Machine Learning

Lecture 7: Support Vector Machine

Fall 2022

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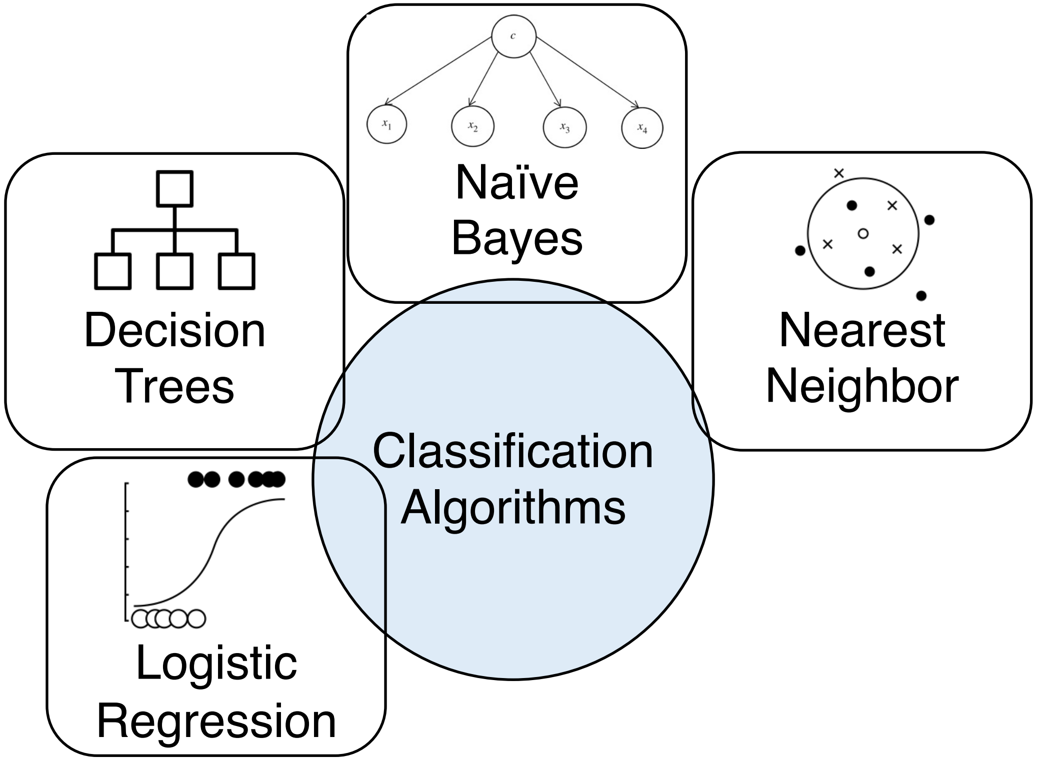
The family of classification

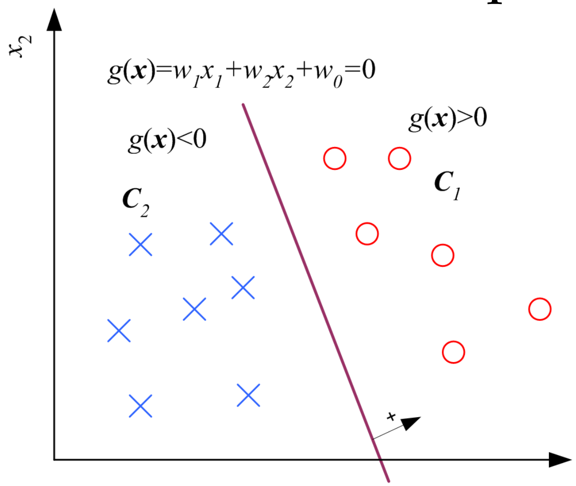


Recall: Linear Classifiers

- **Given**: a training set $\{(x^{(1)},y^{(1)}), \ldots, (x^{(N)}, y^{(N)})\}$ of N samples

$$x^{(\ell)} \in \mathbf{R}^d\text{: input,}\quad y^{(\ell)} \in \{-1, 1\}\text{:target (label)}$$

- Assume that the problem is linearly separable: there exists a linear surface to separate the two classes



