Support Vector Machines: Duality and Leave-One-Out

CS4780/5780 – Machine Learning
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Reading: Schoelkopf/Smola Chapter 7.3, 7.5
Cristianini/Shawe-Taylor Chapter 2-2.1.1

Outline

- Perceptron in dual representation
- Support Vector Machine dual representation
- Analyzing the dual representation
- Bounds on the leave-one-out error of SVMs
- Relationship between expected margin and expected generalization error

(Batch) Perceptron Algorithm

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

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

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 α_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 $y_i(x_i\, w^* + b) = 1$.
  - SVM-light outputs α_i using the "-a" option

Dual SVM Optimization Problem

- Primal Optimization Problem

$$\text{minimize:} \quad P(\vec{w}, b, \vec{\xi}) = \frac{1}{2}\vec{w}\cdot\vec{w} + C\sum_{i=1}^{n}\xi_i$$

$$\text{subject to:} \quad \forall_{i=1}^{n} : y_i[\vec{w}\cdot\vec{x}_i + b] \geq 1 - \xi_i$$

$$\forall_{i=1}^{n} : \xi_i \geq 0$$

- Dual Optimization Problem

$$\text{maximize:} \quad D(\vec{\alpha}) = \sum_{i=1}^{n}\alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} y_i y_j \alpha_i \alpha_j (\vec{x}_i \cdot \vec{x}_j)$$

$$\text{subject to:} \quad \sum_{i=1}^{n} y_i \alpha_i = 0$$

$$\forall_{i=1}^{n} : 0 \leq \alpha_i \leq C$$

- Theorem: If w* is the solution of the Primal and α* 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?

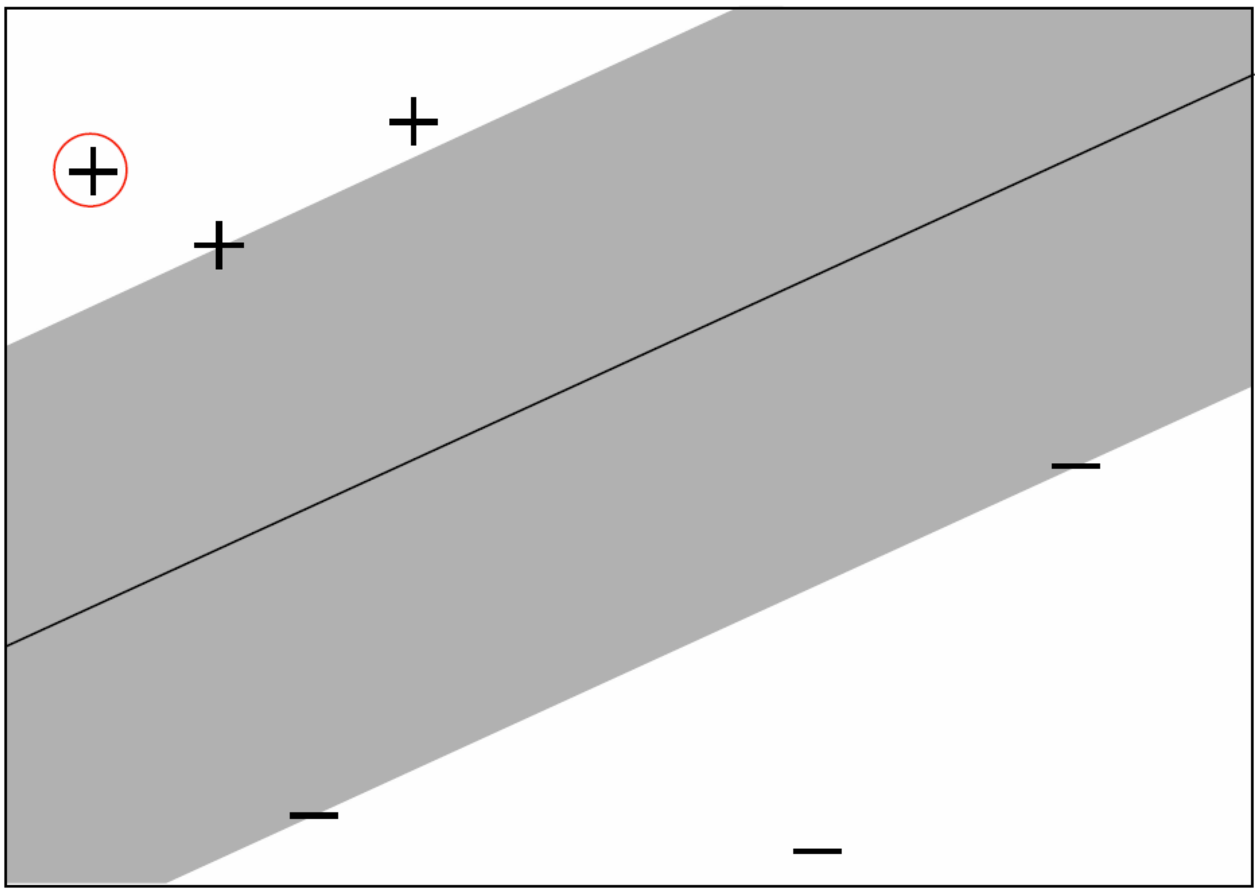
Necessary Condition for Leave-One-Out Error

