Learning Maximum-Margin Hyperplanes: Support Vector Machines

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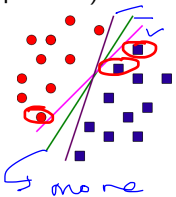
Machine Learning (CS771A)

Aug 24, 2016

Perceptron and (Lack of) Margins

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

2 - class



more preferred

green — max degree of sep

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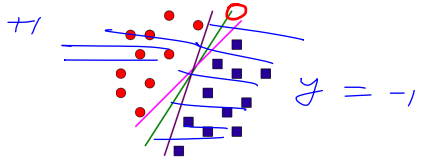

0 Training Error

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

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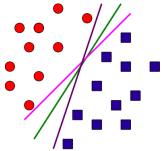


- Standard Perceptron doesn't guarantee any "margin" around the hyperplane
- Note: Possible to "artificially" introduce a margin in the Perceptron

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

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

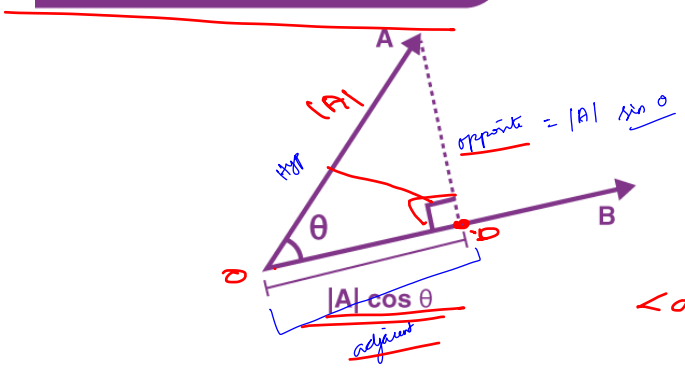
$\vec{a} \cdot \vec{b} = \sum_{2} a_2 b_2 = 2 + 6 = 8$

