Support Vector Machines

CSCI-B455

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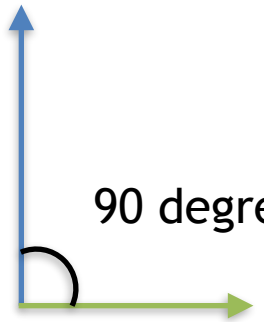
Hyperplanes for SVMs

- For linear classification, would like to separate two classes with a hyperplane
  - Plane characterized by: $\mathbf{w}^\top \mathbf{x} + w_0 = 0$
- We want a hyperplane that separates these classes "the most"
- How do we characterize such a maximal separation?
  - let's talk about vectors in a d-dimensional space
  - let's talk about the distance to a plane

Orthogonality

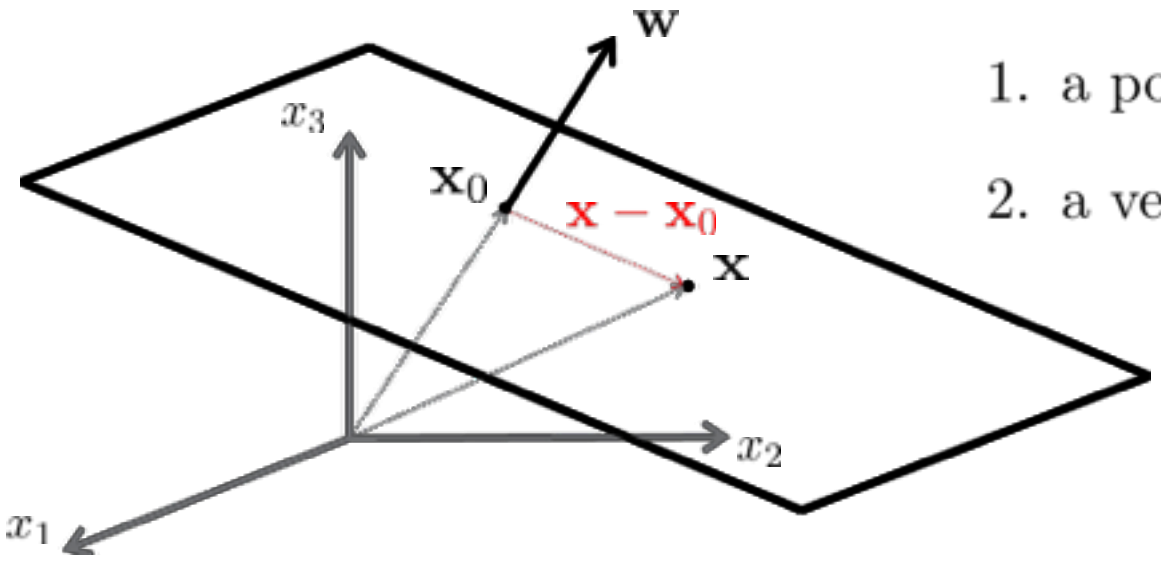
- Two points are orthogonal if dot product is 0
- Cosine similarity: theta angle between w and x

$$\mathbf{w}^\top \mathbf{x} = \|\mathbf{w}\| \|\mathbf{x}\| \cos(\theta)$$



cos(0 degrees) = 0

Equation of the Plane



A plane is defined using:

1. a point $\mathbf{x}_0$ lying in the plane
2. a vector $\mathbf{w}$ normal to the plane

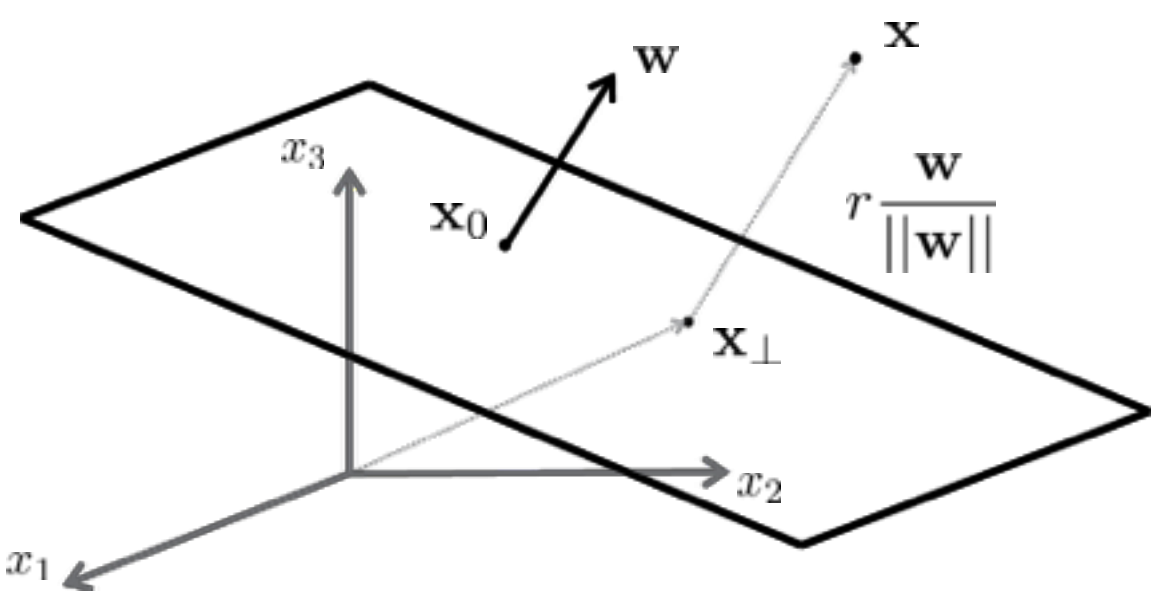
Let $\mathbf{x}$ be on the plane defined by $\mathbf{w}$ and $\mathbf{x}_0$:

