

# Support Vector Machines: Duality and Leave-One-Out

CS4780/5780 – Machine Learning  
Fall 2013

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Reading: Schoelkopf/Smola Chapter 7.3, 7.5  
Cristianini/Shawe-Taylor Chapter 2-2.1.1

# (Batch) Perceptron Algorithm

Input:  $S = ((\vec{x}_1, y_1), \dots, (\vec{x}_n, y_n))$ ,  $\vec{x}_i \in \mathbb{R}^N$ ,  $y_i \in \{-1, 1\}$ ,  
 $I \in [1, 2, \dots]$

Algorithm:

- $\vec{w}_0 = \vec{0}$ ,  $k = 0$
- repeat
  - FOR  $i=1$  TO  $n$ 
    - \* IF  $y_i(\vec{w}_k \cdot \vec{x}_i) \leq 0$  ### makes mistake
      - $\vec{w}_{k+1} = \vec{w}_k + y_i \vec{x}_i$
      - $k = k + 1$
    - \* ENDIF
  - ENDFOR
- until  $I$  iterations reached

# Dual (Batch) Perceptron Algorithm

Input:  $S = ((\vec{x}_1, y_1), \dots, (\vec{x}_n, y_n))$ ,  $\vec{x}_i \in \mathbb{R}^N$ ,  $y_i \in \{-1, 1\}$ ,  
 $I \in [1, 2, \dots]$

Dual Algorithm:

- $\forall i \in [1..n] : \alpha_i = 0$
- repeat
  - FOR  $i=1$  TO  $n$ 
    - \* IF  $y_i \left( \sum_{j=1}^n \alpha_j y_j (\vec{x}_j \cdot \vec{x}_i) \right) \leq 0$ 
      - $\alpha_i = \alpha_i + 1$
    - \* ENDIF
  - ENDFOR
- until  $I$  iterations reached

Primal Algorithm:

- $\vec{w} = \vec{0}$ ,  $k = 0$
- repeat
  - FOR  $i=1$  TO  $n$ 
    - \* IF  $y_i (\vec{w} \cdot \vec{x}_i) \leq 0$ 
      - $\vec{w} = \vec{w} + y_i \vec{x}_i$
    - \* ENDIF
  - ENDFOR
- until  $I$  iterations reached

# SVM Solution as Linear Combination

- Primal OP:

$$\begin{aligned} \text{minimize:} \quad & P(\vec{w}, b, \vec{\xi}) = \frac{1}{2} \vec{w} \cdot \vec{w} + C \sum_{i=1}^n \xi_i \\ \text{subject to:} \quad & \forall_{i=1}^n : y_i [\vec{w} \cdot \vec{x}_i + b] \geq 1 - \xi_i \\ & \forall_{i=1}^n : \xi_i \geq 0 \end{aligned}$$

- Theorem: The solution  $\vec{w}^*$  can always be written as a linear combination

$$\vec{w}^* = \sum_{i=1}^n \alpha_i y_i \vec{x}_i$$

of the training vectors with  $0 \leq \alpha_i \leq C$ .

- Properties:

- Factor  $\alpha_i$  indicates “influence” of training example  $(x_i, y_i)$ .
- If  $\xi_i > 0$ , then  $\alpha_i = C$ .
- If  $0 \leq \alpha_i < C$ , then  $\xi_i = 0$ .
- $(x_i, y_i)$  is a Support Vector, if and only if  $\alpha_i > 0$ .
- If  $0 < \alpha_i < C$ , then  $y_i(x_i \cdot \vec{w}^* + b) = 1$ .
- SVM-light outputs  $\alpha_i$  using the “-a” option

# Dual SVM Optimization Problem

- Primal Optimization Problem

$$\begin{aligned} \text{minimize:} \quad & P(\vec{w}, b, \vec{\xi}) = \frac{1}{2} \vec{w} \cdot \vec{w} + C \sum_{i=1}^n \xi_i \\ \text{subject to:} \quad & \forall_{i=1}^n : y_i [\vec{w} \cdot \vec{x}_i + b] \geq 1 - \xi_i \\ & \forall_{i=1}^n : \xi_i \geq 0 \end{aligned}$$

- Dual Optimization Problem

$$\begin{aligned} \text{maximize:} \quad & D(\vec{\alpha}) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n y_i y_j \alpha_i \alpha_j (\vec{x}_i \cdot \vec{x}_j) \\ \text{subject to:} \quad & \sum_{i=1}^n y_i \alpha_i = 0 \\ & \forall_{i=1}^n : 0 \leq \alpha_i \leq C \end{aligned}$$

- Theorem: If  $\vec{w}^*$  is the solution of the Primal and  $\alpha^*$  is the solution of the Dual, then

$$\vec{w}^* = \sum_{i=1}^n \alpha_i^* y_i \vec{x}_i$$

# Leave-One-Out (i.e. n-fold CV)

- Training Set:  $S = ((x_1, y_1), \dots, (x_n, y_n))$
- Approach: Repeatedly leave one example out for testing.

