

# Boosting on manifolds: adaptive regularization of base classifiers

Balázs Kégl

(joint work with Ligen Wang)

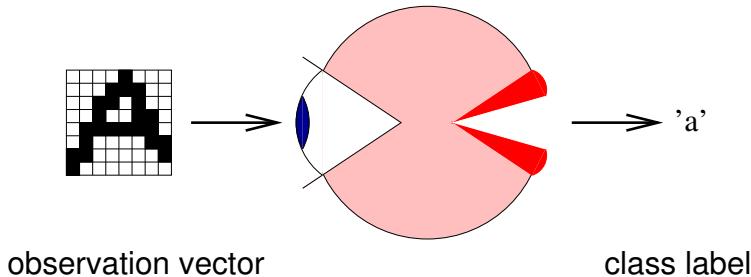
Université de Montréal

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# Outline

- The supervised learning model
- AdaBoost
- RegBoost
- The graph Laplacian regularizer
- Experimental results

# The supervised learning model



- **observation vector:**  $\mathbf{x} \in \mathbb{R}^d$
- **class label:**  $y \in \{-1, 1\}$  – binary classification
- **classifier:**  $g : \mathbb{R}^d \mapsto \{-1, 1\}$

- **discriminant function:**  $f : \mathbb{R}^d \mapsto [-1, 1]$

$$g(\mathbf{x}) = \begin{cases} 1, & \text{if } f(\mathbf{x}) \geq 0, \\ -1, & \text{if } f(\mathbf{x}) < 0 \end{cases}$$

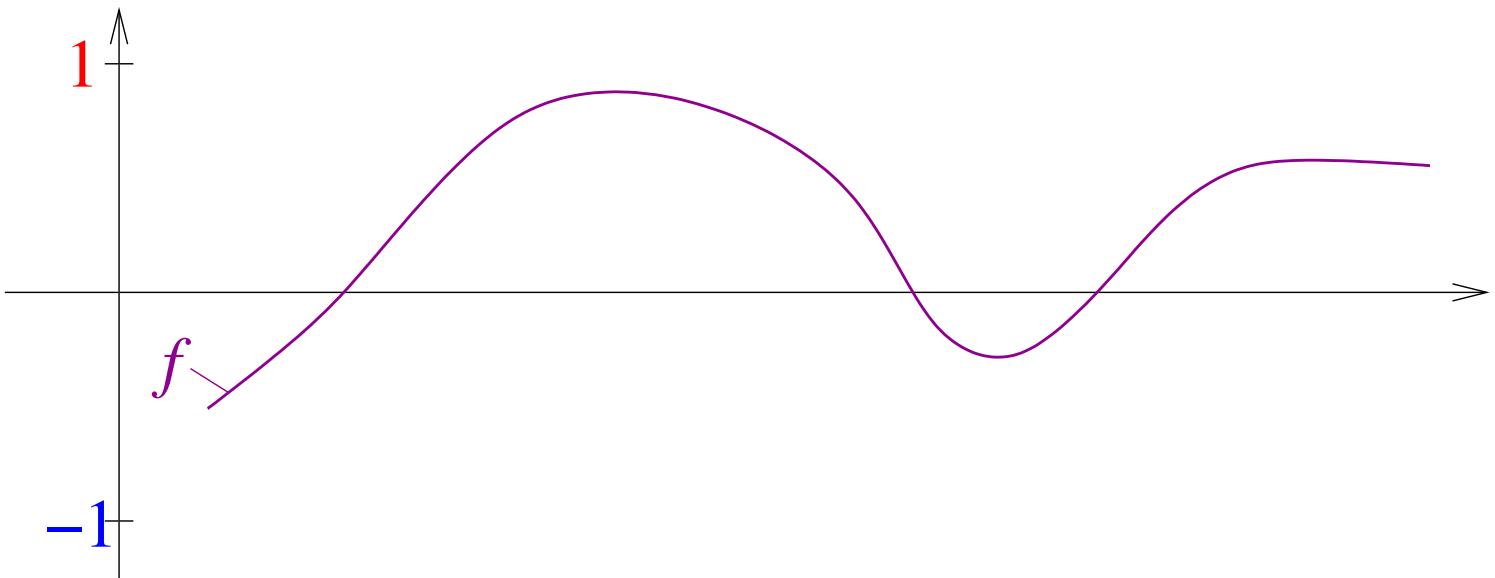
- **decision border:**  $\{\mathbf{x} : f(\mathbf{x}) = 0\}$

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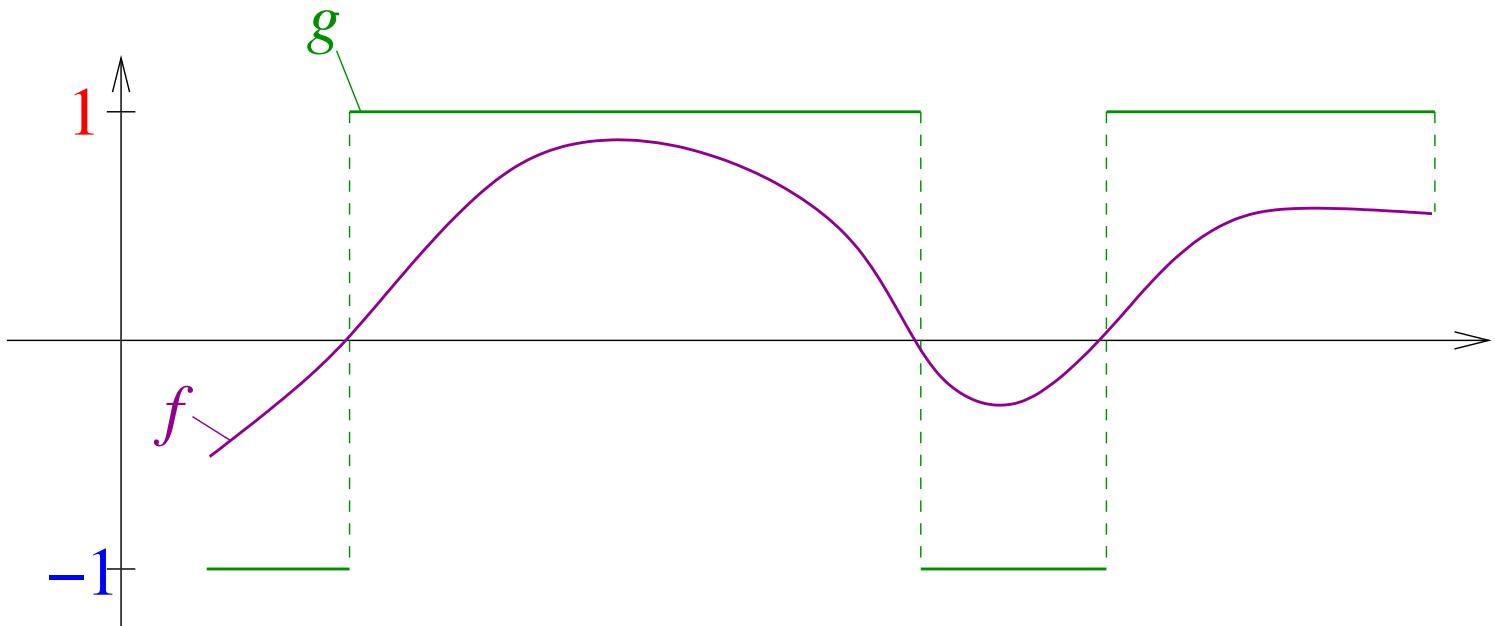
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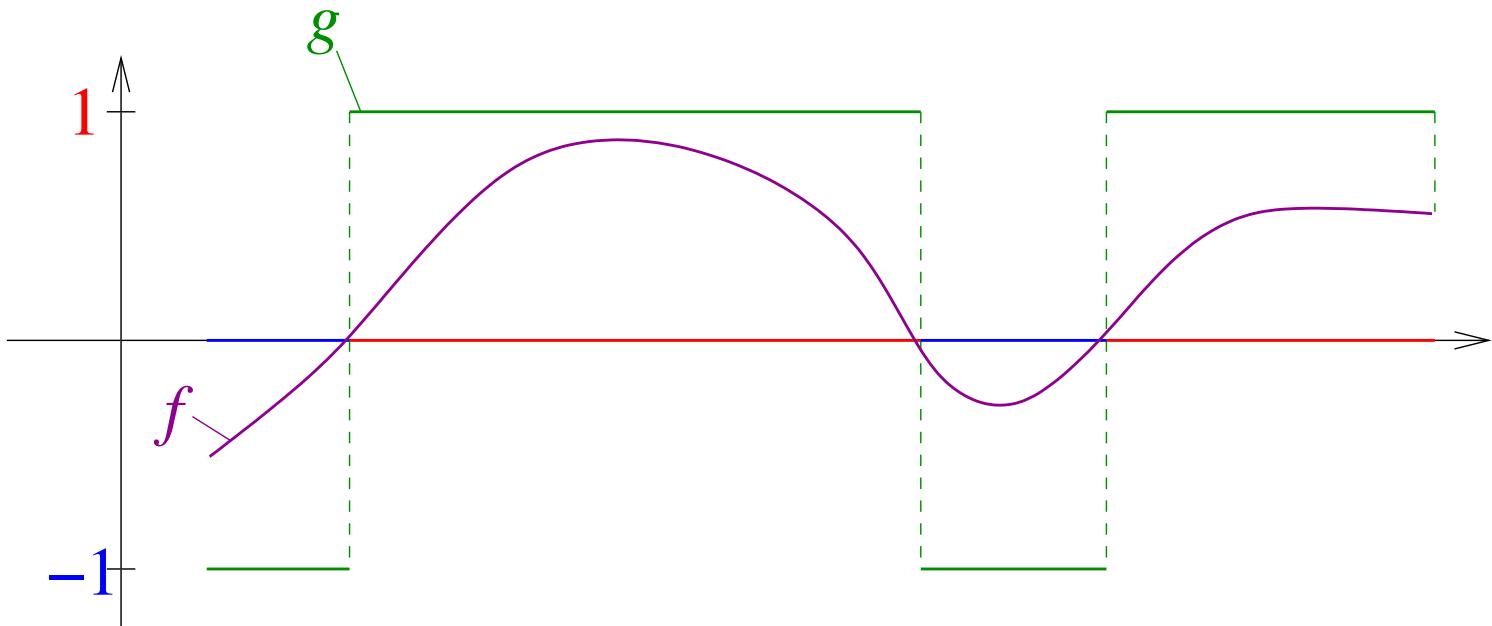


