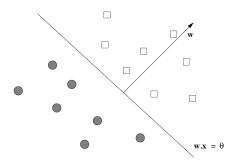
Learning in Big Data Analytics Support Vector Machines

Alexander Schönhuth



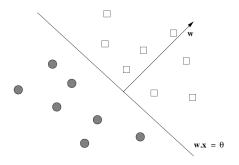
Bielefeld University November 17, 2021 Perceptrons Revisited





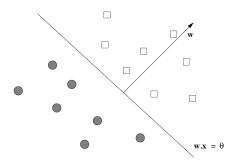
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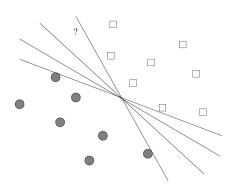




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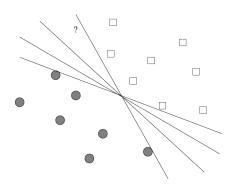




- ► Several half spaces (normal vectors) divide training data
- Question: any half space optimal, in a sensibly defined way?
- ▶ What to do if data cannot be separated (is *non-separable*)?



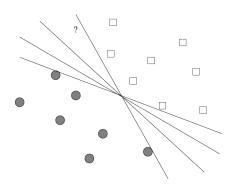




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SUPPORT VECTOR MACHINES: MOTIVATION

- ► Support vector machines (SVM's) address to choose most reasonable half space
- ► SVM's choose half space that maximizes the *margin*, i.e. the distance between data points and half space
- If separable, maximize distance between hyperplane and closest data points
- If not separable, minimize loss function that
 - penalizes misclassified points
 - penalizes points correctly classified but too close to hyperplane (to a lesser extent)



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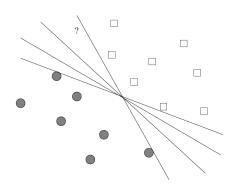
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- ► Outer hyperplanes come very close to data points
- ► So, inner hyperplanes are likely the better choice
- ► ™ Try to make explicit!

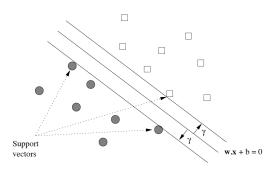




Separable Data



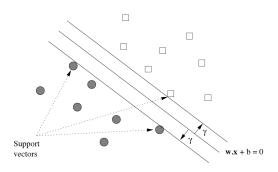
SEPARABLE DATA



- *Goal:* Select hyperplane $\mathbf{w} \cdot \mathbf{x} + b = 0$ that maximizes distance γ
- ► *Intuition*: The further away data from hyperplane, the more certain their classification
- ► Increases chances to correctly classify unseen data (to generalize)



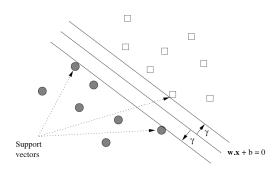
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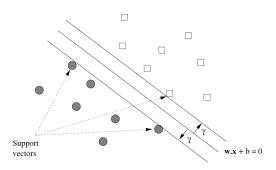
SUPPORT VECTORS



- \blacktriangleright Two parallel hyperplanes at distance γ touch one or more of support vectors
- ▶ In most cases, d-dimensional data set has d + 1 support vectors (but there can be more)



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Let $(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)$ be a training data set, where $\mathbf{x}_i \in \mathbb{R}^d, y_i \in \{-1, +1\}, i = 1, ..., n$.

PROBLEM: By varying \mathbf{w}, b , maximize γ such that

$$y_i(\mathbf{w}\mathbf{x}_i + b) \ge \gamma \quad \text{for all } i = 1, ..., n$$
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- ► Replacing **w** and *b* by 2**w** and 2*b* yields $y_i(2\mathbf{w}\mathbf{x}_i + 2b) \ge 2\gamma$
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Problem badly formulated Try again!



- ▶ Data set (\mathbf{x}_i, y_i) , i = 1, ..., n as before; let $H := \{\mathbf{x} \mid \mathbf{w}\mathbf{x} + b = 0\}$ be the hyperplane given by \mathbf{w} and b.
- ▶ Let

$$d(\mathbf{x}_i, H) := \min_{\mathbf{x}} \{ d(\mathbf{x}_i, \mathbf{x}) \mid \mathbf{w}\mathbf{x} + b = 0 \}$$
 (2)

be the distance between \mathbf{x}_i and H

▶ *Solution*: Impose additional constraint: consider only combinations $\mathbf{w} \in \mathbb{R}^d, b \in \mathbb{R}$ such that for support vectors \mathbf{x}

$$y_i(\mathbf{wx} + b) \in \{-1, +1\}$$
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• *Good Formulation:* By varying \mathbf{w} , b, maximize γ such that

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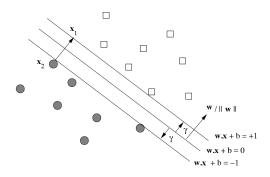
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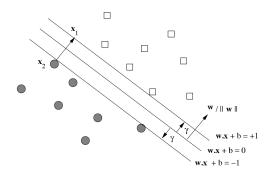


- \mathbf{w} , b, γ determined according to (3),(4)
- $ightharpoonup x_2$ is support vector on lower hyperplane, so by (3), $wx_2 + b = -1$
- Let x_1 be the projection of x_2 onto upper hyperplane:

$$\mathbf{x}_1 = \mathbf{x}_2 + 2\gamma \frac{\mathbf{w}}{||\mathbf{w}||} \tag{5}$$





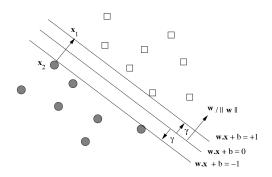


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Because $\mathbf{ww} = ||\mathbf{w}||^2$, and by further regrouping, we conclude that

$$\gamma = \frac{1}{||\mathbf{w}||} \tag{9}$$



Let dataset (\mathbf{x}_i, y_i) , i = 1, ..., n be as before.