Train on	Test on
$(x_2, y_2), (x_3, y_3), (x_4, y_4), \dots, (x_n, y_n)$	$(x_1, y_1)$
$(x_1, y_1), (x_3, y_3), (x_4, y_4), \dots, (x_n, y_n)$	$(x_2, y_2)$
$(x_1, y_1), (x_2, y_2), (x_4, y_4), \dots, (x_n, y_n)$	$(x_3, y_3)$
...	...
$(x_1, y_1), (x_2, y_2), (x_3, y_3), \dots, (x_{n-1}, y_{n-1})$	$(x_n, y_n)$

- Estimate:  $Err_{loo}(A) = \frac{1}{n} \sum_{i=1}^n \Delta(h_i(x_i), y_i)$
- Question: Is there a cheaper way to compute this estimate?

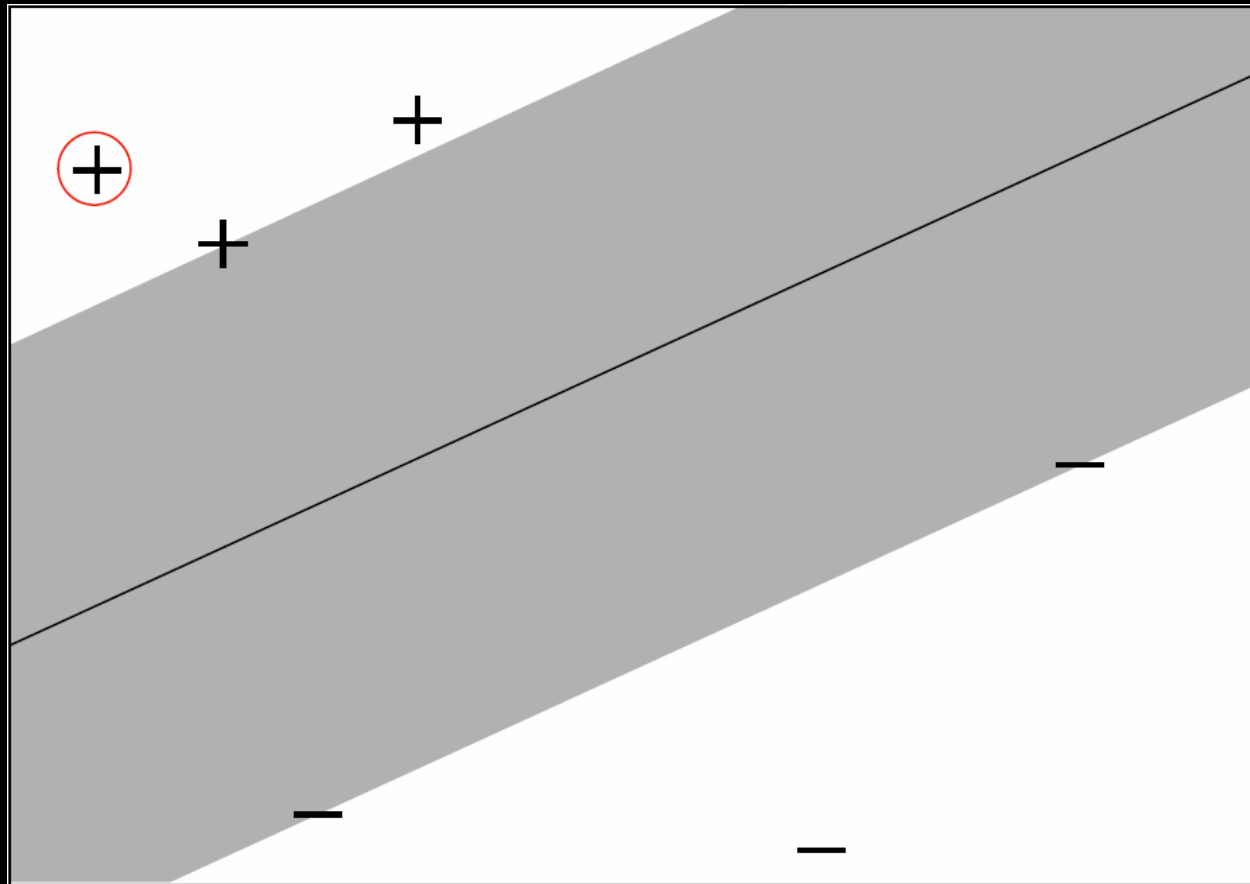
# Necessary Condition for Leave-One-Out Error