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

Value of 2 α_i R^2 + ξ_i	Leave-one-out Error?
0.0	Correct
0.7	Correct
3.5	Error
0.1	Correct
1.3	Correct
…	…

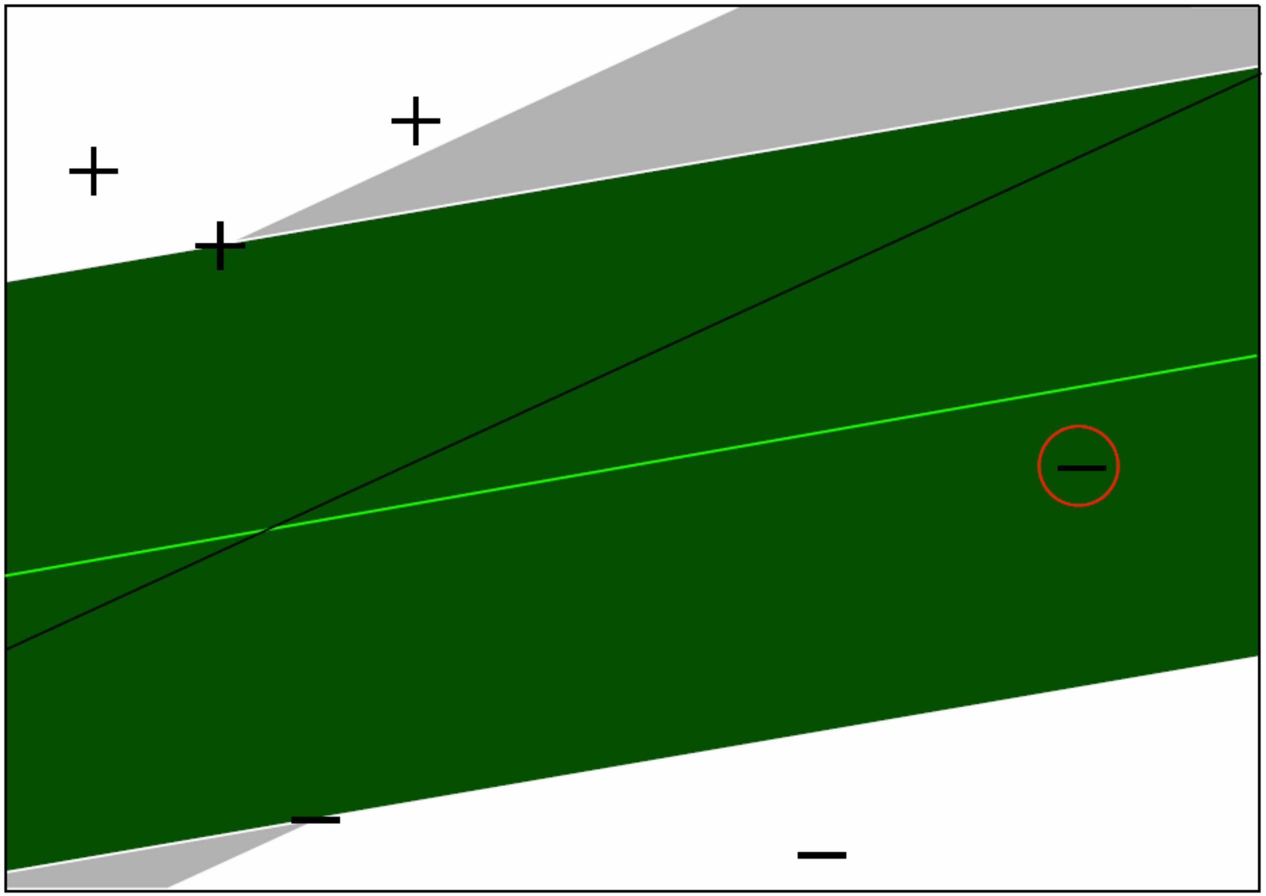
