Introduction to Machine Learning

Lecture 12 Classification - Support Vector Machine

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Outline

Review

- Classification, definition, evaluation
- Linear classifiers (Naïve Bayes classifier, Linear discriminant analysis, Logistic regression)

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- Support-vector machine (SVM)

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Today

- Support-vector machine (SVM)
- Take it easy. Most of the following content can be found at Wikipedia:)
- https://en.wikipedia.org/wiki/Support-vector_machine

Revisit The Principle of Typical Classifiers

Linear determinant analysis

$$\log \frac{p(\boldsymbol{x}|y=1)}{p(\boldsymbol{x}|y=0)}$$

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(What is T for Naïve Bayes?)

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$$p(y=1|\boldsymbol{x}) = \frac{1}{1+\exp(-\boldsymbol{x}^T\boldsymbol{\beta})}$$

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Essentially, they aim at finding a boundary/hyperplane to separate the samples of different classes.

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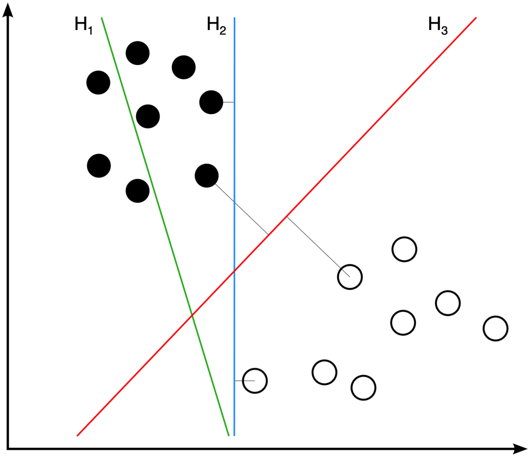
Essentially, they aim at finding a boundary/hyperplane to separate the samples of different classes. (Recall the analytic algebra you learned in your high school.)

Ambiguity of Decision Boundary/Hyperplane



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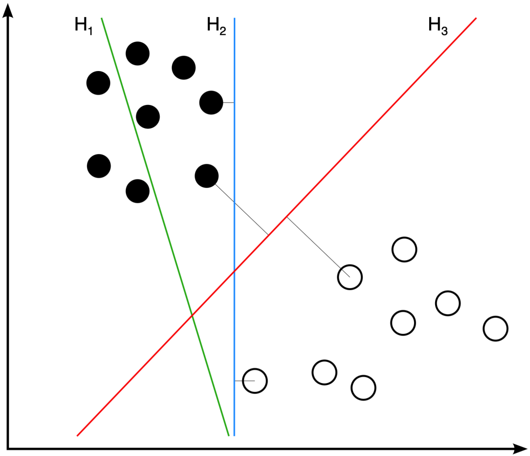

How to find the best decision boundary? What is the criterion?

Support-Vector Machine (SVM)

Motivation:

- Find a hyperplane $\boldsymbol{x}^T\boldsymbol{w} = b$ with maximum-margin/largest separation,

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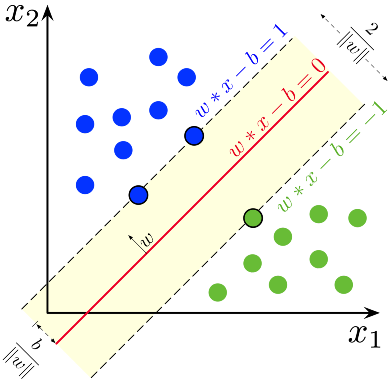
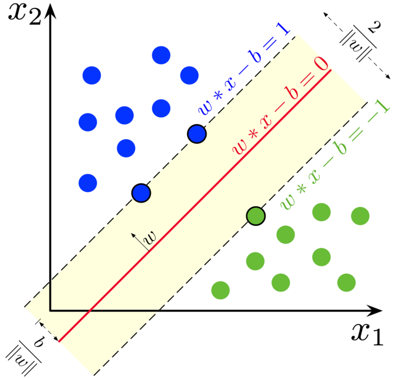


Support-Vector Machine (SVM)