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

dot Products and margin

DOT PRODUCT OF VECTORS

BYJU'S The Learning App



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

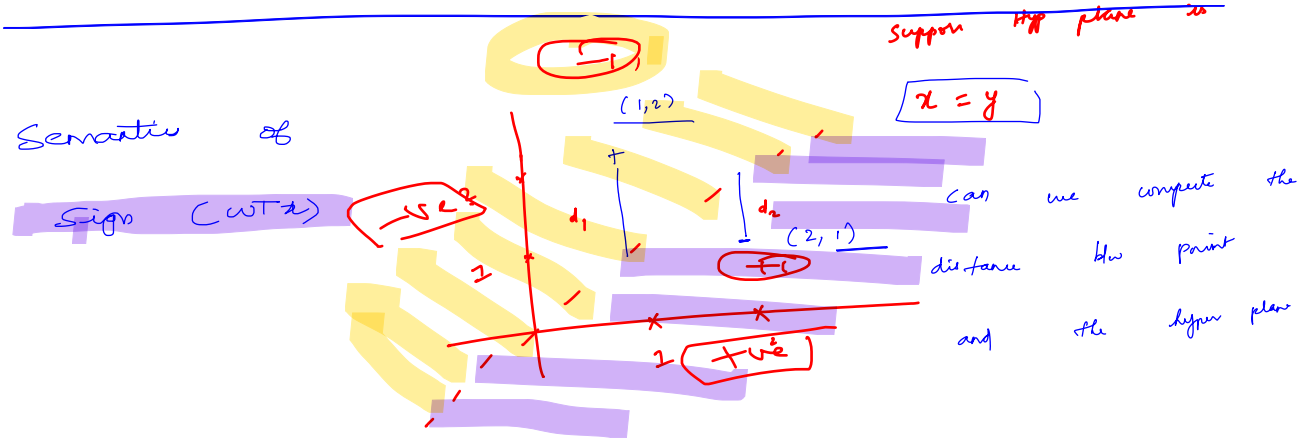
$= \frac{AD}{OA}$

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

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

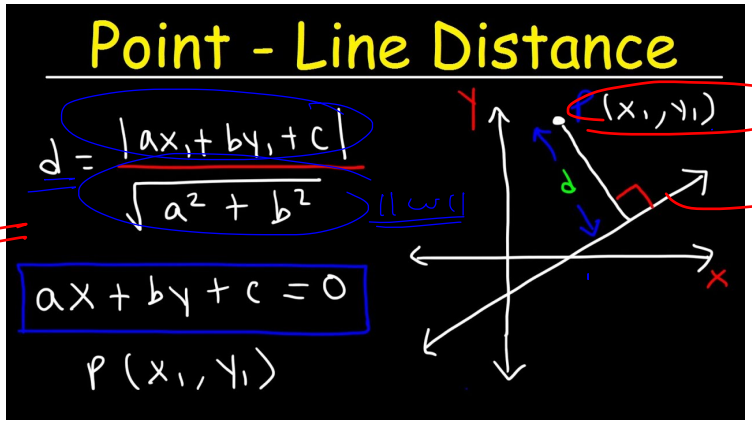
$\langle a, b \rangle =$

Semantics of Sign ($w^T x$)



Support Hyp plane is $x = y$

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



$ax + by + c$

Hyper Plane is $x - y = 0$

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

d_1 d_2

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

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

dot Product b/w line and point

denote $\vec{w}$ as co effecients of the line

$$\vec{w} = [\underset{a}{1}, \underset{b}{-1}, \underset{c}{0}]$$

$P_1 = (1, 1)$

$P_2 = (2, 1)$

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

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

$w^T x_1 = 1 - 2 + 0 = -1$ and $w^T x_2 = 2 - 1 + 0 = 1$

$\frac{-1}{\sqrt{5}}$ $\frac{1}{\sqrt{5}}$

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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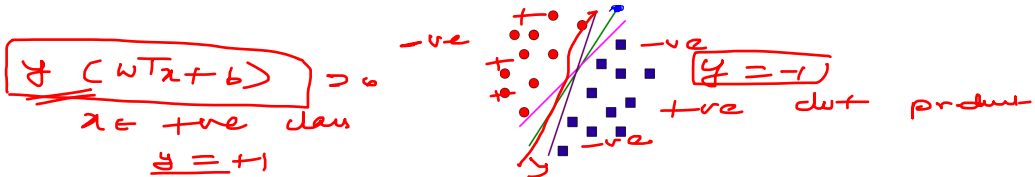

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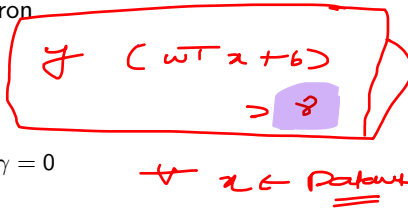
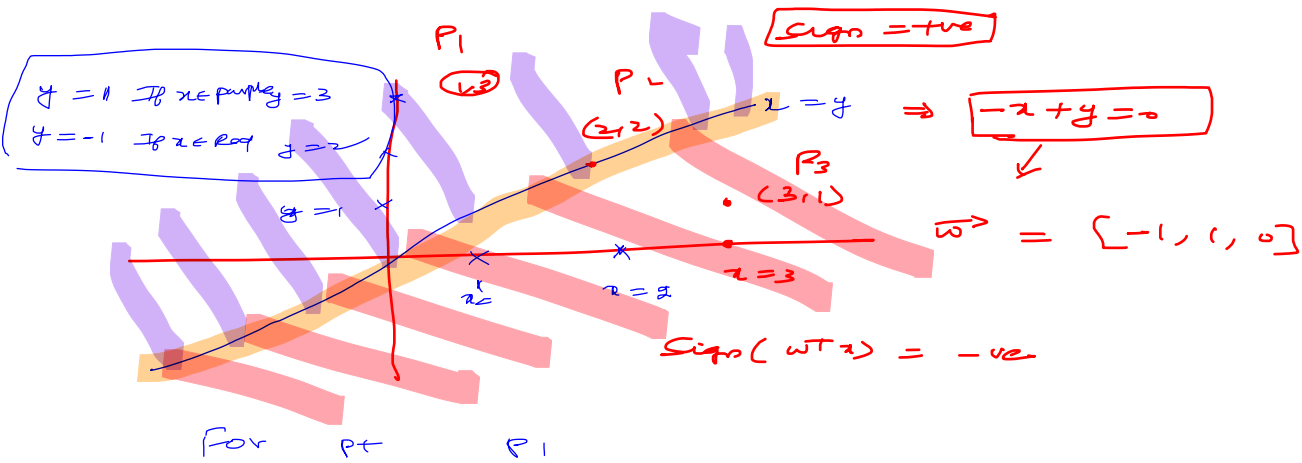
- Note: Possible to "artificially" introduce a margin in the Perceptron
  - Simply change the Perceptron mistake condition to