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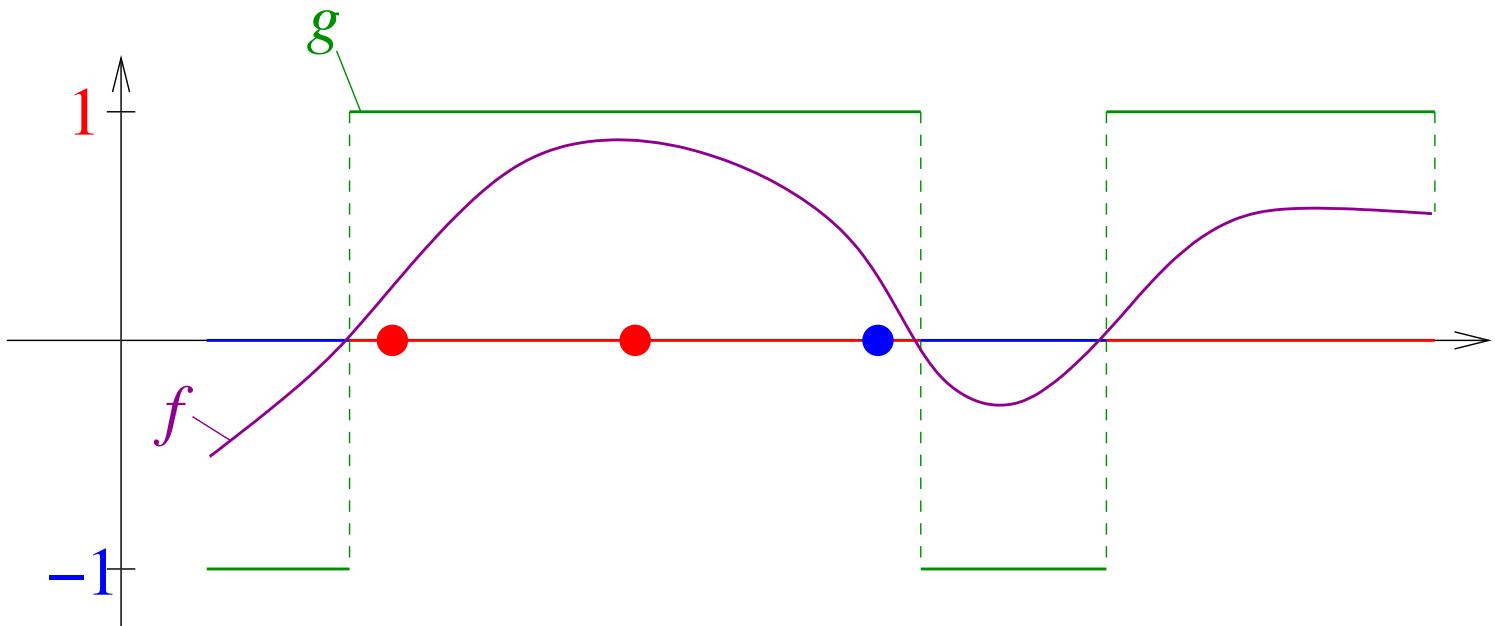


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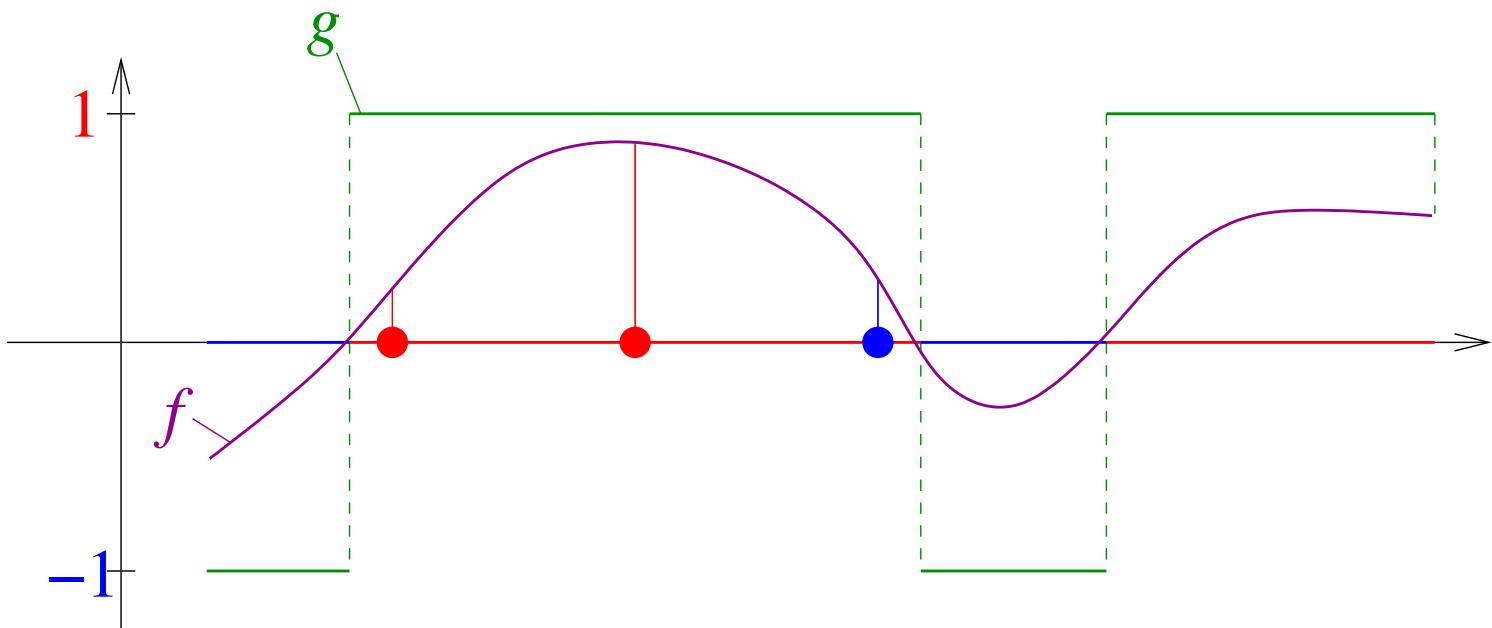
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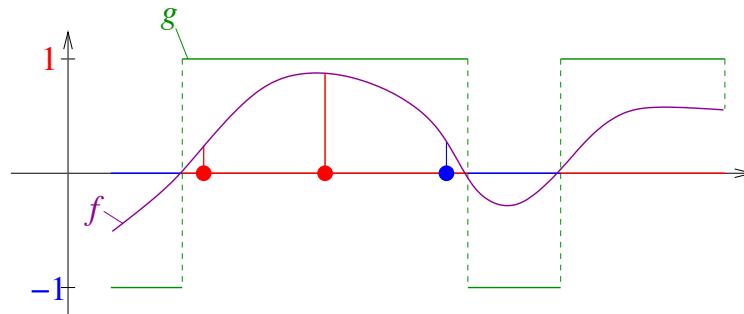


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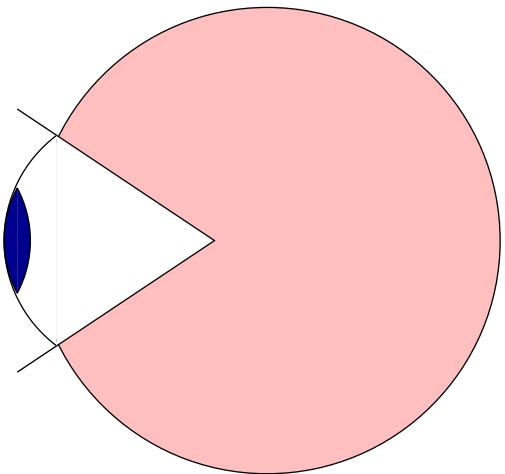
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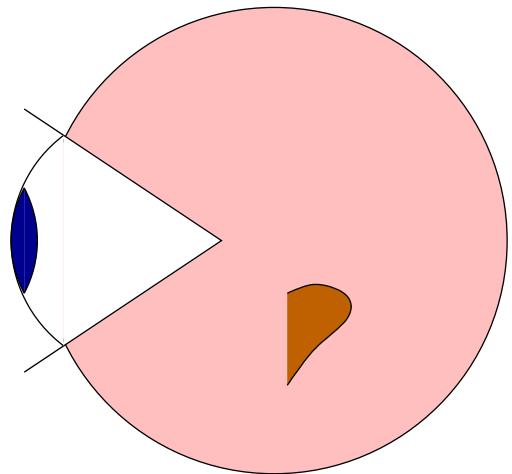


- Margin:  $\rho = y \cdot f(\mathbf{x})$ 
  - classification error = negative margin
  - magnitude of a positive margin quantifies confidence
  - plays an important role in analyzing the generalization performance

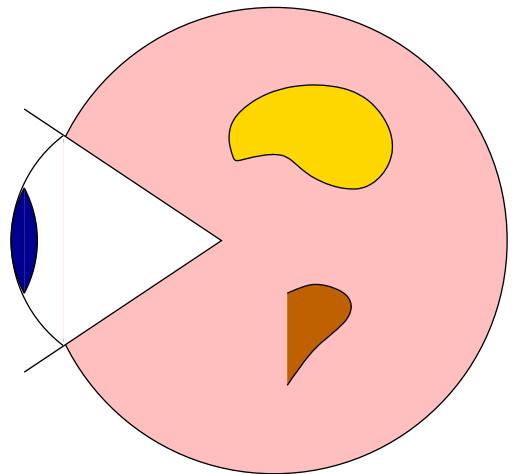
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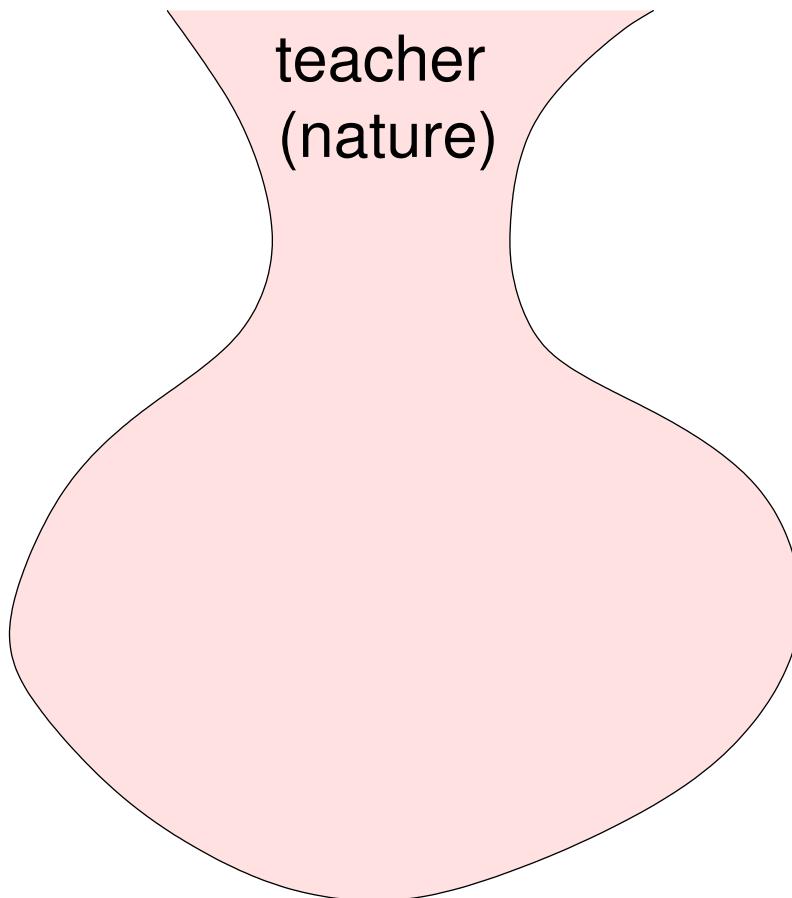


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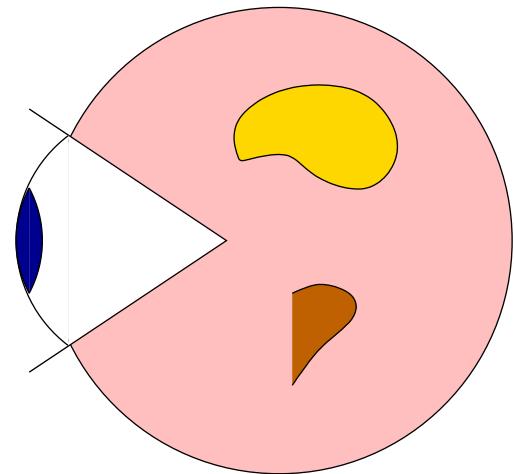


