CSCI567 Machine Learning (Spring 2021)

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Outline

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Logistics

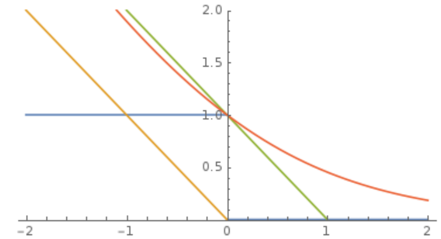
- Quiz 1 is scheduled for March 3, 2021. Details were discussed in the last lecture.

Outline

1. Logistics
2. Review of last lecture
3. A detour of Lagrangian duality
4. Support vector machines (dual formulation)

Primal formulation

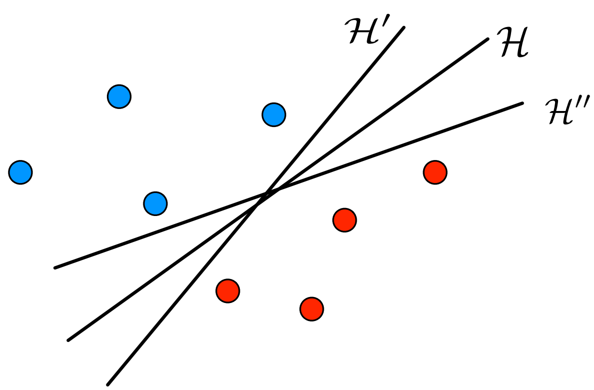
In one sentence: linear model with L2 regularized hinge loss. Recall



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

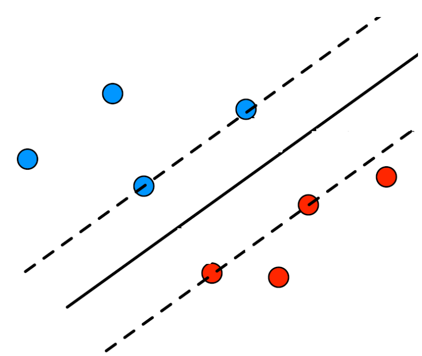
Geometric motivation: separable case

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



Intuition

The further away from data points the better.



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* (*Today's Lecture*)

Outline

Lagrangian duality

Extremely important and powerful tool in analyzing optimizations

We will introduce basic concepts and derive the **KKT conditions**

Applying it to SVM reveals an important aspect of the algorithm

Primal problem

Suppose we want to solve

$$\min_{\boldsymbol{w}} F(\boldsymbol{w}) \quad \text{s.t. } h_j(\boldsymbol{w}) \leq 0 \quad \forall\ j \in [\mathsf{J}]$$

where functions $h_1, \ldots, h_{\mathsf{J}}$ define J **constraints**.

SVM primal formulation is clearly of this form with $\mathsf{J} = 2\mathsf{N}$ constraints:

$$F(\boldsymbol{w}, b, \{\xi_n\}) = C\sum_n \xi_n + \frac{1}{2}\|\boldsymbol{w}\|_2^2$$
$$h_n(\boldsymbol{w}, b, \{\xi_n\}) = 1 - y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b) - \xi_n \quad \forall\ n \in [\mathsf{N}]$$
$$h_{\mathsf{N}+n}(\boldsymbol{w}, b, \{\xi_n\}) = -\xi_n \quad \forall\ n \in [\mathsf{N}]$$

Lagrangian

The **Lagrangian** of the previous problem is defined as:

$$L(\boldsymbol{w}, \{\lambda_j\}) = F(\boldsymbol{w}) + \sum_{j=1}^{\mathsf{J}} \lambda_j h_j(\boldsymbol{w})$$

where $\lambda_1, \ldots, \lambda_{\mathsf{J}} \geq 0$ are called **Lagrangian multipliers**.