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

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





Sign = +ve

$wT\ P_1 = -1 + 3 + 0 = +2$

For pt P_2

$wTP_2 = -2 + 2 = 0$ ($wTP_3 = -2$

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

$$y_i (w^T x_i + b) \geq 1 \quad \forall x_i \in \text{Trn data}$$

$y_i (w^T x_i + b)$ — unnormalized distance

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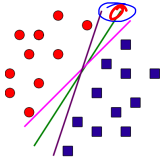

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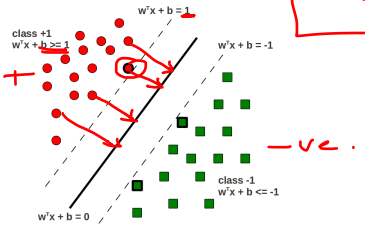
  where $\gamma > 0$ is a pre-specified margin. For standard Perceptron, $\gamma = 0$
  - **Support Vector Machine (SVM)** offers a more principled way of doing this by learning the maximum margin hyperplane

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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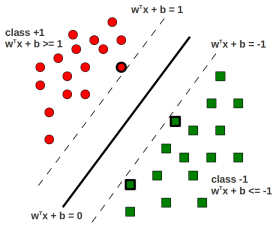

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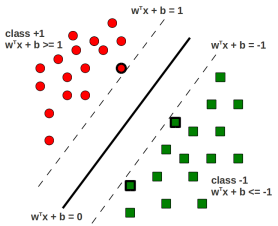

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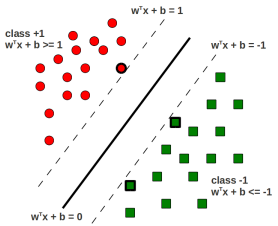

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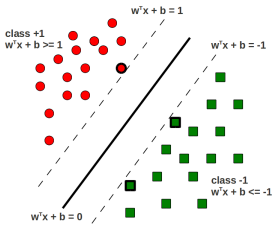

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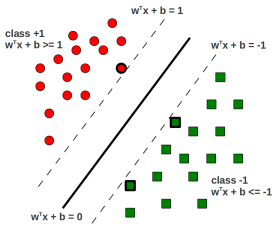

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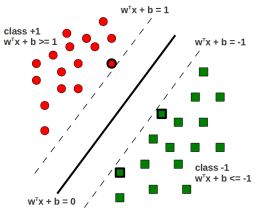
- Reason behind the name "Support Vector Machine"? SVM finds the most important examples (called "support vectors") in the training data
  - These examples also "balance" the margin boundaries (hence called "support"). Also, even if we throw away the remaining training data and re-learn the SVM classifier, we'll get the same hyperplane

Learning a Maximum Margin Hyperplane



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

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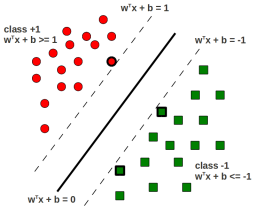

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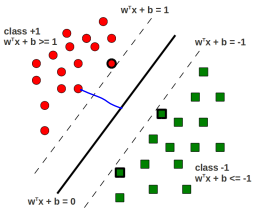