$$\mathbf{w}^T(\mathbf{x} - \mathbf{x}_0) = 0$$

$$\mathbf{w}^T\mathbf{x} - \mathbf{w}^T\mathbf{x}_0 = 0$$

$$\boxed{\mathbf{w}^T\mathbf{x} + w_0 = 0}$$

Distance from Point to the Plane



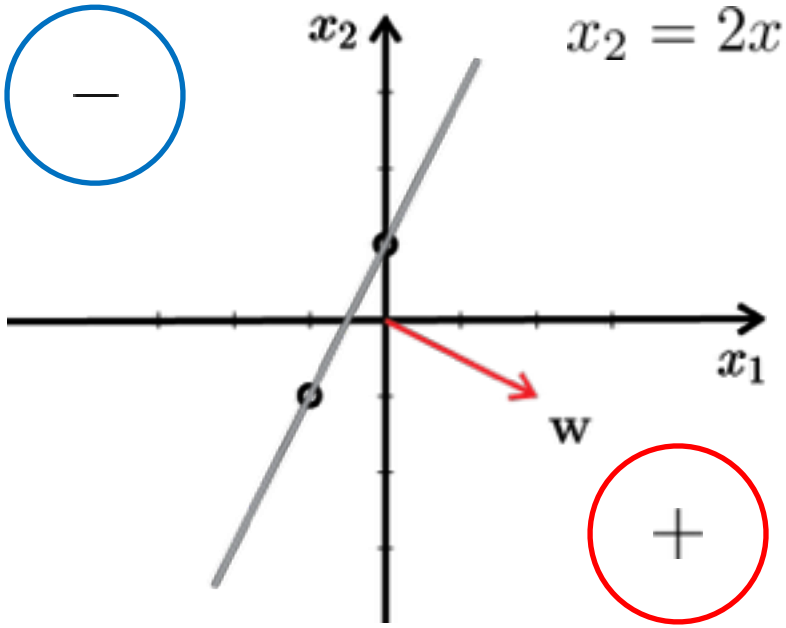
$\mathbf{x}$ = outside the plane

$$\mathbf{x} = \mathbf{x}_\perp + r\frac{\mathbf{w}}{||\mathbf{w}||}$$

$$\mathbf{w}^T\mathbf{x} + w_0 = \underbrace{\mathbf{w}^T\mathbf{x}_\perp + w_0}_{0} + r||\mathbf{w}||$$

$$r = \frac{\mathbf{w}^T\mathbf{x} + w_0}{||\mathbf{w}||}$$

Example



$x_2 = 2x_1 + 1$ or $2x_1 - x_2 + 1 = 0$

$\mathbf{x}, \mathbf{w} \in \mathbb{R}^2$

$\mathbf{w}^T\mathbf{x} + w_0 = 0$
where $\mathbf{w} = (2, -1)$ and $w_0 = 1$.

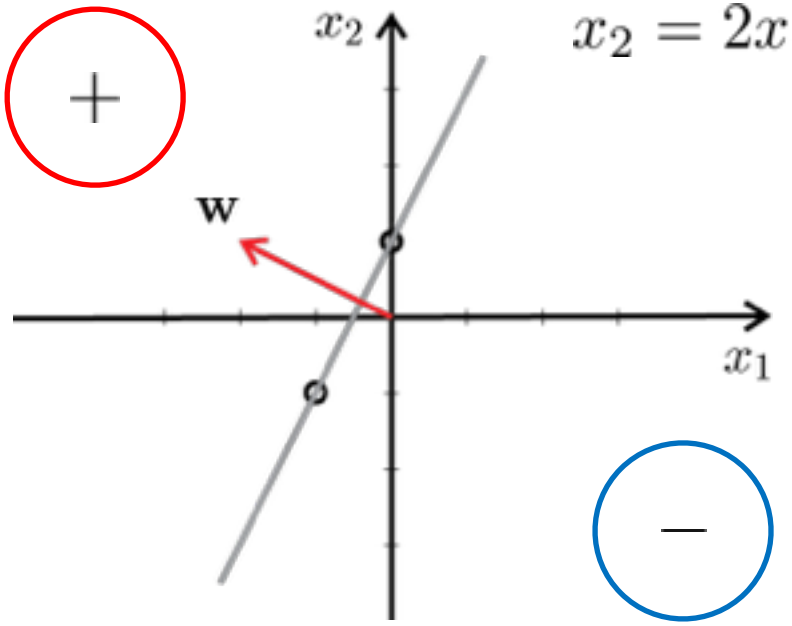
$$r = \frac{\mathbf{w}^T\mathbf{x} + w_0}{||\mathbf{w}||}$$

$\mathbf{x} = (0, 0) \implies r = \frac{1}{\sqrt{5}}$

$\mathbf{x} = (-1, 1) \implies r = -\frac{2}{\sqrt{5}}$

The vector $\mathbf{w}$ defines what side of the plane is positive.

EXAMPLE



$x_2 = 2x_1 + 1$

What if $\mathbf{w} = (-2, 1)$?

