Infinite Ensemble Learning with Support Vector Machinery

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ECML/PKDD, October 4, 2005

Outline

Learning Problem

- notation: example $x \in \mathcal{X} \subseteq \mathbb{R}^D$ and label $y \in \{+1, -1\}$
- hypotheses (classifiers): functions from $\mathcal{X} \to \{+1, -1\}$
- binary classification problem: given training examples and labels $\{(x_i, y_i)\}_{i=1}^N$, find a classifier $g(x) : \mathcal{X} \to \{+1, -1\}$ that predicts the label of unseen x well

Ensemble Learning

$$g(x) : \mathcal{X} \to \{+1, -1\}$$

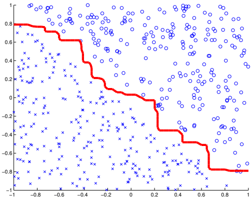
- ensemble learning: popular paradigm (bagging, boosting, etc.)
- ensemble: weighted vote of a committee of hypotheses
  $g(x) = \text{sign}(\sum w_t h_t(x))$
- h_t: base hypotheses, usually chosen from a set $\mathcal{H}$
- w_t: nonnegative weight for h_t
- ensemble usually better than individual $h_t(x)$ in stability/performance

Infinite Ensemble Learning

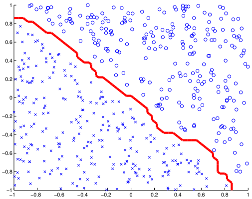
$$g(x) = \text{sign}\left(\sum w_t h_t(x)\right), h_t \in \mathcal{H}, w_t \geq 0$$

- set $\mathcal{H}$ can be of infinite size
- traditional algorithms: assign **finite** number of nonzero w_t

1. is finiteness **regularization** and/or **restriction**?
2. how to handle **infinite** number of nonzero weights?



finite ensemble



infinite ensemble

SVM for Infinite Ensemble Learning

- Support Vector Machine (SVM): large-margin hyperplane in some feature space
- SVM: possibly **infinite** dimensional hyperplane $g(x) = \text{sign}(\sum w_d \phi_d(x) + b)$
- an important machinery to conquer infinity: kernel trick.

> how can we use Support Vector Machinery for **infinite ensemble learning**?

Properties of SVM

$$g(x) = \text{sign}(\sum_{d=1}^{\infty} w_d \phi_d(x) + b) = \text{sign}\left(\sum_{i=1}^{N} \lambda_i y_i \mathcal{K}(x_i, x) + b\right)$$

- a successful large-margin learning algorithm.
- goal: (infinite dimensional) large-margin hyperplane

$$\min_{w,b} \frac{1}{2}\|w\|_2^2 + C\sum_{i=1}^{N} \xi_i, \text{ s.t. } y_i \left(\sum_{d=1}^{\infty} w_d \phi_d(x_i) + b\right) \geq 1 - \xi_i, \xi_i \geq 0$$

- optimal hyperplane: represented through duality
- key for handling infinity: computation with kernel tricks $\mathcal{K}(x, x') = \sum_{d=1}^{\infty} \phi_d(x)\phi_d(x')$
- regularization: controlled with the trade-off parameter C

Properties of AdaBoost

$$g(x) = \text{sign}\left(\sum_{t=1}^{T} w_t h_t(x)\right)$$

- a successful ensemble learning algorithm
- goal: asymptotically, large-margin ensemble

$$\min_{w,h} \|w\|_1, \text{ s.t. } y_i \left(\sum_{t=1}^{\infty} w_t h_t(x_i)\right) \geq 1, w_t \geq 0$$

- optimal ensemble: approximated by finite one
- key for good approximation:
  - finiteness: some $h_{t_1}(x_i) = h_{t_2}(x_i)$ for all i
  - sparsity: optimal ensemble usually has many zero weights
- regularization: finite approximation

