Boosting and Ensemble Learning

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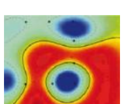


Recap: Statistical Learning setup

Three scenarios: regression, classification & density estimation.
Learn f from examples

$$(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N) \in \mathbf{R}^N \times \mathbf{R}^M \text{ or } \{\pm 1\}, \quad \text{generated from } P(\mathbf{x}, y),$$

such that expected number of errors on test set (drawn from $P(\mathbf{x}, y)$),

$$R[f] = \int \frac{1}{2} |f(\mathbf{x}) - y)|^2 \, dP(\mathbf{x}, y),$$

is minimal *(Risk Minimization (RM))*.

Problem: P is unknown. $\longrightarrow$ need an *induction principle*.

Empirical risk minimization (ERM): replace the average over $P(\mathbf{x}, y)$ by an average over the training sample, i.e. minimize the training error

$$R_{emp}[f] = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{2} |f(\mathbf{x}_i) - y_i|^2$$

Recap: Statistical Learning setup II

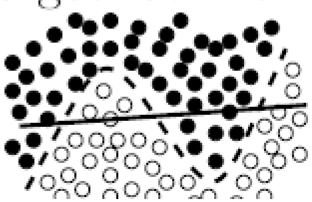
- Law of large numbers: $R_{emp}[f] \to R[f]$ as $N \to \infty$.
  "*consistency*" of ERM: for $N \to \infty$, ERM should lead to the same result as RM?

- No: *uniform* convergence needed (Vapnik) $\to$ VC theory.
  Thm. [classification] (Vapnik 95): with a probability of at least $1 - \eta$,

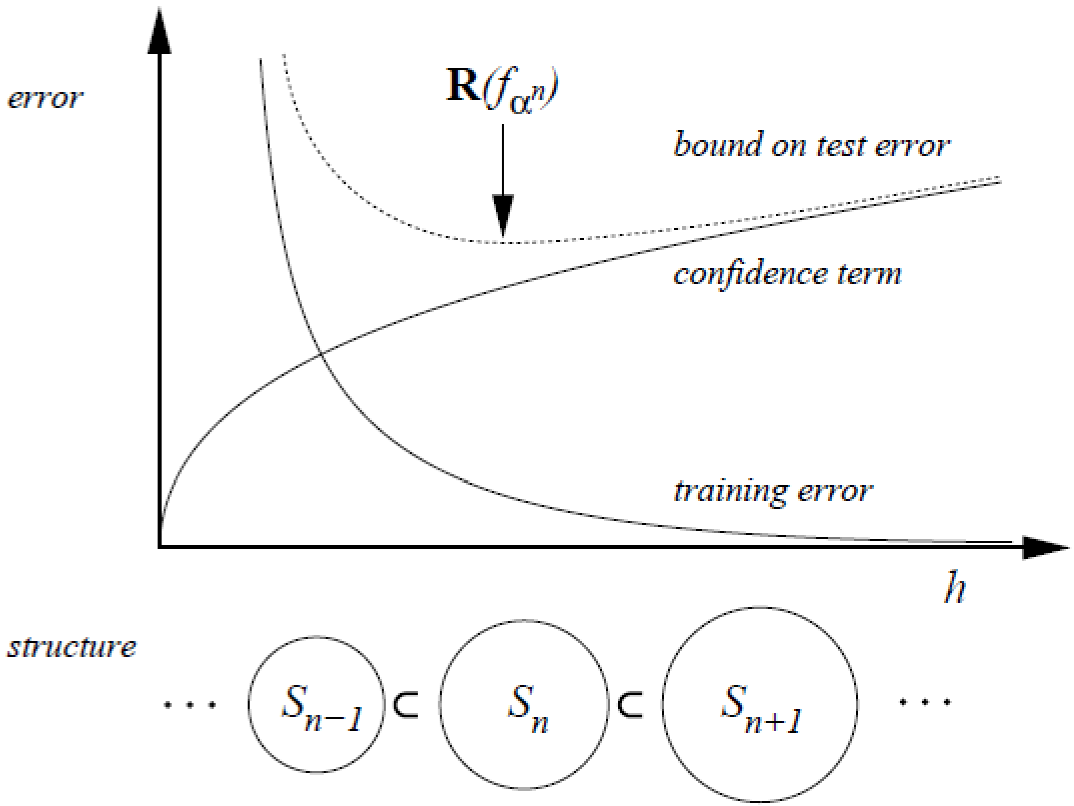
$$R[f] \leq R_{emp}[f] + \sqrt{\frac{d\left(\log\frac{2N}{d} + 1\right) - \log(\eta/4)}{N}}.$$

- Structural risk minimization (SRM): introduce structure on set of functions $\{f_\alpha\}$ & minimize RHS to get low risk! (Vapnik 95)

- d is VC dimension, measuring complexity of function class



SRM- the picture



Learning f requires small training error *and* small complexity of the set $\{f_\alpha\}$.

SVM vs. Boosting

- SVMs

$$R[f] \leq R_{emp}[f] + \mathcal{O}\left(\sqrt{\frac{\log\left(N\theta^2\right)}{\theta^2 N} + \frac{\log(1/\eta)}{N}}\right).$$

- Boosting

$$R[f] \leq R^{\theta}_{emp}[f] + \mathcal{O}\left(\sqrt{\frac{d\log^2\left(\frac{N}{d}\right)}{\theta^2 N} + \frac{\log(1/\delta)}{N}}\right)$$

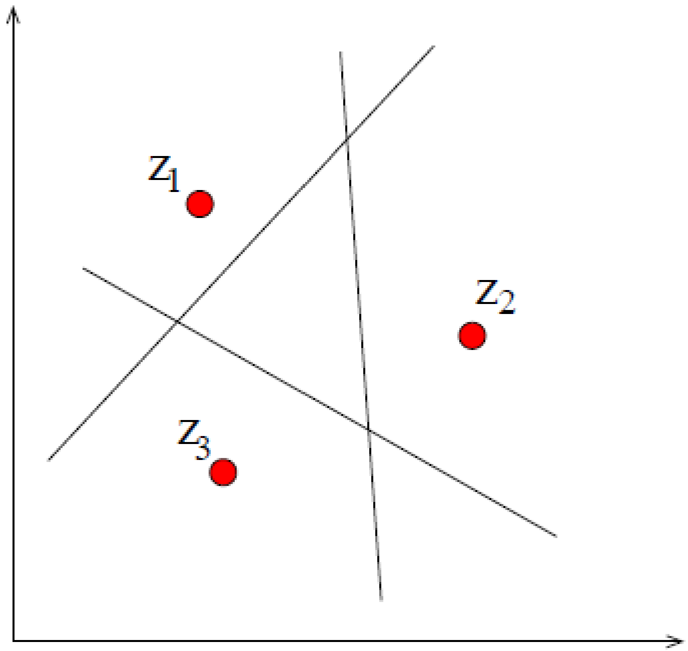
- **independent of the dimensionality of the space!**

VC dimension: example

Half-spaces in $\mathbf{R}^2$:

$$f(x, y) = \operatorname{sgn}(a + bx + cy), \quad \text{with parameters } a, b, c \in \mathbf{R}$$

