CS182 Introduction to Machine Learning

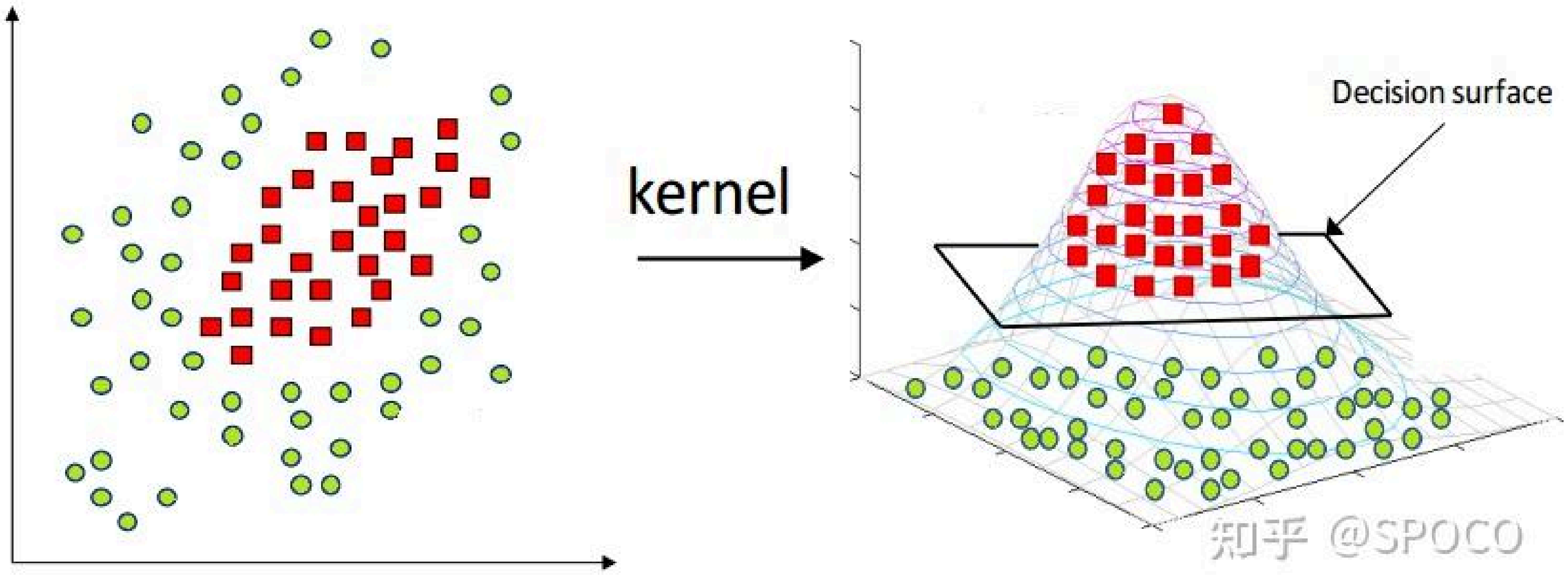
Recitation 4

2025.3.19

Outline

- Kernel Methods
- SVM

Kernel Methods 核方法



Definition: $K(\cdot,\cdot)$ is a kernel if it can be viewed as a legal definition of inner product:

$\exists\phi: K(x,z)=\phi(x)\cdot\phi(y)$

使用时将所有内积$x^\top z$替换为$K(x,z)$

Kernel Methods

> 使用时将所有内积$x^\top z$替换为$K(x, z)$

$\phi : \mathbb{R} \mapsto \mathbb{R}^N$.