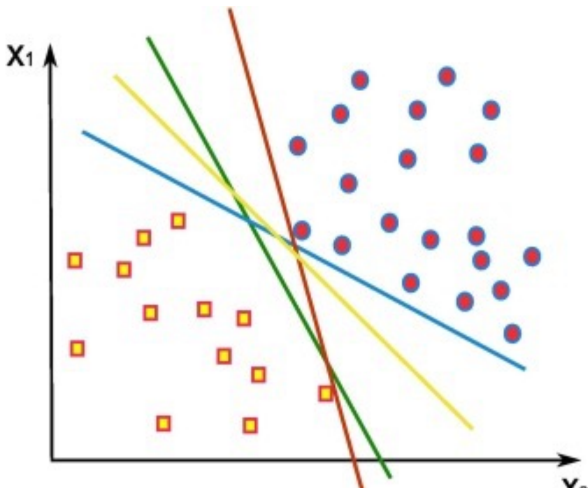
2-D: line;
3-D: plane;
…;
d-D: hyperplane ($\boldsymbol{wx}+w_0=0$)

Goal:

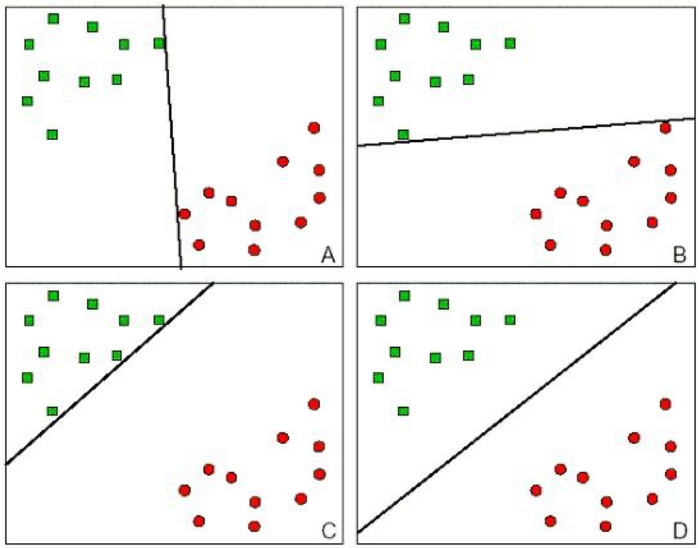
Find $\boldsymbol{wx}+w_0=0$ that perfectly separates the two classes

The Problem

- There can be multiple separating hyperplanes.



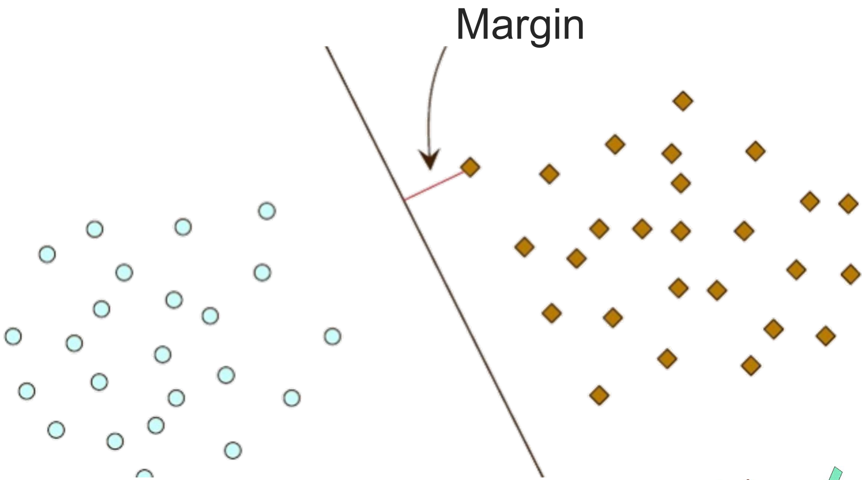
对于这四种情况而言，应该是D项相对更好。
因为D项的划分之后数据分布更加均匀对称，并且没有明显的过拟合，即新的数据点在添加进来时不会那么容易的出现预测错误的情况。



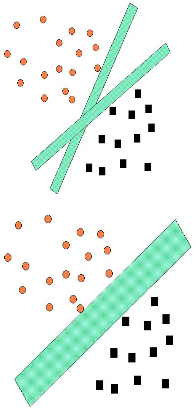
Which one is the best?

The Idea:

- Find a decision boundary that **maximizes the margin** between two classes.