$\mathbf{x}, \mathbf{w} \in \mathbb{R}^2$

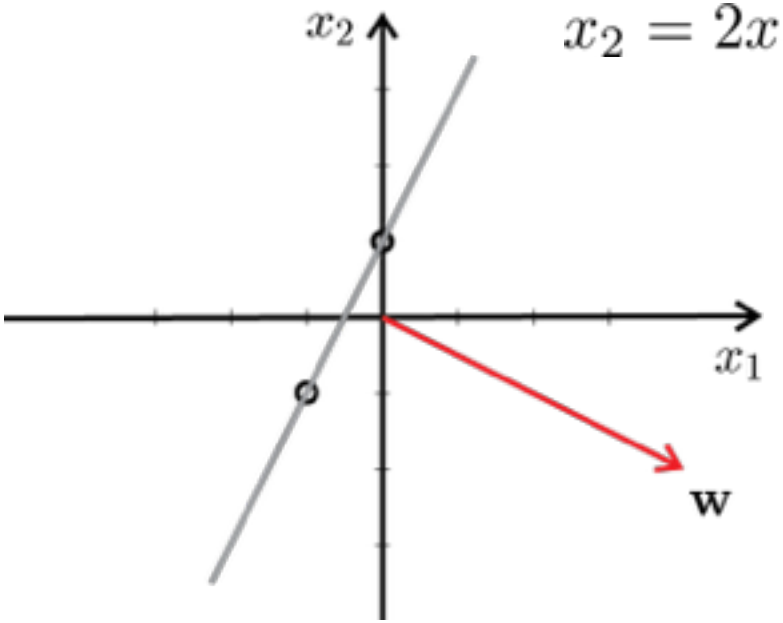
$\mathbf{w}^T\mathbf{x} + w_0 = 0$
where $\mathbf{w} = (-2, 1)$ and $w_0 = -1$.

$$r = \frac{\mathbf{w}^T\mathbf{x} + w_0}{||\mathbf{w}||}$$

$\mathbf{x} = (0, 0) \implies r = -\frac{1}{\sqrt{5}}$

$\mathbf{x} = (-1, 1) \implies r = \frac{2}{\sqrt{5}}$

Example



$x_2 = 2x_1 + 1$

What if $\mathbf{w} = (4, -2)$ and $w_0 = 2$?

$4x_1 - 2x_2 + 2 = 0$

$\mathbf{w}^T\mathbf{x} + w_0$ is "bigger"!!!

$$r = \frac{\mathbf{w}^T\mathbf{x} + w_0}{||\mathbf{w}||}$$

$\mathbf{x} = (0, 0) \implies r = \frac{1}{\sqrt{5}}$

$\mathbf{x} = (-1, 1) \implies r = -\frac{2}{\sqrt{5}}$

Distances are unchanged when $\mathbf{w}$ and w_0 are multiplied by a constant!

Reminders: March 6

- Assignment 3 modification
  - changed dataloader.py to fix a bug with loading census dataset
  - please start early!
- Thought questions due this week
- First Quiz after spring break
  - 45 minutes in class
  - Allowed 2 pages of notes (4 pages front & back)

Example question

- What is the main difference between multi-class and multi-label classification?

Another example

Given dataset $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$, where $\mathbf{x}_i = (x_{i1}, x_{i2})$, the objective is to find parameters of the function

$$f(\mathbf{x}) = \log(w_1 x_1 + w_2 x_2)$$

such that the weighted sum of squared errors between the target and the prediction is minimized, with some of the samples having higher importance than other samples according to importance weights $c_1, \ldots, c_n > 0$.
Provide an algorithm for obtaining the parameter vector $\mathbf{w} = (w_1, w_2)$. If there is a closed form solution, provide the closed-form solution; otherwise, provide an iterative, first-order gradient descent update.

Thought Question

- Why do we use l2 error?
- Related question: how do we deal with outliers
  - e.g., “If a person in our data set whose highest is misrepresented by 3 inches this will contribute 9 times more error to the summed of squared errors that is being minimized than someone whose height is mispredicted by one inch.”

Thought Question

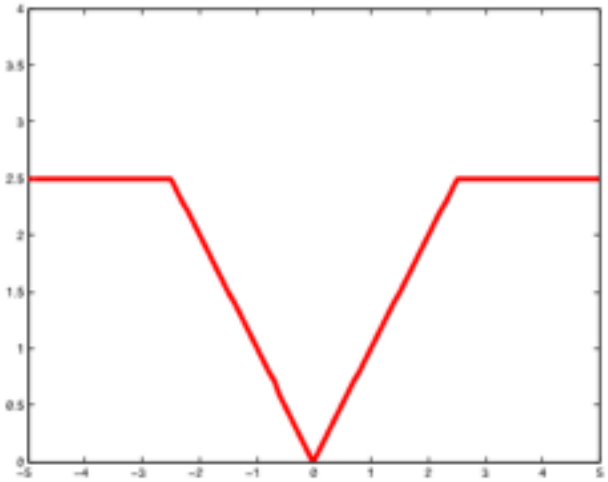
- Why do we use l2 error?
- Related question: how do we deal with outliers
  - e.g., “If a person in our data set whose highest is misrepresented by 3 inches this will contribute 9 times more error to the summed of squared errors that is being minimized than someone whose height is mispredicted by one inch.”

