Learning Maximum-Margin Hyperplanes: Support Vector Machines

soft margin

hard margin

hands on
session

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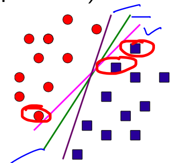
Machine Learning (CS771A)

Aug 24, 2016

Perceptron and (Lack of) Margins

- Perceptron learns a hyperplane (of many possible) that separates the classes

2 - dim



more preferred

green - max degree of sep

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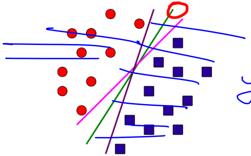
+1



$y = -1$

0 Training Error

- Standard Perceptron doesn't guarantee any "margin" around the hyperplane

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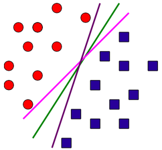


- Standard Perceptron doesn't guarantee any "margin" around the hyperplane
- Note: Possible to "artificially" introduce a margin in the Perceptron

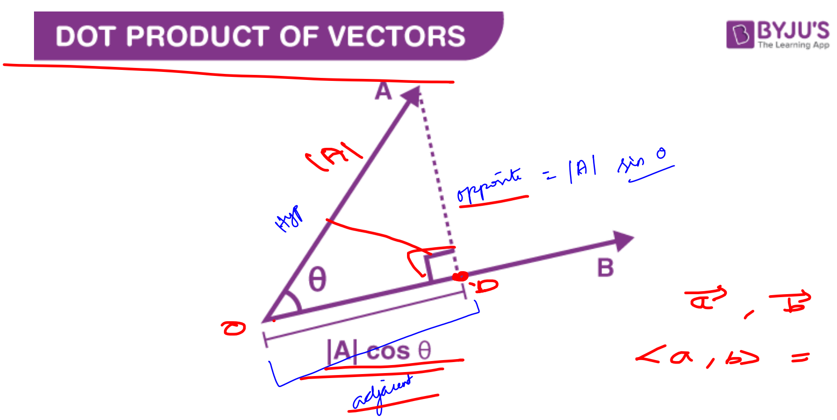
$$\vec{a} = [1, 2]$$

$$\vec{b} = [2, 3]$$

$$\vec{a} \cdot \vec{b} = \sum_i a_i b_i = 2 + 6 = 8$$

$$= \|\vec{a}\| \, \|\vec{b}\| \cos\theta$$

dot Products and margin



$\sin\theta = \frac{opp}{hyp}$

$= \frac{OD}{OA}$

$\cos\theta = \frac{OD}{OA}$

$\vec{a}, \vec{b}$

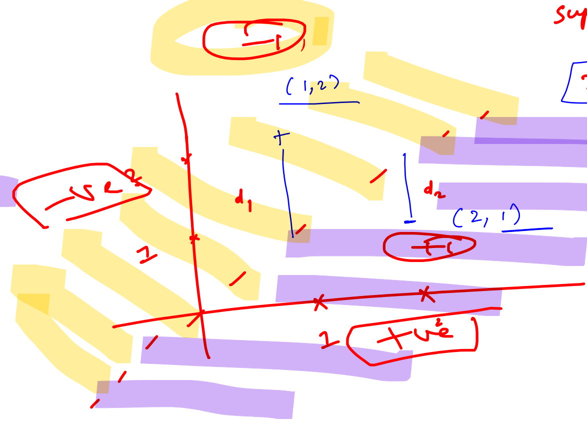
$\langle a, b \rangle =$

suppose Hyp plane is

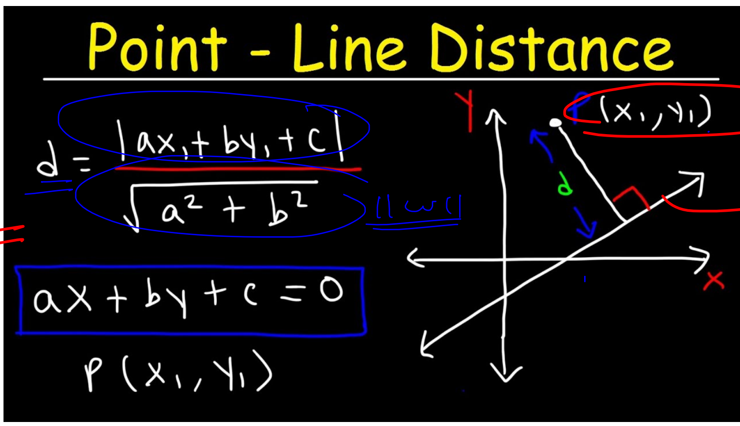
$\boxed{x = y}$

Semantic of

Sign $(w^T x)$



can we compute the distance b/w point and the hyper plane