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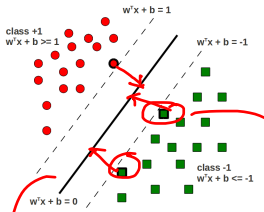

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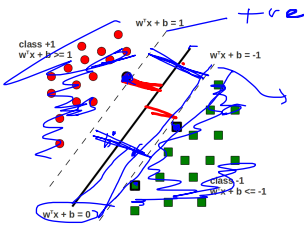

true hyper plane

negative hyper plane

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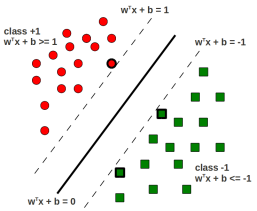

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- Want the hyperplane $(\boldsymbol{w}, b)$ to have the largest possible margin

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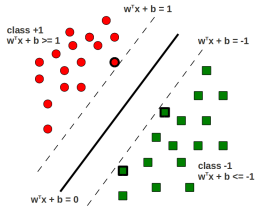
  - Wait until we cover Learning Theory!

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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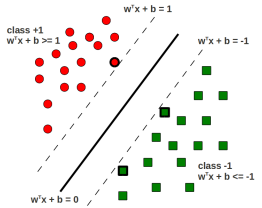

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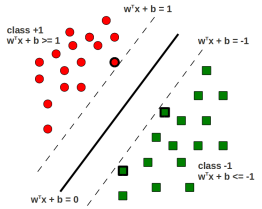

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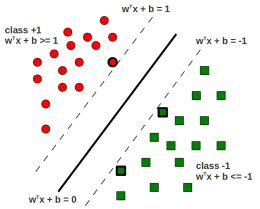

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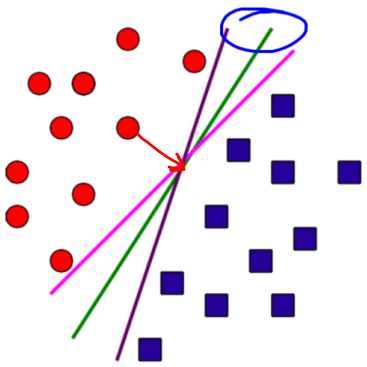
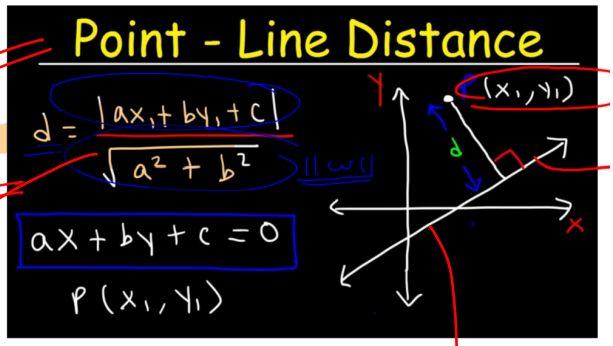
- The objective for hard-margin SVM

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

$$\text{subject to} \quad y_n(\boldsymbol{w}^T\boldsymbol{x}_n + b) \geq 1, \qquad n = 1, \ldots, N$$





$\frac{|\langle w, p \rangle|}{\|w\|_2}$

$ax + by + c = 0$

$\vec{w} = [a \;\; b \;\; c]$

$\vec{p} = [x_1, y_1, 1]$

Recap

① Perceptron returns any arbitrary hyper plane

② we need to prefer green hyp plane.

③ → need to compute the margin

$$\text{margin (point } x \text{ and hyp } w) = \frac{w^T x + b}{\|w\|}$$

So the plan now is to find w so that

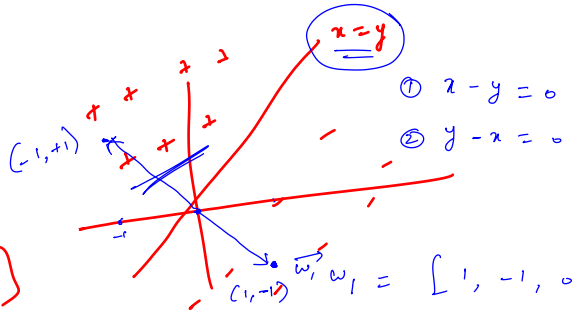
$$w^T x_i + b \geq 1 \quad \forall \; y_i = +1$$