Note that

$$\max_{\{\lambda_j\}\geq 0} L(\boldsymbol{w}, \{\lambda_j\}) = \begin{cases} F(\boldsymbol{w}) & \text{if } h_j(\boldsymbol{w}) \leq 0 \quad \forall\, j \in [\mathsf{J}] \\ +\infty & \text{else} \end{cases}$$

and thus,

$$\min_{\boldsymbol{w}} \max_{\{\lambda_j\}\geq 0} L(\boldsymbol{w}, \{\lambda_j\}) \iff \min_{\boldsymbol{w}} F(\boldsymbol{w}) \ \text{ s.t. } \ h_j(\boldsymbol{w}) \leq 0 \quad \forall\, j \in [\mathsf{J}]$$

Duality

We define the **dual problem** by swapping the min and max:

$$\max_{\{\lambda_j\}\geq 0} \min_{\boldsymbol{w}} L(\boldsymbol{w}, \{\lambda_j\})$$

How are the primal and dual connected? Let $\boldsymbol{w}^*$ and $\{\lambda_j^*\}$ be the primal and dual solutions respectively, then

$$\max_{\{\lambda_j\}\geq 0} \min_{\boldsymbol{w}} L(\boldsymbol{w}, \{\lambda_j\}) = \min_{\boldsymbol{w}} L\left(\boldsymbol{w}, \{\lambda_j^*\}\right) \leq L\left(\boldsymbol{w}^*, \{\lambda_j^*\}\right)$$
$$\leq \max_{\{\lambda_j\}\geq 0} L(\boldsymbol{w}^*, \{\lambda_j\}) = \min_{\boldsymbol{w}} \max_{\{\lambda_j\}\geq 0} L(\boldsymbol{w}, \{\lambda_j\})$$

This is called "**weak duality**".

Strong duality

When $F, h_1, \ldots, h_J$ are convex, under some mild conditions:

$$\min_{\boldsymbol{w}} \max_{\{\lambda_j\}\geq 0} L(\boldsymbol{w}, \{\lambda_j\}) = \max_{\{\lambda_j\}\geq 0} \min_{\boldsymbol{w}} L(\boldsymbol{w}, \{\lambda_j\})$$

This is called "**strong duality**".

Deriving the Karush-Kuhn-Tucker (KKT) conditions

Observe that if strong duality holds:

$$F(\boldsymbol{w}^*) = \min_{\boldsymbol{w}} \max_{\{\lambda_j\}\geq 0} L(\boldsymbol{w}, \{\lambda_j\}) = \max_{\{\lambda_j\}\geq 0} \min_{\boldsymbol{w}} L(\boldsymbol{w}, \{\lambda_j\})$$

$$= \min_{\boldsymbol{w}} L\left(\boldsymbol{w}, \{\lambda_j^*\}\right) \leq L\left(\boldsymbol{w}^*, \{\lambda_j^*\}\right) = F(\boldsymbol{w}^*) + \sum_{j=1}^{\mathsf{J}} \lambda_j^* h_j(\boldsymbol{w}^*) \leq F(\boldsymbol{w}^*)$$

Implications:

- *all inequalities above have to be equalities!*
- last equality implies $\lambda_j^* h_j(\boldsymbol{w}^*) = 0$ for all $j \in [\mathsf{J}]$
- equality $\min_{\boldsymbol{w}} L(\boldsymbol{w}, \{\lambda_j^*\}) = L(\boldsymbol{w}^*, \{\lambda_j^*\})$ implies $\boldsymbol{w}^*$ is a **minimizer** of $L(\boldsymbol{w}, \{\lambda_j^*\})$ and thus has **zero gradient**:

$$\nabla_{\boldsymbol{w}} L(\boldsymbol{w}^*, \{\lambda_j^*\}) = \nabla F(\boldsymbol{w}^*) + \sum_{j=1}^{\mathsf{J}} \lambda_j^* \nabla h_j(\boldsymbol{w}^*) = \boldsymbol{0}$$

