EECS 545: Machine Learning

Lectures 9 & 10. Kernel methods: Support Vector Machines

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Overview

- Support Vector Machine (SVM)
- Soft-margin SVM
- Primal optimization
 - Soft-margin SVM
- Dual optimization (next lecture)
 - hard-margin SVM
 - soft-margin SVM

Support Vector Machines: Motivation and Formulation

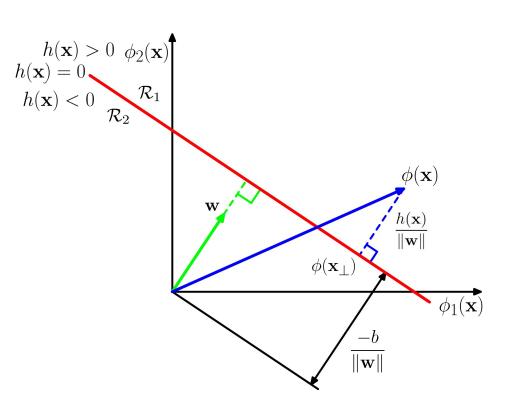
Linear Discriminant Function

$$h(\mathbf{x}) = \mathbf{w}^{\top} \phi(\mathbf{x}) + b$$

 Decision boundary is the hyperplane

$$\mathbf{w}^{\top}\phi(\mathbf{x}) + b = 0$$

- w determines direction
- b determines offset

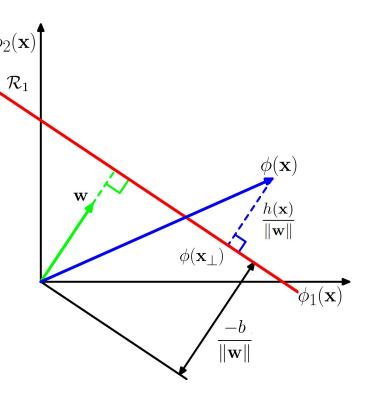


Distance of a point from a hyperplane

- 2D Case:
 - Line: ax + by + c = 0
 - Point: (x_0, y_0)
 - +/- depending on which side of line

$$distance = \frac{ax_0 + by_0 + c}{\sqrt{a^2 + b^2}}$$

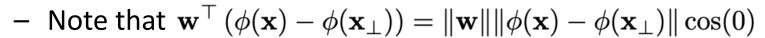
- M dimensional:
 - Hyperplane: $h(\mathbf{x}) = \mathbf{w}^{\top} \phi(\mathbf{x}) + b$
 - Point: $\phi(\mathbf{x})$ distance = $\frac{\mathbf{w}^{\top}\phi(\mathbf{x}) + b}{\|\mathbf{w}\|}$



Distance of a point from a hyperplane

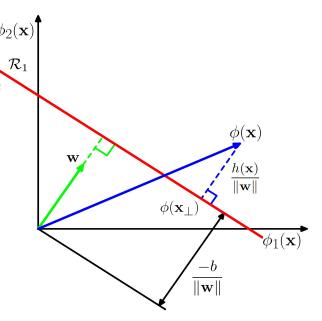
• Derivation:

- Let $\phi(\mathbf{x}_{\perp})$ be the point on the hyperplane closest to $\phi(\mathbf{x})$
- $-\phi(\mathbf{x})-\phi(\mathbf{x}_{\perp})$ is perpendicular to the hyperplane and hence parallel to \mathbf{w}
- Distance = $\pm \|\phi(\mathbf{x}) \phi(\mathbf{x}_{\perp})\|$

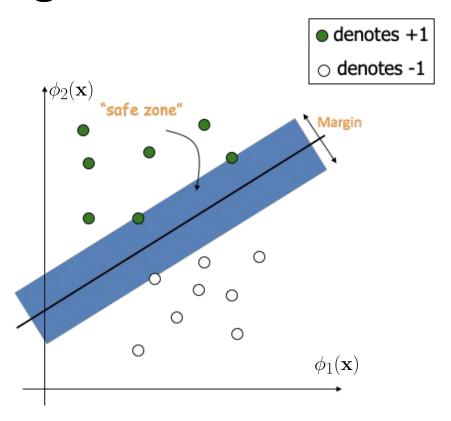


- Thus,
$$\|\phi(\mathbf{x}) - \phi(\mathbf{x}_{\perp})\| = \frac{\mathbf{w}^{\top}\phi(\mathbf{x}) - \mathbf{w}^{\top}\phi(\mathbf{x}_{\perp})}{\|\mathbf{w}\|}$$

$$= \frac{\mathbf{w}^{\top}\phi(\mathbf{x}) + b}{\|\mathbf{w}\|} \quad \because \mathbf{w}^{\top}\phi(\mathbf{x}_{\perp}) + b = 0$$