Some losses

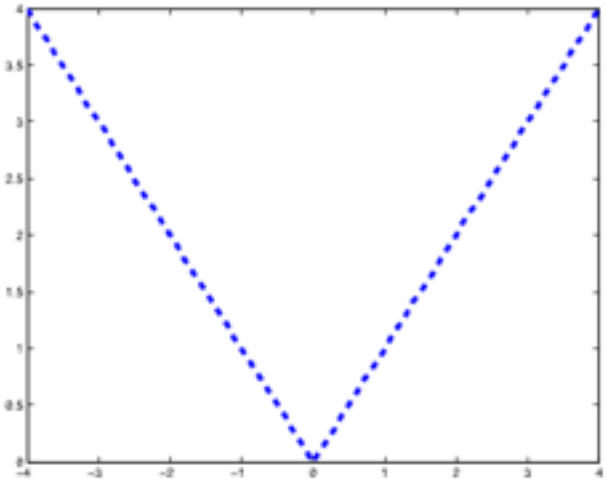
Which ones would be more robust to outliers?

i.e., least-squares loss

l2-norm loss



(a) Capped ℓ_1-norm loss ($\varepsilon = 2.5$)



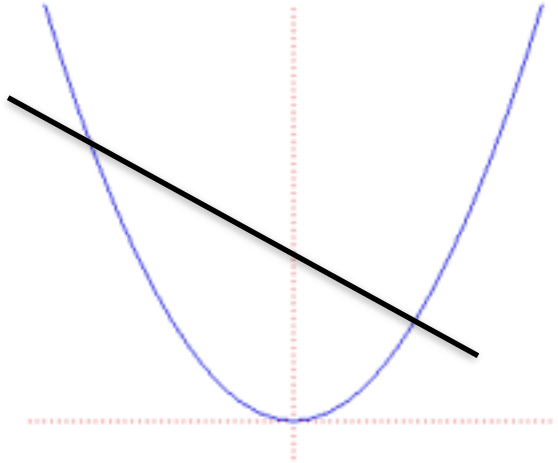
(b) ℓ_1-norm loss

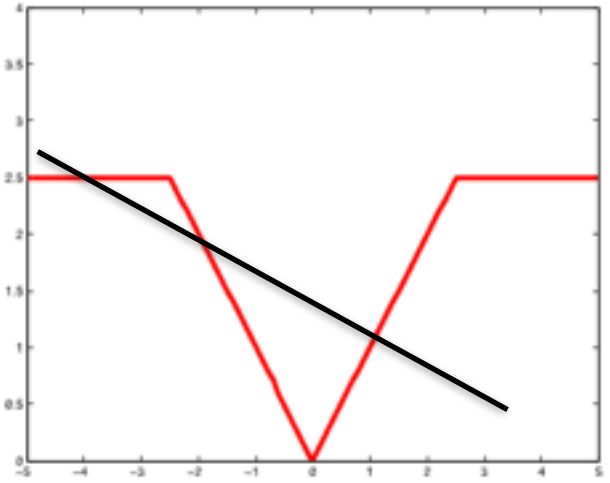
Why the l2?

- The l2 (least-squares) is easy to optimize
- The l1 has a non-differentiable point
  - as you saw in your assignment, you had to use a special proximal update
- The clipped l1 is nonconvex
  - gradient descent may get stuck in local minima or saddlepoints

Convex function

- If you draw a line connecting the function values for two points, that line always lies above the function