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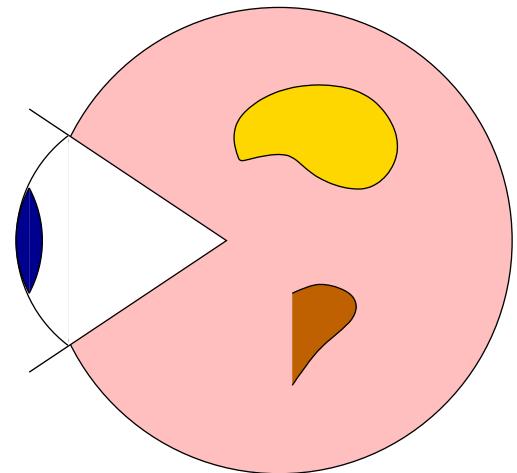
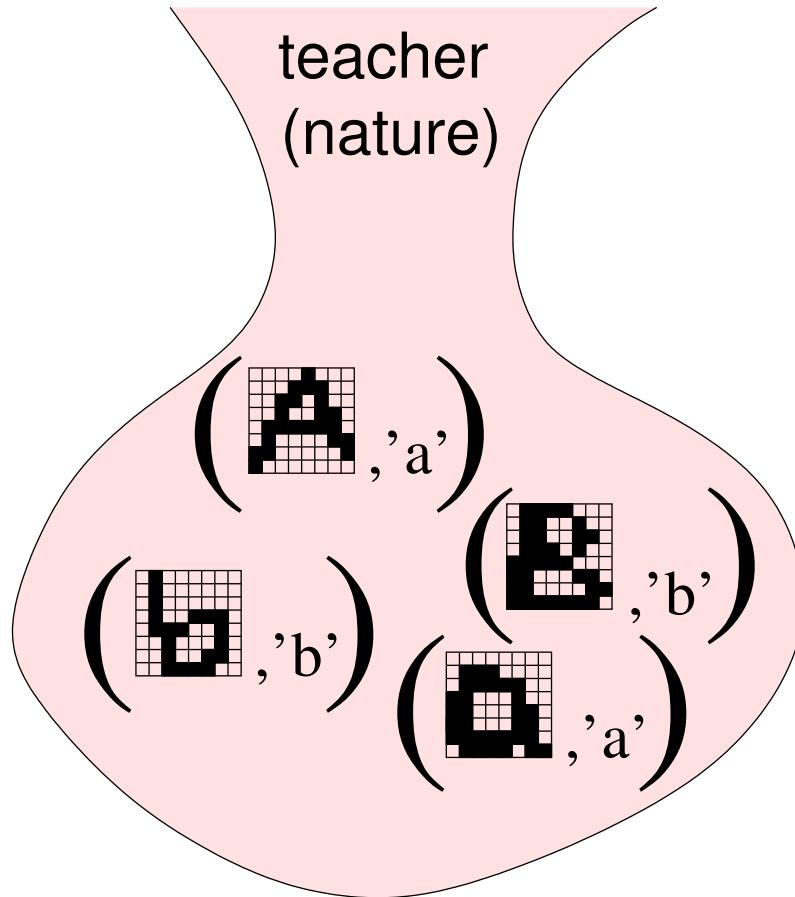


teacher  
(nature)



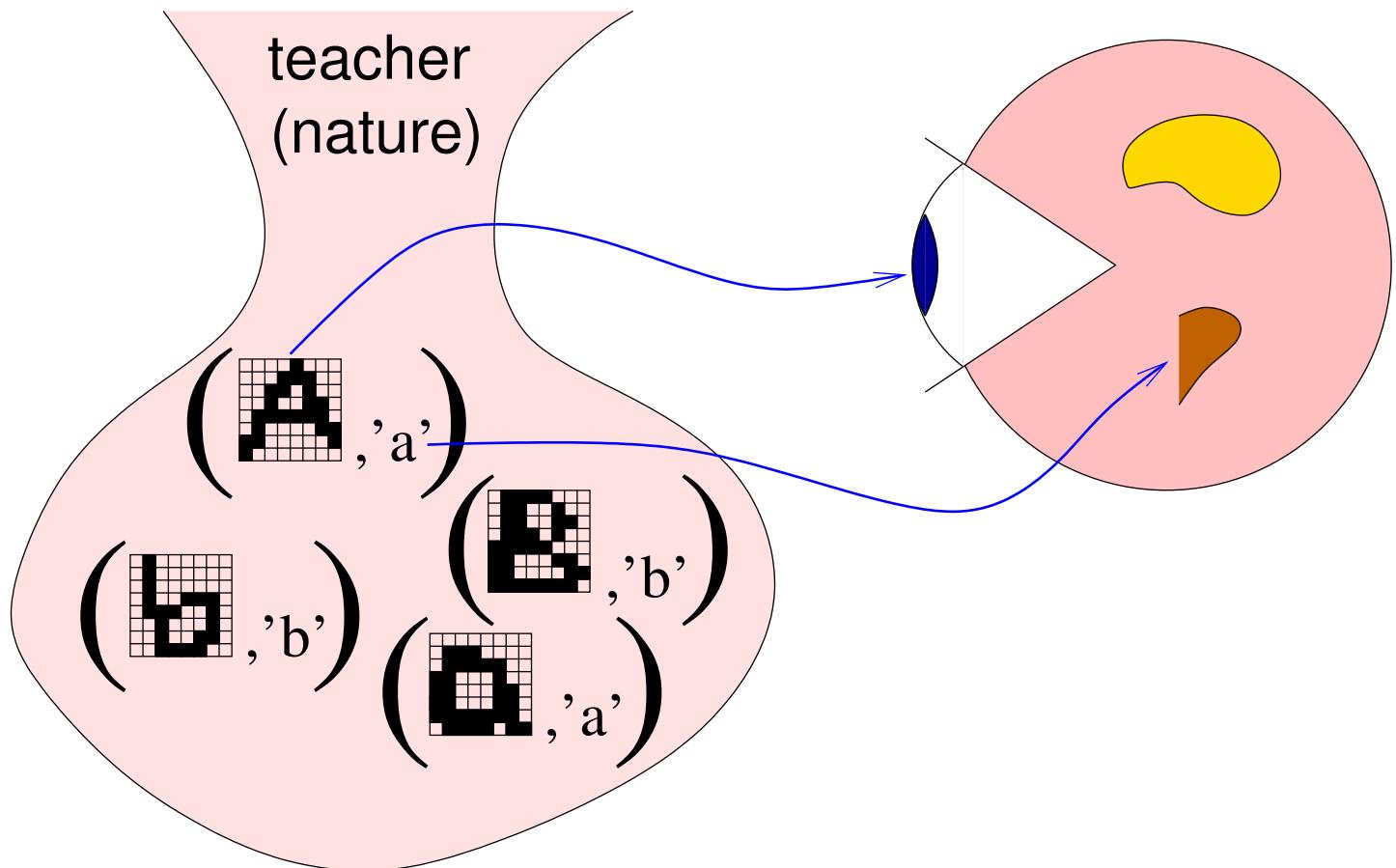
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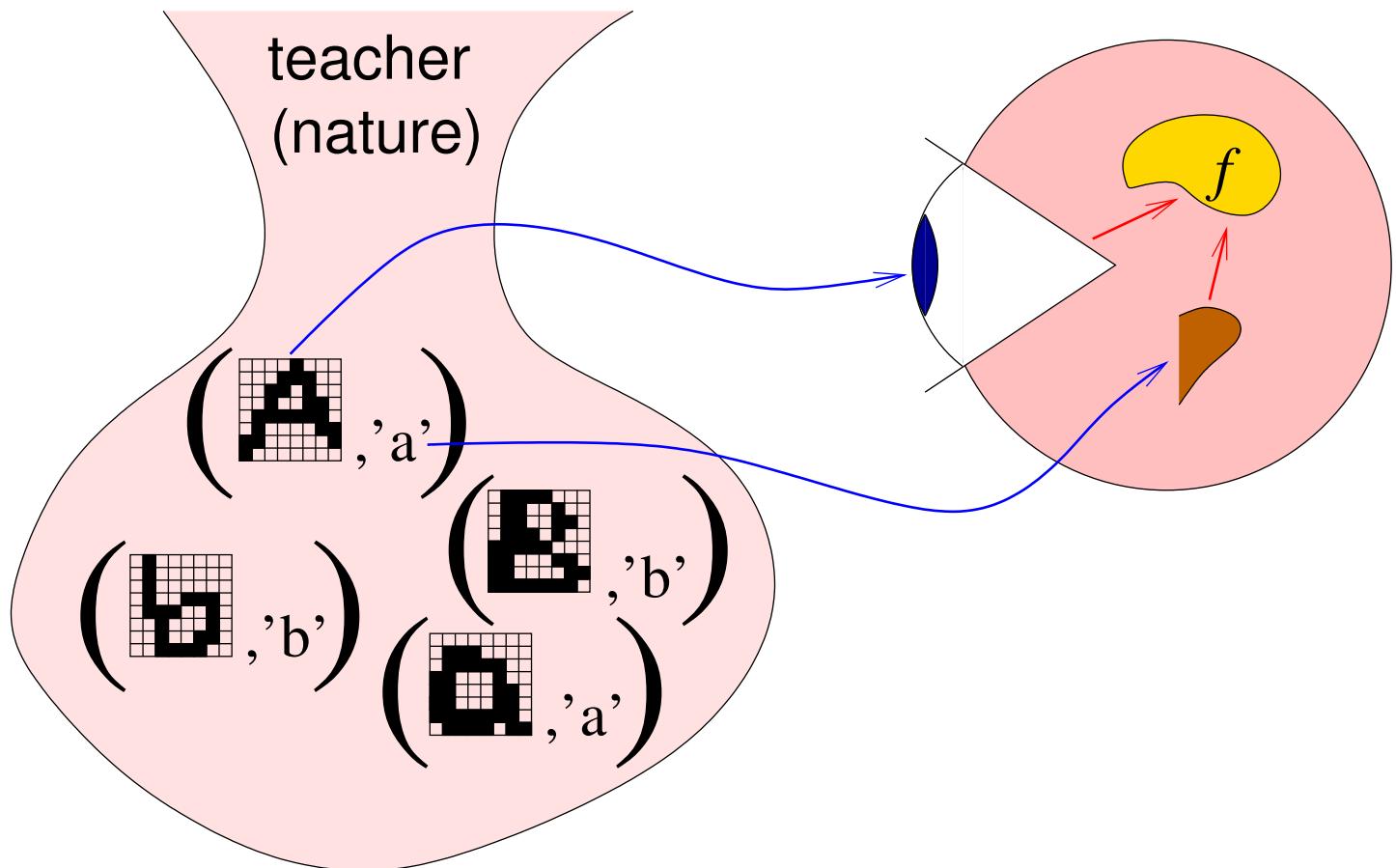
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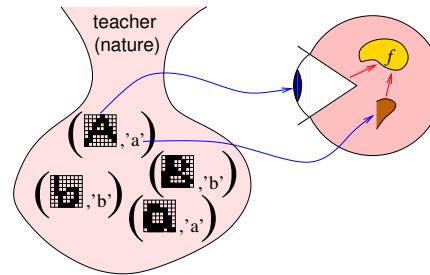


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# The supervised learning model



- Learning

- training sample:  $D_n = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$
- function set:  $\mathcal{F}$
- learning algorithm:  $\text{ALGO} : (\mathbb{R}^d \times \{-1, 1\})^n \mapsto \mathcal{F}$

$$\text{ALGO}(D_n) \rightarrow f$$

- goal: small generalization error  $P[\text{ALGO}(D_n, \mathbf{X}) \neq Y]$

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# AdaBoost

- Model:  $f(\mathbf{x}) = \sum_{j=1}^T \alpha^{(j)} h^{(j)}(\mathbf{x})$ 
  - $h^{(j)}$  can be any “weak” classifier: it has to be only slightly better than a random guess
  - interpretation: weighted vote of “weak” experts
  - [Freund - Schapire '97]