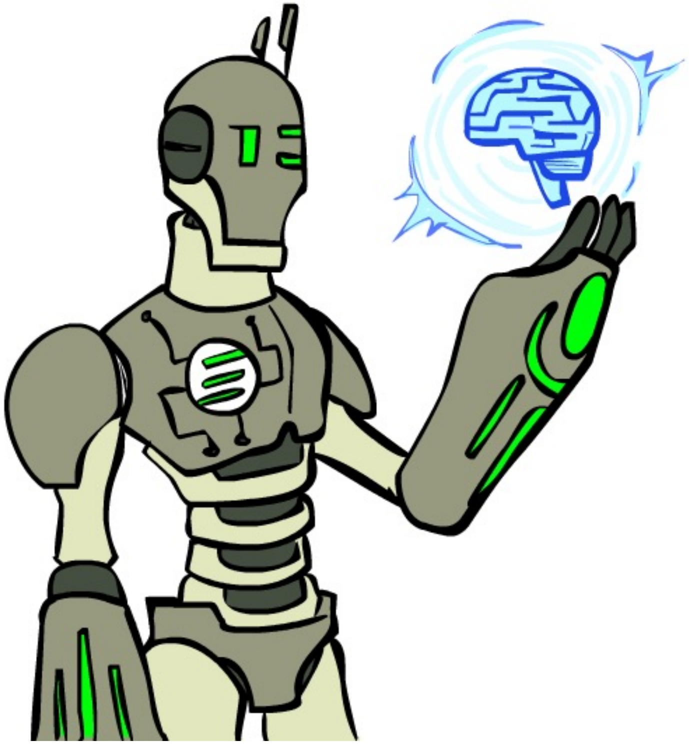
Margin and generalization:
Statistical learning theories have shown that the boundary with the largest margin generalizes best (i.e., has the smallest generalization error).



Today

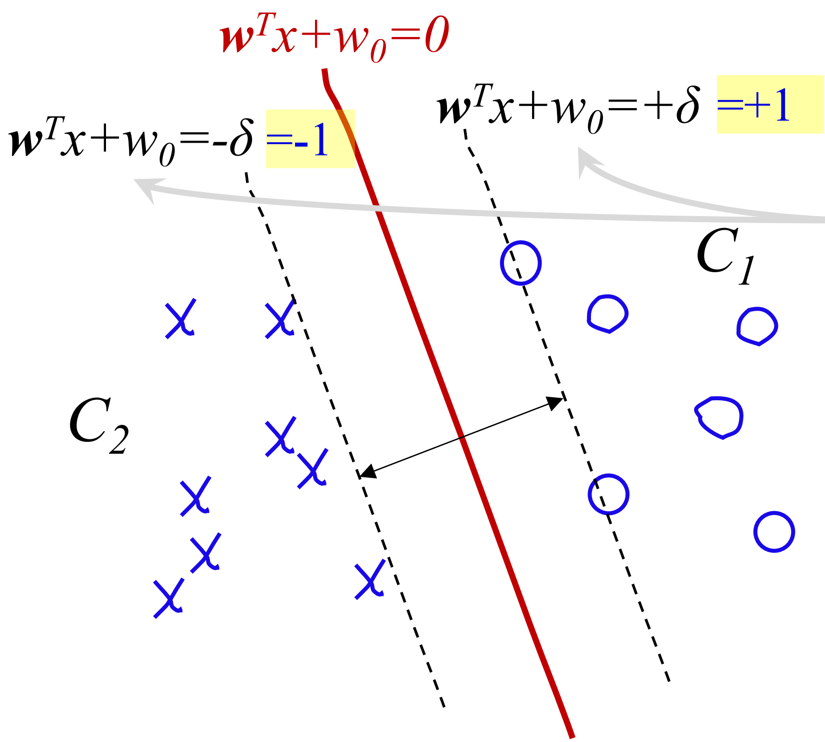
Support Vector Machine

- Problem Formulation
- Dual Problem
- Loss and Optimization



Problem Formulation

- A linear discriminant function models a **linear decision boundary** of two classes.