Case 1: Example is not SV

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



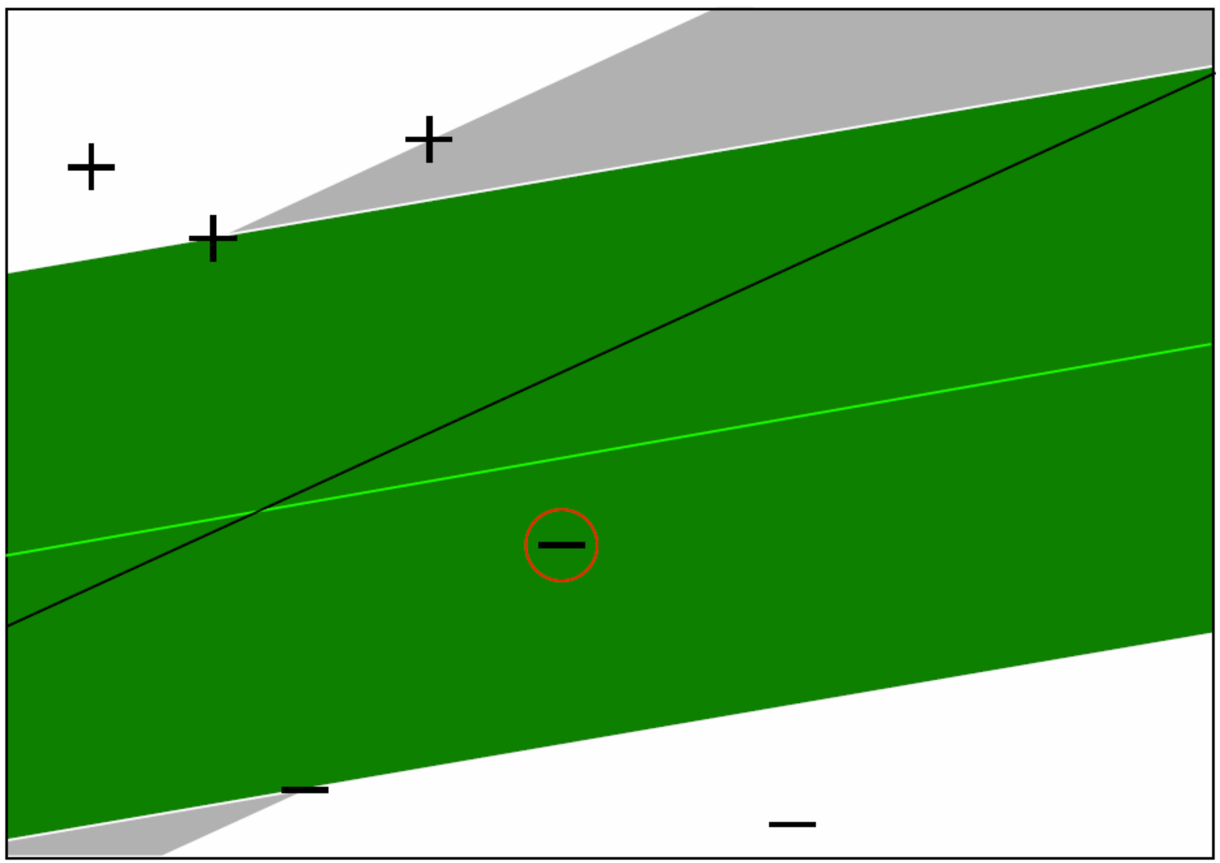
Case 2: Example is SV with Low Influence

