt{3\mu}}{3m} + \sqrt{\frac{3\mu}{m}} \Pr_{S}[yf(x) < \theta] \right] \\ where \\ \mu &= \frac{8}{\theta^{2}} \ln m \ln(2|\mathcal{H}|) + \ln \frac{2|\mathcal{H}|}{\delta}. \end{split}$$

- ✓ Uniformly tighter than Breiman's as well as Schapire et al.' bounds
- ✓ Considers the same factors as Schapire et al. and Breiman

thus, defends the margin theory against Breiman's doubt

[Gao & Zhou, AIJ 2013]



Theorem 9. For any $\delta > 0$, with probability at least $1 - \delta$ over the random choice of sample S with size $m \ge 5$, every voting classifier $f \in C(\mathcal{H})$ satisfies the following bound: $\Pr_{D}[yf(x) < 0] \le \frac{1}{m^{50}} + \inf_{\theta \in (0,1]} \left[\Pr_{S}[yf(x) < \theta] + m^{-2/(1 - E_{S}^{2}[yf(x)] + \theta/9)} + \frac{3\sqrt{\mu}}{m^{3/2}} + \frac{7\mu}{3m} + \sqrt{\frac{3\mu}{m}} \hat{\mathcal{I}}(\theta)\right]$

where

 $\mu = 144 \ln m \ln(2|\mathcal{H}|)/\theta^2 + \ln(2|\mathcal{H}|/\delta), \quad \text{related to} \\ \hat{\mathcal{I}}(\theta) = \Pr_S[yf(x) < \theta] \Pr_S[yf(x) \ge 2\theta/3]. \quad \text{margin variance}$

 $O(\log m / m)$

We should pay attention to not only the average margin, but also the margin variance !

[Gao & Zhou, AIJ 2013]

In practice





Margin variance really important

Figure from [Gao & Zhou, AIJ 2013]

Figure 1: Each curve represents a voting classifier. The X-axis and Y-axis denote example and margin, respectively, and uniform distribution is assumed on the example space. The voting classifiers h_1 , h_2 and h_3 have the same average margin but with different generalization error rates: 1/2, 1/3 and 0.

[Shivaswamy & Jebara, NIPS 2011] tried to design new boosting algorithms by maximizing average margin and minimizing margin variance simultaneously, and the results are encouraging



- 1989, [Kearns & Valiant], open problem
- 1990, [Schapire], proof by construction, the first Boosting algorithm
- 1993, [Freund], another impractical boosting algorithm by voting
- 1995/97, [Freund & Schapire], AdaBoost
- 1998, [Schapire, Freund, Bartlett & Lee], Margin theory
- 1999, [Breiman], serious doubt by minimum margin bound
- 2006, [Reyzin & Schapire], finding the model complexity issue in exps, emphasizing the importance of margin distribution
- 2008, [Wang, Sugiyama, Yang, Zhou & Feng], Emargin bound, believed to be a margin distribution bound
- 2013, [Gao & Zhou], a real margin distribution bound, sheding new insight ; margin theory defensed

Joint work with my student



W. Gao and Z.-H. Zhou. On the doubt about margin explanation of boosting. <u>Artificial Intelligence</u>, 2013, 203: 1-18. (arXiv:1009.3613, Sept.2010)



An easy-to-read article:

Z.-H. Zhou. Large margin distribution learning. <u>ANNPR 2014</u>, Montreal, Canada, LNAI 8774, pp.1-11 (keynote article)