$1/\delta\, \boldsymbol{w}^T x + 1/\delta\, w_0 = 0$ defines the same hyperplane as $\boldsymbol{w}^T x + w_0 = 0$

$$\boldsymbol{w}^T x + w_0 \begin{cases} \geq +1 & x \in C_1 \\ \leq -1 & x \in C_2 \end{cases}$$

Maximizing the Margin

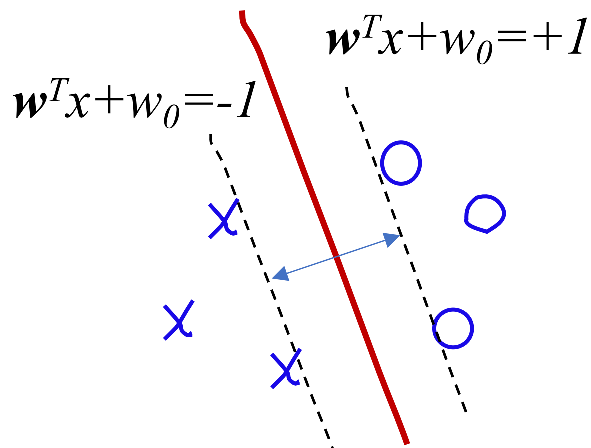
$$\boldsymbol{w}^{\mathrm{T}}x+w_0=\begin{cases}1 & \text{for the closest points on one side}\\ -1 & \text{for the closest points on the other}\end{cases}$$

- Let $x^{(1)}$ and $x^{(2)}$ be two closest points on each side of the hyperplane.
- Note that

$$\boldsymbol{w}^{\mathrm{T}}\, x^{(1)}+w_0=+1$$
$$\boldsymbol{w}^{\mathrm{T}}\, x^{(2)}+w_0=-1$$

which imply

$$\boldsymbol{w}^{\mathrm{T}}(x^{(1)}-x^{(2)})=2.$$



Hence, the margin can be given by

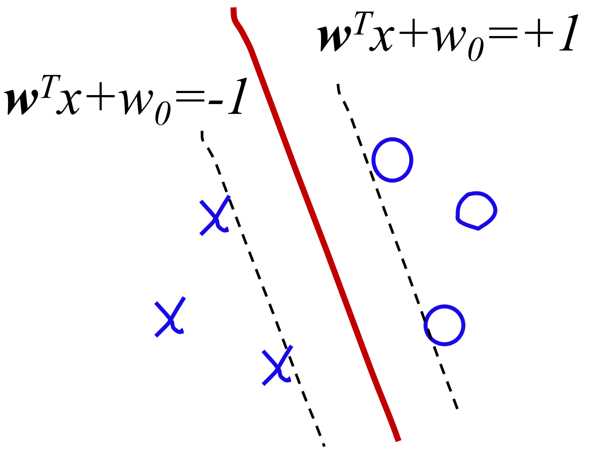
$$\text{margin}=\frac{\boldsymbol{w}^{\mathrm{T}}(x^{(1)}-x^{(2)})}{\|\boldsymbol{w}\|}=\frac{2}{\|\boldsymbol{w}\|}$$ (在向量w方向上的投影)

Maximizing the margin is equivalent to minimizing $\frac{1}{2}\|\boldsymbol{w}\|$

Inequality Constraints

- Given: $D = \{(x^{(\ell)}, y^{(\ell)}), \ldots, (x^{(N)}, y^{(N)})\}$, we want $\boldsymbol{w}$ and w_0 to satisfy

$$\boldsymbol{w}^{\mathrm{T}} x^{(\ell)} + w_0 \begin{cases} \geq +1 & \text{if } y^{(\ell)} = +1 \\ \leq -1 & \text{if } y^{(\ell)} = -1 \end{cases}$$



- Or, equivalently,

$$y^{(\ell)} (\boldsymbol{w}^{\mathrm{T}} x^{(\ell)} + w_0) \geq 1$$

SVM = Solving an Optimization Problem

In summary, SVM aims to solve a constrained optimization problem:

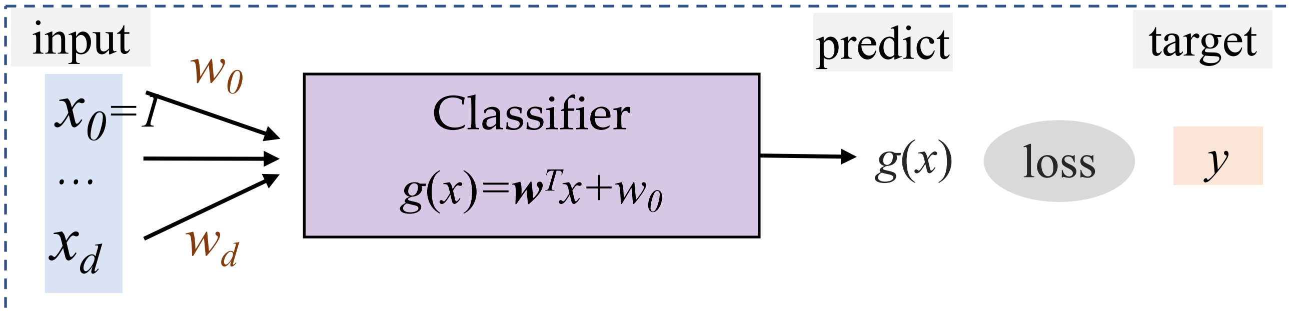
$$\begin{aligned}&\text{minimize} \quad \frac{1}{2}||\boldsymbol{w}||^2\\&\text{subject to} \quad y^{(\ell)}(\boldsymbol{w}^{\mathrm{T}}x^{(\ell)}+w_0)\geq 1,\ \ell=1,\ldots,\mathrm{N}\end{aligned}$$

- This is a quadratic programming (QP) problem, which is one type of convex optimization problem. (凸优化中的二次优化)
- The complexity depends on the dimensionality d of inputs

(因为待优化的参数为w，其是d维的，并且与输入的x的数量N无关)

Model Architecture

- The same architecture as Perceptron.



- Train:
  - optimize the parameters $\boldsymbol{w}$ and w_0 using data
- Test:
  - calculate $g(x) = \boldsymbol{w}^{\mathsf{T}}x+w_0$ and choose C_1 if $g(x) > 1$ or choose C_2 if $g(x)<-1$.

Loss Function

$$\min \ \frac{1}{2}\|\boldsymbol{w}\|^2$$
$$\text{s.t.} \quad y^{(\ell)}(\boldsymbol{w}^{\mathrm{T}}x^{(\ell)}+w_0)\geq 1,\ \ell=1,\ldots,N$$

- For a given input x, the model outputs a score $g(x) = \boldsymbol{w}^{\mathrm{T}}x+w_0$. Let $y \in \{-1, +1\}$ be the label of the real class (y =+1: $x \in C_1$, y = -1: $x \in C_2$):
  - if $y(\boldsymbol{w}^{\mathrm{T}}x+w_0) <1$: we aim to maximize $y(\boldsymbol{w}^{\mathrm{T}}x+w_0)$ until reaching 1, cost is $1-y(\boldsymbol{w}^{\mathrm{T}}x+w_0)$ 极限值一般情况下是在边界上取到
  - if $y(\boldsymbol{w}^{\mathrm{T}}x+w_0) >1$: outlier points, no need to optimize, cost is **0**
- Can writhe this succinctly as a **Hinge** loss:

$$\ell\,(\boldsymbol{w}, w_0 \,|\, x, y) = \max(0,\ 1\text{-}y(\boldsymbol{w}^{\mathrm{T}}x+w_0))$$

- Given: $D = \{(x^{(1)}, r^{(1)}), \ldots, (x^{(N)}, r^{(N)})\}$, the loss over the dataset is defined as:

$$L\,(\boldsymbol{w}, w_0 \,|\, D) = \frac{1}{N}\sum_{\ell=1}^{N} \max(0,\ 1-y^{(\ell)}(\boldsymbol{w}^{\mathrm{T}}x^{(\ell)}+w_0)) + \frac{\lambda}{2}\|\boldsymbol{w}\|^2$$

Optimization – Gradient Descend

$$\boldsymbol{w}_{\text{new}} = \boldsymbol{w}_{\text{old}} + \eta \frac{\partial L}{\partial w}$$

What is $\frac{\partial L}{\partial w}$?

$$L(\boldsymbol{w}, w_0 \mid D) = \begin{cases} \frac{\lambda}{2} \|\boldsymbol{w}\|^2 & \textbf{if} \quad y^{(\ell)}(\boldsymbol{w}^{\mathrm{T}} x^{(\ell)} + w_0) \geq 1 \\ \frac{1}{N} \sum_{\ell=1}^{N} 1 - y^{(\ell)}(\boldsymbol{w}^{\mathrm{T}} x^{(\ell)} + w_0) + \frac{\lambda}{2} \|\boldsymbol{w}\|^2 & \text{otherwise} \end{cases}$$