EQUIVALENT PROBLEM FORMULATION:

By varying \mathbf{w} , b, minimize $||\mathbf{w}||$ subject to

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Optimizing under Constraints

- ► Topic is broadly covered
- Many packages can be used
- ► Target function $(||\mathbf{w}||)^2 = \sum_i w_i^2$ quadratic; well manageable



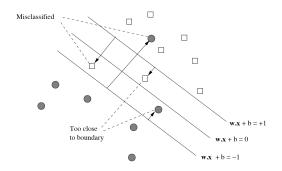
EXAMPLE



Non Separable Data



NON SEPARABLE DATA SETS



Situation:

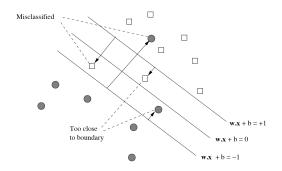
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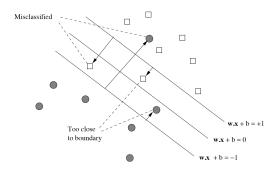
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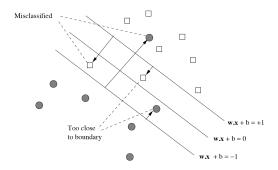






- ► *Situation:* No hyperplane can separate the data points correctly
- ► Approach:
 - Determine appropriate penalties for bad points
 - Solve original problem, by involving penalties

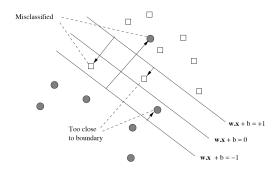




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Let (\mathbf{x}_i, y_i) , i = 1, ...n be training data, where

- $ightharpoonup \mathbf{x}_i = (x_{i1}, ..., x_{id}),$
- ▶ $y_i \in \{-1, +1\}$

and let **w** = $(w_1, ..., w_d)$.



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Minimize the following function:

$$f(\mathbf{w}, b) = \frac{1}{2} \sum_{j=1}^{d} w_j^2 + C \sum_{i=1}^{n} \max\{0, 1 - y_i(\sum_{j=1}^{d} w_j x_{ij} + b)\}$$
 (11)



$$f(\mathbf{w}, b) = \underbrace{\frac{1}{2} \sum_{j=1}^{d} w_j^2}_{\text{Seek minimal } ||\mathbf{w}||} + \underbrace{C \sum_{i=1}^{n} \max\{0, 1 - y_i(\sum_{j=1}^{d} w_j x_{ij} + b)\}}_{\text{Bad point penalty}}$$

- ▶ Minimizing ||w|| equivalent to minimizing monotone function of ||w||
 Minimizing f seeks minimal ||w||
- ▶ Vectors w and training data balanced in terms of basic units:

$$\frac{\partial(||\mathbf{w}||^2/2)}{\partial w_i} = w_i$$
 and $\frac{\partial(\sum_{j=1}^d w_j x_{ij} + b)}{\partial w_i} = x_{ij}$

- C is a regularization parameter
 - Large C: minimize misclassified points, but accept narrow margin
 - Small C: accept misclassified points, but widen margin



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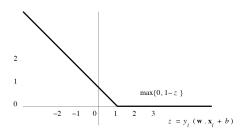
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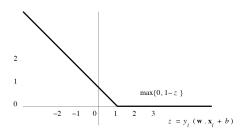
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 (12)



- ▶ $L(\mathbf{x}_i, y_i) = 0$ iff \mathbf{x}_i on the correct side of hyperplane with sufficient margin
- ▶ The worse x_i is located the greater $L(x_i, y_i)$



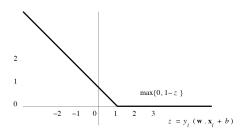
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Let the *hinge function L* be defined by

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Partial derivatives of hinge function:

$$\frac{\partial L}{\partial w_j} = \begin{cases} 0 & \text{if } y_i(\sum_{j=1}^d w_j x_{ij} + b) \ge 1\\ -y_i x_{ij} & \text{otherwise} \end{cases}$$
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Reflecting:

- ▶ If x_i is on right side with sufficient margin: nothing to be done
- ightharpoonup Otherwise adjust w_i to have x_i better placed



Let the *hinge function L* be defined by

$$L(\mathbf{x}_i, y_i) = \max\{0, 1 - y_i(\sum_{j=1}^d w_j x_{ij} + b)\}$$

Partial derivatives of hinge function:

$$\frac{\partial L}{\partial w_j} = \begin{cases} 0 & \text{if } y_i(\sum_{j=1}^d w_j x_{ij} + b) \ge 1\\ -y_i x_{ij} & \text{otherwise} \end{cases}$$
 (13)

Reflecting:

- ▶ If x_i is on right side with sufficient margin: nothing to be done
- ightharpoonup Otherwise adjust w_i to have \mathbf{x}_i better placed

GENERAL / FURTHER READING

Literature

► Mining Massive Datasets, Chapter 12, Section 3: http://infolab.stanford.edu/~ullman/mmds/ch12.pdf



Thank you for listening!