- Algorithm

- simple, no gradient descent, no quadratic optimization
- add base functions one at a time
- set their weights proportionally to their correctness
- train the next expert on data points that were missed by previous experts
- automatically concentrates on training points that are hard to learn

# AdaBoost

**ADABoost**( $D_n = ((\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n))$ , **BASE**( $D_n, \mathbf{w}$ ),  $T$ )

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1    $\mathbf{w} \leftarrow (1/n, \dots, 1/n)$        $\triangleright$  initial weight distribution on the training data
2   for  $t \leftarrow 1$  to  $T$ 
3      $h^{(t)} \leftarrow \text{BASE}(D_n, \mathbf{w})$        $\triangleright$  base classifier
4      $\epsilon \leftarrow \sum_{i=1}^n w_i I\{h^{(t)}(\mathbf{x}_i) \neq y_i\}$        $\triangleright$  weighted error
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6     if  $\alpha^{(t)} \leq 0$        $\triangleright$  equivalent to  $\epsilon \geq 1/2$ 
7       return  $f^{(t-1)}(\cdot) = \sum_{j=1}^{t-1} \alpha^{(j)} h^{(j)}(\cdot)$ 
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1    $\mathbf{w} \leftarrow (1/n, \dots, 1/n)$        $\triangleright$  initial weight distribution on the training data
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4      $\epsilon \leftarrow \sum_{i=1}^n w_i I\{h^{(t)}(\mathbf{x}_i) \neq y_i\}$        $\triangleright$  weighted error
5      $\alpha^{(t)} \leftarrow \frac{1}{2} \log \left( \frac{1-\epsilon}{\epsilon} \right)$        $\triangleright$  weight of base classifier
6     if  $\alpha^{(t)} \leq 0$        $\triangleright$  equivalent to  $\epsilon \geq 1/2$ 
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9       if  $h^{(t)}(\mathbf{x}_i) \neq y_i$  then       $w_i^{(t+1)} \leftarrow w_i^{(t)} \frac{1}{2\epsilon}$       ↑
10      else       $w_i^{(t+1)} \leftarrow w_i^{(t)} \frac{1}{2(1-\epsilon)}$       ↓
11   return  $f^{(T)}(\cdot) = \sum_{t=1}^T \alpha^{(t)} h^{(t)}(\cdot)$ 
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# AdaBoost