$$w^T x_i + b \leq -1 \quad \forall \; y_i = -1$$

$$y_i (w^T x_i + b) \geq 1$$

$$\text{margin} = \frac{w^T x + b}{\|w\|} \rightarrow \text{optimization}$$

→ constraint



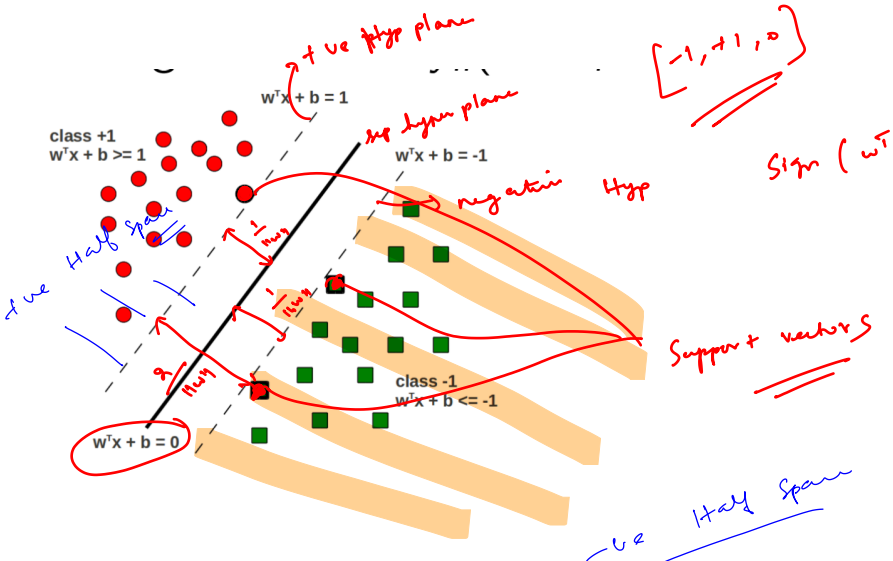
$[-1, +1, 0]$

$w_1 = [1, -1, 0]$

$w_2 = [-1, 1, 0]$

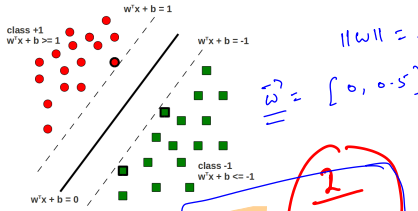
$\text{Sign}(w^T x + b) = +ve$

$= -ve.$



Hard-Margin SVM

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



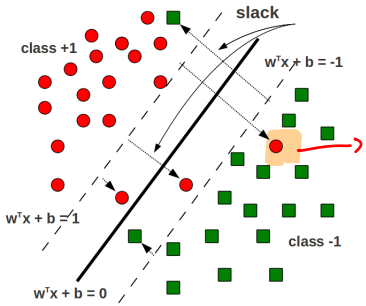
- Also want to maximize the margin $\gamma \propto \frac{1}{||\boldsymbol{w}||}$
  - Equivalent to minimizing $||\boldsymbol{w}||^2$ or $\frac{||\boldsymbol{w}||^2}{2}$
- The objective for hard-margin SVM

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

- 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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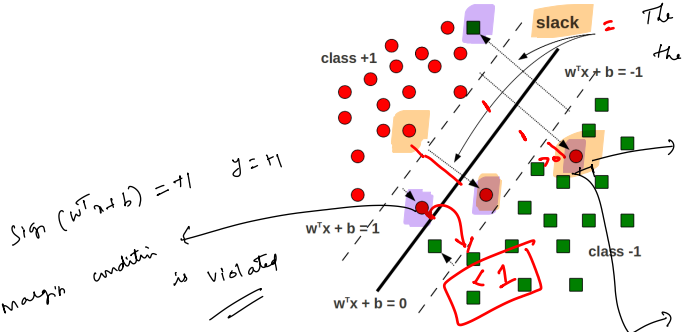

- Each training example $(\boldsymbol{x}_n, y_n)$ given a "slack" $\xi_n \geq 0$ (distance by which it "violates" the margin). If $\xi_n > 1$ then $\boldsymbol{x}_n$ is totally on the wrong side

slack

slack < 1

$\text{sign}(w^T x + b) = y$ — True

slack > 0

is $y_n(w^T x + b) \geq 1$ satisfied ?