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



Case 3: Example has Small Training Error

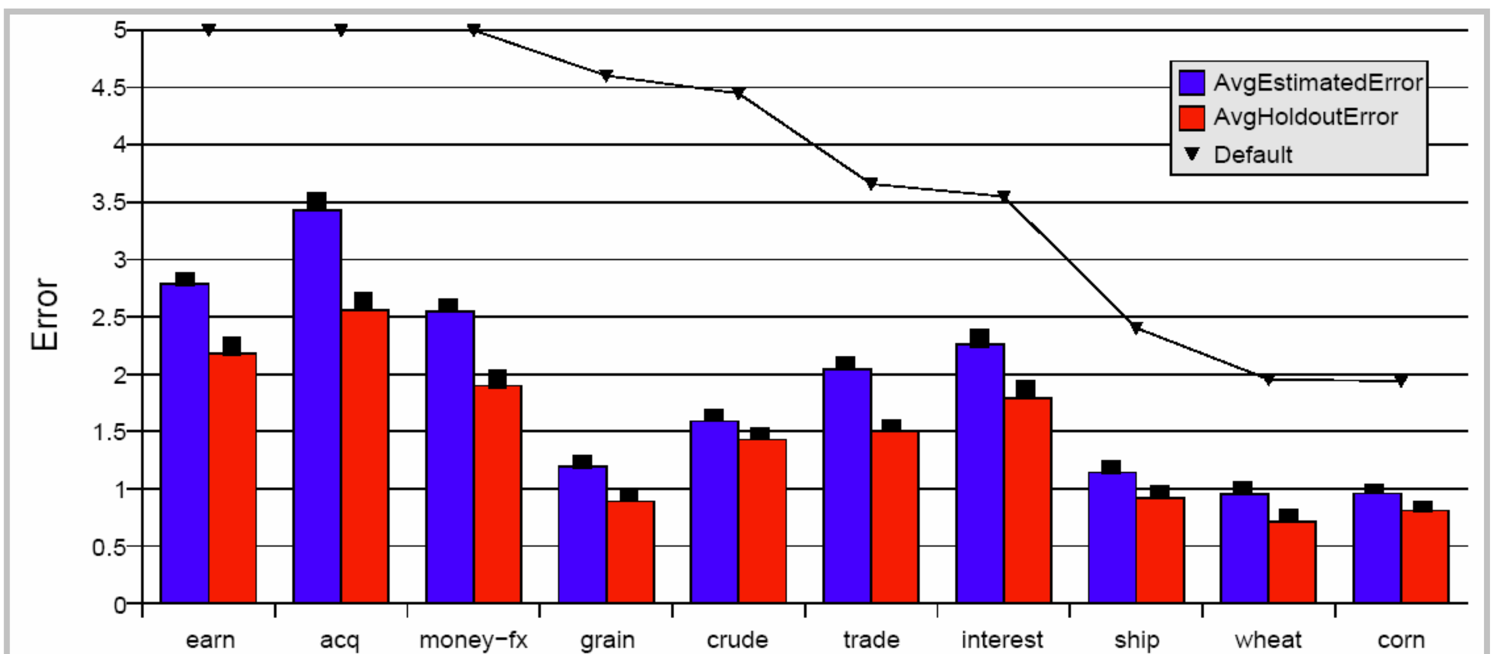
Criterion: $(\alpha_l = C) \Rightarrow (\xi_i < 1\text{-}2CR^2) \Rightarrow (2\alpha_i R^2 + \xi_i < 1) \Rightarrow$ Correct



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:

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