The Karush-Kuhn-Tucker (KKT) conditions

If $\boldsymbol{w}^*$ and $\{\lambda_j^*\}$ are the primal and dual solution respectively, then:

Stationarity:

$$\nabla_{\boldsymbol{w}} L\left(\boldsymbol{w}^*, \{\lambda_j^*\}\right) = \nabla F(\boldsymbol{w}^*) + \sum_{j=1}^{\mathsf{J}} \lambda_j^* \nabla h_j(\boldsymbol{w}^*) = \boldsymbol{0}$$

Complementary slackness:

$$\lambda_j^* h_j(\boldsymbol{w}^*) = 0 \quad \text{for all } j \in [\mathsf{J}]$$

Feasibility:

$$h_j(\boldsymbol{w}^*) \le 0 \quad \text{and} \quad \lambda_j^* \ge 0 \quad \text{for all } j \in [\mathsf{J}]$$

These are *necessary conditions*. They are also *sufficient* when F is convex and $h_1, \ldots, h_{\mathsf{J}}$ are continuously differentiable convex functions.

Outline

Writing down the Lagrangian

Recall the primal formulation

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

Lagrangian is

$$\begin{aligned} L\left(\boldsymbol{w}, b, \{\xi_n\}, \{\alpha_n\}, \{\lambda_n\}\right) = {} & C \sum_n \xi_n + \frac{1}{2}\|\boldsymbol{w}\|_2^2 - \sum_n \lambda_n \xi_n \\ & + \sum_n \alpha_n \left(1 - y_n(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}_n) + b) - \xi_n\right) \end{aligned}$$

where $\alpha_1, \ldots, \alpha_{\mathsf{N}} \ge 0$ and $\lambda_1, \ldots, \lambda_{\mathsf{N}} \ge 0$ are Lagrangian multipliers.

Applying the stationarity condition

$$L = C \sum_n \xi_n + \frac{1}{2}\|\boldsymbol{w}\|_2^2 - \sum_n \lambda_n \xi_n + \sum_n \alpha_n \left(1 - y_n(\boldsymbol{w}^{\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}_n) + b) - \xi_n\right)$$

$\exists$ primal and dual variables $\boldsymbol{w}, b, \{\xi_n\}, \{\alpha_n\}, \{\lambda_n\}$ s.t. $\nabla_{\boldsymbol{w}, b, \{\xi_n\}} L = \boldsymbol{0}$, which means

$$\frac{\partial L}{\partial \boldsymbol{w}} = \boldsymbol{w} - \sum_n y_n \alpha_n \boldsymbol{\phi}(\boldsymbol{x}_n) = \boldsymbol{0} \quad \Longrightarrow \quad \boldsymbol{w} = \sum_n y_n \alpha_n \boldsymbol{\phi}(\boldsymbol{x}_n)$$

$$\frac{\partial L}{\partial b} = -\sum_n \alpha_n y_n = 0 \quad \text{and} \quad \frac{\partial L}{\partial \xi_n} = C - \lambda_n - \alpha_n = 0, \quad \forall\, n$$

Rewrite the Lagrangian in terms of dual variables

Replacing $\boldsymbol{w}$ by $\sum_n y_n \alpha_n \boldsymbol{\phi}(\boldsymbol{x}_n)$ in the Lagrangian gives

$$L = C\sum_n \xi_n + \frac{1}{2}\|\boldsymbol{w}\|_2^2 - \sum_n \lambda_n \xi_n + \sum_n \alpha_n \left(1 - y_n(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) + b) - \xi_n\right)$$

$$= C\sum_n \xi_n + \frac{1}{2}\|\sum_n y_n\alpha_n\boldsymbol{\phi}(\boldsymbol{x}_n)\|_2^2 - \sum_n \lambda_n\xi_n +$$

$$\sum_n \alpha_n \left(1 - y_n\left(\left(\sum_m y_m\alpha_m\boldsymbol{\phi}(\boldsymbol{x}_m)\right)^{\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}_n) + b\right) - \xi_n\right)$$