↳ false!

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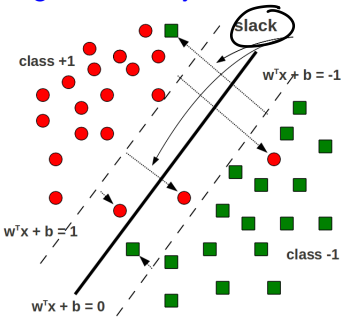
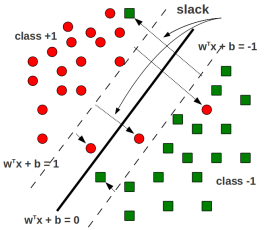


Slack part of opt variables

- Each training example $(\boldsymbol{x}_n, y_n)$ given a "slack" $\xi_n \geq 0$ (distance by which it "violates" the margin). If $\xi_n > 1$ then $\boldsymbol{x}_n$ is totally on the wrong side
  - 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)



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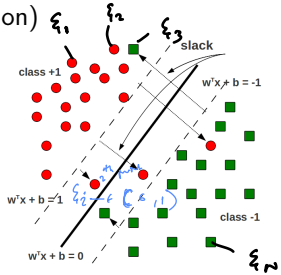

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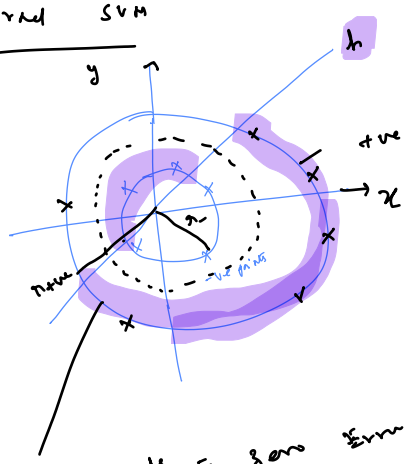
$$\text{subject to constraints} \quad y_n(\boldsymbol{w}^T\boldsymbol{x}_n + b) \geq 1 - \xi_n, \quad \xi_n \geq 0 \qquad n = 1,\ldots,N$$

Large margin

Hard margin SVM

Err [Training data] ≥ 0.5

Kernel SVM



Soft margin SVM on this ds will go crazy.

Deep Neural Nets = zero Error!

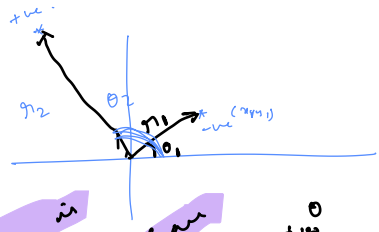
Kernel SVM

$(x, y) \rightarrow \phi(x, y)$ — Kernel Space

↳ Polar coordinate Transformation

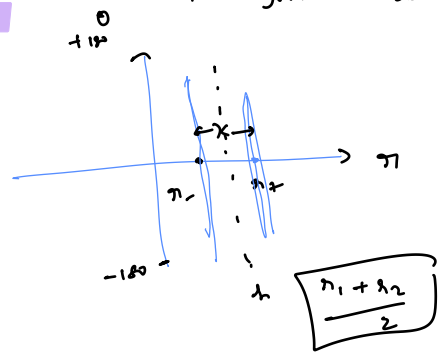
(r, θ)