$ax + by + c$

Hyper plane is $\boxed{x - y = 0}$

$a = 1$ and $b = -1$ $c = 0$

d1 d2

$d_1 = \frac{|1 - 2 + 0|}{\sqrt{1+4}} = \frac{-1}{\sqrt{5}}$

$d_2 = \frac{|2 - 1 + 0|}{\sqrt{5}} = \frac{+1}{\sqrt{5}}$

dot Product b/w line and point

denote $\vec{w}$ as coefficients of the line

$$\vec{w} = \begin{array}{ccc} x & y & c \\ \left[1, \right. & -1, & \left. 0 \right] \\ a & b & c \end{array}$$

$P_1 = (1, 2)$

$P_2 = (2, 1)$

augment each point with 1 towards the end to account for 'c'

$x_1 = [1, 2, 1]$ and $x_2 = [2, 1, 1]$

$w^T x_1 = 1 - 2 + 0 = -1$ $\frac{}{\sqrt{5}}$ and $w^T x_2 = 2 - 1 + 0 = 1$ $\frac{}{\sqrt{5}}$

This is unnormalized signed distance.

[1, 2]

Norm factor $= \frac{1}{\|w\|} = \frac{1}{\sqrt{1^2 + 2^2 + 0^2}} = \frac{1}{\sqrt{5}}$

Sign Indicates the side of the margin

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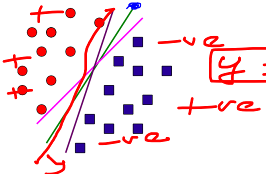
$\boxed{y\,(w^T x + b)} > 0$

$x \in$ +ve class

$y = +1$



$\boxed{y = -1}$

dot product

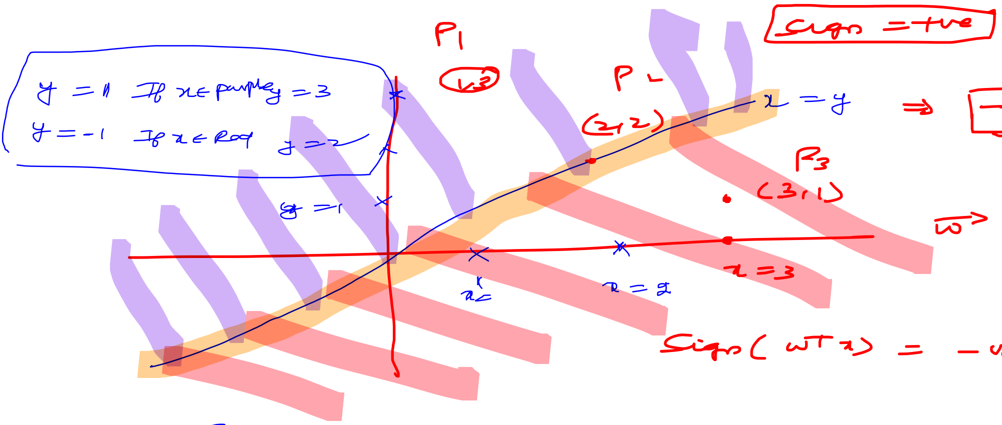
- Standard Perceptron doesn't guarantee any "margin" around the hyperplane
- Note: Possible to "artificially" introduce a margin in the Perceptron
  - Simply change the Perceptron mistake condition to

$$y_n(\boldsymbol{w}^T \boldsymbol{x}_n + b) \leq \gamma$$

where $\gamma > 0$ is a pre-specified margin. For standard Perceptron, $\gamma = 0$