- 升维
- 节省计算复杂度
  (e.g. 下面第二个Polynomial Kernel, 计算复杂度由$O(2^k - 1)$降为$O(d)$)

Kernels

- Polynomial Kernel: $K(x,z) = (x \cdot z)^k$: 只有最高次项
  e.g. $k=2, d=2, x \in \mathbb{R}^d$: $\phi(x) = (x_1^2, x_2^2, x_1x_2, x_2x_1)$ or
  $\phi(x) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$
- Polynomial Kernel: $K(x,z) = (c + x \cdot z)^k$: 最高次项为$k$
  e.g. $k=2, d=2, x \in \mathbb{R}^d$: $\phi(x) = (x_1^2, x_2^2, x_1x_2, x_2x_1, \sqrt{2c}x_1, \sqrt{2c}x_2, c)$
- Gaussian Kernel: $K(x,z) = \exp\left(-\frac{\|x-z\|^2}{2\sigma^2}\right)$

  升到无穷维

> https://zhuanlan.zhihu.com/p/657916972
> https://www.zhihu.com/question/508649281/answer/2293811576
> https://zhuanlan.zhihu.com/p/79717760

Kernel tricks on Ridge Regression

$$\mathcal{L}(\beta) = \frac{1}{2}\|y - X\beta\|^2 + \frac{1}{2}\lambda\|\beta\|^2$$

$$\Rightarrow \beta = \left(X^\top X + \lambda I\right)^{-1} X^\top y$$

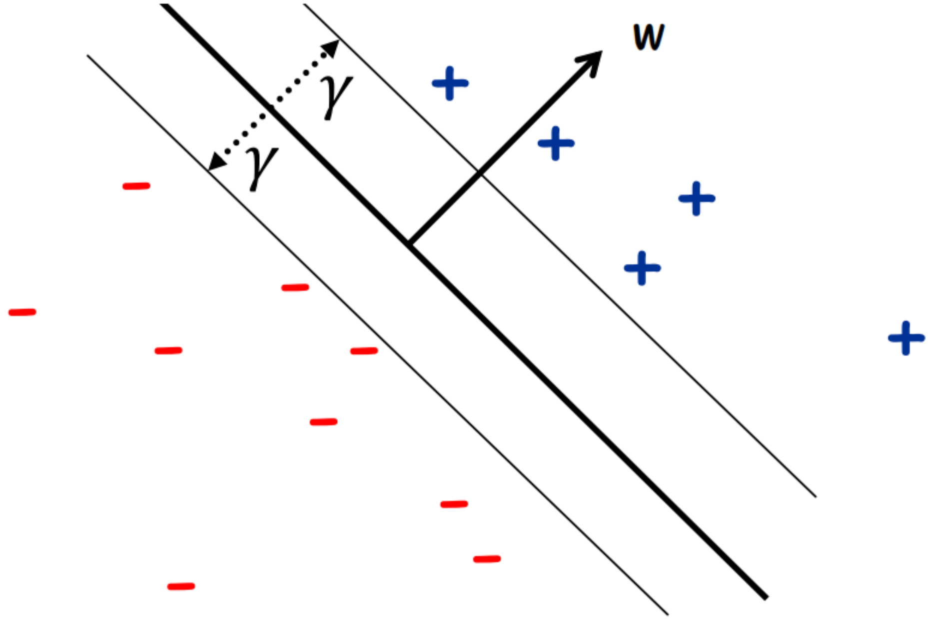
> $X^\top X + \lambda I$ 一定可逆?

Support Vector Machine(SVM) 支持向量机

Max Margin Classifier

Margin γ: **Support Vector** 到 Hyperplane $\mathcal{H}$ 的距离

$\mathcal{H} = \{\mathbf{x} | \mathbf{w}^\top \mathbf{x} = 0\}, \mathbf{x} \in \mathbb{R}^{d+1}$



SVM 优化问题

- Max Margin Classifier
- 点x到Hyperplane $\mathcal{H}=\{\mathbf{x}|\mathbf{w}^\top\mathbf{x}=0\}$的距离公式

$$d=\frac{|\mathbf{w}^\top\mathbf{x}|}{\|w\|}$$

为了方便表示距离, 我们设 $\|w\|=1$, 且假设数据点线性可分:

$$\begin{aligned} \max_{w,\gamma} \quad & \gamma \\ \text{subject to} \quad & \|w\|=1 \\ & y_i x_i\cdot w\geq\gamma,\ \forall i\in\{1,2,\cdots,n\} \end{aligned}$$

> problem: $\|w\|=1$是圆周, 非凸!