Connection between SVM and AdaBoost

$$\phi_d(x) \Leftrightarrow h_t(x)$$

SVM	AdaBoost
$G(x) = \sum_k w_k \phi_k(x) + b$	$G(x) = \sum_k w_k h_k(x)$
	$w_k \geq 0$

hard-goal

$$\min \|w\|_p, \text{ s.t. } y_i G(x_i) \geq 1$$

$p = 2$	$p = 1$

key for infinity

kernel trick	finiteness and sparsity

regularization

soft-margin trade-off	finite approximation

Challenge

- challenge: how to design a good infinite ensemble learning algorithm?
- traditional ensemble learning: iterative and cannot be directly generalized
- our main contribution: **novel and powerful infinite ensemble learning algorithm with Support Vector Machinery**
- our approach: embedding infinite number of hypotheses in SVM kernel, i.e., $\mathcal{K}(x, x') = \sum_{t=1}^{\infty} h_t(x) h_t(x')$
  – then, SVM classifier: $g(x) = \text{sign}(\sum_{t=1}^{\infty} w_t h_t(x) + b)$

1. **does the kernel exist?**
2. **how to ensure $w_t \geq 0$?**

Embedding Hypotheses into the Kernel

Definition

The kernel that embodies $\mathcal{H} = \{h_\alpha \colon \alpha \in \mathcal{C}\}$ is defined as

$$\mathcal{K}_{\mathcal{H},r}(x, x') = \int_{\mathcal{C}} \phi_x(\alpha)\phi_{x'}(\alpha)\, d\alpha,$$

where $\mathcal{C}$ is a measure space, $\phi_x(\alpha) = r(\alpha)h_\alpha(x)$, and $r \colon \mathcal{C} \to \mathbb{R}^+$ is chosen such that the integral always exists

- integral instead of sum: works even for uncountable $\mathcal{H}$
- existence problem handled with a suitable $r(\cdot)$
- $\mathcal{K}_{\mathcal{H},r}(x, x')$: an inner product for ϕ_x and $\phi_{x'}$ in $\mathcal{F} = \mathcal{L}_2(\mathcal{C})$
- the classifier: $g(x) = \text{sign}\left(\int_{\mathcal{C}} w(\alpha)r(\alpha)h_\alpha(x)\, d\alpha + b\right)$

Negation Completeness and Constant Hypotheses

$$g(x) = \text{sign}\left(\int_{\mathcal{C}} w(\alpha) r(\alpha) h_\alpha(x)\, d\alpha + b \right)$$

- not an ensemble classifier yet
- $w(\alpha) \geq 0$?
  - hard to handle: possibly uncountable constraints
  - simple with negation completeness assumption on $\mathcal{H}$ ($h \in \mathcal{H}$ if and only if $(-h) \in \mathcal{H}$)
  - e.g. neural networks, perceptrons, decision trees, etc.
  - for any w, exists nonnegative $\tilde{w}$ that produces same g
- What is b?
  - equivalently, the weight on a constant hypothesis
  - another assumption: $\mathcal{H}$ contains a constant hypothesis
- with mild assumptions, $g(x)$ is equivalent to an ensemble classifier

Framework of Infinite Ensemble Learning

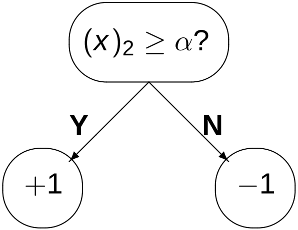
Algorithm

1. Consider a hypothesis set $\mathcal{H}$ (negation complete and contains a constant hypothesis)
2. Construct a kernel $\mathcal{K}_{\mathcal{H},r}$ with proper $r(\cdot)$
3. Properly choose other SVM parameters
4. Train SVM with $\mathcal{K}_{\mathcal{H},r}$ and $\{(x_i, y_i)\}_{i=1}^N$ to obtain λ_i and b
5. Output $g(x) = \text{sign}\left(\sum_{i=1}^N y_i \lambda_i \mathcal{K}_{\mathcal{H}}(x_i, x) + b\right)$

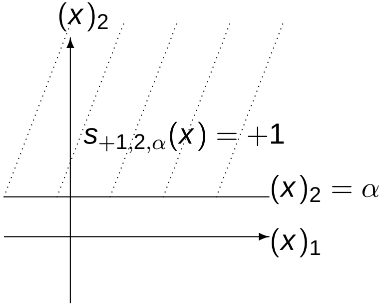
- hard: kernel construction
- SVM as an optimization machinery: training routines are widely available
- SVM as a well-studied learning model: inherit the profound regularization properties

Decision Stump

- decision stump: $s_{q,d,\alpha}(x) = q \cdot \text{sign}((x)_d - \alpha)$
- simplicity: popular for ensemble learning