$$= \sum_n \alpha_n + \frac{1}{2}\|\sum_n y_n\alpha_n\boldsymbol{\phi}(\boldsymbol{x}_n)\|_2^2 - \sum_{m,n}\alpha_n\alpha_m y_m y_n \boldsymbol{\phi}(\boldsymbol{x}_m)^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n)$$

$$(\textstyle\sum_n \alpha_n y_n = 0 \text{ and } C = \lambda_n + \alpha_n)$$

$$= \sum_n \alpha_n - \frac{1}{2}\sum_{m,n}\alpha_n\alpha_m y_m y_n \boldsymbol{\phi}(\boldsymbol{x}_m)^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n)$$

The dual formulation

To find the dual solutions, it amounts to solving

$$\begin{aligned} \max_{\{\alpha_n\},\{\lambda_n\}} \quad & \sum_n \alpha_n - \frac{1}{2}\sum_{m,n} y_m y_n \alpha_m \alpha_n \boldsymbol{\phi}(\boldsymbol{x}_m)^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) \\ \text{s.t.} \quad & \sum_n \alpha_n y_n = 0 \\ & C - \lambda_n - \alpha_n = 0,\ \alpha_n \geq 0,\ \lambda_n \geq 0, \quad \forall\ n \end{aligned}$$

Note the last three constraints can be written as $0 \leq \alpha_n \leq C$ for all n. So the final **dual formulation of SVM** is:

$$\begin{aligned} \max_{\{\alpha_n\}} \quad & \sum_n \alpha_n - \frac{1}{2}\sum_{m,n} y_m y_n \alpha_m \alpha_n \boldsymbol{\phi}(\boldsymbol{x}_m)^{\mathrm{T}}\boldsymbol{\phi}(\boldsymbol{x}_n) \\ \text{s.t.} \quad & \sum_n \alpha_n y_n = 0 \quad \text{and} \quad 0 \leq \alpha_n \leq C, \quad \forall\ n \end{aligned}$$

Kernelizing SVM

Now it is clear that with a **kernel function k** for the mapping ϕ, we can kernelize SVM as:

$$\begin{aligned} \max_{\{\alpha_n\}} \quad & \sum_n \alpha_n - \frac{1}{2}\sum_{m,n} y_m y_n \alpha_m \alpha_n k(\boldsymbol{x}_m, \boldsymbol{x}_n) \\ \text{s.t.} \quad & \sum_n \alpha_n y_n = 0 \quad \text{and} \quad 0 \leq \alpha_n \leq C, \quad \forall\ n \end{aligned}$$

Again, no need to compute $\phi(\boldsymbol{x})$. It is a **quadratic program** and many efficient optimization algorithms exist.

Recover the primal solution

But how do we predict given the dual solution $\{\alpha_n^*\}$? Need to figure out the primal solution $\boldsymbol{w}^*$ and b^*.

Based on previous observation,

$$\boldsymbol{w}^* = \sum_n \alpha_n^* y_n \boldsymbol{\phi}(\boldsymbol{x}_n) = \sum_{n:\alpha_n > 0} \alpha_n^* y_n \boldsymbol{\phi}(\boldsymbol{x}_n)$$

A point with $\alpha_n^* > 0$ is called a "**support vector**". Hence the name SVM.

To identify b^*, we need to apply complementary slackness.

Applying complementary slackness

For all n we should have

$$\lambda_n^* \xi_n^* = 0, \quad \alpha_n^* \left(1 - \xi_n^* - y_n(\boldsymbol{w}^{*\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}_n) + b^*)\right) = 0$$

For any support vector $\boldsymbol{\phi}(\boldsymbol{x}_n)$ with $0 < \alpha_n^* < C$, $\lambda_n^* = C - \alpha_n^* > 0$ holds.