Principle:

- The desired hyperplane has the largest distance to the nearest training-data point of any class (so-called functional margin)



Implementation of SVM (Linearly Separable 2-Class)

- A set of training data $\{\boldsymbol{x}_n, y_n\}_{n=1}^N$, and each $y_n \in \{-1, 1\}$

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- $\boldsymbol{w}$: the normal vector
- $\frac{b}{\|w\|_2}$: the offset of the hyperplane shifting from the original along the normal vector. (Derive Them)

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- Shift the hyperplane along two opposite directions and define classification criteria (margins):

$$\boldsymbol{w}^T\boldsymbol{x} - b = 1 \quad \Rightarrow \quad \text{Any } \boldsymbol{x} \text{ on or above it is labeled by } 1$$

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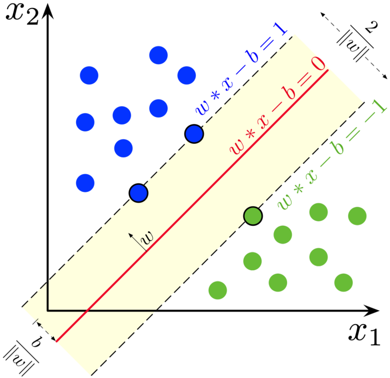
- $\frac{2}{\|\boldsymbol{w}\|_2}$: The distance between these two margins. (Derive It)

Implementation of SVM (Linearly Separable 2-Class)



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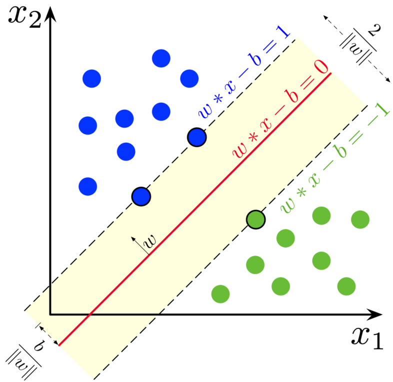

For each $\boldsymbol{x}_n, y_n$, the data point $\boldsymbol{x}_n$ must lie on the correct side of the margin.

$$\boldsymbol{w}^T\boldsymbol{x}_n - b \begin{cases} \geq 1 & \text{if } y_n = 1, \\ \leq -1 & \text{if } y_n = -1. \end{cases}$$

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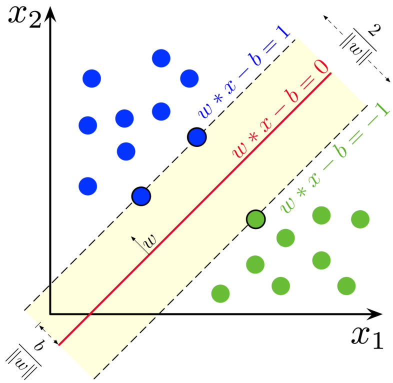

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$$\boldsymbol{w}^T\boldsymbol{x}_n - b \begin{cases} \geq 1 & \text{if } y_n = 1, \\ \leq -1 & \text{if } y_n = -1. \end{cases} \quad \Rightarrow \quad y_n(\boldsymbol{w}^T\boldsymbol{x}_n - b) \geq 1, \ \forall n = 1, .., N. \tag{4}$$

Implementation of SVM (Linearly Separable 2-Class)

Principle:

- Maximize the distance between margins, i.e., max $\frac{2}{\|\boldsymbol{w}\|_2}$

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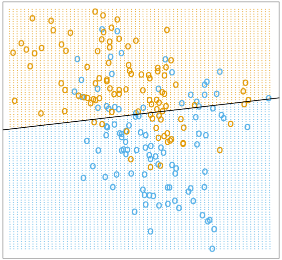
- Equivalently, the problem becomes

$$
\begin{aligned}
&\min_{w,b} \|\boldsymbol{w}\|_2 \\
&s.t.\ y_n(\boldsymbol{w}^T\boldsymbol{x}_n - b) \geq 1,\ \forall\, n = 1, ..., N
\end{aligned}
\tag{5}
$$

How To Deal with Fuzzy Decision Boundary/Hyperplane?