(a) Decision Process



(b) Decision Boundary

Figure: Illustration of the decision stump $s_{+1,2,\alpha}(x)$

Stump Kernel

- consider the set of decision stumps
  $\mathcal{S} = \left\{ s_{q,d,\alpha_d} \colon q \in \{+1,-1\}, d \in \{1,\ldots,D\}, \alpha_d \in [L_d, R_d] \right\}$
- when $\mathcal{X} \subseteq [L_1, R_1] \times [L_2, R_2] \times \cdots \times [L_D, R_D]$, $\mathcal{S}$ is negation complete, and contains a constant hypothesis

Definition

The stump kernel $\mathcal{K}_\mathcal{S}$ is defined for $\mathcal{S}$ with $r(q, d, \alpha_d) = \frac{1}{2}$

$$\mathcal{K}_\mathcal{S}(x, x') = \Delta_\mathcal{S} - \sum_{d=1}^{D} \left| (x)_d - (x')_d \right| = \Delta_\mathcal{S} - \|x - x'\|_1,$$

where $\Delta_\mathcal{S} = \frac{1}{2} \sum_{d=1}^{D} (R_d - L_d)$ is a constant

Properties of Stump Kernel

- simple to compute: can even use a simpler one $\tilde{\mathcal{K}}_{\mathcal{S}}(x, x') = -\|x - x'\|_1$ while getting the same solution
  - under the dual constraint $\sum_i y_i \lambda_i = 0$, using $\mathcal{K}_{\mathcal{S}}$ or $\tilde{\mathcal{K}}_{\mathcal{S}}$ is the same
  - feature space explanation for ℓ_1-norm distance
- infinite power: under mild assumptions, SVM-Stump with $C = \infty$ can perfectly classify all training examples
  - if there is a dimension for which all feature values are different, the kernel matrix K with $K_{ij} = \mathcal{K}(x_i, x_j)$ is strictly positive definite
  - similar power to the popular Gaussian kernel $\exp(-\gamma \|x - x'\|_2^2)$
    – suitable control on the power leads to good performance

Properties of Stump Kernel (Cont'd)

- fast automatic parameter selection: only needs to search for a good soft-margin parameter C
  - scaling the stump kernel is equivalent to scaling soft-margin parameter C
  - Gaussian kernel depends on a good (γ, C) pair (10 times slower)
- well suited in some specific applications:
  cancer prediction with gene expressions
  (Lin and Li, ECML/PKDD Discovery Challenge, 2005)

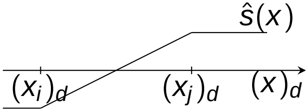
Infinite Decision Stump Ensemble

$$g(x) = \operatorname{sign}\left(\sum_{q \in \{+1,-1\}} \sum_{d=1}^{D} \int_{L_d}^{R_d} w_{q,d}(\alpha) s_{q,d,\alpha}(x)\, d\alpha + b \right)$$

- each $s_{q,d,\alpha}$: infinitesimal influence $w_{q,d}(\alpha)\, d\alpha$
- equivalently,

$$g(x) = \operatorname{sign}\left(\sum_{q \in \{+1,-1\}} \sum_{d=1}^{D} \sum_{a=0}^{A_d} \hat{w}_{q,d,a} \hat{s}_{q,d,a}(x) + b \right)$$

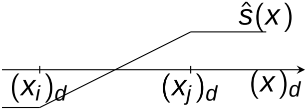
- $\hat{s}$: a smoother variant of decision stump



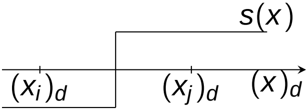
Infinitesimal Influence

$$g(x) = \operatorname{sign}\left(\sum_{q \in \{+1,-1\}} \sum_{d=1}^{D} \sum_{a=0}^{A_d} \hat{w}_{q,d,a} \hat{s}_{q,d,a}(x) + b \right)$$

- infinity $\rightarrow$ dense combination of finite number of smooth stumps
- infinitesimal influence $\rightarrow$ concrete weight of the smooth stumps