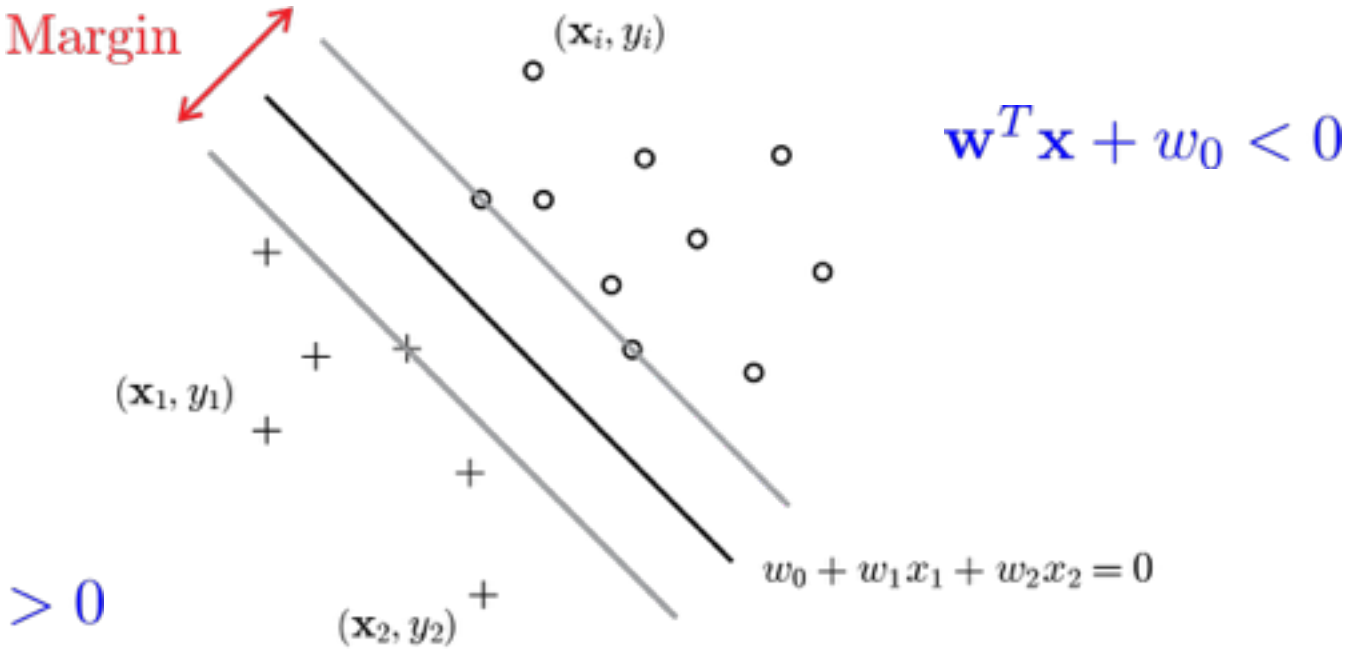




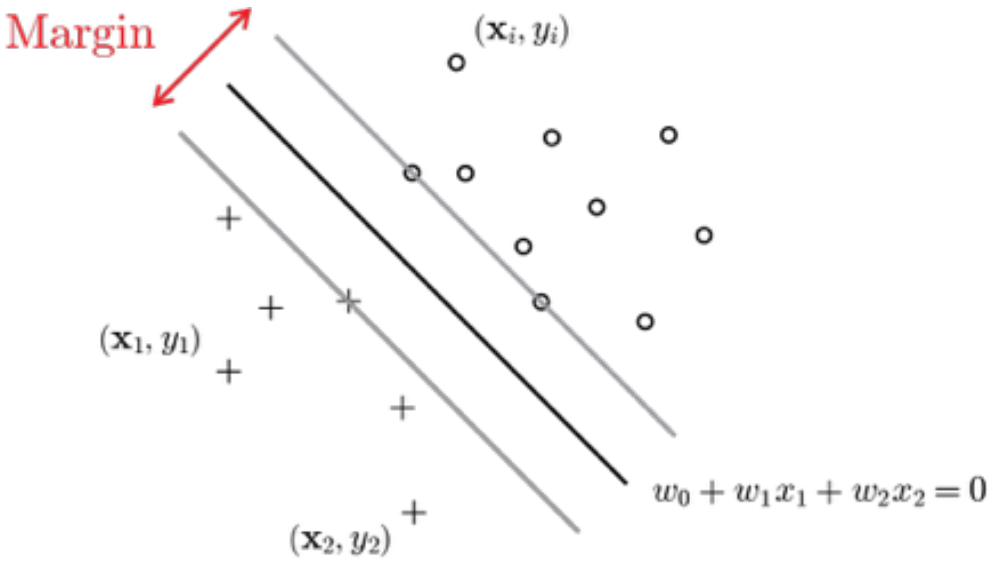
Problem Formulation

Given: $\mathcal{D} = \{(\mathbf{x}_i, y_i\}_{i=1}^{n}$, where $\mathbf{x}_i \in \mathbb{R}^k$ and $y_i \in \{-1, +1\}$.
Data is linearly separable.

Objective: Find hyperplane such that the minimum distance from any data point to the hyperplane is maximized.



Maximizing Margin



$$\mathbf{w}^T\mathbf{x}_i + w_0 > 0 \implies y_i = +1$$
$$\mathbf{w}^T\mathbf{x}_i + w_0 < 0 \implies y_i = -1$$

$$y_i(\mathbf{w}^T\mathbf{x}_i + w_0) > 0$$

$$i \in \{1, 2, \ldots, n\}$$

Idea: find $\mathbf{w}$ to maximize unsigned distance $d_i = \dfrac{y_i(\mathbf{w}^T\mathbf{x} + w_0)}{||\mathbf{w}||}$

$$(\mathbf{w}^*, w_0^*) = \arg\max_{\mathbf{w}, w_0} \left\{ \frac{1}{||\mathbf{w}||} \min_i \left(y_i(\mathbf{w}^T\mathbf{x}_i + w_0) \right) \right\}$$

Reformulating the Problem

$$(\mathbf{w}^*, w_0^*) = \arg\max_{\mathbf{w}, w_0} \left\{ \frac{1}{||\mathbf{w}||} \min_i \left(y_i(\mathbf{w}^T \mathbf{x}_i + w_0) \right) \right\}$$

Scale $\mathbf{w}$ and w_0 such that $\min_i y_i(\mathbf{w}^\top \mathbf{x}_i + w_0) = 1$

$$\mathbf{w} \leftarrow k \cdot \mathbf{w}$$
$$w_0 \leftarrow k \cdot w_0$$

Equivalence class of w, since distance is the same for all of these points, goal is the same even if w shorter or longer

So

$$y_i(\mathbf{w}^T \mathbf{x}_i + w_0) \geq 1 \quad \forall i \in \{1, 2, \ldots, n\}$$

And

$$\arg\max_{\mathbf{w}} \|\mathbf{w}\|^{-1} = \arg\min_{\mathbf{w}} \|\mathbf{w}\|$$

Reformulating the Problem

$$(\mathbf{w}^*, w_0^*) = \arg\max_{\mathbf{w}, w_0} \left\{ \frac{1}{||\mathbf{w}||} \min_i \left(y_i(\mathbf{w}^T \mathbf{x}_i + w_0) \right) \right\}$$

