CSCI567 Machine Learning (Spring 2021)

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Outline

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Logistics

- HW 3 was assigned.
- We will discuss quiz specifics at the end of the lecture today.

Outline

1. Logistics
2. Review of last lecture
3. Support vector machines (primal formulation)
4. Quiz 1 Specifics

Kernel functions

Definition: a function $k : \mathbb{R}^{\mathsf{D}} \times \mathbb{R}^{\mathsf{D}} \rightarrow \mathbb{R}$ is called a *(positive semidefinite) kernel function* if there exists a function $\boldsymbol{\phi} : \mathbb{R}^{\mathsf{D}} \rightarrow \mathbb{R}^{\mathsf{M}}$ so that for any $\boldsymbol{x}, \boldsymbol{x}' \in \mathbb{R}^{\mathsf{D}}$,

$$k(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{\phi}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}')$$

Examples we have seen

$$k(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x}^{\mathrm{T}}\boldsymbol{x}')^2$$

$$k(\boldsymbol{x}, \boldsymbol{x}') = \sum_{d=1}^{\mathsf{D}} \frac{\sin(2\pi(x_d - x'_d))}{x_d - x'_d}$$

$$k(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x}^{\mathrm{T}}\boldsymbol{x}' + c)^d \qquad \textbf{(polynomial kernel)}$$

$$k(\boldsymbol{x}, \boldsymbol{x}') = e^{-\frac{\|\boldsymbol{x}-\boldsymbol{x}'\|_2^2}{2\sigma^2}} \qquad \textbf{(Gaussian/RBF kernel)}$$

Kernelizing ML algorithms

Feasible as long as **only inner products are required**:

- regularized linear regression (dual formulation)

$$\boldsymbol{\phi}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{w}^* = \boldsymbol{\phi}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{\Phi}^{\mathrm{T}}(\boldsymbol{K} + \lambda\boldsymbol{I})^{-1}\boldsymbol{y} \quad (\boldsymbol{K} = \boldsymbol{\Phi}\boldsymbol{\Phi}^{\mathrm{T}} \text{ is } \textit{kernel matrix})$$

- nearest neighbor classifier with L2 distance

$$\|\boldsymbol{\phi}(\boldsymbol{x}) - \boldsymbol{\phi}(\boldsymbol{x}')\|_2^2 = k(\boldsymbol{x}, \boldsymbol{x}) + k(\boldsymbol{x}', \boldsymbol{x}') - 2k(\boldsymbol{x}, \boldsymbol{x}')$$

- perceptron, logistic regression, SVM, . . .

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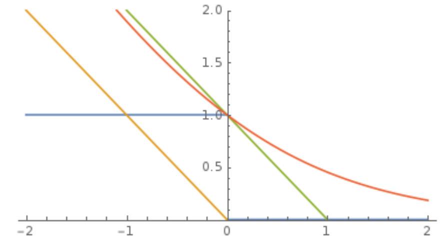
Support vector machines (SVM)

- One of the most commonly used classification algorithms
- Works well with the kernel trick
- Strong theoretical guarantees

We focus on **binary classification** here.

Primal formulation

In one sentence: linear model with L2 regularized hinge loss. Recall



- perceptron loss $\ell_{\text{perceptron}}(z) = \max\{0, -z\}$ → Perceptron
- logistic loss $\ell_{\text{logistic}}(z) = \log(1 + \exp(-z))$ → logistic regression
- hinge loss $\ell_{\text{hinge}}(z) = \max\{0, 1 - z\}$ → **SVM**

Primal formulation

For a linear model $(\boldsymbol{w}, b)$, this means

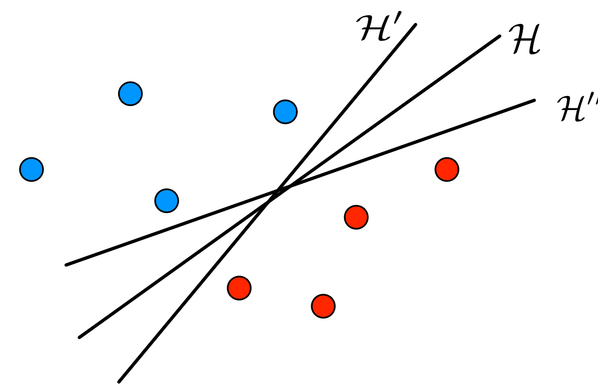
$$\min_{\boldsymbol{w},b} \sum_n \max\left\{0, 1 - y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b)\right\} + \frac{\lambda}{2}\|\boldsymbol{w}\|_2^2$$

- recall $y_n \in \{-1, +1\}$
- a nonlinear mapping $\boldsymbol{\phi}$ is applied
- the bias/intercept term b is used explicitly (think about why after this lecture)

So why L2 regularized hinge loss?