$\boxed{y\,(w^T x + b) > \gamma}$

$\forall\, x \in$ Dataset



$\Rightarrow \boxed{-x + y = 0}$

$\vec{w} = [-1, 1, 0]$

$\text{sign}(w^T x) = -ve$

For pt P_1

$$w^T P_1 = -1 + 3 + 0 = +2$$

For pt P_2

$$w^T P_2 = -2 + 2 = 0$$

$\{ \; w^T P_3 = -2$

Solve for a $\vec{w}$ such that

$$\boxed{y\,(w^T x + b) \geq \, ?} \quad \forall x \in \text{Trn data}$$

$(w^T x + b)$: unnormalized distance

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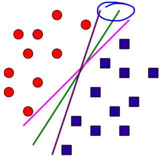

$\gamma \geq 0$

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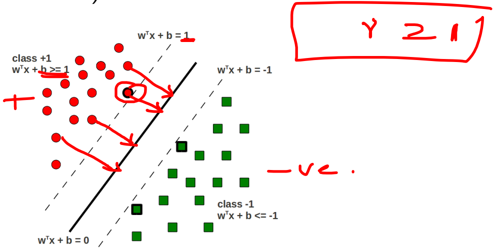
    where $\gamma > 0$ is a pre-specified margin. For standard Perceptron, $\gamma = 0$
    - **Support Vector Machine (SVM)** offers a more principled way of doing this by learning the maximum margin hyperplane

Support Vector Machine (SVM)

- Learns a hyperplane such that the positive and negative class training examples are as far away as possible from it (ensures good generalization)



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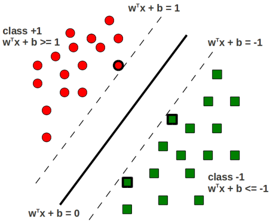

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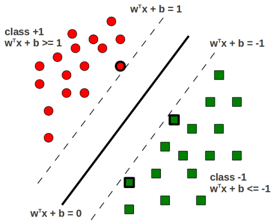

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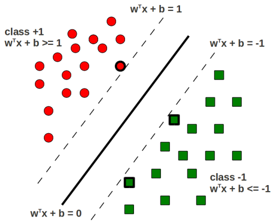

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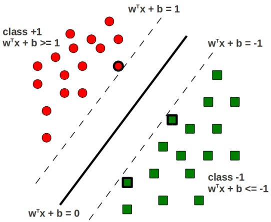

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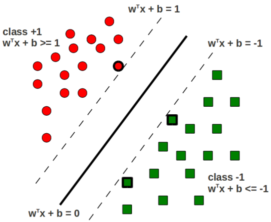
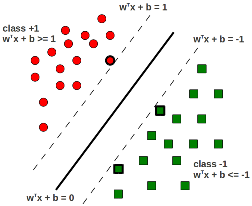


- SVMs can also learn nonlinear decision boundaries using **kernels** (though the idea of kernels is not specific to SVMs and is more generally applicable)
- Reason behind the name "Support Vector Machine"? SVM finds the most important examples (called "support vectors") in the training data
  - These examples also "balance" the margin boundaries (hence called "support"). Also, even if we throw away the remaining training data and re-learn the SVM classifier, we'll get the same hyperplane

Learning a Maximum Margin Hyperplane



$(\vec{w}, b)$

- *Suppose* there exists a hyperplane $\boldsymbol{w}^\top \boldsymbol{x} + b = 0$ such that
  - $\boldsymbol{w}^T \boldsymbol{x}_n + b \geq 1$ for $y_n = +1$
  - $\boldsymbol{w}^T \boldsymbol{x}_n + b \leq -1$ for $y_n = -1$