- The linear discriminant function (classifier) with the maximum margin is a good classifier.
- Margin is defined as the width that the boundary could be increased by before hitting a data point
- Why is it the "good" one?
 - Robust to outliers and thus strong generalization ability

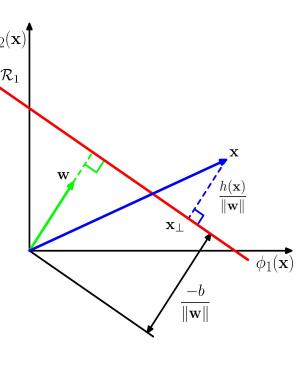


• Distance from $\phi(\mathbf{x})$ to the hyperplane $\mathbf{w}^{\top}\phi(\mathbf{x})+b=0$ $h(\mathbf{x})>0$ $\phi_2(\mathbf{x})$ (assuming data is linearly separable, $\mathbf{y}\in\{-1,1\}$) $h(\mathbf{x})<0$ \mathcal{R}_2 $y(\mathbf{w}^{\top}\phi(\mathbf{x})+b)$

$$\frac{y(\mathbf{w}^{\top}\phi(\mathbf{x}) + b)}{\|\mathbf{w}\|}$$

Margin (defined over training data):

$$\min_n \frac{y^{(n)}(\mathbf{w}^{\top}\phi(\mathbf{x}^{(n)}) + b)}{\|\mathbf{w}\|}$$



Optimization problem:

$$\underset{\mathbf{w},b}{\operatorname{argmax}} \left\{ \frac{1}{\|\mathbf{w}\|} \min_{n} \left[y^{(n)} \left(\mathbf{w}^{\top} \phi \left(\mathbf{x}^{(n)} \right) + b \right) \right] \right\}$$

Rescale w and b such that:

$$y^{(n)}\left(\mathbf{w}^{\top}\phi\left(\mathbf{x}^{(n)}\right)+b\right) \geq 1$$
 $n=1,...,N$

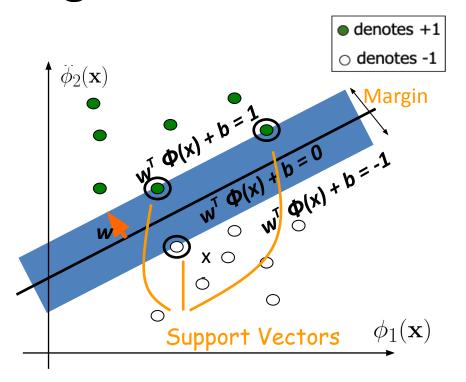
• Optimization is equivalent to:

$$\underset{\mathbf{w},b}{\operatorname{argmin}} \frac{1}{2} \|\mathbf{w}\|^2$$
 subject to $y^{(n)} \left(\mathbf{w}^{\top} \phi \left(\mathbf{x}^{(n)}\right) + b\right) \geq 1$ $n=1,...,N$

Optimization problem:

$$\operatorname*{argmin}_{\mathbf{w},b} \frac{1}{2} \|\mathbf{w}\|^2$$
 subject to

For
$$y^{(n)} = 1$$
, $\mathbf{w}^{\top} \phi \left(\mathbf{x}^{(n)} \right) + b \ge 1$
For $y^{(n)} = -1$, $\mathbf{w}^{\top} \phi \left(\mathbf{x}^{(n)} \right) + b \le -1$



Solving the optimization problem

Optimization problem (Hard SVM):

$$\underset{\mathbf{w},b}{\operatorname{argmin}} \frac{1}{2} \|\mathbf{w}\|^2$$
 subject to $y^{(n)} \left(\mathbf{w}^{\top} \phi \left(\mathbf{x}^{(n)}\right) + b\right) \geq 1$ $n = 1, ..., N$

- This is a constrained optimization problem.
 - We solve this using Lagrange multipliers (convex optimization).
- Problem of "Hard SVM":
 - formulation is based on the assumption that the training data linearly separable
 - What happens if this assumption is not satisfied?
 - Note: Hard-margin SVM is not practically useful.