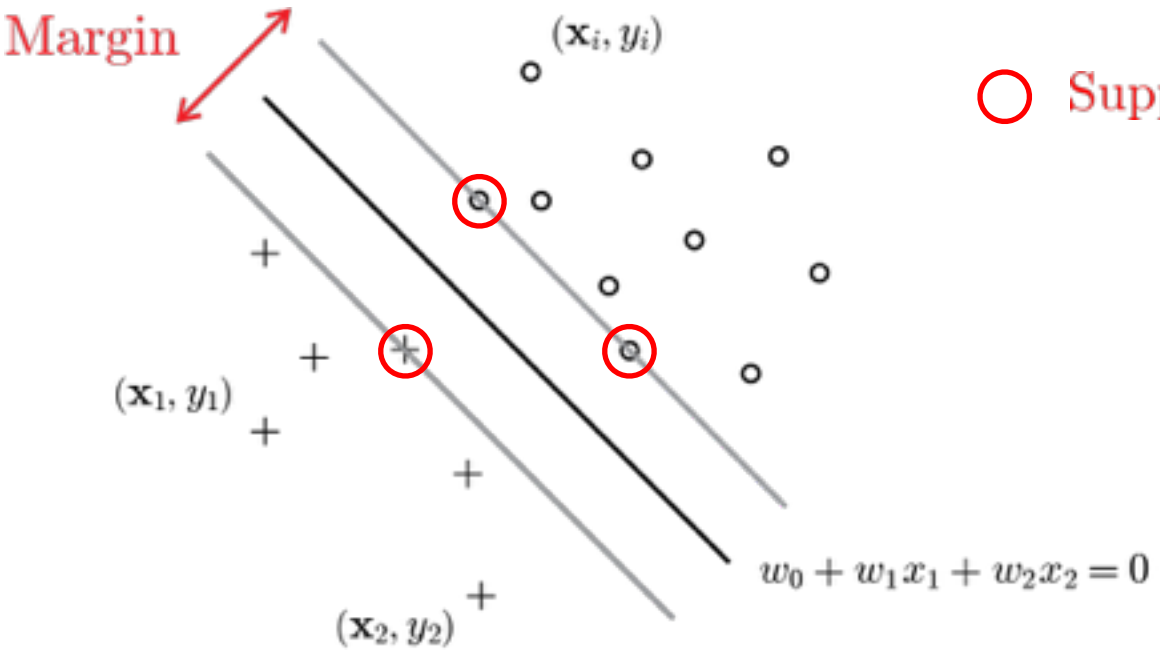
Scale $\mathbf{w}$ and w_0 such that $\min_i y_i(\mathbf{w}^\top \mathbf{x}_i + w_0) = 1$

$$(\mathbf{w}^*, w_0^*) = \arg\min_{\mathbf{w}} \{||\mathbf{w}||\}$$

Subject to:

$$y_i(\mathbf{w}^T \mathbf{x}_i + w_0) \geq 1 \quad \forall i \in \{1, 2, \ldots, n\}$$

Final Problem Formulation



$$(\mathbf{w}^*, w_0^*) = \arg\min_{\mathbf{w}} \left\{ \frac{1}{2} \mathbf{w}^T \mathbf{w} \right\}$$

← Convex function!

Subject to:

$$y_i(\mathbf{w}^T \mathbf{x}_i + w_0) \geq 1 \quad \forall i \in \{1, 2, \ldots, n\}$$

← Linear constraints!

How can We Solve it?

$$(\mathbf{w}^*, w_0^*) = \arg\min_{\mathbf{w}} \left\{ \frac{1}{2} \mathbf{w}^T \mathbf{w} \right\}$$

Subject to:

$$y_i(\mathbf{w}^T \mathbf{x}_i + w_0) \geq 1 \quad \forall i \in \{1, 2, \ldots, n\}$$

Need to know more about constrained optimization

Constrained Optimization

Objective: solve the following optimization problem

$$\mathbf{x}^* = \arg\max_{\mathbf{x}} \{f(\mathbf{x})\}$$

Subject to:

$$g_i(\mathbf{x}) = 0 \qquad \forall i \in \{1, 2, \ldots, m\}$$

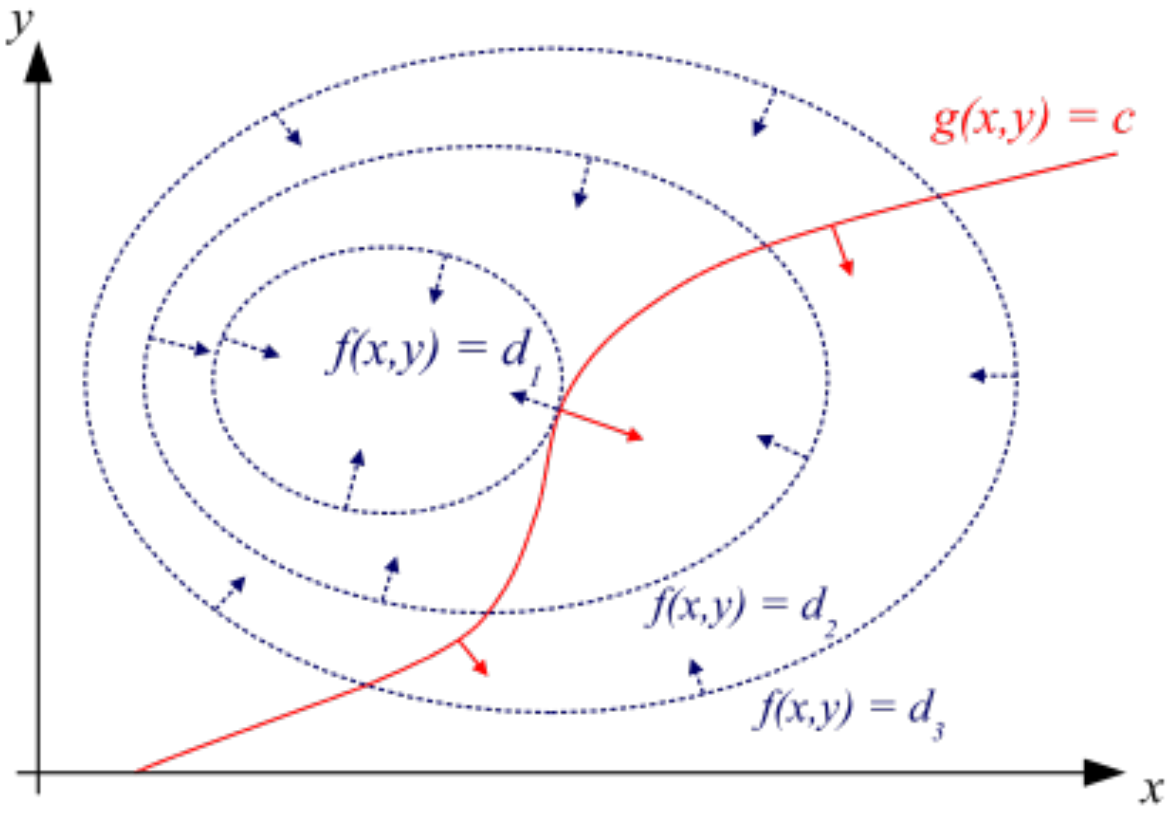
$$h_j(\mathbf{x}) \geq 0 \qquad \forall j \in \{1, 2, \ldots, n\}$$