SVM 凸优化问题

$$
\begin{aligned}
\max_{w,\gamma} \quad & \gamma \\
\text{subject to} \quad & \|w\| = 1 \\
& y_i x_i \cdot w \geq \gamma, \ \forall i \in \{1, 2, \cdots, n\}
\end{aligned}
$$

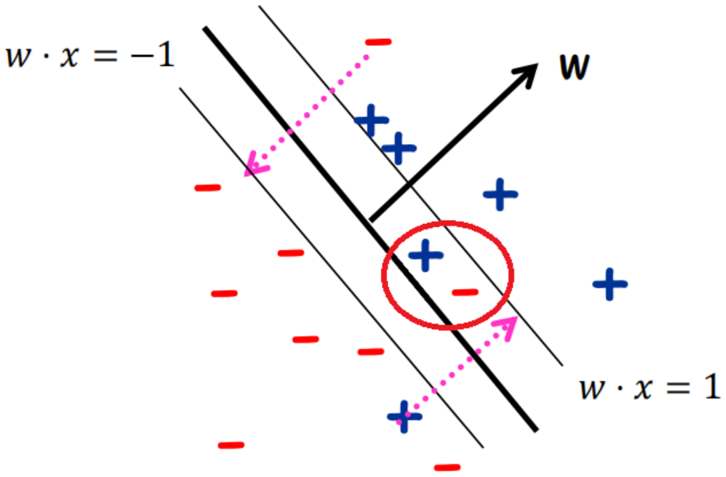
$$\Downarrow$$

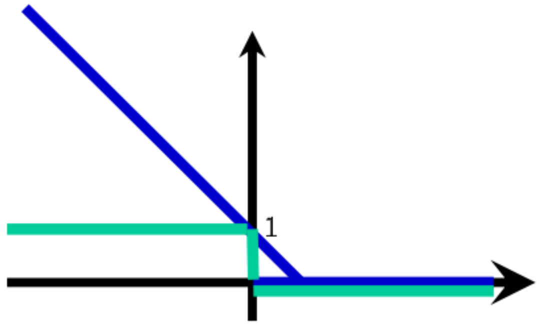
$$
\begin{aligned}
\min_{w'} \quad & \|w'\|^2 \\
\text{subject to} \quad & y_i (x_i \cdot w') \geq 1, \ \forall i \in \{1, 2, \cdots, n\}
\end{aligned}
$$

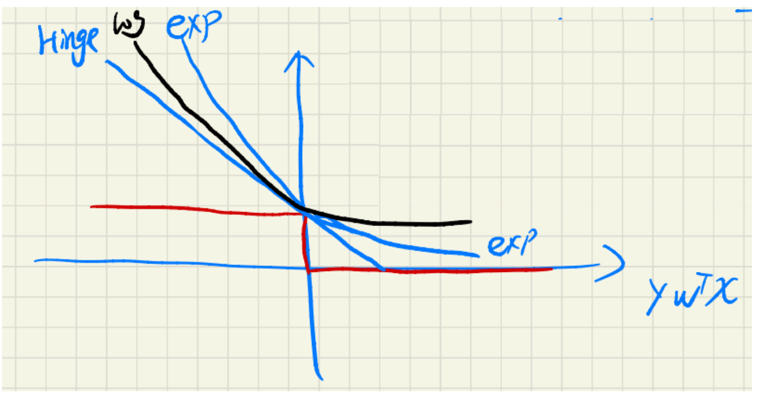
> 此时已经是凸优化问题, 可以用优化算法求解

SVM 线性不可分

- 01 loss: 分类正确为0, 分类错误为1. 枚举所有的情况: NP-hard
  Hinge loss(折页损失): $\max(0, 1 - y_i w^\top x_i)$, 01 loss的上界