- Lemma: For SVM,  $[h_i(\vec{x}_i) \neq y_i] \Rightarrow [2\alpha_i R^2 + \xi_i \geq 1]$
- Input:
  - $\alpha_i$  dual variable of example  $i$
  - $\xi_i$  slack variable of example  $i$
  - $\|\vec{x}_i\| \leq R$  bound on length
- Example:

Value of $2\alpha_i R^2 + \xi_i$	Leave-one-out Error?
0.0	Must be Correct
0.7	Must be Correct
3.5	Error
0.1	Must be Correct
1.3	Correct
...	...

# Case 1: Example is not SV

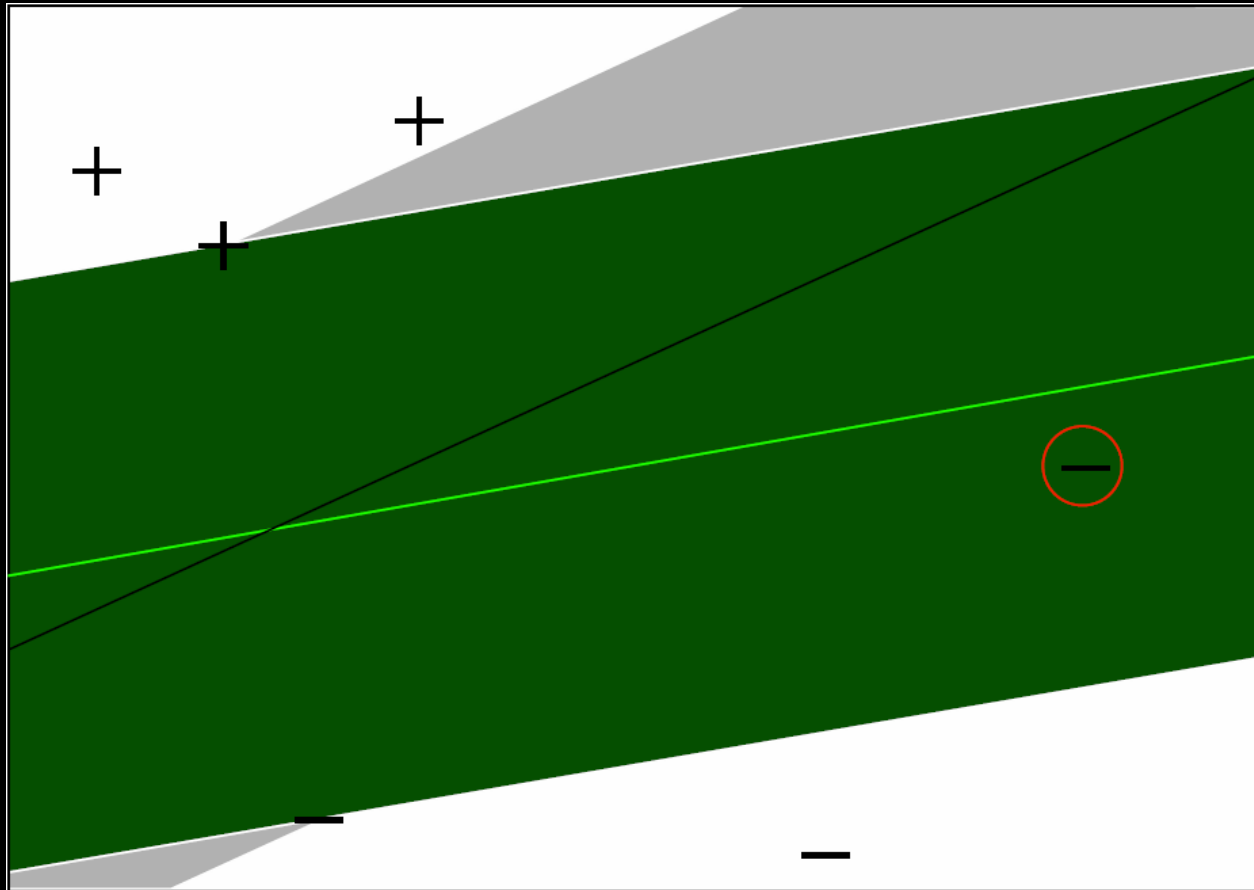
Criterion:  $(\alpha_i = 0) \Rightarrow (\xi_i = 0) \Rightarrow (2 \alpha_i R^2 + \xi_i < 1) \Rightarrow \text{Correct}$