Or, in a shorter notation, to:

$$\mathbf{g}(\mathbf{x}) = \mathbf{0}$$

$$\mathbf{h}(\mathbf{x}) \geq \mathbf{0}$$

INTUITION ON LAGRANGE MULTIPLIERS



Lagrange Multipliers

Taylor's expansion for $g(\mathbf{x})$, where $\mathbf{x}+\boldsymbol{\epsilon}$ is on the surface of $g(\mathbf{x})$

$$g(\mathbf{x}+\boldsymbol{\epsilon}) \approx g(\mathbf{x}) + \boldsymbol{\epsilon}^T \nabla g(\mathbf{x})$$

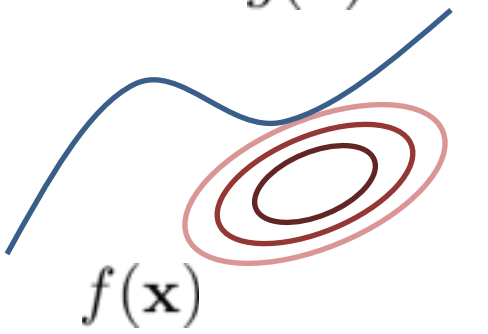
We know that $g(\mathbf{x}) = g(\mathbf{x}+\boldsymbol{\epsilon})$

$$\boldsymbol{\epsilon}^T \nabla g(\mathbf{x}) \approx 0$$

when $\boldsymbol{\epsilon} \to \mathbf{0}$

$$\boldsymbol{\epsilon}^T \nabla g(\mathbf{x}) = 0$$

$\Longrightarrow$ $\nabla g(\mathbf{x})$ is orthogonal to the surface



$\nabla g(\mathbf{x})$ and $\nabla f(\mathbf{x})$ are parallel!

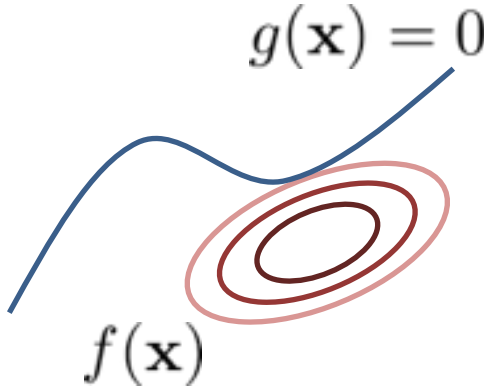
$$\nabla f(\mathbf{x}) + \alpha \nabla g(\mathbf{x}) = 0 \qquad \alpha \neq 0$$

$$L(\mathbf{x}, \alpha) = f(\mathbf{x}) + \alpha g(\mathbf{x})$$

Not a step-size
This is a Lagrange multiplier

More intuition on Lagrange multipliers

The two gradients are parallel,
but not necessarily of the same magnitude
The Lagrange multiplier adapts to
this difference in magnitude



$\nabla g(\mathbf{x})$ and $\nabla f(\mathbf{x})$ are parallel!

$$\nabla f(\mathbf{x}) + \alpha \nabla g(\mathbf{x}) = 0$$

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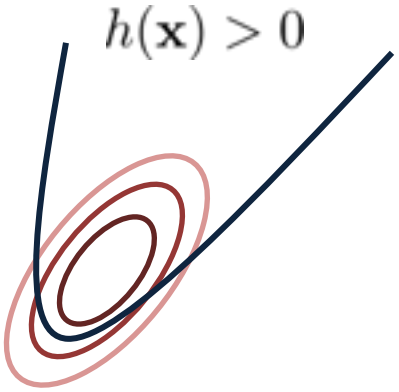
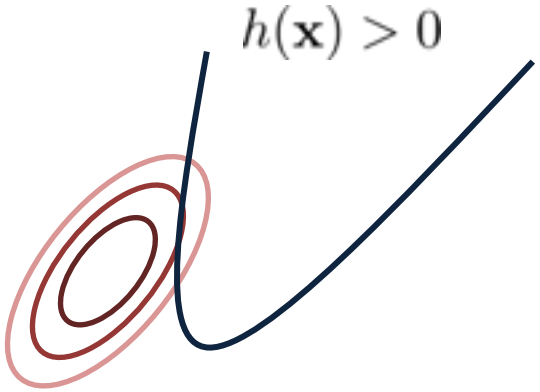
Lagrange Multipliers

Inactive constraint



$$\nabla f(\mathbf{x}) = 0$$

Active constraint



$$\nabla f(\mathbf{x}) = -\mu \nabla h(\mathbf{x}) \qquad \mu > 0$$

It holds that:

$$h(\mathbf{x}) \geq 0$$
$$\mu \geq 0$$
$$\mu \cdot h(\mathbf{x}) = 0$$

Karush-Kuhn-Tucker (KKT) conditions

Note: alpha rather than mu is used for inequality constraint in SVMs; an unfortunate historical choice, but we stick with it next

$$L(\mathbf{x}, \boldsymbol{\alpha}, \boldsymbol{\mu}) = f(\mathbf{x}) + \boldsymbol{\alpha}^T \mathbf{g}(\mathbf{x}) + \boldsymbol{\mu}^T \mathbf{h}(\mathbf{x})$$