- first condition implies $\xi_n^* = 0$.
- second condition implies $1 = y_n(\boldsymbol{w}^{*\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}_n) + b^*)$ and thus

$$b^* = y_n - \boldsymbol{w}^{*\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}_n) = y_n - \sum_m y_m \alpha_m^* k(\boldsymbol{x}_m, \boldsymbol{x}_n)$$

Since $y_n \in \{-1, +1\}$, we write $1/y_n = y_n$. Usually *average* over all n with $0 < \alpha_n^* < C$ to stabilize computation.

The prediction on a new point $\boldsymbol{x}$ is therefore

$$\mathrm{SGN}\left(\boldsymbol{w}^{*\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}) + b^*\right) = \mathrm{SGN}\left(\sum_m y_m \alpha_m^* k(\boldsymbol{x}_m, \boldsymbol{x}) + b^*\right)$$

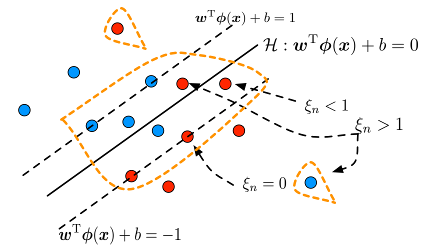
Geometric interpretation of support vectors

A support vector satisfies $\alpha_n^* \neq 0$ and

$$1 - \xi_n^* - y_n(\boldsymbol{w}^{*\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}_n) + b^*) = 0$$

When

- $\xi_n^* = 0$, $y_n(\boldsymbol{w}^{*\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}_n) + b^*) = 1$ and thus the point is $1/\|\boldsymbol{w}^*\|_2$ away from the hyperplane.
- $\xi_n^* < 1$, the point is classified correctly but does not satisfy the large margin constraint.
- $\xi_n^* > 1$, the point is misclassified.

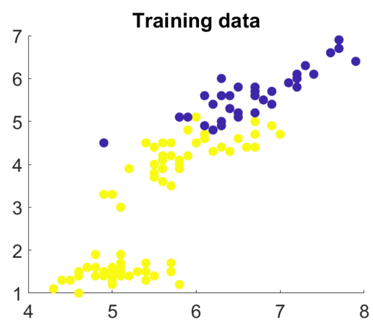


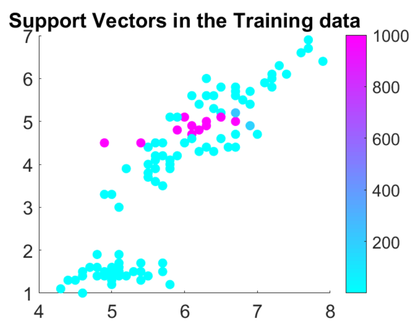
Support vectors (circled with the orange line) are *the only points that matter!*

An example

One drawback of kernel method: **non-parametric**, need to keep all training points potentially

For SVM, very often #support vectors $\ll$ N





Summary

SVM: **max-margin linear classifier**

Primal (equivalent to minimizing L2 regularized hinge loss):

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

Dual (kernelizable, reveals what training points are support vectors):

$$\begin{aligned} \max_{\{\alpha_n\}} \quad & \sum_n \alpha_n - \frac{1}{2} \sum_{m,n} y_m y_n \alpha_m \alpha_n \boldsymbol{\phi}(\boldsymbol{x}_m)^{\mathrm{T}} \boldsymbol{\phi}(\boldsymbol{x}_n) \\ \text{s.t.} \quad & \sum_n \alpha_n y_n = 0 \quad \text{and} \quad 0 \leq \alpha_n \leq C, \quad \forall\, n \end{aligned}$$

Summary

Typical steps of applying Lagrangian duality

- start with a primal problem
- write down the Lagrangian (one dual variable per constraint)
- apply KKT conditions to find the connections between primal and dual solutions
- eliminate primal variables and arrive at the dual formulation
- maximize the Lagrangian with respect to dual variables
- recover the primal solutions from the dual solutions