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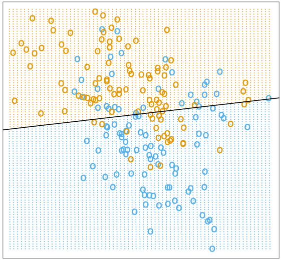

Soft-margin SVM: for noisy linearly-separable classes

$$\min_{w,b,\boldsymbol{\xi}} \lambda \|\boldsymbol{w}\|_2^2 + \frac{1}{N} \sum_{n=1}^{N} \xi_n$$

$$s.t.\ y_n(\boldsymbol{w}^T \boldsymbol{x}_n - b) \geq 1 - \xi_n,\ \xi_n \geq 0,\ \ \forall\, n = 1, \ldots, N$$

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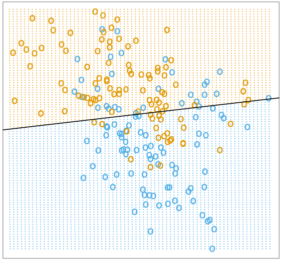

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where $\xi_n = \max\{0, 1 - y_n(\boldsymbol{w}^T\boldsymbol{x}_n - b)\}$, i.e., the smallest nonnegative number satisfying $y_n(\boldsymbol{w}^T\boldsymbol{x}_n - b) \geq 1 - \xi_n$.

Solve Soft-margin SVM (Primal Problem)

- The Primal Problem of Soft-margin SVM:

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- Plug the definition $\xi_n = \max\{0, 1 - y_n(\boldsymbol{w}^T\boldsymbol{x}_n - b)\}$ into (7):

$$\min_{w,b}\ \underbrace{\lambda\|\boldsymbol{w}\|_2^2}_{\text{Tikhonov reg.}} + \frac{1}{N}\sum_{n=1}^{N} \underbrace{\max\{0, 1 - y_n(\boldsymbol{w}^T\boldsymbol{x}_n - b)\}}_{\text{Hinge loss}}$$

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- The objective function is convex (but non-smooth) w.r.t. $\boldsymbol{w}$ and b, so GD or SGD can be applied.

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- The objective function is convex (but non-smooth) w.r.t. $\boldsymbol{w}$ and b, so GD or SGD can be applied.
- Derive the gradient of Hinge loss

Solve Soft-margin SVM (Dual Problem)

Because the Primal problem is convex optimization, we can solve it equivalently via solving its dual problem.

- Recall the Primal Problem of Soft-margin SVM:

$$\min_{w,b,\boldsymbol{\xi}} \lambda \|\boldsymbol{w}\|_2^2 + \frac{1}{N}\sum_{n=1}^{N} \xi_n$$

$$s.t.\ \underbrace{y_n(\boldsymbol{w}^T\boldsymbol{x}_n - b) \geq 1 - \xi_n}_{\text{Constraint 1}},\ \underbrace{\xi_n \geq 0}_{\text{Constraint 2}},\ \forall\, n = 1, \ldots, N$$

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\end{aligned}
\tag{9}
$$

- The Lagrangian dual of (9): Introduce dual variables $\{c_n\}_{n=1}^N$ for the first N constraints, and $\{\tau_n\}_{n=1}^N$ for the second N constraints

$$
\max_{\{c_n,\tau_n\}_{n=1}^N} \left(\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \lambda\|\boldsymbol{w}\|_2^2 + \sum_{n=1}^{N} \left(\frac{1}{N}\xi_n + c_n(1 - \xi_n - y_n(\boldsymbol{w}^T\boldsymbol{x}_n - b)) - \tau_n\xi_n \right) \right)
$$

$$
s.t.\ c_n \geq 0,\ \tau_n \geq 0,\ \forall n = 1, ..., N
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$$

$s.t.\ c_n \geq 0,\ \tau_n \geq 0,\ \forall n = 1, ..., N$

- Looks terrible... but simple actually;)

Solve Soft-margin SVM (Dual Problem)