- Clearly, we can shatter three non-collinear points.
- But we can never shatter four points.
- Hence the VC dimension is $d = 3$
- in n dimensions: VC dimension is $d = n + 1$



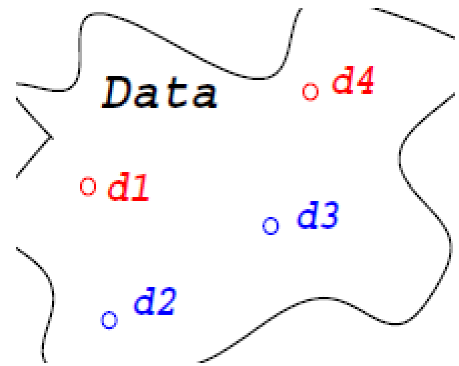
The Basic idea behind boosting

Ensemble Learning and Classification

- Ensemble for binary classification consists of
  - Hypotheses (basis functions) $\{h_t(\mathbf{x}) : t = 1, \ldots, T\}$
    - of some hypothesis ("concept") set
      $\mathcal{H} = \{h \mid h(\mathbf{x}) \mapsto \{\pm 1\}\}$
  - Weights $\boldsymbol{\alpha} = [\alpha_1, \ldots, \alpha_T]$
    - satisfying $\alpha_t \geq 0$
- Classification Output: weighted majority of the votes
  - $f_{\mathrm{Ens}}(\mathbf{x}) = \sum_{t=1}^{T} \alpha_t h_t(\mathbf{x})$
- How to find the hypotheses and their weights?
  - Bagging (Breiman, 1996): $\alpha_t = 1/T$
  - AdaBoost (Freund & Schapire, 1994)

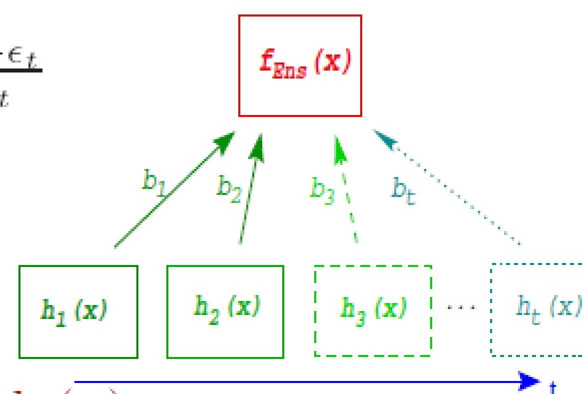
The Adaboost Algorithm

Input: N examples $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$
Initialize: $d_i^{(1)} = 1/N$ for all $i = 1 \ldots N$
Do for $t = 1, \ldots, T$,



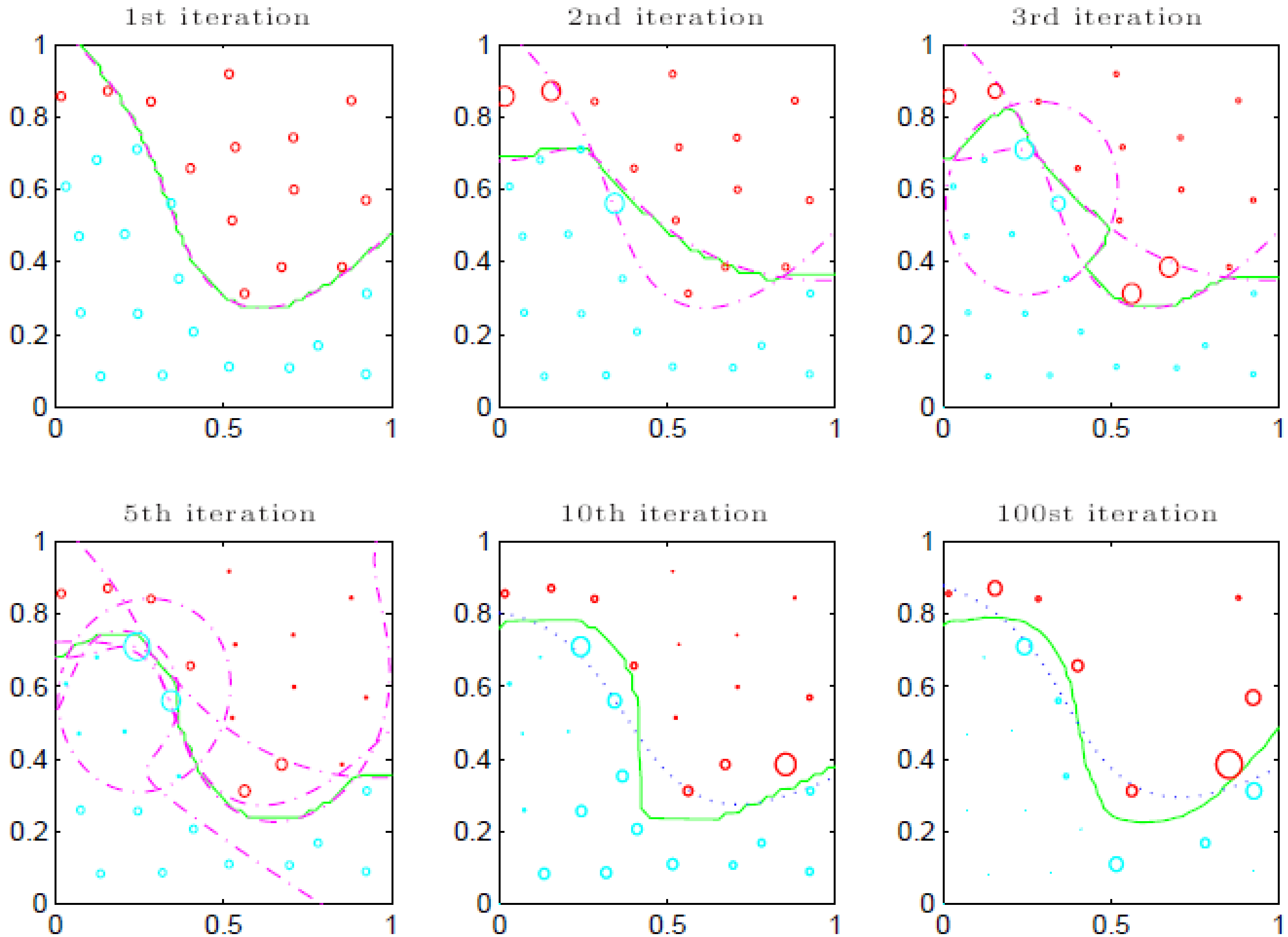
1. Train base learner according to example distribution $\mathbf{d}^{(t)}$ and obtain hypothesis $h_t : \mathbf{x} \mapsto \{\pm 1\}$.
2. compute weighted error $\epsilon_t = \sum_{i=1}^{N} d_i^{(t)} \mathrm{I}(y_i \neq h_t(\mathbf{x}_i))$
3. compute hypothesis weight $\alpha_t = \frac{1}{2} \log \frac{1-\epsilon_t}{\epsilon_t}$
4. update example distribution

$$d_i^{(t+1)} = d_i^{(t)} \exp\left(-\alpha_t y_i h_t(\mathbf{x}_i)\right) / Z_t$$