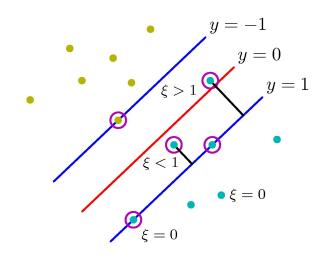
Support Vector Machines

 Hard SVM requires separable sets

$$y^{(n)}h\left(\mathbf{x}^{(n)}\right) - 1 \ge 0$$

Soft SVM introduces
 slack variables for each
 data point

$$y^{(n)}h\left(\mathbf{x}^{(n)}\right) \ge 1 - \xi^{(n)}$$



Recall:
$$h\left(\mathbf{x}\right) = \mathbf{w}^{\top}\phi\left(\mathbf{x}\right) + b$$

Formulation of soft-margin SVM

- Maximize the margin, and also penalize for the slack variables
- Primal optimization
 - Optimization w.r.t $\min_{\mathbf{w},b,\xi} C \sum_{i} \xi^{(n)} + \frac{1}{2} \|\mathbf{w}\|^2$

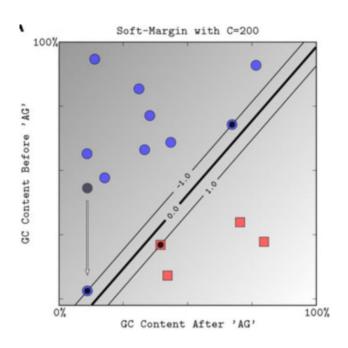
subject to
$$y^{(n)}h\left(\mathbf{x}^{(n)}\right) \geq 1 - \xi^{(n)}, \forall n$$

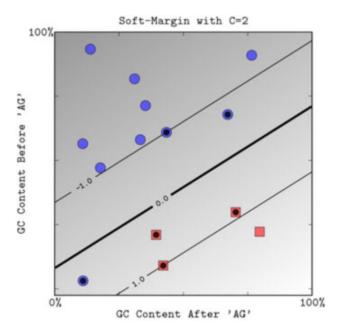
$$\xi^{(n)} \geq 0, \forall n$$

Recall:
$$h\left(\mathbf{x}\right) = \mathbf{w}^{\top}\phi\left(\mathbf{x}\right) + b$$

Soft SVM

• A little slack can give much better margin.





Primal optimization

Optimization

- We can directly optimize the SVM objective function using gradient descent or stochastic gradient
 - Applicable when we have direct access to feature vectors $\phi(\mathbf{x})$
 - This is also called "linear SVM" (due to the use of linear kernels).

- Main idea
 - Convert the constraint into a penalty function

Converting constraints into penalty

• Note: objective is dependent on

$$\min_{\mathbf{w},b,\xi} C \sum_{n=1}^{N} \xi^{(n)} + \frac{1}{2} \|\mathbf{w}\|^{2}$$
subject to $y^{(n)} h\left(\mathbf{x}^{(n)}\right) \ge 1 - \xi^{(n)}, \forall n$

$$\xi^{(n)} > 0, \forall n$$

– We want to minimize $\xi^{(n)}$ under the constraints

Recall:
$$h(\mathbf{x}) = \mathbf{w}^{\top} \phi(\mathbf{x}) + b$$

Converting constraints into penalty

• Note: objective is dependent on $\xi^{(n)}$

$$\min_{\mathbf{w},b,\xi} C \sum_{n=1}^{N} \xi^{(n)} + \frac{1}{2} \|\mathbf{w}\|^2$$
 subject to $y^{(n)}h\left(\mathbf{x}^{(n)}\right) \geq 1 - \xi^{(n)}, \forall n$

$$\xi^{(n)} \geq 0, \forall n$$
— We want to minimize $f(n)$ under the constraint

- We want to minimize $\xi^{(n)}$ under the constraints
- Rewriting the constraints: for each n,

When equality holds, all constraints are satisfied and the objective is minimized!