Original dual problem:

$$\max_{\{c_n,\tau_n\}_{n=1}^N} \left(\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \lambda\|\boldsymbol{w}\|_2^2 + \sum\nolimits_{n=1}^N \left(\frac{1}{N}\xi_n + c_n(1-\xi_n - y_n(\boldsymbol{w}^T\boldsymbol{x}_n - b)) - \tau_n\xi_n \right) \right) \tag{11}$$

$$s.t.\ c_n \geq 0,\ \tau_n \geq 0,\ \forall n = 1, ..., N$$

- **Firstly, we can ignore $\{\tau_n\}_{n=1}^N$ because $\tau_n^* = 0$ (Why?)**

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- **Firstly, we can ignore $\{\tau_n\}_{n=1}^N$ because $\tau_n^* = 0$ (Why?)**
  - $\xi_n \geq 0$ and $\tau_n \geq 0$
  - Objective function: $\max_{\tau_n \geq 0} \min_{\xi_n \geq 0} -\tau_n\xi_n = 0$ when $\tau_n^* = 0$

Solve Soft-margin SVM (Dual Problem)

Original dual problem:

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$$s.t.\ c_n \geq 0,\ \tau_n \geq 0,\ \forall n = 1, ..., N$$

- **Firstly, we can ignore $\{\tau_n\}_{n=1}^N$ because $\tau_n^* = 0$ (Why?)**
  - $\xi_n \geq 0$ and $\tau_n \geq 0$
  - Objective function: $\max_{\tau_n \geq 0} \min_{\xi_n \geq 0} -\tau_n\xi_n = 0$ when $\tau_n^* = 0$
- So, rewrite (11) as

$$\max_{\{c_n\}_{n=1}^N} \left(\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \lambda \|\boldsymbol{w}\|_2^2 + \sum_{n=1}^N \left(\frac{1}{N}\xi_n + {\color{red}c_n}(1 - \xi_n - y_n(\boldsymbol{w}^T\boldsymbol{x}_n - b)) \right) \right) \tag{12}$$

$$s.t.\ c_n \geq 0,\ \forall n = 1, ..., N$$

Solve Soft-margin SVM (Dual Problem)

Modified dual problem (Version 1):

$$\max_{\{c_n\}_{n=1}^N} \left(\min_{\boldsymbol{w}, b, \boldsymbol{\xi}} \lambda \|\boldsymbol{w}\|_2^2 + \sum_{n=1}^N \left(\frac{1}{N} \xi_n + c_n (1 - \xi_n - y_n (\boldsymbol{w}^T \boldsymbol{x}_n - b)) \right) \right) \tag{13}$$

$$s.t.\ c_n \geq 0,\ \forall n = 1, ..., N$$

- **Secondly, the problem can be re-scale to**

$$\max_{\{c_n\}_{n=1}^N} \left(\min_{\boldsymbol{w}, b, \boldsymbol{\xi}} \frac{1}{2} \|\boldsymbol{w}\|_2^2 + \sum_{n=1}^N \left(\frac{1}{2N\lambda} \xi_n + c_n (1 - \xi_n - y_n (\boldsymbol{w}^T \boldsymbol{x}_n - b)) \right) \right) \tag{14}$$

$$s.t.\ c_n \geq 0,\ \forall n = 1, ..., N$$

(Why?)

Solve Soft-margin SVM (Dual Problem)

Modified dual problem (Version 2):

$$\max_{\{c_n\}_{n=1}^N} \left(\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \underbrace{\frac{1}{2}\|\boldsymbol{w}\|_2^2 + \sum_{n=1}^{N} \left(\frac{1}{2N\lambda}\xi_n + c_n(1 - \xi_n - y_n(\boldsymbol{w}^T\boldsymbol{x}_n - b)) \right)}_{L(\boldsymbol{w},b,\boldsymbol{\xi},\boldsymbol{c})} \right) \tag{15}$$

$$s.t.\ c_n \geq 0,\ \forall n = 1, ..., N$$

- **Thirdly, consider the optimality condition of inner problem:**

$$\frac{\partial L}{\partial \boldsymbol{w}} = 0$$

Solve Soft-margin SVM (Dual Problem)