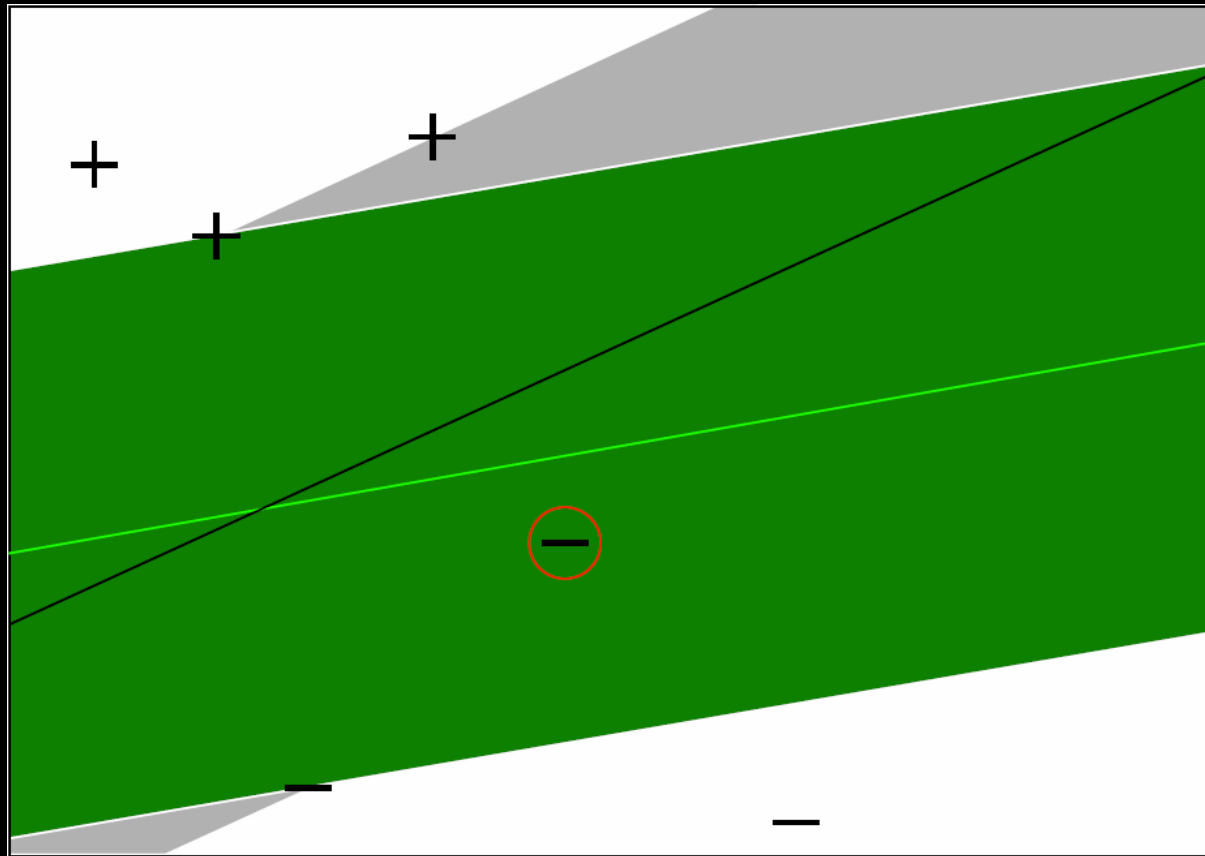
# Case 2: Example is SV with Low Influence

Criterion:  $(\alpha_i < 0.5/R^2 < C) \Rightarrow (\xi_i = 0) \Rightarrow (2\alpha_i R^2 + \xi_i < 1) \Rightarrow \text{Correct}$