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5      $\alpha^{(t)} \leftarrow \frac{1}{2} \log \left( \frac{1 - \epsilon}{\epsilon} \right)$        $\triangleright$  weight of base classifier
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4      $\gamma \leftarrow \sum_{i=1}^n w_i h^{(t)}(\mathbf{x}_i) y_i = 1 - 2\epsilon$      $\triangleright$  edge
5      $\alpha^{(t)} \leftarrow \frac{1}{2} \log \left( \frac{1+\gamma}{1-\gamma} \right)$      $\triangleright$  weight of base classifier
6     if  $\alpha^{(t)} \leq 0$          $\triangleright$  equivalent to  $\gamma \geq 0$ 
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10    return  $f^{(T)}(\cdot) = \sum_{t=1}^T \alpha^{(t)} h^{(t)}(\cdot)$ 
```

# AdaBoost

- Analysis

- margin:  $\rho_i = f(\mathbf{x}_i)y_i$
- normalized margin:  $\tilde{\rho}_i = \frac{\rho_i}{\|\alpha\|_1} = \frac{\sum_{t=1}^T \alpha^{(t)} h^{(t)}(\mathbf{x}_i) y_i}{\sum_{t=1}^T \alpha^{(t)}}$
- AdaBoost directly minimizes the exponential risk

$$\widehat{R}^{(e)}(f) = \frac{1}{n} \sum_{i=1}^n e^{-\rho_i}$$

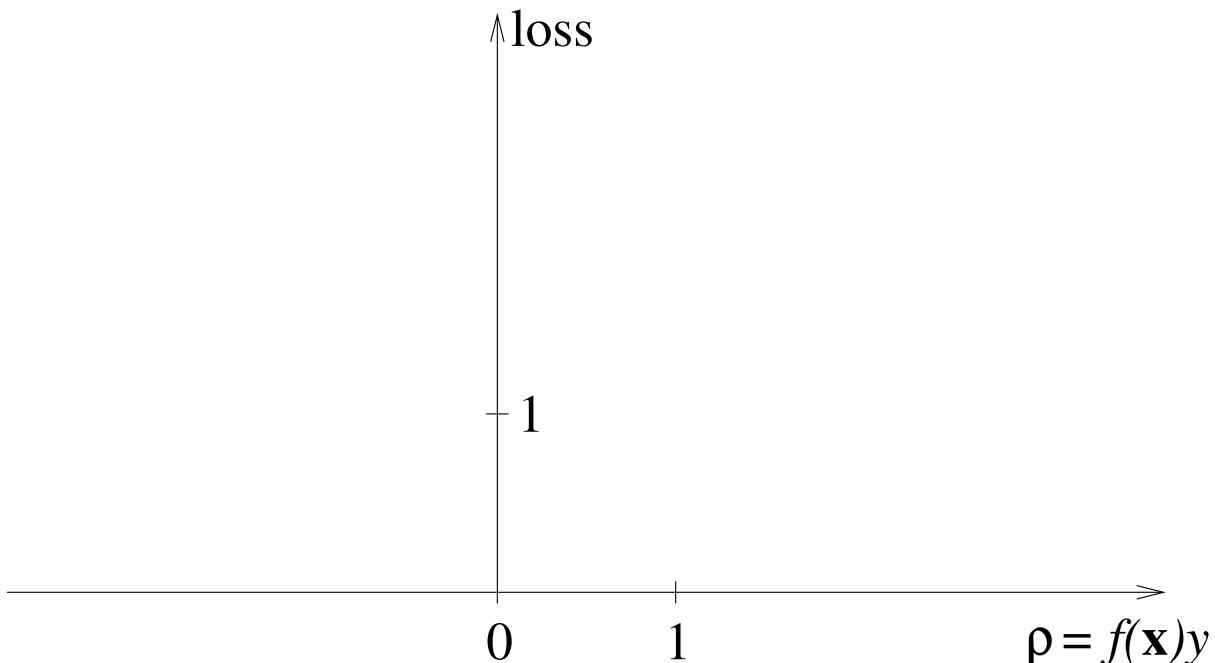
- AdaBoost indirectly minimizes the training error

$$\widehat{R}(f) = \frac{1}{n} \sum_{i=1}^n I\{\rho_i < 0\}$$

# AdaBoost

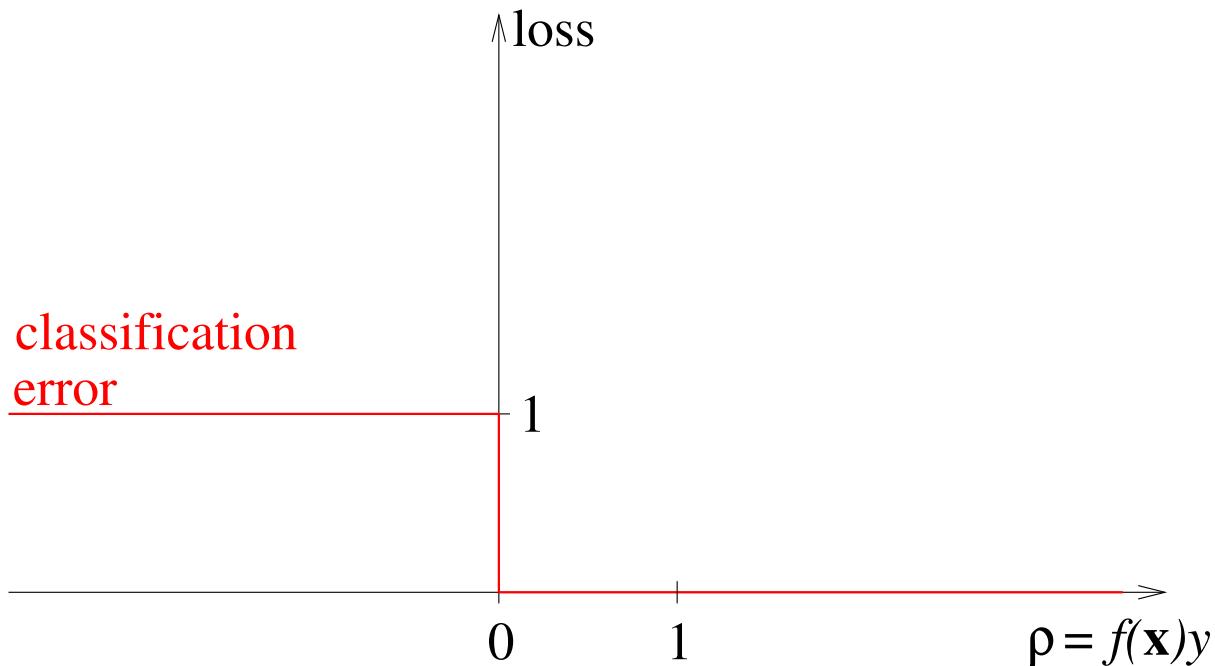
41

- Loss functions



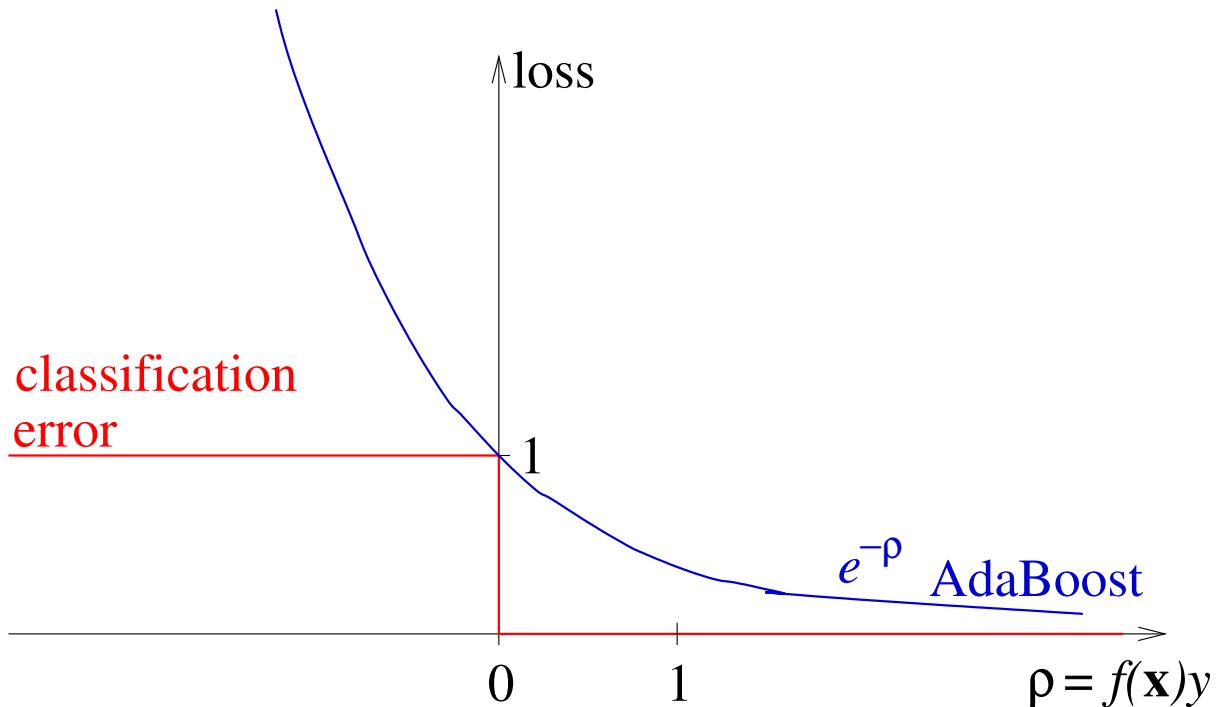
# AdaBoost

- Loss functions



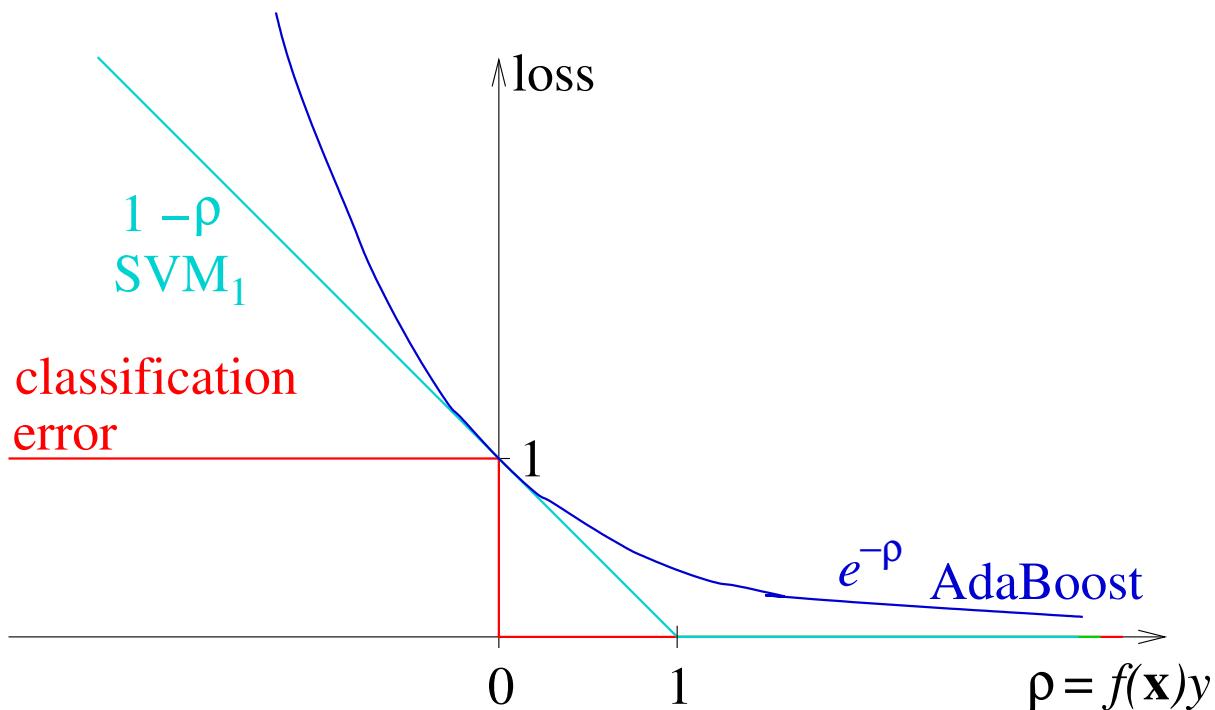
# AdaBoost

- Loss functions



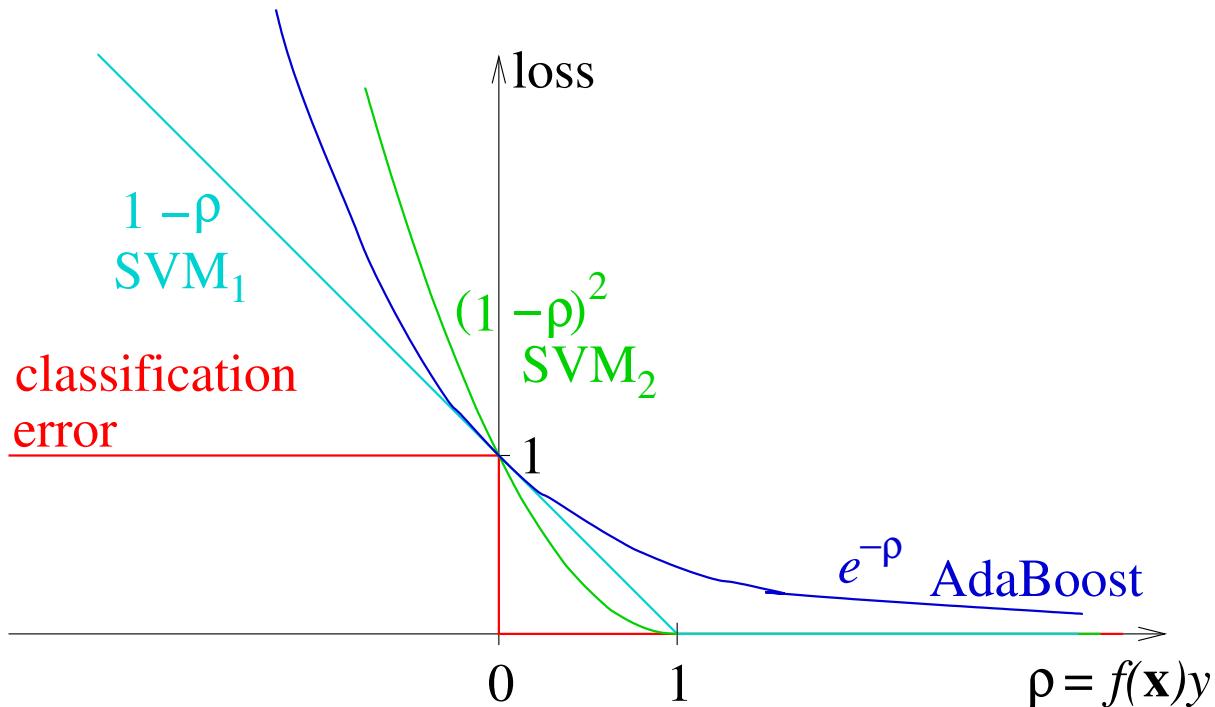
# AdaBoost

- Loss functions



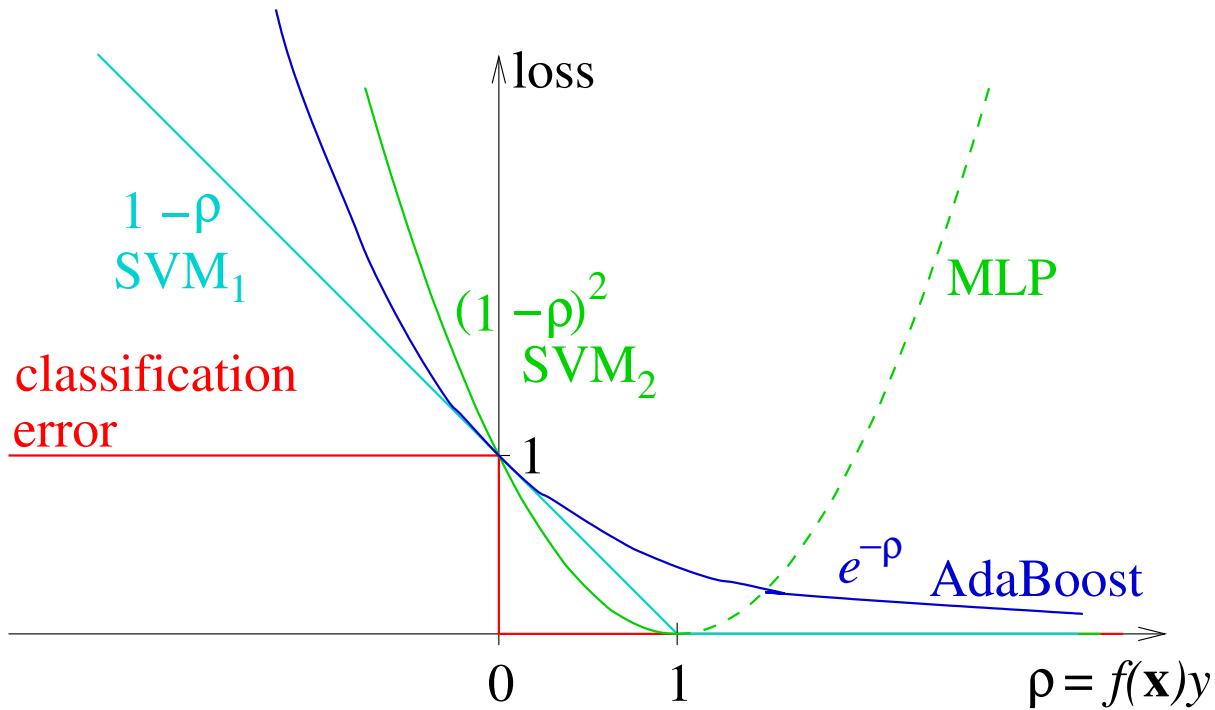
# AdaBoost

- Loss functions



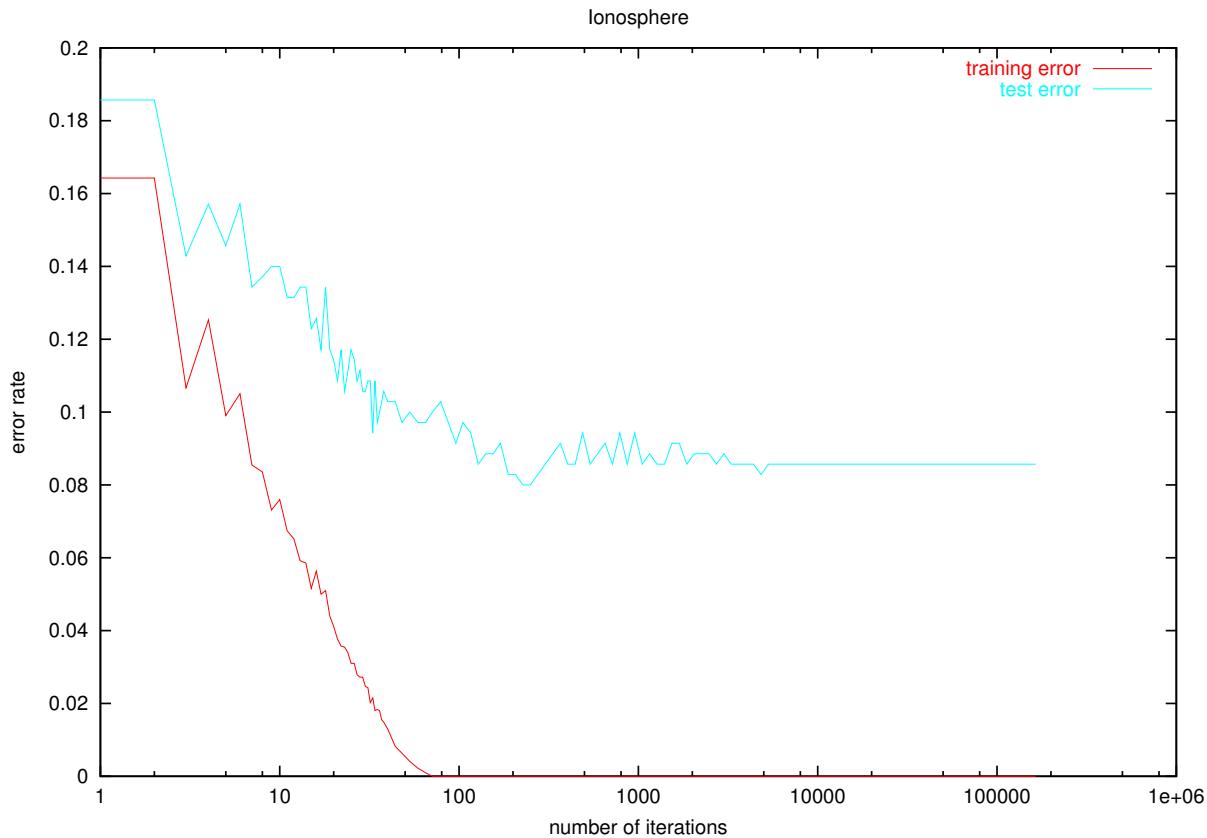
# AdaBoost

- Loss functions



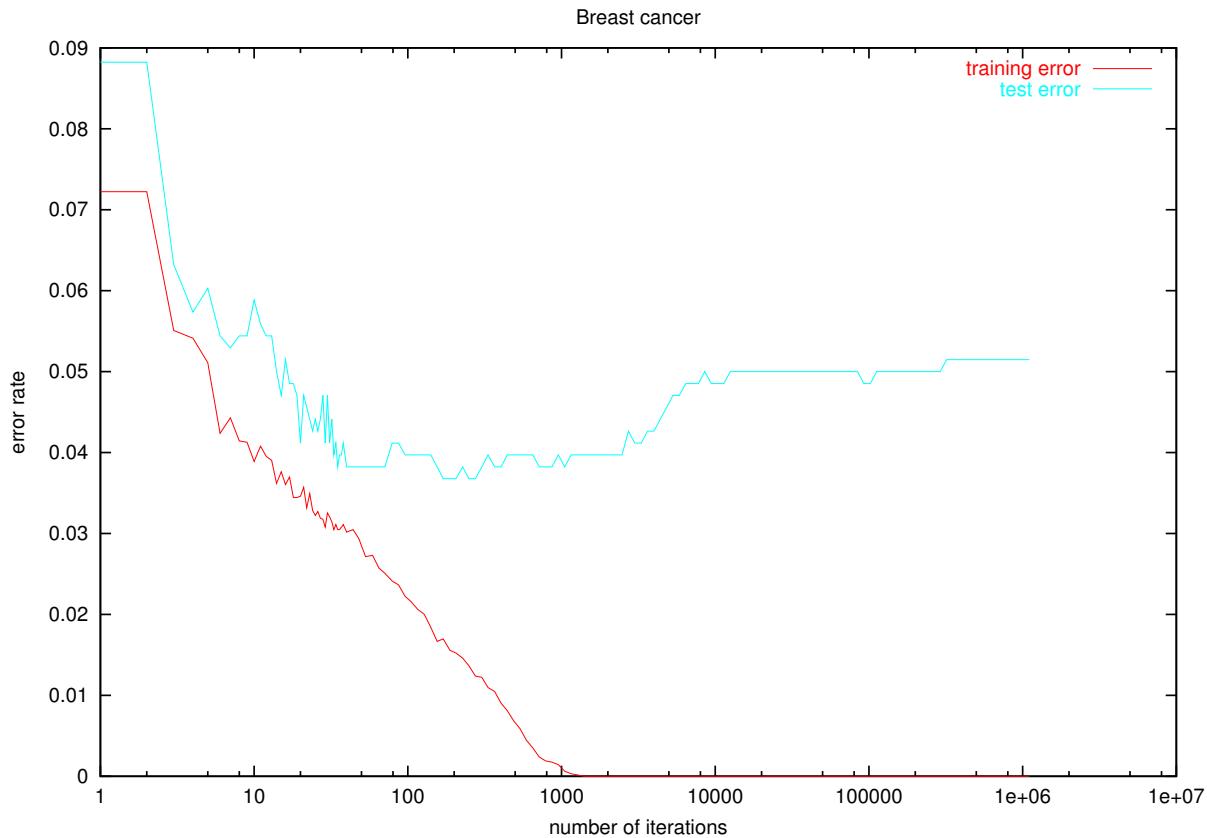
# AdaBoost

- Learning curves



# AdaBoost

- Learning curves



# Marginal AdaBoost

- Theory suggests:
  - minimization of the robust (marginal) training error

$$\widehat{R}_\theta(f) = \frac{1}{n} \sum_{i=1}^n I\{\tilde{p}_i < \theta\}$$

improves generalization.

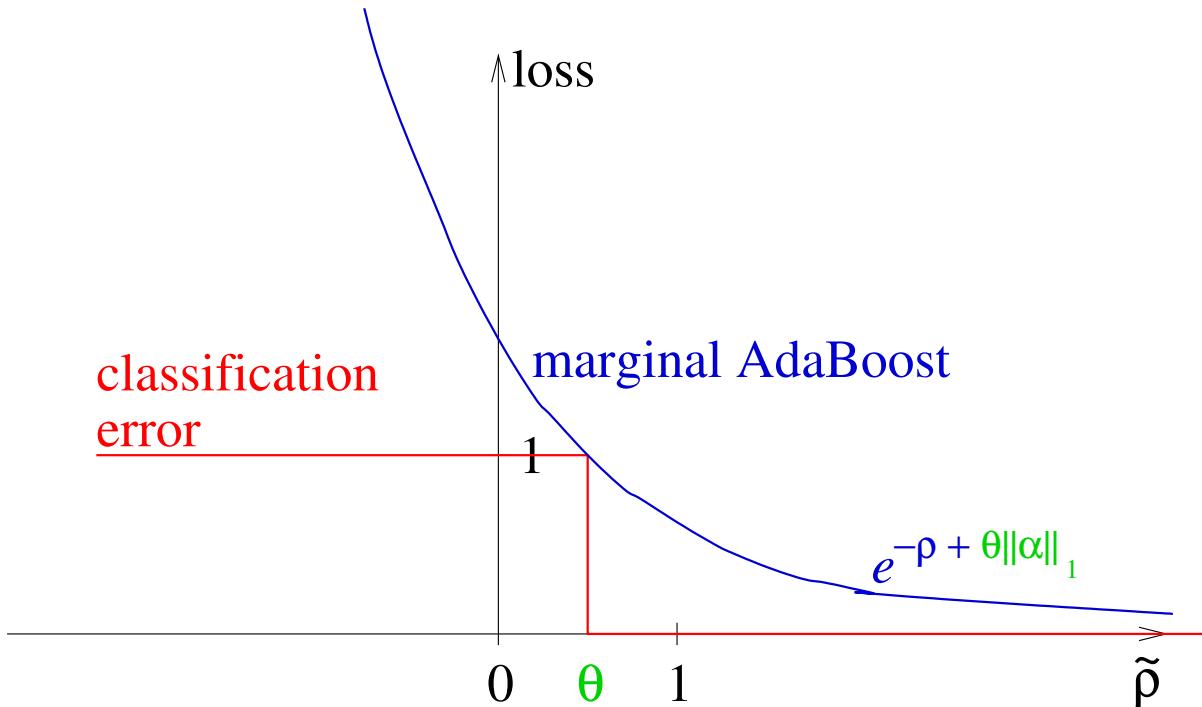
- Idea [Breiman '99, Rätsch - Warmuth '02]
  - directly minimize the exponential marginal risk

$$\widehat{R}_\theta^{(e)}(f) = \frac{1}{n} \sum_{i=1}^n e^{-\rho_i + \theta \|\alpha\|_1}$$

# Marginal AdaBoost

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- Loss functions



# Marginal AdaBoost

**MARGINALADABoost**( $D_n = ((\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n))$ ,  $\text{BASE}(D_n, \mathbf{w})$ ,  $\theta$ ,  $T$ )