$\boxed{y_n(w^T x_n + b) \geq 1}$

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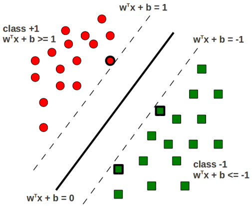

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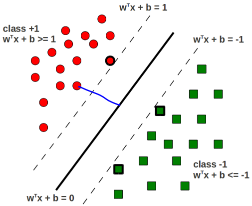

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  - Also note that $\min_{1 \leq n \leq N} |\boldsymbol{w}^T \boldsymbol{x}_n + b| = 1$

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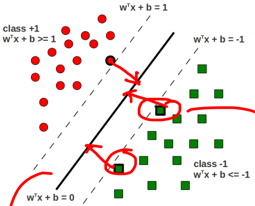

$|w^T x + b|$ = unnorm distance

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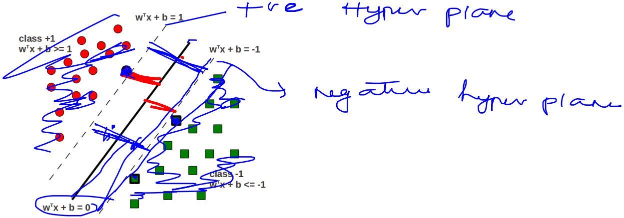
  - Also note that $\min_{1 \leq n \leq N} |\boldsymbol{w}^T \boldsymbol{x}_n + b| = 1$
  - Thus margin on each side: $\gamma = \min_{1 \leq n \leq N} \frac{|\boldsymbol{w}^T \boldsymbol{x}_n + b|}{||\boldsymbol{w}||} = \frac{1}{||\boldsymbol{w}||}$

$\max \frac{1}{||w||}$

s.t. $y_n(w^T x_n + b) \geq 1 \quad \forall n$

Learning a Maximum Margin Hyperplane



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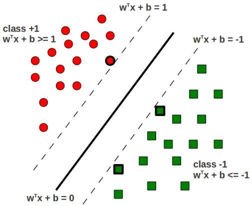

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- Want the hyperplane $(\boldsymbol{w}, b)$ to have the largest possible margin

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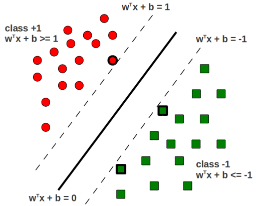
    - Wait until we cover Learning Theory!

Hard-Margin SVM

- Every training example has to fulfil the margin condition $y_n(\boldsymbol{w}^T\boldsymbol{x}_n + b) \geq 1$



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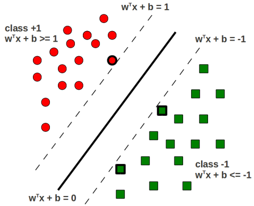

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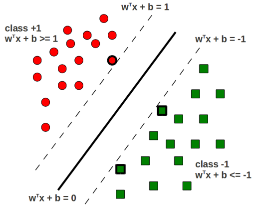

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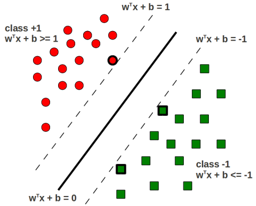

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- The objective for hard-margin SVM

opt pblm to be solved

$$\boxed{\begin{aligned} &\min_{\boldsymbol{w},b} \quad f(\boldsymbol{w}, b) = \frac{||\boldsymbol{w}||^2}{2} \\ &\text{subject to} \quad y_n(\boldsymbol{w}^T\boldsymbol{x}_n + b) \geq 1, \qquad n = 1, \ldots, N \end{aligned}}$$

→ quadratic cost function

→ linear constraint function

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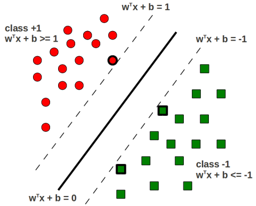