Output: final hypothesis $f_{\text{Ens}}(\mathbf{x}) = \sum_{t=1}^{T} \alpha_t h_t(\mathbf{x})$

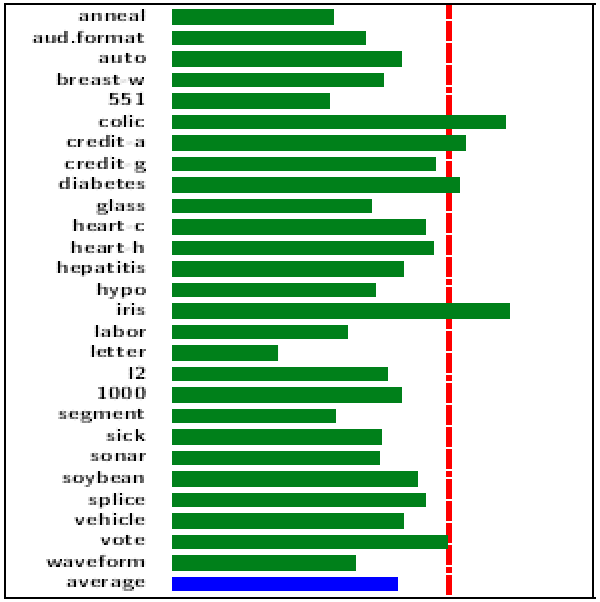
Adaboost Algorithm: illustration



Experimental Motivation

Architecture	Test Error
LeNet 1	1.7%
LeNet 4	1.1%
LeNet 5	0.9%
SVM polynom.	1.4%
SVM virt. SV	0.8%
boosted LeNet 4	**0.7%**

Comparison on NIST handwritten character recognition data set (LeCun et al. (1995))



Comparison on UCI repository data (Quinlan (1998))

Error Function of Adaboost

- AdaBoost stepwise minimizes a function of $y_i f_{\boldsymbol{\alpha}}(x_i) = y_i \sum_t \alpha_t h_t(\mathbf{x}_i)$

$$\mathcal{G}(\boldsymbol{\alpha}) = \sum_{i=1}^{N} \exp\{-y_i f_{\boldsymbol{\alpha}}(\mathbf{x}_i)\}$$

- The gradient of $\mathcal{G}(\boldsymbol{\alpha}^{(t)})$ gives exactly the example weights used for AdaBoost:

$$\frac{\partial \mathcal{G}(\boldsymbol{\alpha}^{(t)})}{\partial f(\mathbf{x}_i)} \sim \exp\{-y_i f_{\boldsymbol{\alpha}}(\mathbf{x}_i)\} \sim d_i^{(t+1)}$$

- The hypothesis coefficient α_t is chosen, such that $\mathcal{G}(\boldsymbol{\alpha}^{(t)})$ is minimized:

$$\alpha_t = \operatorname*{argmin}_{\alpha_t \geq 0} \mathcal{G}(\boldsymbol{\alpha}^{(t)}) = \frac{1}{2} \log \frac{1-\epsilon_t}{\epsilon_t}$$

- **AdaBoost is a gradient descent method to minimizes $\mathcal{G}(\boldsymbol{\alpha})$.**
  $\Longrightarrow$ Bregman Divergences (Entropy Projections, ...)
  $\Longrightarrow$ Coordinate Descent Methods & Column Generation

Theoretical Motivation PAC boosting

PAC Boosting – exponential convergence

Theorem 1 (Schapire et al. 1997) *Suppose AdaBoost generates hypotheses with weighted training errors* $\epsilon_1, \ldots, \epsilon_T$*. Then we have*

$$\sum_{i=1}^{N} \mathrm{I}(y_i \neq \mathrm{sign}(f_{Ens}(\mathbf{x}_i))) \leq 2^T \prod_{t=1}^{T} \sqrt{\epsilon_t(1-\epsilon_t)}$$

If $\epsilon_t < \frac{1}{2} - \frac{1}{2}\gamma$ (for all $t = 1, \ldots, T$), then the training error will decrease exponentially fast, i.e. will be **zero** after only

$$\frac{2\log(N)}{\gamma^2} = \mathcal{O}(\log(N))$$

iterations.

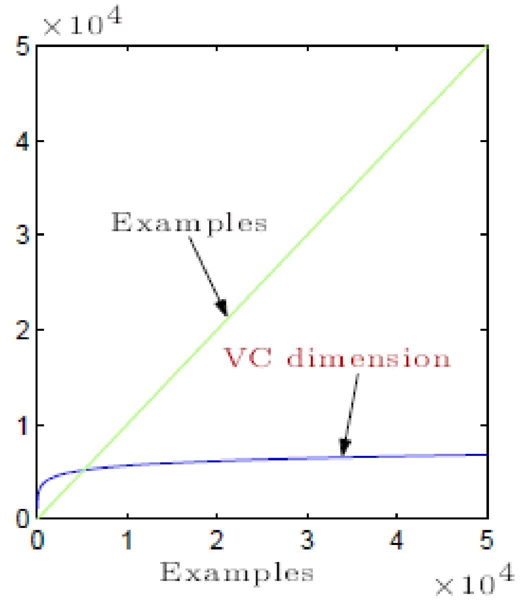
PAC Boosting – VC dimension of combined Hypothesis

Let d be the VC dimension of the base hypothesis class $\mathcal{H}$.
Then the VC dimension of the class of combined functions is

$$d_{Ens}(N,\gamma) = \mathcal{O}\left(\underbrace{d\,\frac{\log(N)}{\gamma^2}}_{\sim T} \log\left(\frac{\log(N)}{\gamma^2}\right)\right) = \mathcal{O}\left(d \log(N) \log^2(N)\right).$$

An Example

- VC dimension $d = 2$
  (e.g. decision stumps)
- $\epsilon_t \leq 0.4 = \frac{1}{2} - \frac{1}{2}\gamma$
  $\Rightarrow \gamma \geq 0.2$

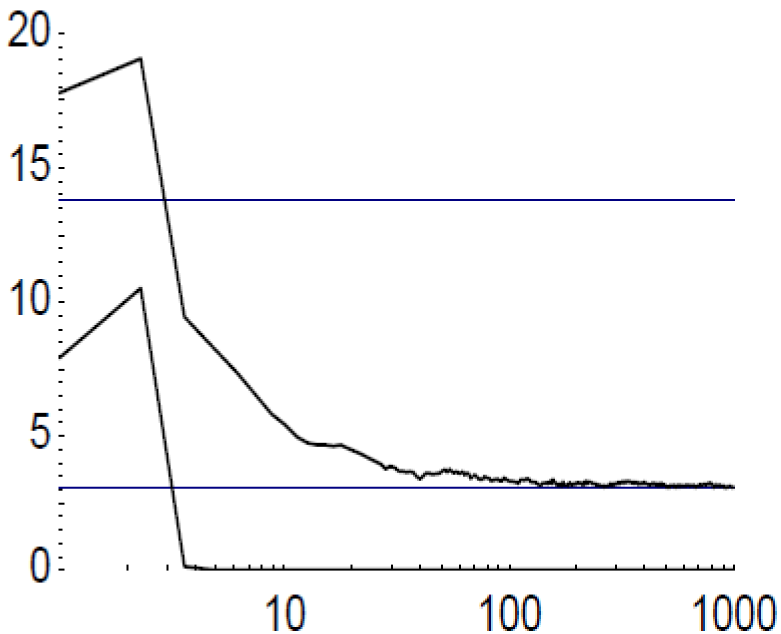


PAC Boosting – Digestion

- properties of weak learner imply exponential convergence to a consistent hypothesis
- Fast convergence ensures small VC dimension of the combined hypothesis
- small VC implies small deviation from the empirical risk
- for any $\varepsilon > 0$ and $\delta > 0$ exists a sample size N, such that with probability $1 - \delta$ the expected risk is smaller than ε
- Any weak learner can be boosted to achieve an arbitrary high accuracy! ($\rightsquigarrow$ strong learner)

A strange Phenomenon

boosting C4.5 on "letter" data



- test error does not increase
  $\rightsquigarrow$ even after 1000 iterations!
- it continues to drop
  $\rightsquigarrow$ even after training error is 0!
- Occam's razor predicts simpler rule is better
  $\rightsquigarrow$ wrong in this case!?