```

1    $\mathbf{w} \leftarrow (1/n, \dots, 1/n)$      $\triangleright$  initial weight distribution on the training data
2   for  $t \leftarrow 1$  to  $T$ 
3      $h^{(t)} \leftarrow \text{BASE}(D_n, \mathbf{w})$      $\triangleright$  base classifier
4      $\gamma \leftarrow \sum_{i=1}^n w_i h^{(t)}(\mathbf{x}_i) y_i$      $\triangleright$  edge
5      $\alpha^{(t)} \leftarrow \frac{1}{2} \log \left( \frac{1+\gamma}{1-\gamma} \right) - \frac{1}{2} \log \left( \frac{1+\theta}{1-\theta} \right)$      $\triangleright$  weight of base classifier
6     if  $\alpha^{(t)} \leq 0$      $\triangleright$  equivalent to  $\gamma \geq \theta$ 
7       return  $f^{(t-1)}(\cdot) = \sum_{j=1}^{t-1} \alpha^{(j)} h^{(j)}(\cdot)$ 
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```

# Outline

- The supervised learning model
- AdaBoost
- RegBoost
- The graph Laplacian regularizer
- Experimental results

# RegBoost

- Idea: let  $\theta$  depend on the complexity of the base classifier

$$\theta = 2\lambda P(h)$$

- $P(h)$  is an arbitrary penalty functional
- $\lambda$  is a penalty coefficient
- Base objective

- minimize

$$R_1(h) = \varepsilon + \lambda P(h)$$

- standard regularized error minimization

# RegBoost

**REGBOOST** $\left(D_n, \text{BASE}(D_n, \mathbf{w}, \mathbf{P}), \mathbf{P}(h), \lambda, T\right)$

```

1    $\mathbf{w} \leftarrow (1/n, \dots, 1/n)$        $\triangleright$  initial weight distribution on the training data
2   for  $t \leftarrow 1$  to  $T$ 
3      $h^{(t)} \leftarrow \text{BASE}(D_n, \mathbf{w}, \mathbf{P})$        $\triangleright$  base classifier
4      $\gamma \leftarrow \sum_{i=1}^n w_i h^{(t)}(\mathbf{x}_i) y_i$        $\triangleright$  edge
5      $\theta \leftarrow 2\lambda P(h^{(t)})$        $\triangleright$  edge offset
6      $\alpha^{(t)} \leftarrow \frac{1}{2} \log \left( \frac{1+\gamma}{1-\gamma} \right) - \frac{1}{2} \log \left( \frac{1+\theta}{1-\theta} \right)$        $\triangleright$  weight of base classifier
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11   return  $f^{(T)}(\cdot) = \sum_{t=1}^T \alpha^{(t)} h^{(t)}(\cdot)$ 

```

# RegBoost

- Interpretation 1:  $L_1$  weight decay

- average edge offset ( $\sim$  average penalty)

$$\bar{\theta} = \frac{\sum_{t=1}^T \alpha^{(t)} \theta^{(t)}}{\sum_{t=1}^T \alpha^{(t)}}$$