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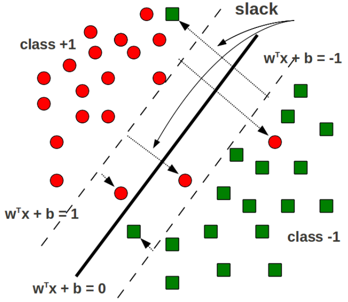
- Thus the hard-margin SVM minimizes a convex objective function which is a Quadratic Program (QP) with N linear inequality constraints

Soft-Margin SVM (More Commonly Used)

- Allow some training examples to fall **within** the margin region, or be even misclassified (i.e., fall on the wrong side). Preferable if training data is noisy



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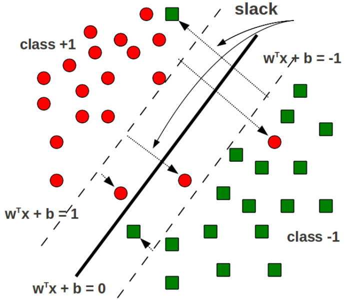

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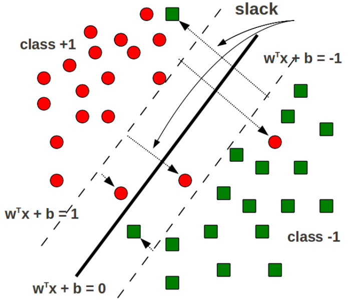

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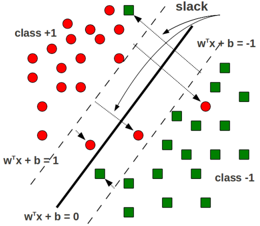
  - Basically, we want a soft-margin condition: $y_n(\boldsymbol{w}^T \boldsymbol{x}_n + b) \geq 1 - \xi_n, \quad \xi_n \geq 0$

Soft-Margin SVM (More Commonly Used)

- Goal: Maximize the margin, while also minimizing the sum of slacks (don't want too many training examples violating the margin condition)



Soft-Margin SVM (More Commonly Used)

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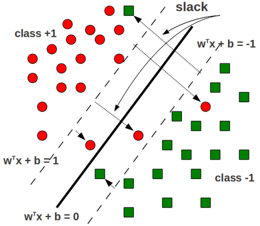

- The primal objective for soft-margin SVM can thus be written as

$$\min_{\boldsymbol{w}, b, \boldsymbol{\xi}} \quad f(\boldsymbol{w}, b, \boldsymbol{\xi}) = \frac{||\boldsymbol{w}||^2}{2} + C \sum_{n=1}^{N} \xi_n$$

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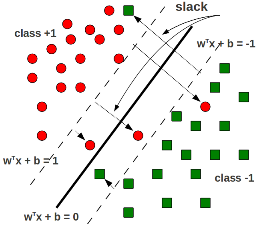

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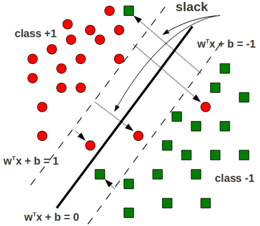

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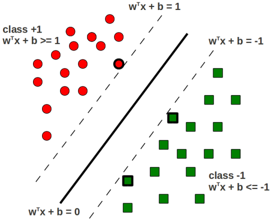
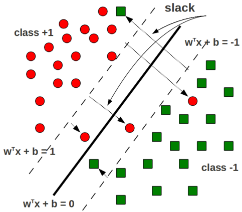
- Param. C controls the trade-off between large margin vs small training error

Summary: Hard-Margin SVM vs Soft-Margin SVM





- Objective for the hard-margin SVM (unknowns are $\boldsymbol{w}$ and b)

$$\min_{\boldsymbol{w},b} \quad f(\boldsymbol{w},b) = \frac{||\boldsymbol{w}||^2}{2}$$

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- In either case, we have to solve constrained, convex optimization problem