For each $\boldsymbol{w}_j$ ($j = 0, \ldots, d$):

$$\frac{\partial L}{\partial w_j} = \begin{cases} \lambda w_j & \text{if } y^{(\ell)}(\boldsymbol{w}^{\mathrm{T}} x^{(\ell)} + w_0) \geq 1 \\ \lambda w_j - y^{(\ell)} x^{(\ell)} & \text{o.w.} \end{cases}$$

$$\frac{\partial L}{\partial w_0} = \begin{cases} 0 & \text{if } y^{(\ell)}(\boldsymbol{w}^{\mathrm{T}} x^{(\ell)} + w_0) \geq 1 \\ -y^{(\ell)} & \text{o.w.} \end{cases}$$

这里的w_0指的是
y=wx+w_0中的w_0

The Algorithm

Gradient Descend for SVM

Input: $D = \{(\mathrm{x}^{(l)}, \mathrm{y}^{(l)})\}$ $(l = 1{:}N)$

for $j = 0, \ldots, d$

$\quad \boldsymbol{w}_{\mathrm{j}} \leftarrow rand\,(-0.01, 0.01)$

repeat

$\quad$ **for** $j = 0, \ldots, d$

$\quad\quad \Delta\boldsymbol{w}_{\mathrm{j}} \leftarrow 0$

$\quad$ **for** $l = 1, \ldots, N$

$\quad\quad a \leftarrow 0$

$\quad\quad$ **for** $j = 0, \ldots, d$

$\quad\quad\quad a \leftarrow a + \boldsymbol{w}_{\mathrm{j}} x_{\mathrm{j}}^{(l)}$

$\quad\quad$ **for** $j = 0, \ldots, d$

$\quad\quad\quad \Delta\boldsymbol{w}_{\mathrm{j}} \leftarrow \Delta\boldsymbol{w}_{\mathrm{j}} + \lambda\boldsymbol{w}_{\mathrm{j}}$

$\quad\quad\quad \Delta\boldsymbol{w}_0 \leftarrow 0$

$\quad\quad\quad$ **if** $y^{(l)}a<1$: $\Delta\boldsymbol{w}_{\mathrm{j}} \leftarrow \Delta\boldsymbol{w}_{\mathrm{j}} - y^{(l)}x^{(l)}$

$\quad \Delta\boldsymbol{w}_{\mathrm{j}} = \Delta\boldsymbol{w}_{\mathrm{j}} / \mathrm{N}$

$\quad$ **for** $j = 0, \ldots, d$

$\quad\quad w_{\mathrm{j}} \leftarrow w_{\mathrm{j}} + \eta\Delta w_{\mathrm{j}}$

until convergence

Lagrangian

- The primal optimization problem:

$$\begin{aligned}&\text{minimize } \tfrac{1}{2}\|w\|^2\\&\text{subject to } y^{(\ell)}(\boldsymbol{w}x^{(\ell)}+w_0) \geq 1,\ \forall \boldsymbol{\ell}\end{aligned}$$

- **Lagrangian**: $\mathcal{L}= \tfrac{1}{2}\|\boldsymbol{w}\|^2 - \Sigma_\ell \alpha_\ell (y^{(\ell)}(\boldsymbol{w}x^{(\ell)}+w_0) - 1)$

$$\nabla_{\boldsymbol{w},w_0}\mathcal{L}=0 \Rightarrow \begin{cases} \dfrac{\partial \mathcal{L}}{\partial \boldsymbol{w}} = 0 \Rightarrow \boldsymbol{w} = \sum_{\ell=1}^{N} \alpha_\ell y^{(\ell)} x^{(\ell)} \\ \dfrac{\partial \mathcal{L}}{\partial w_0} = 0 \Rightarrow \sum_{\ell=1}^{N} \alpha_\ell y^{(\ell)} = 0 \end{cases}$$

- Substitute back in the primal to get the dual

$$\begin{aligned}&\textbf{maximize}\ \ \mathcal{L}(\alpha)=\Sigma_\ell \alpha_\ell - \tfrac{1}{2}\sum_{l=1}^{N}\sum_{l'=1}^{N} \alpha_l \alpha_{l'} y^{(l)} y^{(l')} (x^{(l)})^{\mathrm{T}} x^{(l')}\\&\textbf{subject to}\ \ \alpha_\ell \geq 0,\ \sum_{\ell=1}^{N} \alpha_\ell y^{(\ell)} = 0\end{aligned}$$

