CSCI567 Machine Learning (Spring 2021)

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Outline

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

Outline

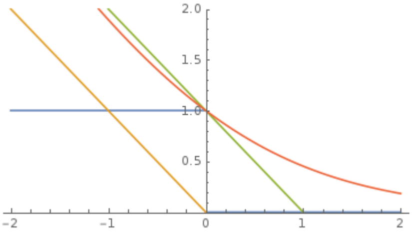
Logistics

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

Outline

Primal formulation

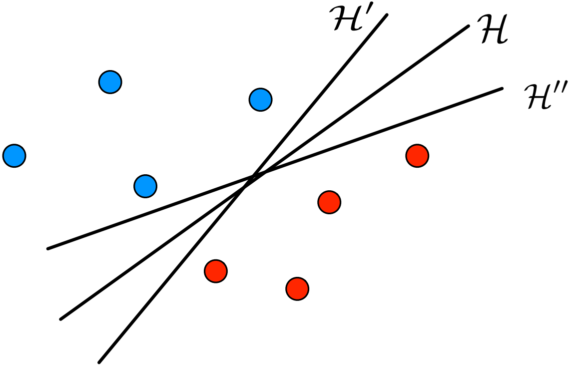
In one sentence: linear model with L2 regularized hinge loss. Recall



- 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**

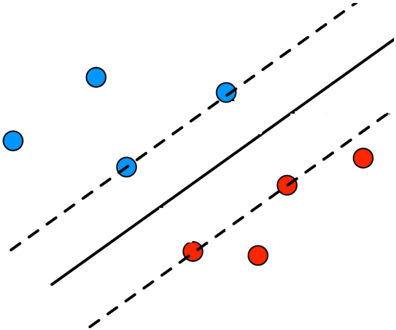
Geometric motivation: separable case

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



Intuition

The further away from data points the better.



Optimization

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

- 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*)

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Lagrangian duality

Extremely important and powerful tool in analyzing optimizations

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

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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**.

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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**.

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Note that

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

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and thus,

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

Duality

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

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

Strong duality

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

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

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Observe that if strong duality holds:

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

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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

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

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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 $\alpha_1, \ldots, \alpha_\mathsf{N} \geq 0$ and $\lambda_1, \ldots, \lambda_\mathsf{N} \geq 0$ 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. $\nabla_{\boldsymbol{w},b,\{\xi_n\}} L = \mathbf{0}$,

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$$\frac{\partial L}{\partial b} = -\sum_n \alpha_n y_n = 0$$

Applying the stationarity condition

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

Rewrite the Lagrangian in terms of dual variables

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

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

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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:

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

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

Recover the primal solution

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

Applying complementary slackness

For all n we should have

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

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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

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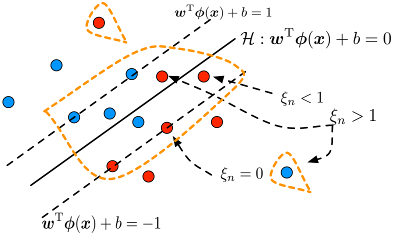

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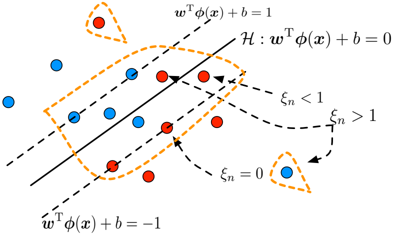

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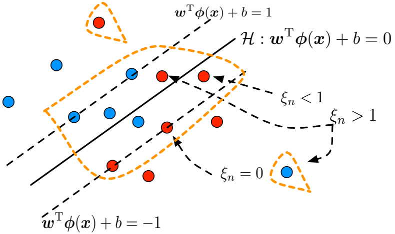

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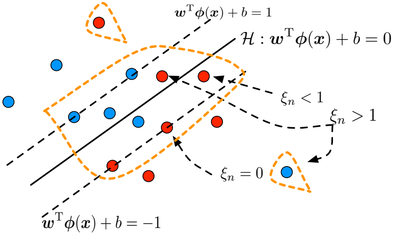

Support vectors (circled with the orange line) are *the only points that matter!*

An example

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

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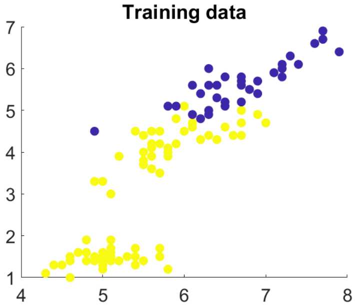

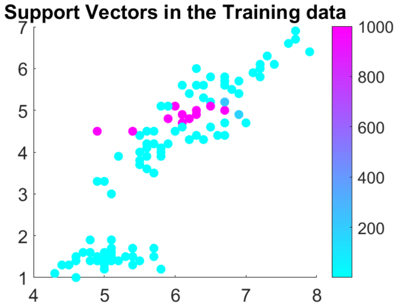

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Dual (kernelizable, reveals what training points are support vectors):

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

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