Brief Detour: Solving Constrained Optimization Problems

Constrained Optimization via Lagrangian

- Consider optimizing the following objective, subject to some constraints

$$
\begin{aligned}
&\min_{\boldsymbol{w}} \quad f(\boldsymbol{w}) \\
&\text{s.t} \quad g_n(\boldsymbol{w}) \leq 0, \quad n = 1, \ldots, N \\
&\qquad \cancel{h_m(\boldsymbol{w}) = 0, \quad m = 1, \ldots, M}
\end{aligned}
$$

let us Ignore the Equality constraints since SVM

does not have them

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\mathcal{L}(\boldsymbol{w}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = f(\boldsymbol{w}) + \sum_{n=1}^{N} \alpha_n g_n(\boldsymbol{w}) + \cancel{\sum_{m=1}^{N} \beta_n h_n(\boldsymbol{w})}
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  - $\mathcal{L}_P(\boldsymbol{w}) = \infty$ if $\boldsymbol{w}$ violates any of the constraints (g's or h's)

assume $g_n(w)$ is violated

$\Rightarrow \quad g_n(w) > 0$

Now when we max$_{\alpha_n}$ $\alpha_n g_n(w)$ we can trivially

set $\alpha_n = +\infty$ and the obj is maximized

Constrained Optimization via Lagrangian

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  - $\mathcal{L}_P(\boldsymbol{w}) = f(\boldsymbol{w})$ if $\boldsymbol{w}$ satisfies all the constraints (g's and h's)

$g_n(w) \leq 0$

what is α_n in $\max_{\alpha_n} \alpha_n g_n(w)$?

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- Thus $\min_{\boldsymbol{w}} \mathcal{L}_P(\boldsymbol{w}) = \min_{\boldsymbol{w}} \max_{\boldsymbol{\alpha} \geq 0, \boldsymbol{\beta}} \mathcal{L}(\boldsymbol{w}, \boldsymbol{\alpha}, \boldsymbol{\beta})$ solves the same problem as the original problem and will have the same solution. For convex f, g, h, the order of min and max is interchangeable.

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- Karush-Kuhn-Tucker (KKT) Conditions: At the optimal solution, $\alpha_n g_n(\boldsymbol{w}) = 0$ (note the $\max_\alpha$)

Solving Hard-Margin SVM

Solving Hard-Margin SVM

- The hard-margin SVM optimization problem is:

$$\boxed{\begin{aligned} &\min_{\boldsymbol{w},b} \quad f(\boldsymbol{w},b) = \frac{||\boldsymbol{w}||^2}{2} \\ &\text{subject to} \quad 1 - y_n(\boldsymbol{w}^T\boldsymbol{x}_n + b) \leq 0, \qquad n = 1,\ldots,N \end{aligned}}$$

- A constrained optimization problem. Can solve using Lagrange's method

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- Note: $\boldsymbol{\alpha} = [\alpha_1,\ldots,\alpha_N]$ is the vector of Lagrange multipliers
- We will solve this Lagrangian by solving a dual problem (eliminate $\boldsymbol{w}$ and b and solve for the "dual variables" $\boldsymbol{\alpha}$)

Solving Hard-Margin SVM

- The original Lagrangian is

$$\boxed{\min_{\boldsymbol{w},b} \max_{\boldsymbol{\alpha}\geq 0} \mathcal{L}(\boldsymbol{w},b,\boldsymbol{\alpha}) = \frac{\boldsymbol{w}^\top \boldsymbol{w}}{2} + \sum_{n=1}^{N} \alpha_n\{1 - y_n(\boldsymbol{w}^T \boldsymbol{x}_n + b)\}}$$

For convex function $\min_{w,b} \max_{\alpha} = \max_{\alpha} \min_{w}$

Interested students can further read on "strong duality".