# Case 3: Example has Small Training Error

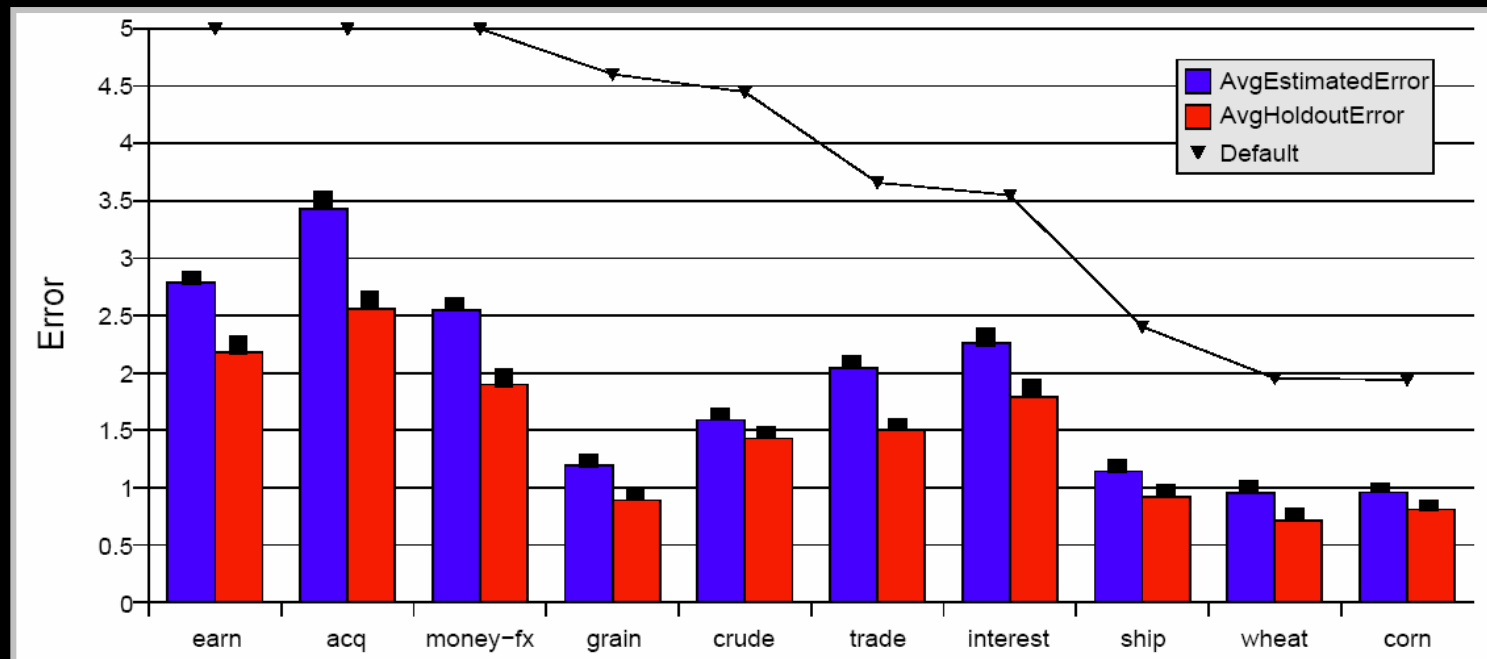
Criterion:  $(\alpha_i = C) \Rightarrow (\xi_i < 1 - 2CR^2) \Rightarrow (2\alpha_i R^2 + \xi_i < 1) \Rightarrow \text{Correct}$



# Experiment: Reuters Text Classification

## Experiment Setup

- 6451 Training Examples
- 6451 Validation Examples to estimate true Prediction Error
- Comparison between Leave-One-Out upper bound and error on Validation Set (average over 10 test/validation splits)



# Fast Leave-One-Out Estimation for SVMs

Lemma: Training errors are always Leave-One-Out Errors.

Algorithm:

- $(R, \alpha, \xi) = \text{trainSVM}(S_{\text{train}})$
- FOR  $(x_i, y_i) \in S_{\text{train}}$ 
  - IF  $\xi_i > 1$  THEN  $\text{loo}++$ ;
  - ELSE IF  $(2 \alpha_i R^2 + \xi_i < 1)$  THEN  $\text{loo} = \text{loo}$ ;
  - ELSE  $\text{trainSVM}(S_{\text{train}} \setminus \{(x_i, y_i)\})$  and test explicitly

Experiment:

Training Data	Retraining Steps (%)	CPU-Time (sec)
Reuters (n=6451)	0.58%	32.3
WebKB (n=2092)	20.42%	235.4
Ohsumed (n=10000)	2.56%	1132.3