Needs a better explanation!

Theoretical Motivation margin distributions

Margin Distributions - definitions

- Function set used in boosting: Convex Hull of $\mathcal{H}$

$$S := \left\{ f : \mathbf{x} \mapsto \sum_{h \in \mathcal{H}} \alpha_h h(\mathbf{x}) \;\middle|\; \alpha_h \geq 0, \sum_{h \in \mathcal{H}} \alpha_h = 1 \right\}$$

- the α's are the parameters

- Find a hyperplane in the Feature Space spanned by the hypotheses set $\mathcal{H} = \{h_1, h_2, \dots\}$

- Margin ρ for an example $(\mathbf{x}_i, y_i)$ by

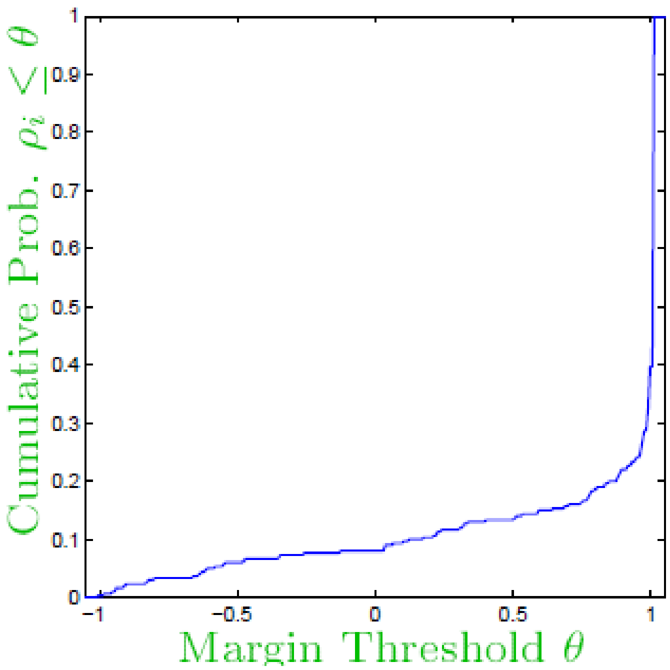
$$\rho_i(\boldsymbol{\alpha}) := y_i f_{\mathrm{Ens}}(\mathbf{x}_i) = y_i \sum_{t=1}^{T} \frac{\alpha_t}{\sum_t \alpha_t} h_t(\mathbf{x}_i)$$

- Margin ϱ for a function f_{Ens} by $\varrho(\boldsymbol{\alpha}) := \min_{i=1,\dots,N} \rho_i(\boldsymbol{\alpha})$

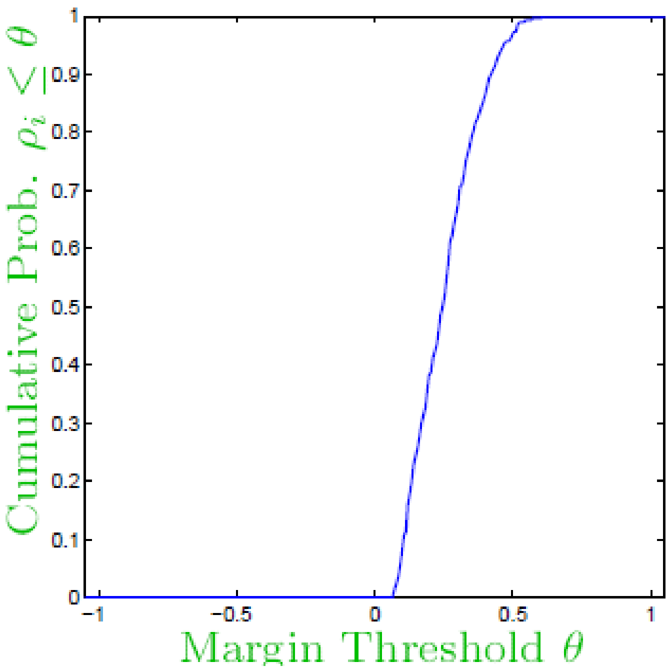
Margin Distributions - illustration

AdaBoost tends to increase small margins, while decreasing large margins

Bagging



AdaBoost



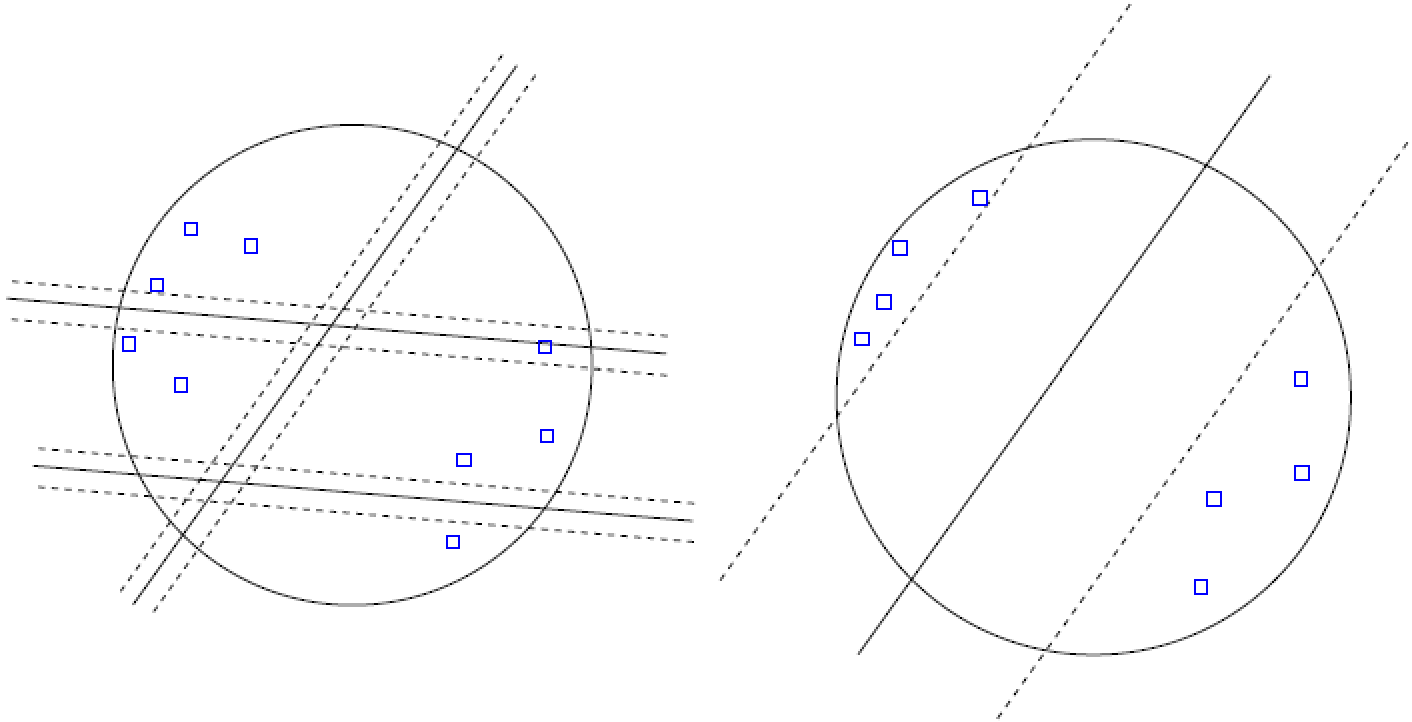
Margin Distributions – lower bounding the margin