Geometric motivation: separable case

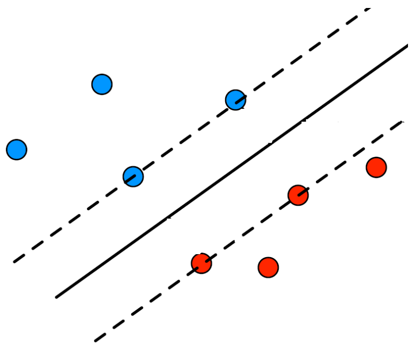
When data is **linearly separable**, there are *infinitely many hyperplanes with zero training error*:



So which one should we choose?

Intuition

The further away from data points the better.



How to formalize this intuition?

Distance to hyperplane

What is the **distance** from a point $\boldsymbol{x}$ to a hyperplane $\{\boldsymbol{x} : \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} + b = 0\}$?

Assume the **projection** is $\boldsymbol{x} - \ell\frac{\boldsymbol{w}}{\|\boldsymbol{w}\|_2}$, then

$$0 = \boldsymbol{w}^{\mathrm{T}}\left(\boldsymbol{x} - \ell\frac{\boldsymbol{w}}{\|\boldsymbol{w}\|_2}\right) + b = \boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} - \ell\|\boldsymbol{w}\| + b$$

and thus $\ell = \frac{\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}+b}{\|\boldsymbol{w}\|_2}$.

Therefore the distance is

$$\frac{|\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} + b|}{\|\boldsymbol{w}\|_2}$$

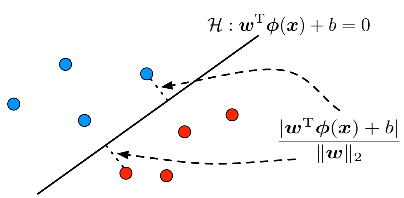
For a hyperplane that correctly classifies $(\boldsymbol{x}, y)$, the distance becomes

$$\frac{y(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x} + b)}{\|\boldsymbol{w}\|_2}$$

Maximizing margin

Margin: the *smallest* distance from all training points to the hyperplane

$$\textsc{margin of } (\boldsymbol{w},\, b) = \min_n \frac{y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b)}{\|\boldsymbol{w}\|_2}$$



The intuition "**the further away the better**" translates to solving

$$\max_{\boldsymbol{w},b} \min_n \frac{y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b)}{\|\boldsymbol{w}\|_2} = \max_{\boldsymbol{w},b} \frac{1}{\|\boldsymbol{w}\|_2} \min_n y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b)$$

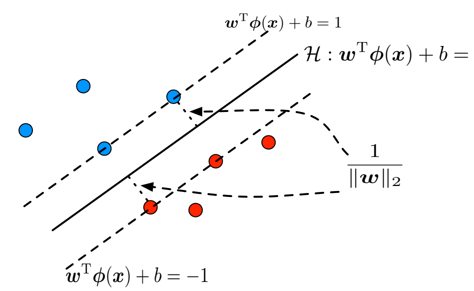
Rescaling

Note: rescaling $(\boldsymbol{w}, b)$ does not change the hyperplane at all.

We can thus always scale $(\boldsymbol{w}, b)$ s.t. $\min_n y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b) = 1$

The margin then becomes

$$\begin{aligned}
&\textsc{margin of } (\boldsymbol{w},\, b) \\
&= \frac{1}{\|\boldsymbol{w}\|_2} \min_n y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b) \\
&= \frac{1}{\|\boldsymbol{w}\|_2}
\end{aligned}$$



Summary for separable data

For a separable training set, we aim to solve

$$\max_{\boldsymbol{w},b} \frac{1}{\|\boldsymbol{w}\|_2} \quad \text{s.t.} \quad \min_n y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n)+b)=1$$

This is equivalent to

$$\begin{aligned} \min_{\boldsymbol{w},b} \quad & \frac{1}{2}\|\boldsymbol{w}\|_2^2 \\ \text{s.t.} \quad & y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n)+b) \geq 1, \quad \forall\ n \end{aligned}$$

SVM is thus also called *max-margin* classifier. The constraints above are called *hard-margin* constraints.