Converting constraints into penalty

Original optimization problem

$$\begin{split} \min_{\mathbf{w},b,\xi} C \sum_{n=1}^{N} \xi^{(n)} + \frac{1}{2} \|\mathbf{w}\|^2 \\ \text{subject to} \ \ y^{(n)} h\left(\mathbf{x}^{(n)}\right) \geq 1 - \xi^{(n)}, \forall n \\ \xi^{(n)} \geq 0, \forall n \\ \end{split} \qquad \qquad \text{Recall:} \qquad h\left(\mathbf{x}\right) = \mathbf{w}^{\top} \phi\left(\mathbf{x}\right) + b \end{split}$$

An equivalent optimization problem

$$\min_{\mathbf{w},b} C \sum_{1}^{N} \max \left(0, \ 1 - y^{(n)} h\left(\mathbf{x}^{(n)}\right) \right) + \frac{1}{2} \|\mathbf{w}\|^{2}$$

This can be optimized using gradient-based methods!
 (batch/stochastic gradient descent)

Gradients

Computing the (sub) gradient with respect to w and b:

- Recall:
$$h(\mathbf{x}) = \mathbf{w}^{\top} \phi(\mathbf{x}) + b$$

$$\min_{\mathbf{w}, b} C \sum_{n=1}^{N} \max \left(0, 1 - y^{(n)} h\left(\mathbf{x}^{(n)}\right)\right) + \frac{1}{2} \|\mathbf{w}\|^{2}$$

$$\nabla_{\mathbf{w}} \mathcal{L} = -C \sum_{n=1}^{N} y^{(n)} \phi\left(\mathbf{x}^{(n)}\right) \mathbb{I}\left(1 - y^{(n)} h\left(\mathbf{x}^{(n)}\right) \ge 0\right) + \mathbf{w}$$

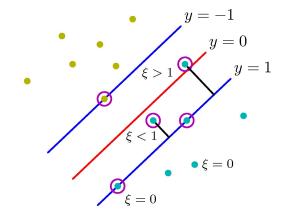
$$\nabla_{b} \mathcal{L} = -C \sum_{n=1}^{N} y^{(n)} \mathbb{I}\left(1 - y^{(n)} h\left(\mathbf{x}^{(n)}\right) \ge 0\right)$$

- The gradient can be used to optimize w over the training data
 - Similar trick can be applied for stochastic gradient.

Support vectors

• In SVM, only the training points that have margin of 1 or less actually affect the final solution (**w**, b).

These are called "support vectors"



Summary

Hard SVM (Max Margin classifier): Assumes data is separable in feature space

$$\underset{\mathbf{w},b}{\operatorname{argmax}} \left\{ \frac{1}{\|\mathbf{w}\|} \min_{n} \left[y^{(n)} \left(\mathbf{w}^{\top} \phi \left(\mathbf{x}^{(n)} \right) + b \right) \right] \right\} \qquad \qquad \underset{\mathbf{x},b}{\operatorname{argmin}} \frac{1}{2} \|\mathbf{w}\|^{2}$$

$$\text{s.t. } y^{(n)} \left(\mathbf{w}^{\top} \phi \left(\mathbf{x}^{(n)} \right) + b \right) \geq 1 \quad n = 1, ..., N$$

Need to use constrained convex optimization to solve this problem



Relax the constraints

Soft SVM: No separability assumption: adding slack variables (for better robustness)

$$\min_{\mathbf{w},b,\xi} C \sum_{n=1}^{N} \xi^{(n)} + \frac{1}{2} \|\mathbf{w}\|^{2}$$
subject to $y^{(n)}h\left(\mathbf{x}^{(n)}\right) \ge 1 - \xi^{(n)}, \forall n$

$$\xi^{(n)} > 0, \forall n$$

$$\min_{\mathbf{w},b} C \sum_{n=1}^{N} \max\left(0, \ 1 - y^{(n)}h\left(\mathbf{x}^{(n)}\right)\right) + \frac{1}{2} \|\mathbf{w}\|^{2}$$

Primal problem can be solved using gradient methods.

Any feedback (about lecture, slide, homework, project, etc.)?

(via anonymous google form: https://forms.gle/fpYmiBtG9Me5qbP37)



Change Log of lecture slides:

https://docs.google.com/document/d/e/2PACX-1vSSIHJjklypK7rKFSR1-5GYXyBCEW8UPtpSfCR9AR6M1l7K9ZQEmxfFwaWaW7kLDxusthsF8WlCyZJ-/pub