Theorem 2 *Suppose the base learning algorithm generates hypothesis with weighted training errors* $\epsilon_1, \ldots, \epsilon_T$. *Then we have for any* θ

$$P_{\mathbf{Z}}(y f_{Ens}(\mathbf{x}) \leq \theta) \leq 2^T \prod_{t=1}^{T} \sqrt{\epsilon_t^{1-\theta}(1-\epsilon_t)^{1+\theta}}$$

Corollary 3 *If the base learning algorithm always achives* $\epsilon_t \leq \frac{1}{2} - \frac{1}{2}\gamma$ *then AdaBoost will generate a combined hyperplane with margin at least* $\frac{1}{2}\gamma$.

Margin Distributions - Large Margin Hyperplanes



Margin Distributions – a bound

Theorem 4 *Let D be a distribution over $X \times \{\pm 1\}$ and let $\mathbf{Z}$ be a sample of N examples chosen independently at random according to D. Suppose the base-hypothesis space $\mathcal{H}$ has VC-dimension d, and let $\delta > 0$. Then with probability at least $1 - \delta$, the expected risk is bounded for $\theta > 0$ by*

$$R[f_{Ens}] \leq P_{\mathbf{Z}}(y f_{Ens}(\mathbf{x}) \leq \theta) + \mathcal{O}\left(\sqrt{\frac{d \log^2(N/d)}{N\theta^2} + \frac{\log(1/\delta)}{N}}\right)$$

SVM vs. Boosting

- SVMs

$$R[f] \leq R_{emp}[f] + \mathcal{O}\left(\sqrt{\frac{\log\left(N\theta^2\right)}{\theta^2 N} + \frac{\log(1/\eta)}{N}}\right).$$

- Boosting

$$R[f] \leq R^{\theta}_{emp}[f] + \mathcal{O}\left(\sqrt{\frac{d\log^2\left(\frac{N}{d}\right)}{\theta^2 N} + \frac{\log(1/\delta)}{N}}\right)$$

- **independent of the dimensionality of the space!**

Boosting in the limit

An error function for Adaboost

- AdaBoost stepwise minimizes a function of $y_i f_{\boldsymbol{\alpha}}(x_i) = y_i \sum_t \alpha_t h_t(\mathbf{x}_i)$

$$\mathcal{G}(\boldsymbol{\alpha}) = \sum_{i=1}^{N} \exp\{-y_i f_{\boldsymbol{\alpha}}(\mathbf{x}_i)\}$$

- The gradient of $\mathcal{G}(\boldsymbol{\alpha}^{(t)})$ gives exactly the example weights used for AdaBoost:

$$\frac{\partial \mathcal{G}(\boldsymbol{\alpha}^{(t)})}{\partial f(\mathbf{x}_i)} \sim \exp\{-y_i f_{\boldsymbol{\alpha}}(\mathbf{x}_i)\} \sim d_i^{(t+1)}$$

- The hypothesis coefficient α_t is chosen, such that $\mathcal{G}(\boldsymbol{\alpha}^{(t)})$ is minimized:

$$\alpha_t = \underset{\alpha_t \geq 0}{\operatorname{argmin}}\, \mathcal{G}(\boldsymbol{\alpha}^{(t)}) = \frac{1}{2} \log \frac{1-\epsilon_t}{\epsilon_t}$$

- **AdaBoost is a coordinate gradient descent method which minimizes $\mathcal{G}(\alpha)$ stepwise.**

What happens in the long run?

- Explicit expression for $d_i^{(t+1)}$:

$$d_i^{(t+1)} = \frac{\exp\left\{-\rho_i(\boldsymbol{\alpha}^{(t)})\right\}^{\|\boldsymbol{\alpha}^{(t)}\|}}{\sum_{j=1}^{N} \exp\left\{-\rho_j(\boldsymbol{\alpha}^{(t)})\right\}^{\|\boldsymbol{\alpha}^{(t)}\|}}$$

$\rightsquigarrow$ **Soft-Max Function** with parameter $\|\boldsymbol{\alpha}^{(t)}\|_1$

- $\|\boldsymbol{\alpha}\|_1$ will increase monotonicaly ($\sim$ linear)

$\rightsquigarrow$ the d's concentrate on a **few** difficult patterns

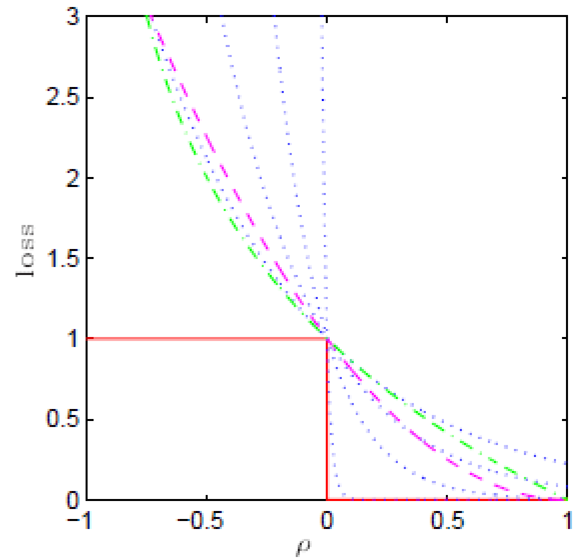
$\rightarrow$ **Support Patters**

$\rightsquigarrow$ Annealing Process:

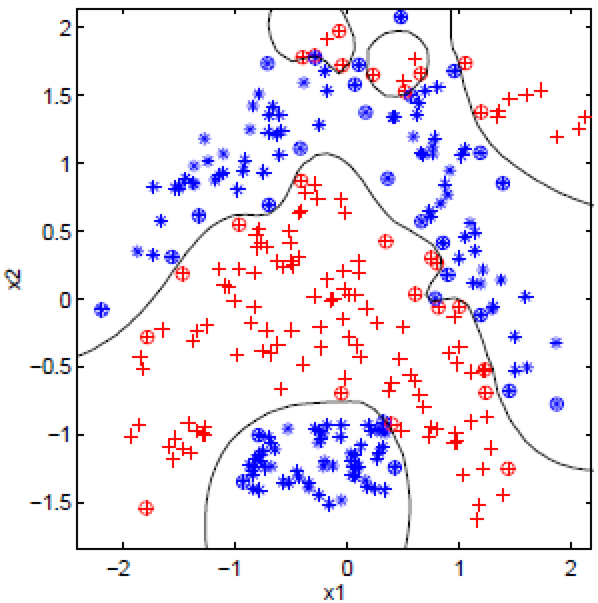
$$\mathcal{G}(\boldsymbol{\alpha}) = \sum \exp\left\{-\rho_i(\boldsymbol{\alpha})\right\}^{\|\boldsymbol{\alpha}\|_1}$$

$\rightarrow$ $0/\infty$-Loss approximated asymptoticaly

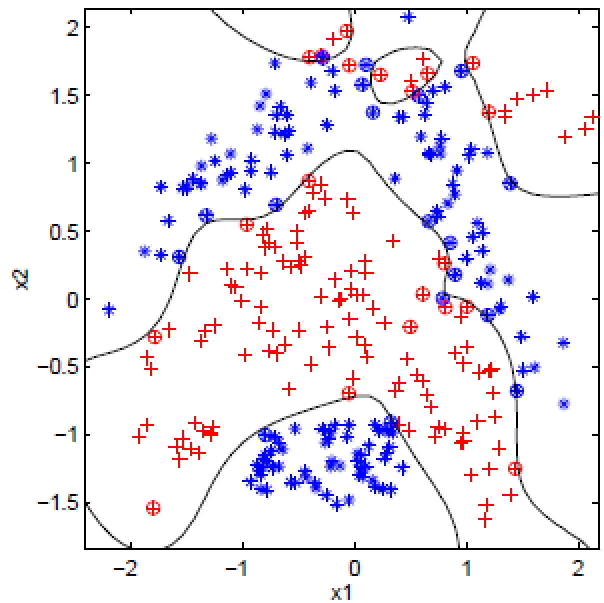
$\rightarrow$ **Barrier Optimization**



Support Vector vs Support Patterns



AdaBoost's decision line



SVM's decision line

These decision lines are for a low noise case with similar generalisation errors. In AdaBoost, RBF networks with 13 centers were used.

Mathematical Programs: SVMs vs. Boosting

Mathematical Program Formulation- SVMs

The SVM minimization of

$$\begin{aligned} \min_{\mathbf{w}\in\mathcal{F}_\Phi} \quad & \tfrac{1}{2}\|\mathbf{w}\|^2 \\ \text{subject to} \quad & y_i\langle\mathbf{w},\Phi(\mathbf{x}_i)\rangle \geq 1, \quad i=1,\ldots,N. \end{aligned} \tag{1}$$

reformulate as maximization of the margin ρ

$$\begin{aligned} \max_{\mathbf{w}\in\mathcal{F}_\Phi,\rho\in\mathbf{R}_+} \quad & \rho \\ \text{subject to} \quad & y_i\sum_{j=1}^{D} w_j\Phi_j(\mathbf{x}_i) \geq \rho \quad \text{for} \quad i=1,\ldots,N \\ & \|\mathbf{w}\|_2 = 1, \end{aligned} \tag{2}$$

where $D=\dim(\mathcal{F})$ and Φ_j is the j-th component of Φ in feature space:

$$\Phi_j = P_j[\Phi]$$

Boosting as a Mathematical Program

- master hypothesis

$$f(\mathbf{x}) = \sum_{t=1}^{T} \frac{w_t}{\|\mathbf{w}\|_1} h_t(\mathbf{x})$$

- base hypotheses h_t produced by the base learning algorithm.

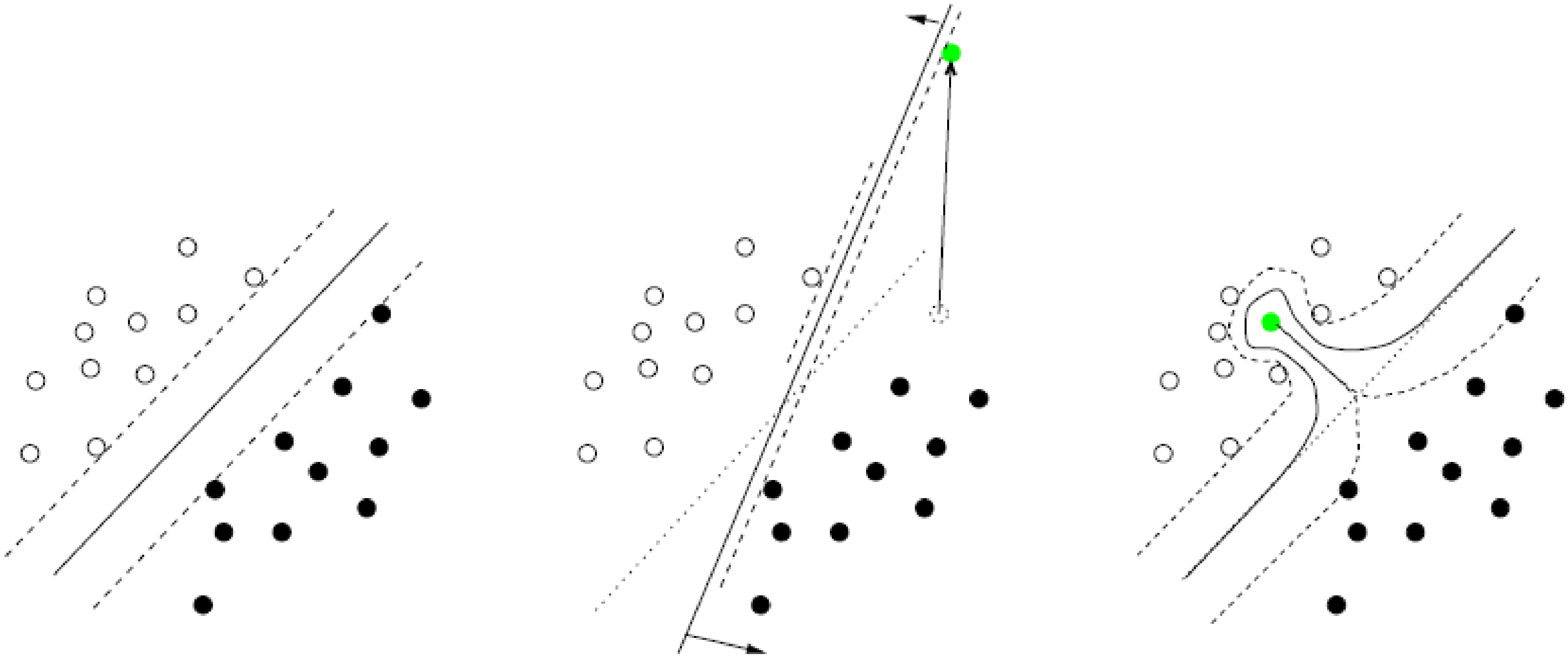
Arc-GV solution is asymptotically the same as linear program solution, maximizing smallest margin ρ:

$$\begin{aligned} \max_{\mathbf{w}\in\mathbf{R}^J, \rho\in\mathbf{R}_+} \quad & \rho \\ \text{subject to} \quad & y_i \sum_{j=1}^{J} w_j h_j(\mathbf{x}_i) \geq \rho \quad \text{for} \quad i = 1, \ldots, N \\ & \|\mathbf{w}\|_1 = 1, \end{aligned} \tag{3}$$

where J is the number of hypotheses in $\mathcal{H}$.