Modified dual problem (Version 2):

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$$\frac{\partial L}{\partial \boldsymbol{w}} = 0 \quad \Rightarrow \quad \boldsymbol{w}^* = \sum_{n=1}^N c_n y_n \boldsymbol{x}_n \quad \text{Relation between opt. primal and dual}$$

Solve Soft-margin SVM (Dual Problem)

Modified dual problem (Version 2):

$$\max_{\{c_n\}_{n=1}^N} \left(\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \underbrace{\frac{1}{2}\|\boldsymbol{w}\|_2^2 + \sum_{n=1}^N \left(\frac{1}{2N\lambda}\xi_n + c_n(1 - \xi_n - y_n(\boldsymbol{w}^T\boldsymbol{x}_n - b)) \right)}_{L(\boldsymbol{w},b,\boldsymbol{\xi},\boldsymbol{c})} \right) \tag{15}$$

$$s.t.\ c_n \geq 0,\ \forall n = 1, ..., N$$

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$$\frac{\mathrm{d}L}{\mathrm{d}b} = 0$$

Solve Soft-margin SVM (Dual Problem)

Modified dual problem (Version 2):

$$\max_{\{c_n\}_{n=1}^N} \left(\underbrace{\min_{\boldsymbol{w},b,\boldsymbol{\xi}} \frac{1}{2}\|\boldsymbol{w}\|_2^2 + \sum_{n=1}^N \left(\frac{1}{2N\lambda}\xi_n + c_n(1 - \xi_n - y_n(\boldsymbol{w}^T\boldsymbol{x}_n - b)) \right)}_{L(\boldsymbol{w},b,\boldsymbol{\xi},\boldsymbol{c})} \right) \tag{15}$$

$$s.t.\ c_n \geq 0,\ \forall n = 1, ..., N$$

- **Thirdly, consider the optimality condition of inner problem:**

$$\frac{\partial L}{\partial \boldsymbol{w}} = 0 \quad \Rightarrow \quad \boldsymbol{w}^* = \sum_{n=1}^N c_n y_n \boldsymbol{x}_n \quad \text{Relation between opt. primal and dual}$$

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$$\frac{\mathrm{d}L}{\mathrm{d}\xi_n} = \frac{1}{2N\lambda} - c_n \geq 0 \quad \text{(Inequality constraints of dual variables, why?)}$$

Solve Soft-margin SVM (Dual Problem)

- **Finally, plugging the relation and the constraints into (15), we obtain the final dual problem:**

$$
\max_{\{c_n\}_{n=1}^N} \sum_{n=1}^{N} c_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} y_n c_n (\boldsymbol{x}_n^T \boldsymbol{x}_m) y_m c_m
$$

$$
s.t. \sum_{n=1}^{N} c_n y_n = 0, \quad 0 \leq c_n \leq \frac{1}{2N\lambda}, \; \forall n = 1, ..., N.
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- Why are the terms of ξ_n's ignored?

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\end{aligned} \tag{17}
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- Derive it and write it in a matrix form.
- Why are the terms of ξ_n's ignored?
- This problem can be solved by GD or Coordinate Gradient Descent.

Revisit Dual SVM as Kernel Methods

- Key relation:

$$\boldsymbol{w}^* = \sum_{n=1}^{N} c_n y_n \boldsymbol{x}_n$$

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- The dual SVM can be treated as applying a linear kernel function:

$$\begin{aligned} &\max_{\{c_n\}_{n=1}^N} \sum_{n=1}^{N} c_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} y_n c_n \big(\underbrace{\boldsymbol{x}_n^T \boldsymbol{x}_m}_{K(\boldsymbol{x}_n, \boldsymbol{x}_m)} \big) y_m c_m \\ &s.t. \sum_{n=1}^{N} c_n y_n = 0, \quad 0 \le c_n \le \frac{1}{2N\lambda}, \ \forall n = 1, ..., N. \end{aligned} \tag{19}$$