General non-separable case

If data is not linearly separable, the previous constraint

$$y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n)+b) \geq 1, \quad \forall\ n$$

is obviously *not feasible*.

To deal with this issue, we relax them to **soft-margin** constraints:

$$y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n)+b) \geq 1-\xi_n, \quad \forall\ n$$

where we introduce **slack variables** $\xi_n \geq 0$.

SVM Primal formulation

We want ξ_n to be as small as possible too. The objective becomes

$$\begin{aligned} \min_{\boldsymbol{w},b,\{\xi_n\}} \quad & \frac{1}{2}\|\boldsymbol{w}\|_2^2 + C\sum_n \xi_n \\ \text{s.t.} \quad & y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n)+b) \geq 1-\xi_n, \quad \forall\ n \\ & \xi_n \geq 0, \quad \forall\ n \end{aligned}$$

where C is a hyperparameter to balance the two goals.

Equivalent form

Formulation

$$\begin{aligned} \min_{\boldsymbol{w},b,\{\xi_n\}} \quad & C\sum_n \xi_n + \frac{1}{2}\|\boldsymbol{w}\|_2^2 \\ \text{s.t.} \quad & 1-y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n)+b) \leq \xi_n, \quad \forall\ n \\ & \xi_n \geq 0, \quad \forall\ n \end{aligned}$$

is equivalent to

$$\begin{aligned} \min_{\boldsymbol{w},b,\{\xi_n\}} \quad & C\sum_n \xi_n + \frac{1}{2}\|\boldsymbol{w}\|_2^2 \\ \text{s.t.} \quad & \max\left\{0, 1-y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n)+b)\right\} = \xi_n, \quad \forall\ n \end{aligned}$$

Equivalent form

$$\min_{\boldsymbol{w},b,\{\xi_n\}} \quad C\sum_n \xi_n + \frac{1}{2}\|\boldsymbol{w}\|_2^2$$
$$\text{s.t.} \quad \max\left\{0, 1 - y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b)\right\} = \xi_n, \quad \forall\, n$$

is equivalent to

$$\min_{\boldsymbol{w},b} \; C\sum_n \max\left\{0, 1 - y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b)\right\} + \frac{1}{2}\|\boldsymbol{w}\|_2^2$$

and

$$\min_{\boldsymbol{w},b} \; \sum_n \max\left\{0, 1 - y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b)\right\} + \frac{\lambda}{2}\|\boldsymbol{w}\|_2^2$$

with $\lambda = 1/C$. *This is exactly minimizing L2 regularized hinge loss!*

Optimization

$$\min_{\boldsymbol{w},b,\{\xi_n\}} \quad C\sum_n \xi_n + \frac{1}{2}\|\boldsymbol{w}\|_2^2$$
$$\text{s.t.} \quad 1 - y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b) \leq \xi_n, \quad \forall\, n$$
$$\xi_n \geq 0, \quad \forall\, n$$

- It is a convex (**quadratic** in fact) problem
- thus can apply any convex optimization algorithms, e.g. SGD
- there are **more specialized and efficient** algorithms
- but usually we apply kernel trick, which requires solving the *dual problem*

Outline

Logistics

- Quiz 1 is scheduled for March 3, 2021 from 10:00 – 12:00 PM. It is an in-class, open book and notes exam (no other resources are allowed).
- We will be using CrowdMark and WebEx to administer the exam.
- CrowdMark link: `https://app.crowdmark.com/sign-in/usc`
- We'll be releasing some questions (and solutions) for the topics covered in HW3 on Friday using CrowdMark. *Make sure you get familiar with the platform*.
- **Topics:** All topics covered till the next lecture.

On Quiz day

- Join $\sim$15 min prior to the class time.
- We'll assign the exam 5 minutes before 10:00 AM on CrowdMark.
- You will have 10:00 – 11:45 AM for the exam, and the last 15 minutes are for you to upload your solutions.
- You will upload the pictures for each question separately.
- Join via the WebEx link on DEN@USC, *required to have video ON*.
- We'll be recording the video via WebEx.
- You may ask your questions privately to the teaching staff using WebEx chat, cannot communicate with fellow students in any way.