Soft Margins

Hard Margin Classification



- The problem of finding a maximum margin "hyper-plane" on reliable data (left), data with outlier (middle) and a mislabeled pattern (right). The hard margin implies **noise sensitivity**.

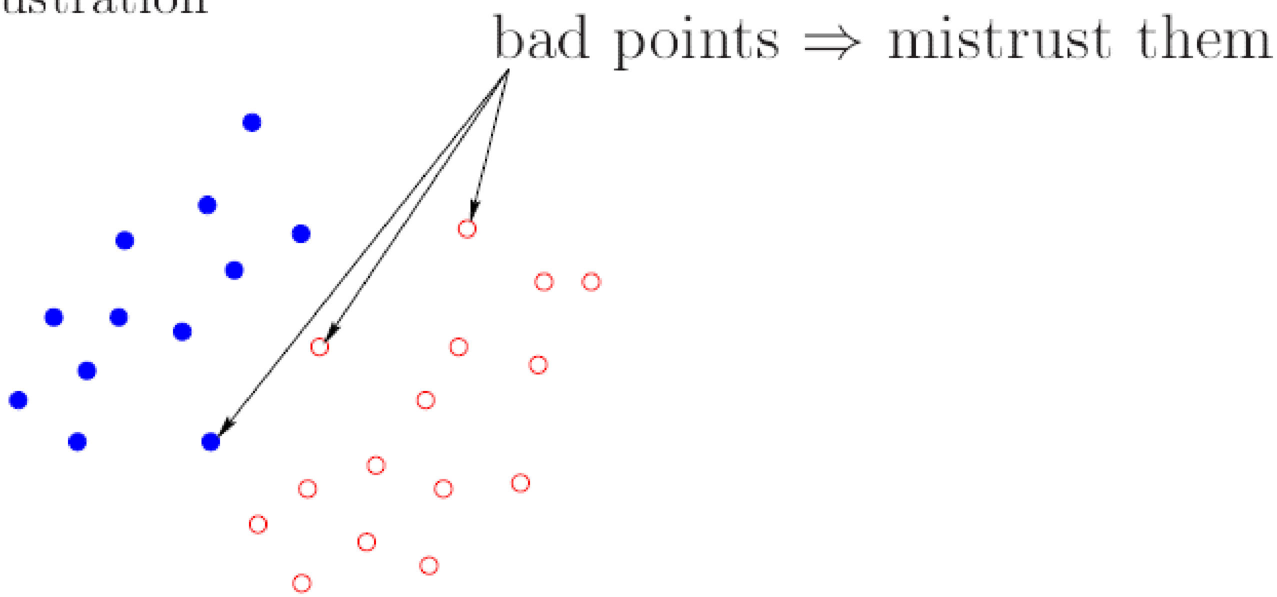
Adaboost with Soft Margins

- Define a Soft Margin

$$\tilde{\rho}_n(\boldsymbol{\alpha}) = \rho_n(\boldsymbol{\alpha}) + \zeta_n,$$

  - where ζ_n is the amount of uncertainty in example $(\mathbf{x}_n, y_n)$

- Illustration



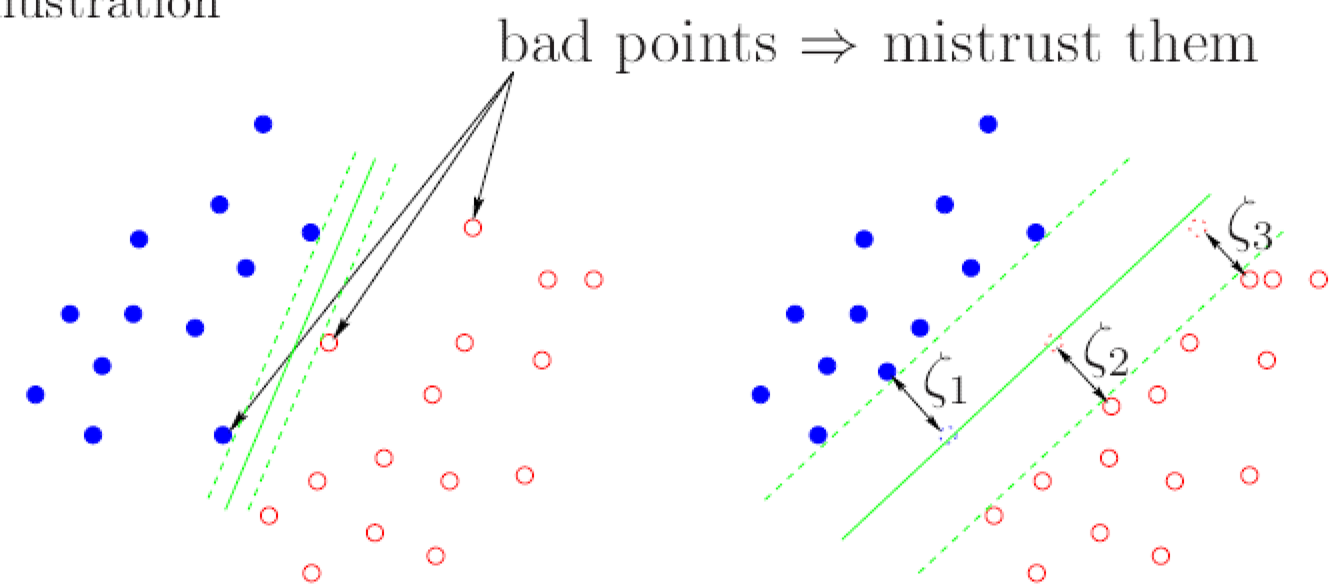
Adaboost with Soft Margins

- Define a Soft Margin

$$\tilde{\rho}_n(\boldsymbol{\alpha}) = \rho_n(\boldsymbol{\alpha}) + \zeta_n$$

  - where ζ_n is the amount of uncertainty in pattern $\mathbf{z}_n$

- Illustration



Adaboost with Soft Margins

- Once we have defined the uncertainity measure ζ_n, we can easily get a new regularized Boosting algorithm.

