Support Vector Machines: Soft Margin and Duality

CS6780 – Advanced Machine Learning
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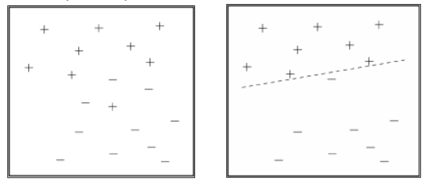
Reading: Schoelkopf/Smola Chapter 7.3, 7.5
Cristianini/Shawe-Taylor Chapter 2-2.1.1

Non-Separable Training Data

- Limitations of hard-margin formulation
  - For some training data, there is no separating hyperplane.
  - Complete separation (i.e. zero training error) can lead to suboptimal prediction error.



Soft-Margin Separation

Idea: Maximize margin and minimize training

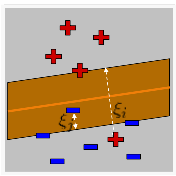
Hard-Margin OP (Primal):

$$\min_{\vec{w},b} \frac{1}{2}\vec{w}\cdot\vec{w}$$
$$s.t.\quad y_1(\vec{w}\cdot\vec{x}_1+b)\geq 1$$
$$\dots$$
$$y_n(\vec{w}\cdot\vec{x}_n+b)\geq 1$$

Soft-Margin OP (Primal):

$$\min_{\vec{w},\vec{\xi},b} \frac{1}{2}\vec{w}\cdot\vec{w}+C\sum_{i=1}^{n}\xi_i$$
$$s.t.\quad y_1(\vec{w}\cdot\vec{x}_1+b)\geq 1-\xi_1 \wedge \xi_1\geq 0$$
$$\dots$$
$$y_n(\vec{w}\cdot\vec{x}_n+b)\geq 1-\xi_n \wedge \xi_n\geq 0$$

- Slack variable ξ_i measures by how much (x_i,y_i) fails to achieve margin δ
- $\Sigma\xi_i$ is upper bound on number of training errors
- C is a parameter that controls trade-off between margin and training error.

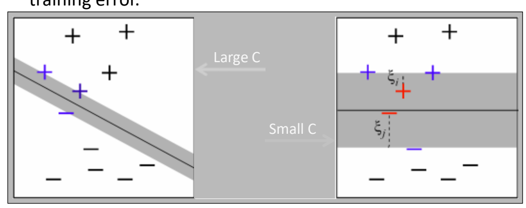


Controlling Soft-Margin Separation

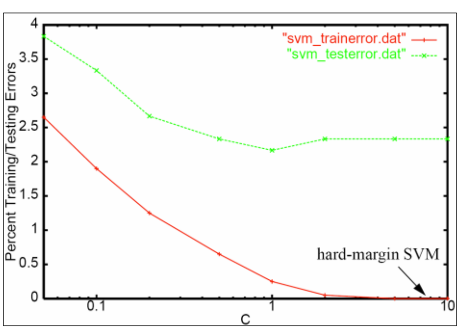
- $\Sigma\xi_i$ is upper bound on number of training errors
- C is a parameter that controls trade-off between margin and training error.

Soft-Margin OP (Primal):

$$\min_{\vec{w},\vec{\xi},b} \frac{1}{2}\vec{w}\cdot\vec{w}+C\sum_{i=1}^{n}\xi_i$$
$$s.t.\quad y_1(\vec{w}\cdot\vec{x}_1+b)\geq 1-\xi_1 \wedge \xi_1\geq 0$$
$$\dots$$
$$y_n(\vec{w}\cdot\vec{x}_n+b)\geq 1-\xi_n \wedge \xi_n\geq 0$$



Example Reuters “acq”: Varying C



Example: Margin in High-Dimension

Training Sample S_{train}	x_1	x_2	x_3	x_4	x_5	x_6	x_7	y
	1	0	0	1	0	0	0	1
	1	0	0	0	1	0	0	1
	0	1	0	0	0	1	0	-1
	0	1	0	0	0	0	1	-1
	w_1	w_2	w_3	w_4	w_5	w_6	w_7	**b**
Hyperplane 1	1	1	0	0	0	0	0	2
Hyperplane 2	0	0	0	1	1	-1	-1	0
Hyperplane 3	1	-1	1	0	0	0	0	0
Hyperplane 4	0.5	-0.5	0	0	0	0	0	0
Hyperplane 5	1	-1	0	0	0	0	0	0
Hyperplane 6	0.95	-0.95	0	0.05	0.05	-0.05	-0.05	0
Hyperplane 7	0.67	-0.67	0	0.33	0.33	-0.33	-0.33	0

(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:

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

- 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).
  - (x_i, y_i) is a Support Vector, if and only if $\alpha_i > 0$.
  - If $\xi_i > 0$, then $\alpha_i = C$.
  - If $0 \leq \alpha_i < C$, then $\xi_i = 0$.
  - 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

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

- Dual Optimization Problem

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

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

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

$\rightarrow h_i$ is the rule learned on $S \setminus \{(x_i, y_i)\}$

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

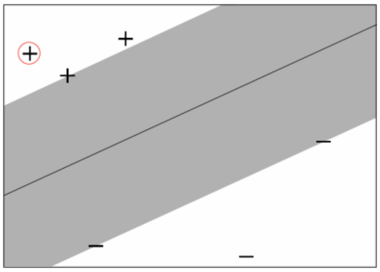
Necessary Condition for Leave-One-Out Error

- 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 $2\alpha_i R^2 + \xi_i$	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
…	…

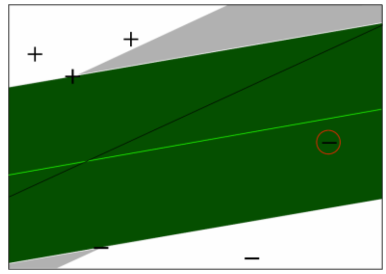
Case 1: Example is not SV

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



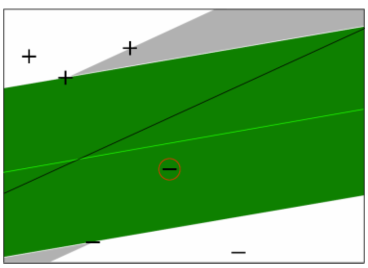
Case 2: Example is SV with Low Influence

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

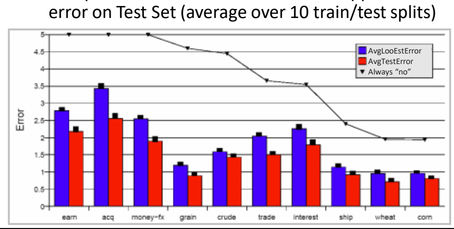
Criterion: $(\alpha_I = C)$ and $(\xi_i < 1\text{-}2CR^2) \rightarrow (2\alpha_i R^2+\xi_i < 1) \rightarrow$ Correct



Experiment: Reuters Text Classification

Experiment Setup

- 6451 Training Examples
- 6451 Test Examples to estimate true Prediction Error
- Comparison between Leave-One-Out upper bound and error on Test Set (average over 10 train/test 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 $\text{trainSVM}(S_{train} \setminus \{(x_i,y_i)\})$ 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