Solving Hard-Margin SVM

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- Take (partial) derivatives of $\mathcal{L}$ w.r.t. $\boldsymbol{w}$, b and set them to zero

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{w}} = 0 \Rightarrow \boxed{\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y_n \boldsymbol{x}_n} \qquad \frac{\partial \mathcal{L}}{\partial b} = 0 \Rightarrow \sum_{n=1}^{N} \alpha_n y_n = 0$$

This means that $\vec{w}$ = weighted sum of I/p points

$\parallel^{r}$ to perceptron

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- Important: Note the form of the solution $\boldsymbol{w}$ - it is simply a weighted sum of all the training inputs $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$ (and α_n is like the "importance" of $\boldsymbol{x}_n$)
- Substituting $\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y_n \boldsymbol{x}_n$ in Lagrangian and also using $\sum_{n=1}^{N} \alpha_n y_n = 0$

$$\boxed{\max_{\boldsymbol{\alpha}\geq 0} \ \mathcal{L}_D(\boldsymbol{\alpha}) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{m,n=1}^{N} \alpha_m \alpha_n y_m y_n (\boldsymbol{x}_m^T \boldsymbol{x}_n) \qquad \text{s.t.} \quad \sum_{n=1}^{N} \alpha_n y_n = 0}$$

Solving Hard-Margin SVM

- Can write the objective more compactly in vector/matrix form as

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where $\mathbf{G}$ is an $N \times N$ matrix with $G_{mn} = y_m y_n \boldsymbol{x}_m^\top \boldsymbol{x}_n$, and $\mathbf{1}$ is a vector of 1s

† If interested in more details of the solver, see: "Support Vector Machine Solvers" by Bottou and Lin

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  - Using (projected) gradient methods (projection needed because the α's are constrained). Gradient methods will usually be much faster than QP methods.

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Hard-Margin SVM: The Solution

- Once we have the α_n's, $\boldsymbol{w}$ and b can be computed as:

$$\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y_n \boldsymbol{x}_n$$

$$b = -\frac{1}{2}\left(\min_{n:y_n=+1} \boldsymbol{w}^T \boldsymbol{x}_n + \max_{n:y_n=-1} \boldsymbol{w}^T \boldsymbol{x}_n\right)$$

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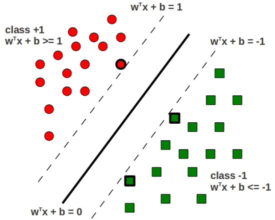

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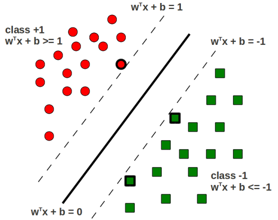

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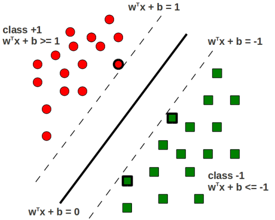
$$\boldsymbol{w} = \sum_{n=1}^{N} \alpha_n y_n \boldsymbol{x}_n$$

$$b = -\frac{1}{2}\left(\min_{n:y_n=+1} \boldsymbol{w}^T\boldsymbol{x}_n + \max_{n:y_n=-1} \boldsymbol{w}^T\boldsymbol{x}_n\right)$$

- **A nice property:** Most α_n's in the solution will be zero (sparse solution)



- Reason: Karush-Kuhn-Tucker (KKT) conditions
- For the optimal α_n's

$$\alpha_n\{1 - y_n(\boldsymbol{w}^T\boldsymbol{x}_n + b)\} = 0$$

- α_n is non-zero only if $\boldsymbol{x}_n$

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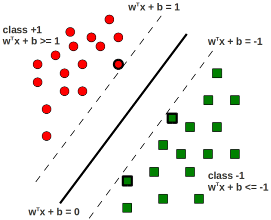

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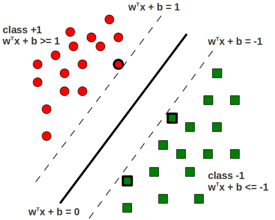

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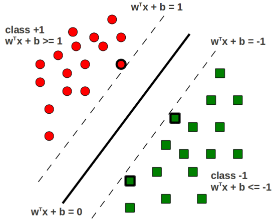

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- Recall the support vectors "support" the margin boundaries