  $\Rightarrow$ Improve the Error Function by plugging-in the Soft Margin

$$\tilde{G}(\boldsymbol{\alpha}) = \sum_{n=1}^{N} \exp\{-\|\boldsymbol{\alpha}\|_1 \tilde{\rho}_n(\boldsymbol{\alpha})\}$$

$$d_n^{t+1} = \frac{\partial \tilde{G}(\boldsymbol{\alpha})}{\partial f_{\boldsymbol{\alpha}}(\mathbf{x}_n))}$$

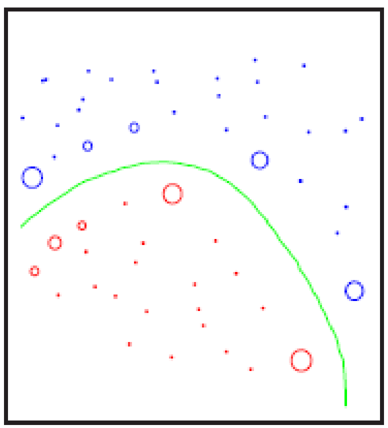
$$\alpha_t = \operatorname*{argmin}_{\alpha_t \geq 0} \tilde{G}(\boldsymbol{\alpha})$$

Regularizing Adaboost – Reducing the *Influence*

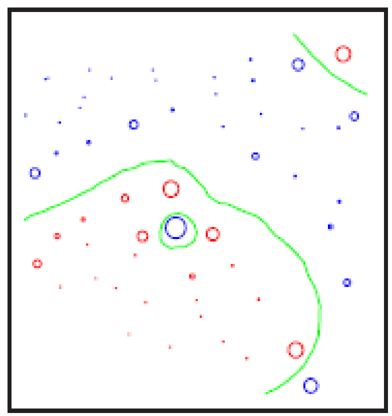
- How can we know which patterns are unreliable?

  AdaBoost focuses on difficult-to-learn patterns by assigning high pattern weights d_n that we can exploit. Hence, we define the Influence of a pattern

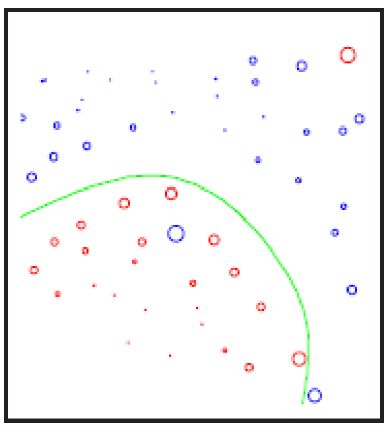
$$\mu_n^t = \sum_{r=1}^{t} \frac{\alpha_r}{\|\boldsymbol{\alpha}\|_1} d_n^r \qquad \zeta_n = C(\mu_n^t)^2$$



AdaBoost without “Noise”



AdaBoost with “Noise”



AdaBoost$_{Reg}$ with “Noise”

Regularizing Adaboost

Positive:

- first algorithm that addresses overfitting in Boostin
- much improved results

Negative:

- Modification on algorithmic level
- hard to analyze
  - which optimization problem is solved
  - no generalization results

Idea:

- go back to beginning and redesign optimization problem
- use convergence results for leveraging
- apply margin bounds

Benchmark Comparison

- 10 datasets (from UCI, DELVE and STATLOG repositories)
- Non binary problems partitioned into two-class problems.
- 100 partitions into test and training set (about 60%:40%).
- On each data sets we trained and tested all classifiers. Results are average test errors over 100 runs and standard deviations.
- Parameters estimated by 5-fold cross validation on first 5 realizations of dataset.
- For SVM we used Gaussian kernel
- For Boosting we used RBF networks as base learner

Experimental Results

	KNN	C4.5	RBF	AB	AB_R	SVM
Banana	$15.0_{\pm 1.0}$	$16.1_{\pm 2.8}$	$10.8_{\pm 0.6}$	$12.3_{\pm 0.7}$	$10.9_{\pm 0.4}$	$11.5_{\pm 0.7}$
B.Cancer	$28.4_{\pm 4.4}$	$24.6_{\pm 4.5}$	$27.6_{\pm 4.7}$	$30.4_{\pm 4.7}$	$26.5_{\pm 4.5}$	$26.0_{\pm 4.7}$
Diabetes	$28.9_{\pm 2.4}$	$26.0_{\pm 2.4}$	$24.3_{\pm 1.9}$	$26.5_{\pm 2.3}$	$23.8_{\pm 1.8}$	$23.5_{\pm 1.7}$
German	$28.9_{\pm 1.9}$	$28.1_{\pm 2.4}$	$24.7_{\pm 2.4}$	$27.5_{\pm 2.5}$	$24.3_{\pm 2.1}$	$23.6_{\pm 2.1}$
Heart	$15.8_{\pm 3.3}$	$20.4_{\pm 4.6}$	$17.6_{\pm 3.3}$	$20.3_{\pm 3.4}$	$16.5_{\pm 3.5}$	$16.0_{\pm 3.3}$
Ringnorm	$35.9_{\pm 1.3}$	$15.3_{\pm 1.5}$	$1.7_{\pm 0.2}$	$1.9_{\pm 0.3}$	$1.6_{\pm 0.1}$	$1.7_{\pm 0.1}$
F.Solar	$37.8_{\pm 2.8}$	$33.2_{\pm 1.9}$	$34.4_{\pm 2.0}$	$35.7_{\pm 1.8}$	$34.2_{\pm 2.2}$	$32.4_{\pm 1.8}$
Thyroid	$5.8_{\pm 2.8}$	$8.7_{\pm 3.3}$	$4.5_{\pm 2.1}$	$4.4_{\pm 2.2}$	$4.6_{\pm 2.2}$	$4.8_{\pm 2.2}$
Titanic	$25.5_{\pm 3.8}$	$22.9_{\pm 1.5}$	$23.3_{\pm 1.3}$	$22.6_{\pm 1.2}$	$22.6_{\pm 1.2}$	$22.4_{\pm 1.0}$
Waveform	$11.4_{\pm 0.8}$	$17.8_{\pm 1.0}$	$10.7_{\pm 1.1}$	$10.8_{\pm 0.6}$	$9.8_{\pm 0.8}$	$9.9_{\pm 0.4}$
Mean%	$2400_{\pm 6800}$	$1200_{\pm 2700}$	$5.8_{\pm 3.7}$	$13.4_{\pm 9.2}$	$2.7_{\pm 2.5}$	$2.9_{\pm 3.5}$

Other Applications

Some examples:

Text classification	Schapire and Singer - Used stumps with normalized term frequency and multi-class encoding
OCR	Schwenk and Bengio (neural networks)
Natural language Processing	Collins; Haruno, Shirai and Ooyama
Image retrieval	Thieu and Viola
Medical diagnosis	Merle *et al.*
Fraud Detection	Rätsch & Müller 2001
Drug Discovery	Rätsch, Demiriz, Bennett 2002
Elect. Power Monitoring	Onoda, Rätsch & Müller 2000

Fuller list: Schapire's 2002, Meir & Rätsch 2003 review

Recently more…

Conclusions

- Boosting algorithms
  - AdaBoost
  - PAC Motivation
  - Boosting with Large Margins
  - Strategies for Dealing with High Dimensional Spaces
  - Relations to Mathematical Programming & SVMs

`Boosting Homepage:` **http://www.boosting.org**

Sources of Information

Internet http://www.boosting.org

http://www.cs.princeton.edu/~schapire/boost.html

Conferences Computational Learning Theory (COLT), Neural Information Processing Systems (NIPS), Int. Conference on Machine Learning (ICML), . . .

Journals Machine Learning, Journal of Machine Learning Research, Information and Computation, Annals of Statistics

People List available at http://www.boosting.org

Software Only few implementations (algorithms 'too simple') (cf. http://www.boosting.org)

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