Revisit Dual SVM as Kernel Methods

- Kernel SVM = Applying Linear Dual SVM in the feature space $\mathcal{F}$ defined by the kernel function:

$$K(\boldsymbol{x}, \boldsymbol{x}') = \langle \phi(\boldsymbol{x}), \phi(\boldsymbol{x}') \rangle_{\mathcal{F}}, \quad \phi : \mathcal{X} \mapsto \mathcal{F}.$$

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$$\boldsymbol{w}^* = \sum_{n=1}^{N} c_n y_n \phi(\boldsymbol{x}_n) \in \mathcal{F}$$

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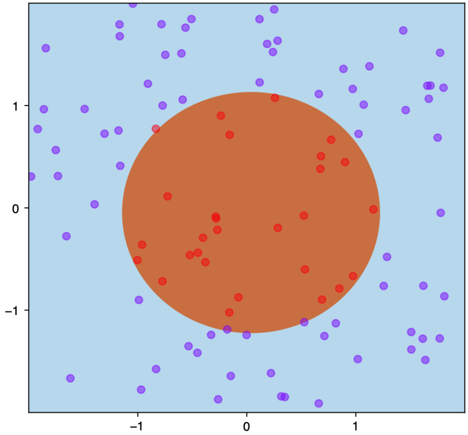
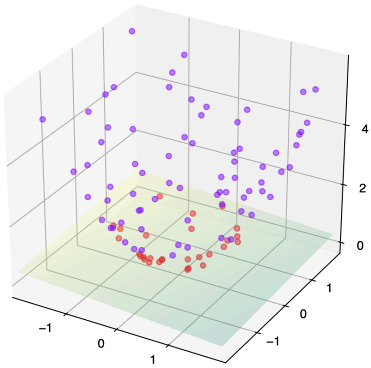
- Kernel SVM:

$$\begin{aligned} &\max_{\{c_n\}_{n=1}^N} \sum_{n=1}^{N} c_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} y_n c_n \underbrace{\langle \phi(\boldsymbol{x}_n), \phi(\boldsymbol{x}_m) \rangle_{\mathcal{F}}}_{K(\boldsymbol{x}_n, \boldsymbol{x}_m)} y_m c_m \\ &s.t. \sum_{n=1}^{N} c_n y_n = 0, \quad 0 \le c_n \le \frac{1}{2N\lambda}, \ \forall n = 1, \ldots, N. \end{aligned} \tag{22}$$

Similar to other kernel method, we don't have to find ϕ explicitly — just define K.

Revisit Dual SVM as Kernel Methods





Extensions of SVM

Multi-class SVM

- Like LDA, “one against the rest” or pairwise classification

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Support-Vector Regression (SVR)

$$\begin{aligned} &\min_{\boldsymbol{w},b} \frac{1}{2}\|\boldsymbol{w}\|_2^2 \\ &s.t.\ \ |y_n - \boldsymbol{w}^T\boldsymbol{x}_n - b| \le \epsilon \end{aligned} \tag{23}$$

In Summary

- Support-vector machine (SVM)
- Kernelized SVM

Next...

- Information theory in Statistic ML
- Decision tree model

HW 4: DDL June 3, 2022

Python Programming

1. Lab # 9 (4 Pts)
2. Lab # 10 (4 Pts)

Questions for Tech Report (6 Pts, $\leq$ 3 Pages)

1. Given $\boldsymbol{X} \in \mathbb{R}^{N \times D}$ and $\boldsymbol{Y} \in \mathbb{R}^{N \times C}$, where each row of $\boldsymbol{X}$ is a D-dimensional feature, and each row of $\boldsymbol{Y}$ is a one-hot vector indicating one of the C classes. **Can we solve classification as regression?** e.g.,

$$\min_{\boldsymbol{W}} \|\boldsymbol{Y} - \boldsymbol{X}\boldsymbol{W}\|_F^2 \tag{24}$$

   If it does not work well in general, when it works? (Hint: Find the answer in ESL) (3 Pts)

2. Derive from (15) to (17) in details, and demonstrate that the terms related to ξ_n's are ignorable (Hint: consider the objective function in (15)). (3 Pts)