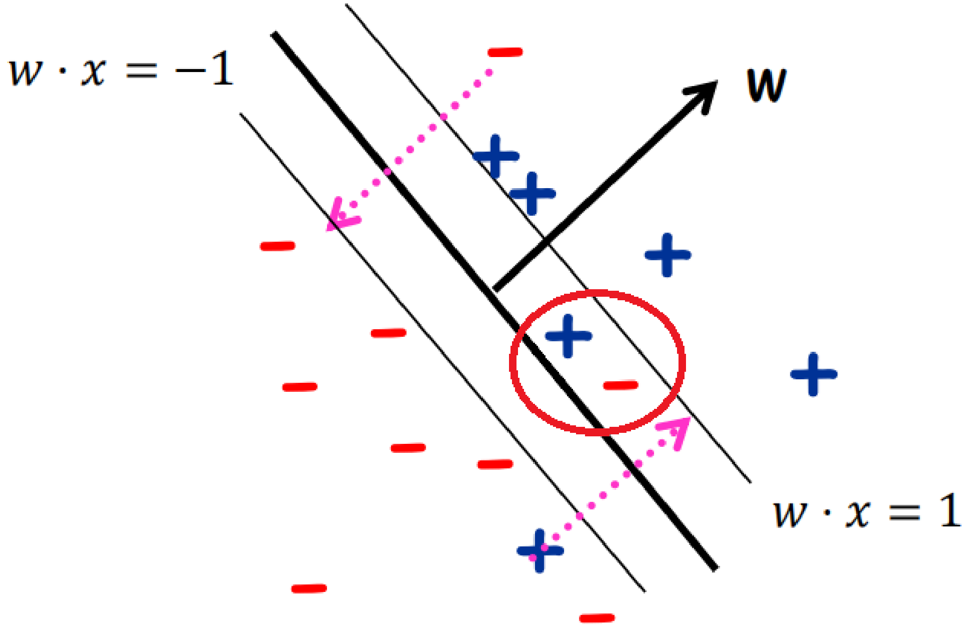






SVM 线性不可分

$$
\begin{aligned}
\min_{w,\xi} \quad & \|w\|^2 + \lambda \sum_{i=1}^{n} \xi_i \\
\text{subject to} \quad & y_i(x_i \cdot w) \geq 1 - \xi_i, \ \forall i \in \{1, 2, \cdots, n\} \\
& \xi_i \geq 0, \ \forall i \in \{1, 2, \cdots, n\}
\end{aligned}
$$



Kernel SVM!

- primal problem

$$\begin{aligned} \min_{w,\xi} \quad & \|w\|^2 + \lambda \sum_{i=1}^{n} \xi_i \\ \text{subject to} \quad & y_i(x_i \cdot w) \geq 1 - \xi_i,\ \forall i \in \{1, 2, \cdots, n\} \\ & \xi_i \geq 0,\ \forall i \in \{1, 2, \cdots, n\} \end{aligned}$$

> $\mathcal{L}(w, \xi, \alpha, \beta) = ?$

Dual problem

$$\mathcal{L}(w,\xi,\alpha,\beta)=\frac{1}{2}\|w\|^2+\lambda\sum_{i=1}^{n}\xi_i+\sum_{i=1}^{n}\alpha_i(1-\xi_i-y_iw^\top x_i)-\sum_{i=1}^{n}\beta_i\xi_i$$

- dual problem

$$\begin{aligned}\max_{\alpha,\beta}\quad & g(\alpha,\beta)\\ \text{subject to}\quad & \alpha\succeq 0\\ & \beta\succeq 0\\ & g(\alpha,\beta)\text{取到}\min_{w,\xi}\mathcal{L}(w,\xi,\alpha,\beta)\end{aligned}$$

Dual problem

$$
\begin{aligned}
\max_{\alpha} \quad & -\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j y_i y_j x_i^\top x_j + \sum_{i=1}^{n}\alpha_i \\
\text{subject to} \quad & \alpha \succeq 0 \\
& \lambda\mathbf{1} - \alpha \succeq 0
\end{aligned}
$$

- 出现$x_i^\top x_j$, 可以用kernel method $\Rightarrow K(x_i, x_j)$
- 变量个数 $n + d + 1 \to n$

Multi-class SVM

类似于其他二分类问题拓展成多(n)分类问题的方法

- 训练n个二分类器
- 第i个分类器将第i类作为正类，其他类作为负类
- 预测时，选择最大的分类器的结果作为预测结果