SVM: dense combination of smoothed stumps

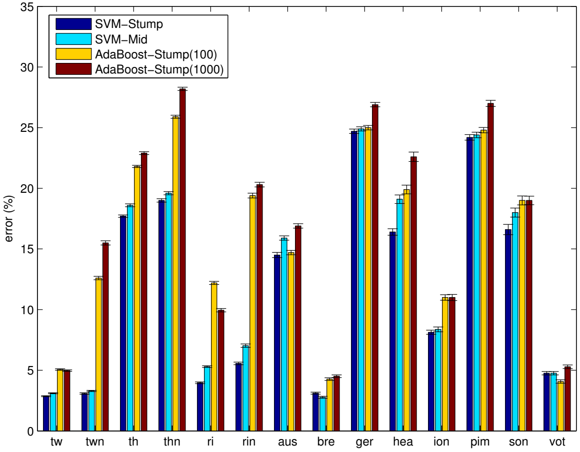


AdaBoost: sparse combination of middle stumps

Experiment Setting

- ensemble learning algorithms:
  - SVM-Stump: infinite ensemble of decision stumps (dense ensemble of smooth stumps)
  - SVM-Mid: dense ensemble of middle stumps
  - AdaBoost-Stump: sparse ensemble of middle stumps
- SVM algorithms: SVM-Stump versus SVM-Gauss
- artificial, noisy, and realworld datasets
- cross-validation for automatic parameter selection of SVM
- evaluate on hold-out test set and averaged over 100 different splits

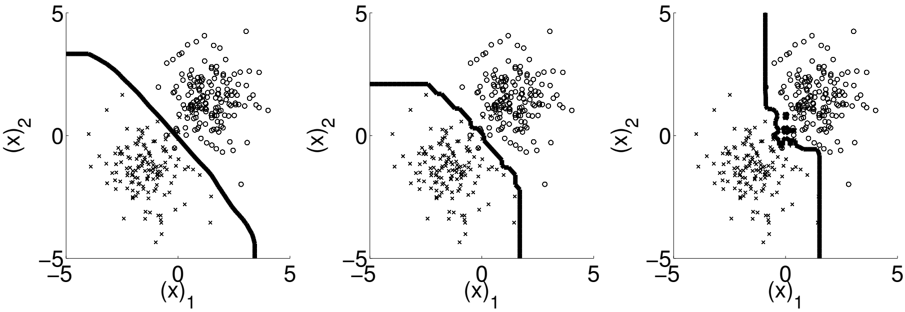
Comparison between SVM and AdaBoost



Results

- fair comparison between AdaBoost and SVM
- SVM-Stump is usually best – benefits to go to infinity
- SVM-Mid is also good – benefits to have dense ensemble
- sparsity and finiteness are **restrictions**

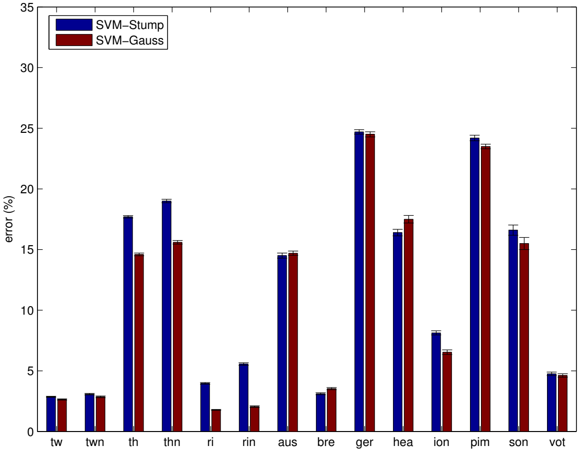
Comparison between SVM and AdaBoost (Cont'd)



left to right: SVM-Stump, SVM-Mid, AdaBoost-Stump

- smoother boundary with infinite ensemble (SVM-Stump)
- still fits well with dense ensemble (SVM-Mid)
- cannot fit well when sparse and finite (AdaBoost-Stump)

Comparison of SVM Kernels



Results

- SVM-Stump is only a bit worse than SVM-Gauss
- still benefit with faster parameter selection in some applications

Conclusion

- novel and powerful framework for infinite ensemble learning
- derived a new and meaningful kernel
  – stump kernel: succeeded in specific applications
- infinite ensemble learning could be better – existing AdaBoost-Stump applications may switch
- not the only kernel:
  - perceptron kernel $\longrightarrow$ infinite ensemble of perceptrons
  - Laplacian kernel $\longrightarrow$ infinite ensemble of decision trees
- SVM: our machinery for conquering infinity
  – possible to apply similar machinery to areas that need infinite or lots of aggregation