The Dual Problem

Dual optimization problem:

$$\text{maximize} \quad \sum_{\ell=1}^{N} \alpha_\ell - \frac{1}{2}\sum_{\ell=1}^{N}\sum_{\ell'=1}^{N} \alpha_\ell \alpha_{\ell'} y^{(\ell)} y^{(\ell')} (x^{(\ell)})^{\mathrm{T}} x^{(\ell')}$$

$$\text{subject to} \quad \sum_{\ell=1}^{N} \alpha_\ell y^{(\ell)} = 0$$

$$\alpha_\ell \geq 0, \ \ell = 1 \ldots \mathrm{N}$$

- This is also a QP problem, but its complexity depends on the sample size N (rather than the input dimensionality d)

Primal and Dual

Primal

$$\min \ \frac{1}{2}||\boldsymbol{w}||^2$$
$$\text{s.t.} \quad y^{(l)}(\boldsymbol{w}^{\mathrm{T}}\mathrm{x}^{(l)}+w_0)\geq 1, \ \forall l$$

The complexity depends on the dimensionality d of inputs

Dual

$$\max \ \Sigma_l \alpha_l - \tfrac{1}{2}\Sigma_l \Sigma_{l'} \alpha_l \alpha_{l'} y^{(l)} y^{(l')} (x^{(l)})^{\mathrm{T}} x^{(l')}$$
$$\text{s.t.} \quad \Sigma_l \alpha_l y^{(l)} = 0$$
$$\alpha_l \geq 0, \quad l = 1 \ldots \mathrm{N}$$

The complexity depends on the sample size N

- **It turns out to be more convenient to solve the dual problem** than solving the **primal problem** ($N < d$)
- We can firstly solve **Dual** to obtain $\{\alpha_\ell\}$, and then obtain the W in **Primal**

Training (Dual)

- Given: $D = \{(x^{(\ell)}, y^{(\ell)}), \dots, (x^{(N)}, y^{(N)})\}$
- minimize the **loss function** $L(\alpha)$ using any general purpose optimization toolkits (e.g., Matlab)
- But SVM is usually optimized using the **SMO** (sequential minimal optimization)

> - **Goal:**
>
> $$\min_\alpha L(\boldsymbol{\alpha})$$
>
> - **Iteration:**
>
> Update two variables each time until convergence {
> 1. Select an α_1 that violates the KKT condition
> 2. Pick a second multiplier α_2 and optimize $L(\alpha)$ w.r.t. α_1 and α_2
>
> }

Support Vectors

Suppose the optimal $\{\alpha_\ell\}$ have been obtained

- Patterns for which $y^{(\ell)}(\boldsymbol{w}x^{(\ell)}+w_0) > 1$

即这个数据点没有起到约束作用

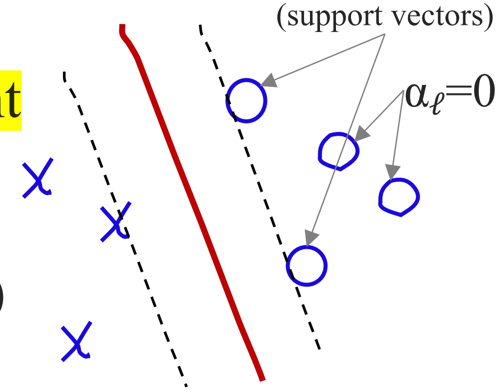
$\alpha_\ell=0$ (inactive constraints) $\Rightarrow x^{(\ell)}$ irrelevant

recall complimentary slackness: $\lambda_i^* g_i(x^*)=0$

- Patterns that have $\alpha_\ell>0$ (active constraints)

互补松弛条件一般都是由对偶问题系数和约束条件中的不等式的乘积构成的。

$y^{(\ell)}(\boldsymbol{w}x^{(\ell)}+w_0) = 1 \Rightarrow x^{(\ell)}$ lies on margin