- REGBOOST minimizes

$$\frac{1}{n} \sum_{i=1}^n \exp(-\rho_i + \bar{\theta} \|\alpha\|_1)$$

- weight decay coefficient  $\bar{\theta}$  is adaptive

# RegBoost

- Interpretation 2: adaptive marginal error minimization

- REGBOOST minimizes

$$\frac{1}{n} \sum_{i=1}^n I\{\tilde{\rho}_i < \bar{\theta}\}$$

- margin parameter  $\bar{\theta}$  is adaptive

- Interpretation 3: pool reduction

- decreased number (complexity) of base classifiers:

$$\#\{h : \gamma > \theta\} < \#\{h : \gamma > 0\}$$

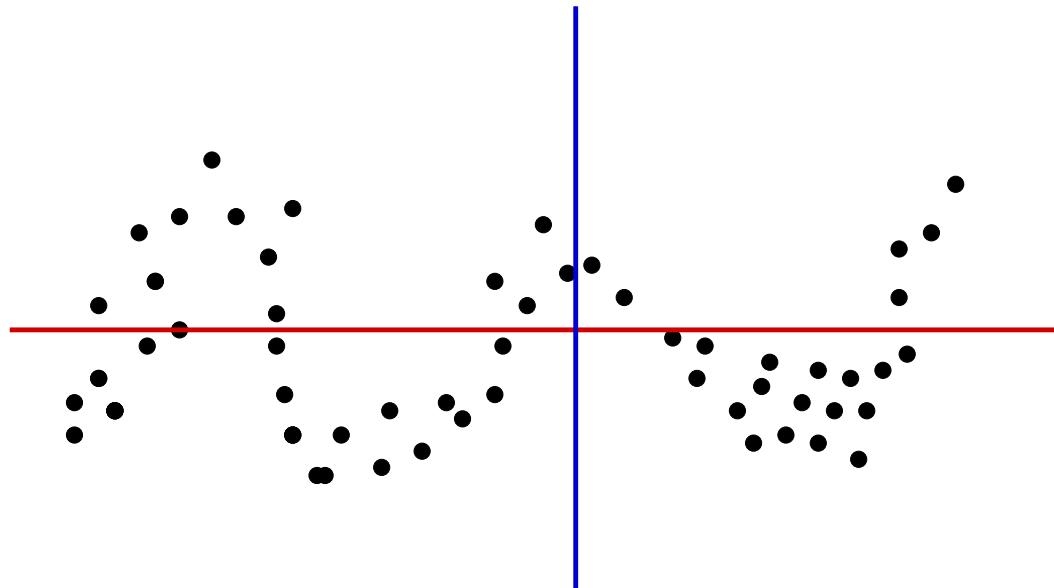
# Outline

- The supervised learning model
- AdaBoost
- RegBoost
- The graph Laplacian regularizer
- Experimental results

# The graph Laplacian regularizer

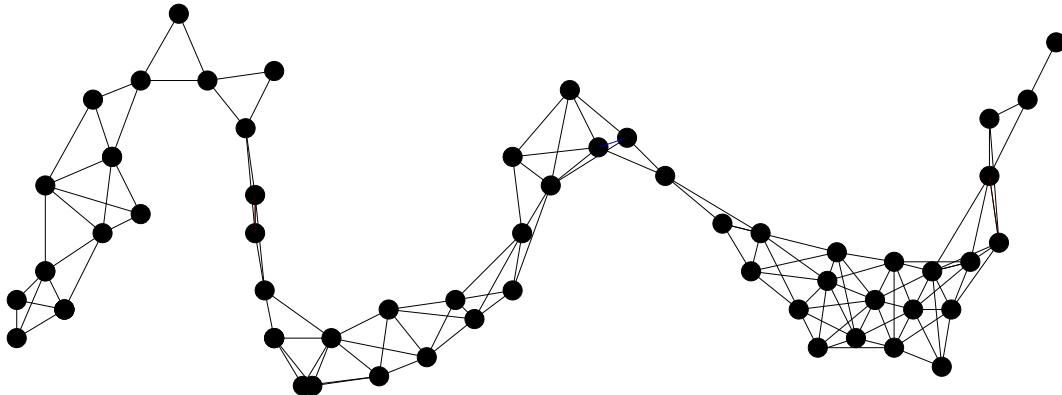
58

- Motivation:



# The graph Laplacian regularizer

- The neighborhood graph:



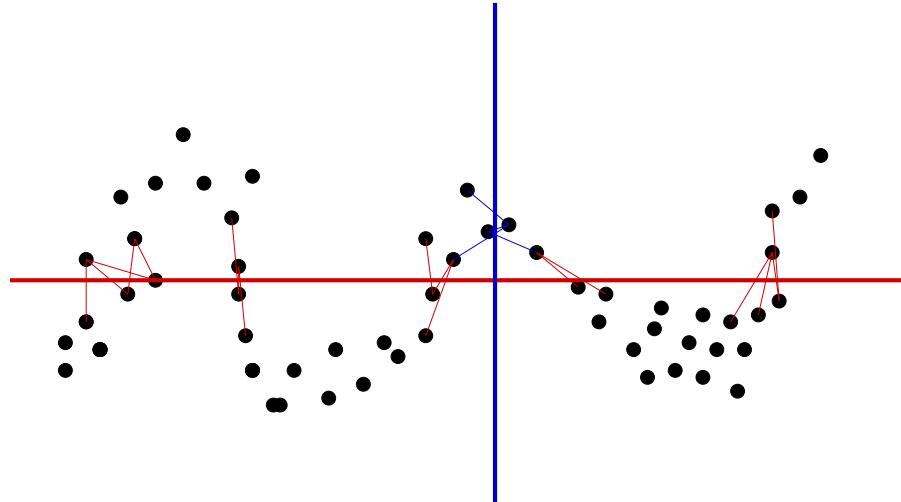
- $G = (\mathcal{V}, \mathcal{E})$
- $\mathcal{V} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$
- $\mathcal{E} = \{(\mathbf{x}_i, \mathbf{x}_j) : \|\mathbf{x}_i - \mathbf{x}_j\| < r\}$  (or  $k$  nearest neighbors)
- adjacency matrix:  $W_{ij} = I\{(\mathbf{x}_i, \mathbf{x}_j) \in \mathcal{E}\}$

# The graph Laplacian regularizer

- The penalty:

$$P_{\mathcal{L}}(h) = \sum_{i=1}^n \sum_{j=i+1}^n (h(\mathbf{x}_i) - h(\mathbf{x}_j))^2 W_{ij},$$

- $P_{\mathcal{L}}(h)$  is proportional to the number of neighbors that  $h$  separates



- related to dimensionality reduction [Belkin - Niyogi '03] and spectral clustering [Shi - Malik '00]

# Outline

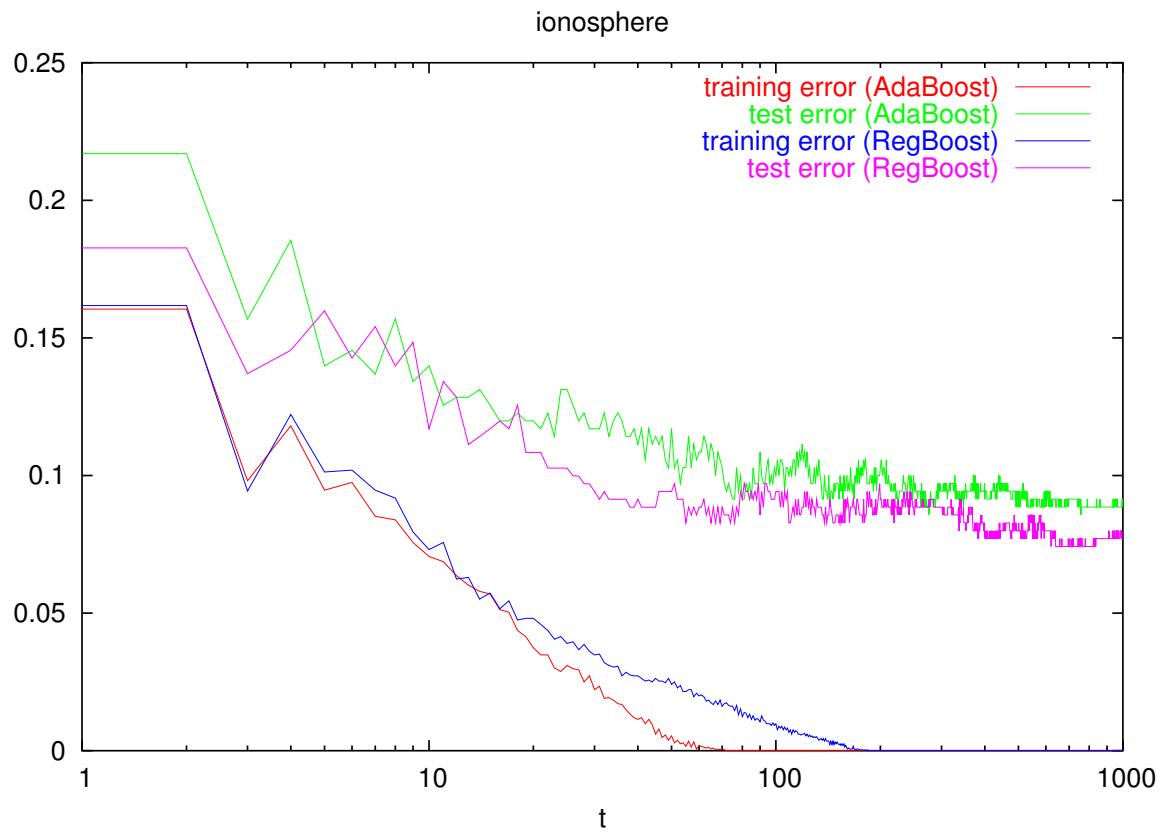
- The supervised learning model
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# Experimental results

- Setup
  - decision stumps
  - 8 nearest neighbors
  - $5 \times$  CV for  $\lambda$
  - $10 \times$  CV for test
  - UCI datasets