How can We Solve it?

$$(\mathbf{w}^*, w_0^*) = \arg\min_{\mathbf{w}} \left\{ \frac{1}{2}\mathbf{w}^T\mathbf{w} \right\}$$

Subject to:

$$y_i(\mathbf{w}^T\mathbf{x}_i + w_0) \geq 1 \quad \forall i \in \{1, 2, \ldots, n\}$$

Solution: use Lagrangian multipliers!

$$L(\mathbf{w}, w_0, \boldsymbol{\alpha}) = \frac{1}{2}\mathbf{w}^T\mathbf{w} - \sum_{i=1}^{n} \alpha_i \left(y_i \left(\mathbf{w}^T\mathbf{x}_i + w_0 \right) - 1 \right)$$

$$\max_{\alpha} \min_{\mathbf{w}, w_0} L(\mathbf{w}, w_0, \boldsymbol{\alpha}) \qquad \alpha_i \geq 0$$

Solving it

$$\frac{\partial}{\partial w_j} L(\mathbf{w}, w_0, \boldsymbol{\alpha}) = 0 \quad \Longrightarrow \quad w_j = \sum_{i=1}^{n} \alpha_i y_i x_{ij}$$

$$\Longrightarrow \quad \mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$$

$$\frac{\partial}{\partial w_0} L(\mathbf{w}, w_0, \boldsymbol{\alpha}) = 0 \quad \Longrightarrow \quad \sum_{i=1}^{n} \alpha_i y_i = 0$$

Dual Problem

$$\sum_{i=1}^{n} \alpha_i y_i = 0 \qquad \mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$$

$$\begin{aligned}
L(\mathbf{w}, w_0, \boldsymbol{\alpha}) &= \frac{1}{2}\mathbf{w}^T\mathbf{w} - \sum_{i=1}^{n} \alpha_i y_i \mathbf{w}^T\mathbf{x}_i - \sum_{i=1}^{n} \alpha_i y_i w_0 + \sum_{i=1}^{n} \alpha_i \\
&= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T\mathbf{x}_j - \sum_{i=1}^{n} \alpha_i y_i (\sum_{j=1}^{n} \alpha_j y_j \mathbf{x}_j)^T \mathbf{x}_i + \sum_{i=1}^{n} \alpha_i \\
&= \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T\mathbf{x}_j \\
&= \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j k(\mathbf{x}_i, \mathbf{x}_j)
\end{aligned}$$

kernel property

$$k(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^\top \mathbf{x}_j$$

Subject to:

$$\alpha_i \geq 0 \qquad \forall i \in \{1, 2, \ldots, n\}$$

$$\sum_{i=1}^{n} \alpha_i y_i = 0$$

Solving the Dual Problem

Use quadratic programming to solve for $\boldsymbol{\alpha}$

Then set

$$\Longrightarrow \qquad \mathbf{w} = \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i$$

$$k(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^\top \mathbf{x}_j$$

$$\Longrightarrow \qquad f(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + w_0$$

$$= \frac{1}{2} \sum_{i=1}^{n} \alpha_i y_i k(\mathbf{x}, \mathbf{x}_i) + w_0$$

Analysis of the Solution

Karush-Kuhn-Tucker (KKT) conditions:

$$\alpha_i \geq 0$$

$$y_i(\mathbf{w}^T\mathbf{x}_i + w_0) - 1 \geq 0 \qquad \forall i \in \{1, 2, \ldots, n\}$$

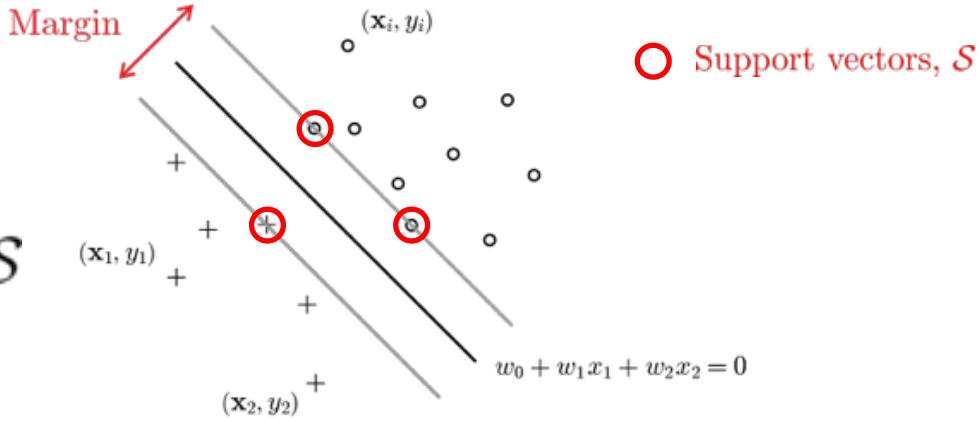
$$\alpha_i \left(y_i \left(\mathbf{w}^T\mathbf{x}_i + w_0\right) - 1\right) = 0$$

This means that for $\forall i$, either $\alpha_i = 0$ or $y_i \left(\mathbf{w}^T\mathbf{x}_i + w_0\right) = 1$

$\alpha_i = 0$ for all vectors that are not support vectors

$$f(\mathbf{x}) = \sum_{\mathbf{x}_i \in \mathcal{S}} \alpha_i y_i k(\mathbf{x}, \mathbf{x}_i) + w_0$$

$w_0 = 1 - \mathbf{w}^T\mathbf{x}_s$, where $\mathbf{x}_s \in \mathcal{S}$



A Support Vector Machine