- Most of the dual variables vanish with $\alpha_\ell=0$. They are points lying beyond the margin with **no effect** on the hyperplane.
- Solution is only determined by the examples on the margin (support vectors), i.e., $x^{(\ell)}$ with $\alpha_\ell>0$, hence the name **support vector machine (SVM).**

support vectors：即满足互补松弛条件中系数不为零的那些边界点

Computation of Primal Variables

- Having obtained the optimal $\boldsymbol{\alpha}$, we can obtain $\boldsymbol{w}$:

$$\boxed{\mathbf{w} = \sum_{\ell=1}^{N} \alpha_\ell y^{(\ell)} \mathbf{x}^{(\ell)} = \sum_{\mathbf{x}^{(\ell)} \in \mathcal{SV}} \alpha_\ell y^{(\ell)} \mathbf{x}^{(\ell)}}$$

where $\mathcal{SV}$ denotes the set of support vectors.

- The support vectors must lie on the margin, so they should satisfy $y^{(\ell)}(\mathbf{w}^T \mathbf{x}^{(\ell)} + w_0) = 1$ or $w_0 = y^{(\ell)} - \mathbf{w}^T \mathbf{x}^{(\ell)}$
- For numerical stability, all support vectors are used to compute w_0:

$$\boxed{w_0 = \frac{1}{|\mathcal{SV}|} \sum_{\mathbf{x}^{(\ell)} \in \mathcal{SV}} \left(y^{(\ell)} - \mathbf{w}^T \mathbf{x}^{(\ell)} \right)}$$

Prediction

- **Discriminant Function:**

$$
\begin{aligned}
g(\mathbf{x}) &= \mathbf{w}^T\mathbf{x} + w_0 \\
&= \left(\sum_{\mathbf{x}^{(\ell)} \in \mathcal{SV}} \alpha_\ell y^{(\ell)} \mathbf{x}^{(\ell)}\right)^T \mathbf{x} + \frac{1}{|\mathcal{SV}|} \sum_{\mathbf{x}^{(\ell)} \in \mathcal{SV}} \left(y^{(\ell)} - \mathbf{w}^T \mathbf{x}^{(\ell)}\right)
\end{aligned}
$$

- **Decision Rule:**

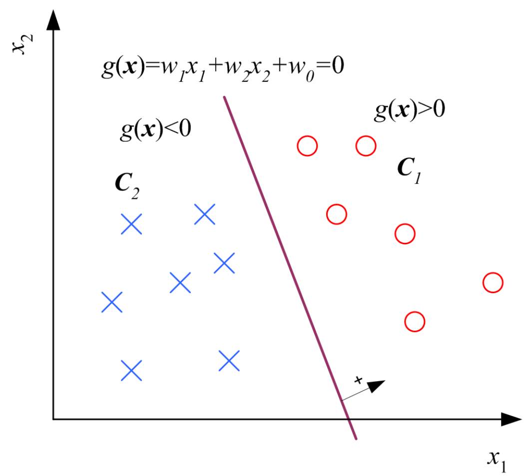
$$
\text{Choose } \begin{cases} C_1 & \text{if } g(\mathbf{x}) > 0 \\ C_2 & \text{otherwise} \end{cases}
$$

A Python Tutorial

https://towardsdatascience.com/implementing-svm-from-scratch-784e4ad0bc6a

https://www.kaggle.com/code/misbahbilgili/svm-from-scratch-with-explanation/notebook

What’s Next



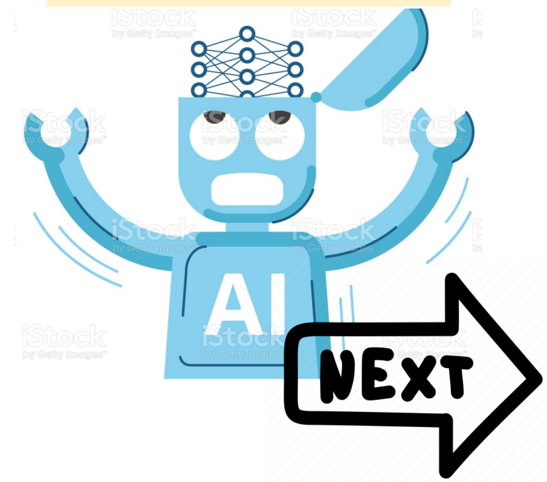
Perceprton

Logistic Regression

SVM

I can approximate any non-linear functions !

Neural Networks



The curse of nonlinearity