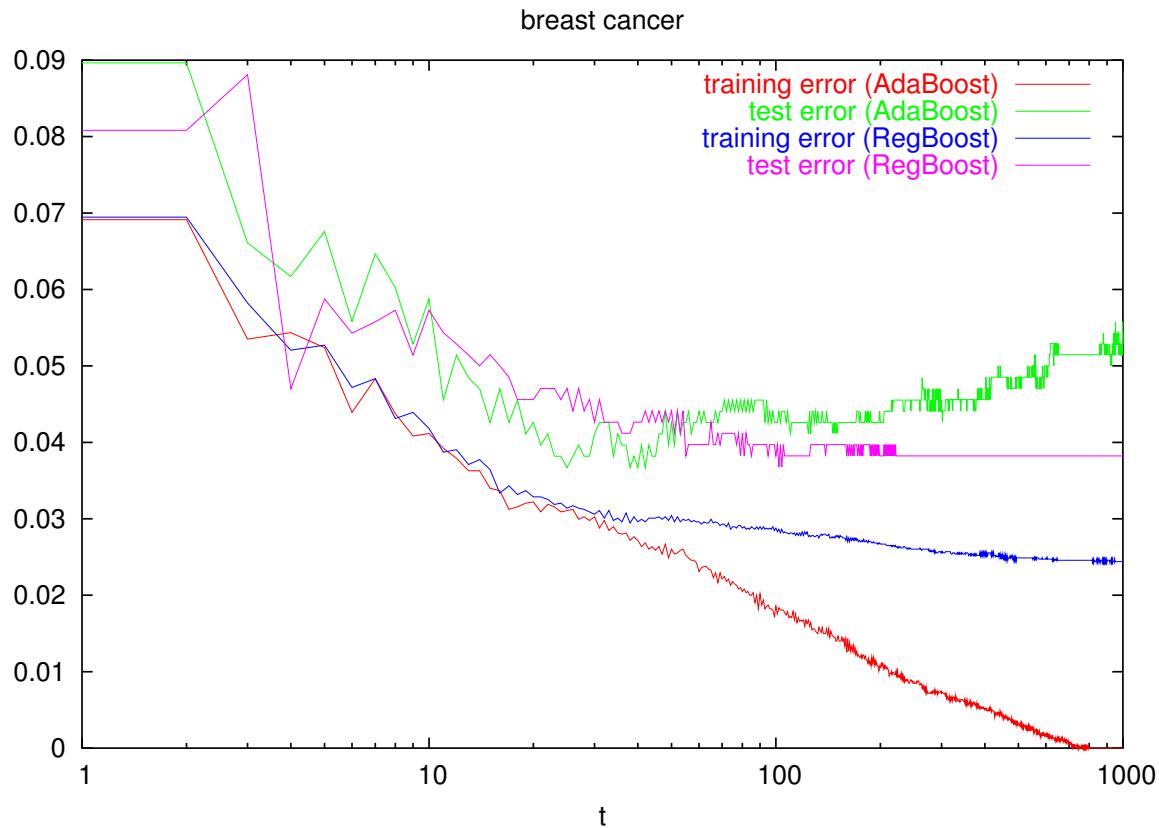
# Experimental results

- Ionosphere



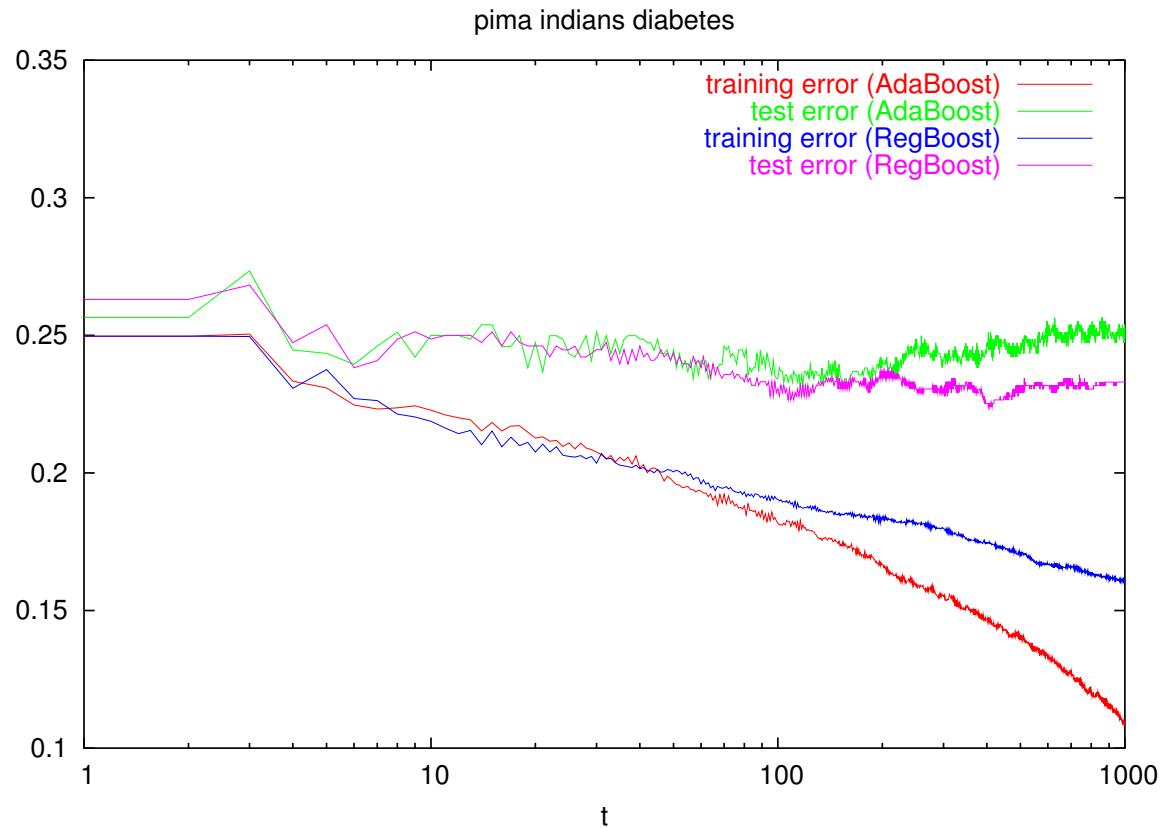
# Experimental results

- Breast cancer



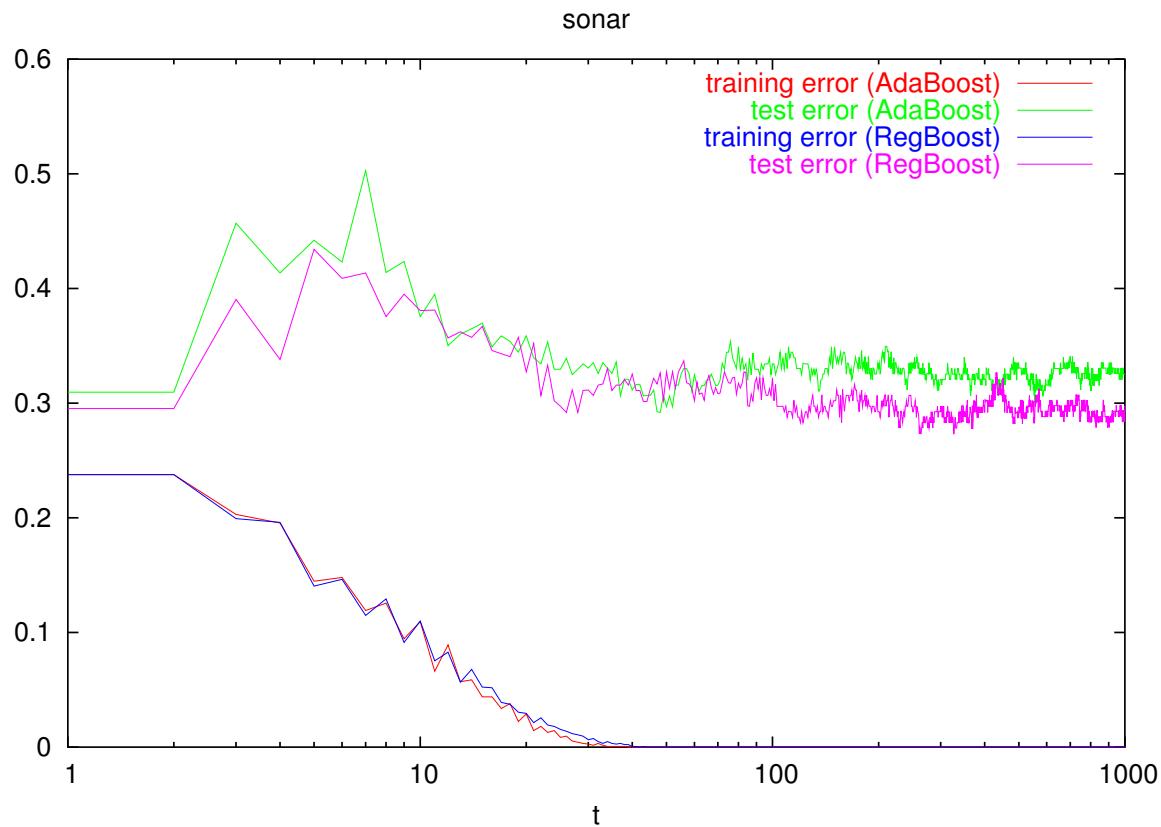
# Experimental results

- Pima Indians diabetes



# Experimental results

- Sonar



# Experimental results

- Discussion

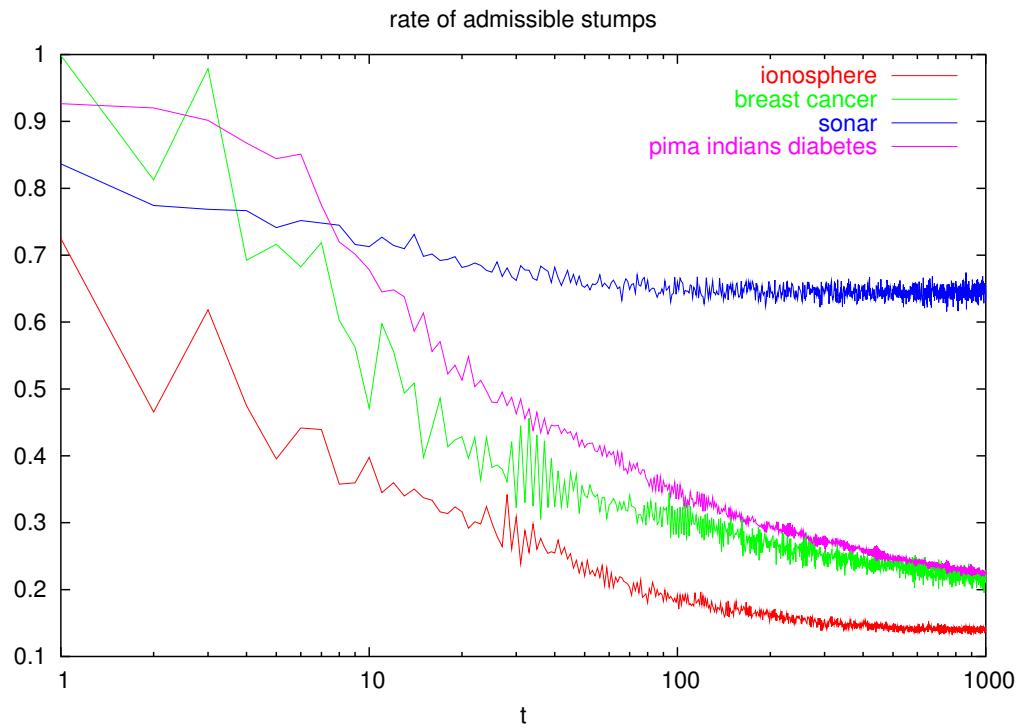
- test error is always better, although not significantly
- the difference between test and training errors decreases significantly
- final classifier is significantly sparser

data set	# of stumps ( $T = 1000$ )	
	ADABOOST	REGBOOST
ionosphere	182	114
breast cancer	58	30
pima Indians diabetes	175	91
sonar	233	199

# Experimental results

- Pool reduction

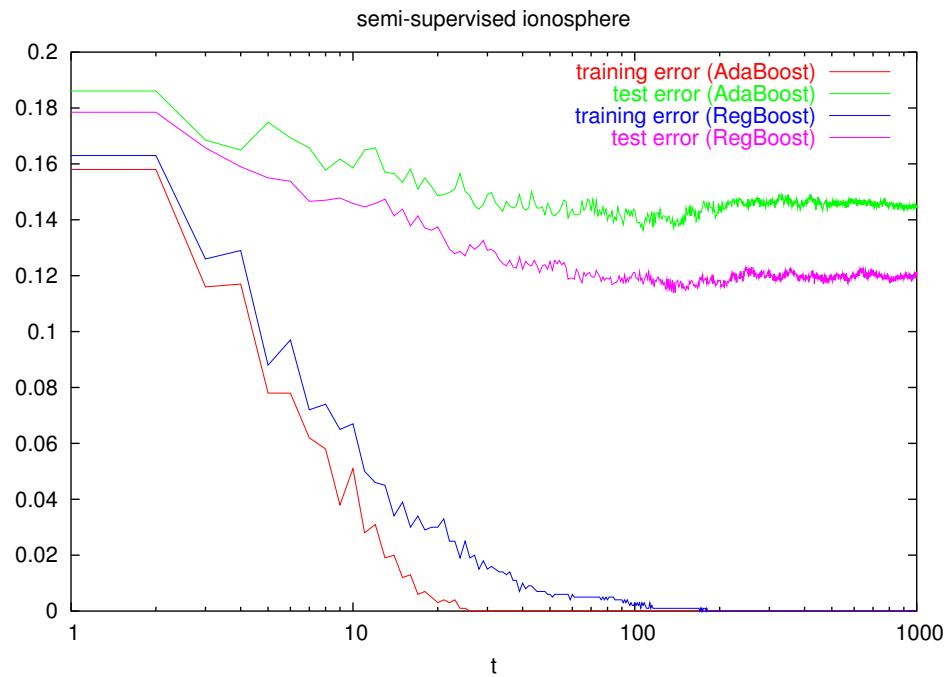
- the number of admissible stumps drops significantly



# Experimental results

- Semi-supervised learning

- the penalty can be calculated on **unlabeled points**
- ionosphere, 100 labeled, 251 unlabeled



# Conclusion

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- Combination of two powerful ideas, boosting and manifold learning
- Simple modification to AdaBoost
- Improves generalization, sparsity
- Semi-supervised approach: improves on AdaBoost and beats other manifold-based semi-supervised algorithms by far