In general ϕ is very complicated function



Transformed space is in 2-dimensional space

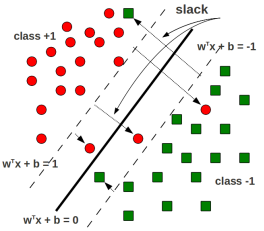
Transformed data



$\frac{r_1 + r_2}{2}$

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)



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- Thus the soft-margin SVM also minimizes a convex objective function which is a Quadratic Program (QP) with $2N$ linear inequality constraints

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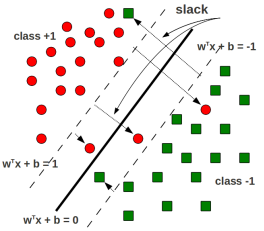

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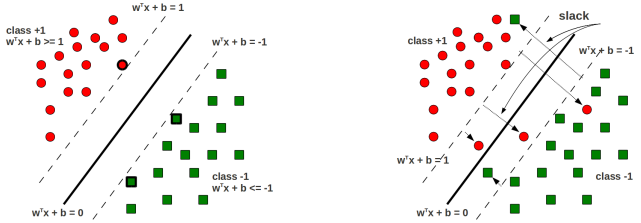
- Thus the soft-margin SVM also minimizes a convex objective function which is a Quadratic Program (QP) with $2N$ linear inequality constraints
- Param. C controls the trade-off between large margin vs small training error

Summary: Hard-Margin SVM vs Soft-Margin SVM



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

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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

$$\min_{\boldsymbol{w}} \; f(\boldsymbol{w})$$
$$\text{s.t} \quad g_n(\boldsymbol{w}) \leq 0, \quad n = 1, \ldots, N$$
$$h_m(\boldsymbol{w}) = 0, \quad m = 1, \ldots, M$$

let us Ignore the Eq uality constraints since SVM does not have them

Constrained Optimization via Lagrangian

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- Introduce Lagrange multipliers $\boldsymbol{\alpha} = \{\alpha_n\}_{n=1}^N$, $\alpha_n \geq 0$, and $\boldsymbol{\beta} = \{\beta_m\}_{m=1}^M$, one for each constraint, and construct the following Lagrangian

$$\mathcal{L}(\boldsymbol{w}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = f(\boldsymbol{w}) + \sum_{n=1}^{N} \alpha_n g_n(\boldsymbol{w}) + \sum_{m=1}^{N} \beta_n h_n(\boldsymbol{w})$$

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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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If $g_n(w)$ is satisfied

$g_n(w) \leq 0$

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

Constrained Optimization via Lagrangian

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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:

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

- 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

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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

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

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

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

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

$\boldsymbol{w}$ to perceptron

Solving Hard-Margin SVM

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

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

- 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 $\sum_{n=1}^{N} \alpha_n y_n = 0$

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

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Hard-Margin SVM: The Solution

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

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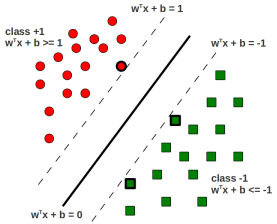

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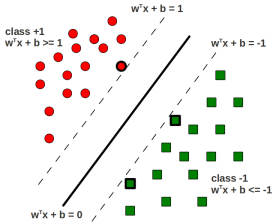

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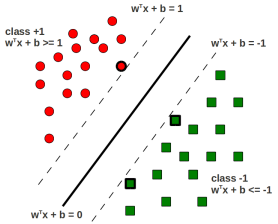

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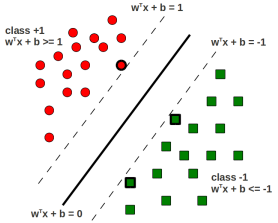

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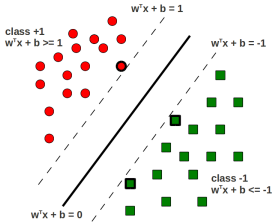

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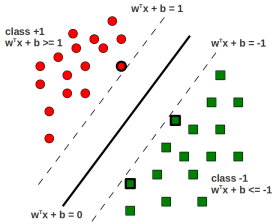

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- Recall the support vectors "support" the margin boundaries