EECS 545: Machine Learning

Lecture 9 & 10. Kernel methods: support vector machines

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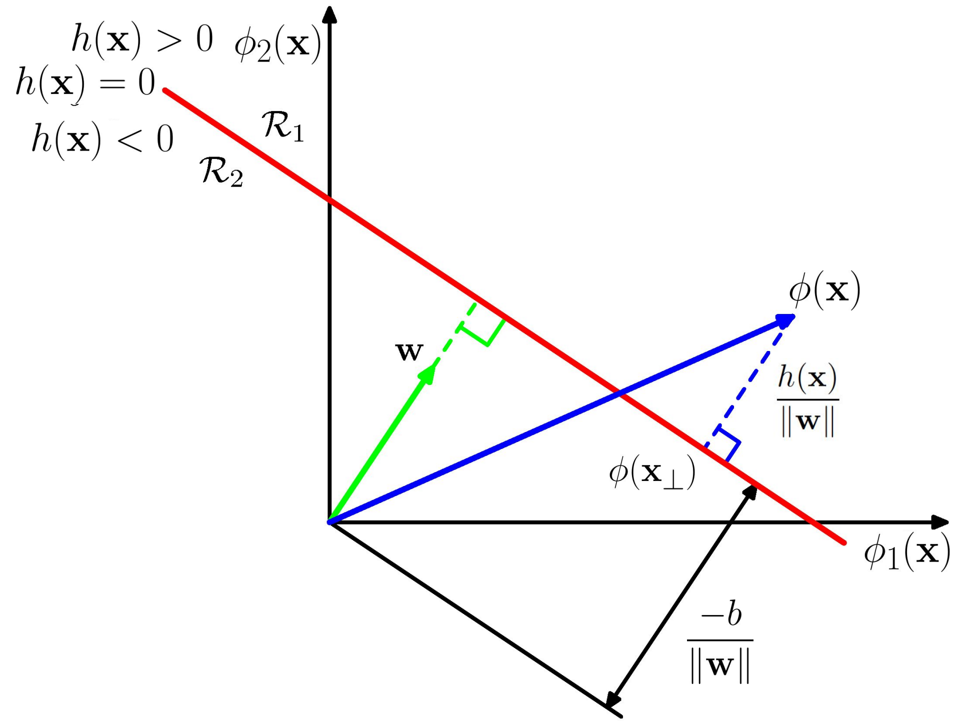
Overview

- 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

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



- Decision boundary is the hyperplane

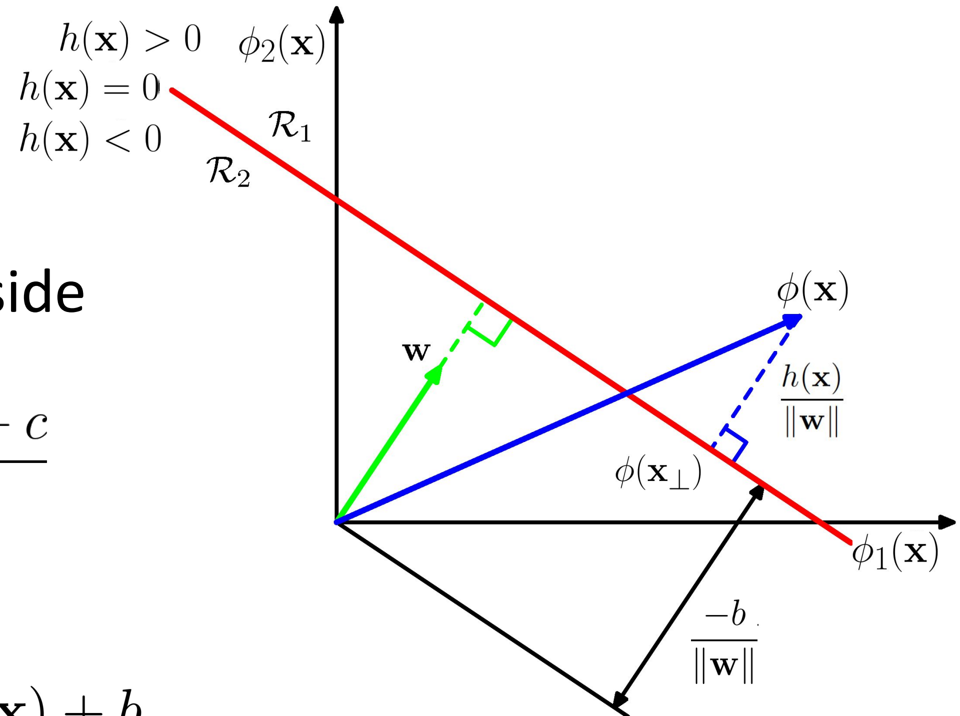
  $$\mathbf{w}^T \phi(\mathbf{x}) + b = 0.$$

  - **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

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

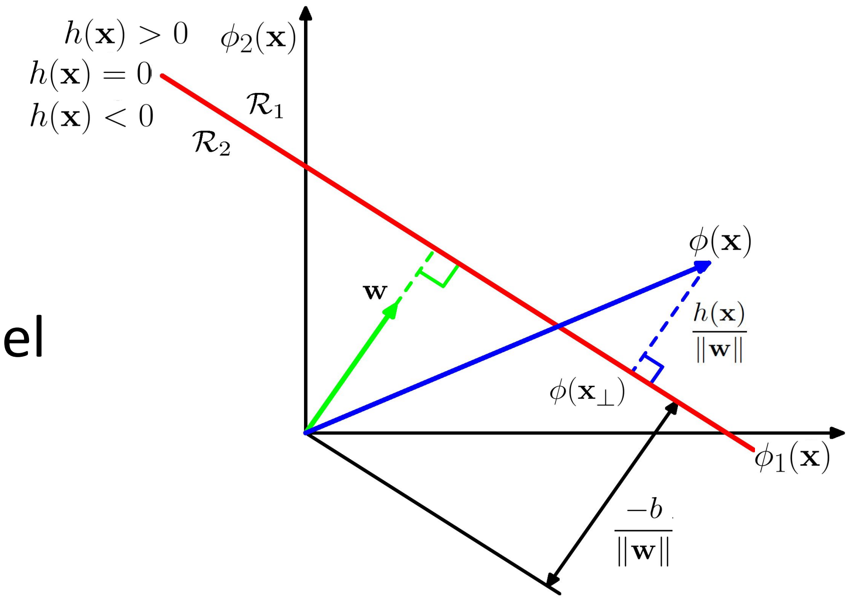


- M - dimensional:
  - Hyperplane: $h(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) + b$
  - Point: $\phi(\mathbf{x})$

$$\textbf{distance} = \frac{\mathbf{w}^T \phi(\mathbf{x}) + b}{\|\mathbf{w}\|}$$

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 = ± $\|\phi(\mathbf{x}) - \phi(\mathbf{x}_\perp)\|$



  - Note that $\mathbf{w}^T\big(\phi(\mathbf{x}) - \phi(\mathbf{x}_\perp)\big) = \|\mathbf{w}\|\,\|\phi(\mathbf{x}) - \phi(\mathbf{x}_\perp)\|\cos(0)$
  - Thus, $\|\phi(\mathbf{x}) - \phi(\mathbf{x}_\perp)\| = \dfrac{\mathbf{w}^T\phi(\mathbf{x}) - \mathbf{w}^T\phi(\mathbf{x}_\perp)}{\|\mathbf{w}\|}$

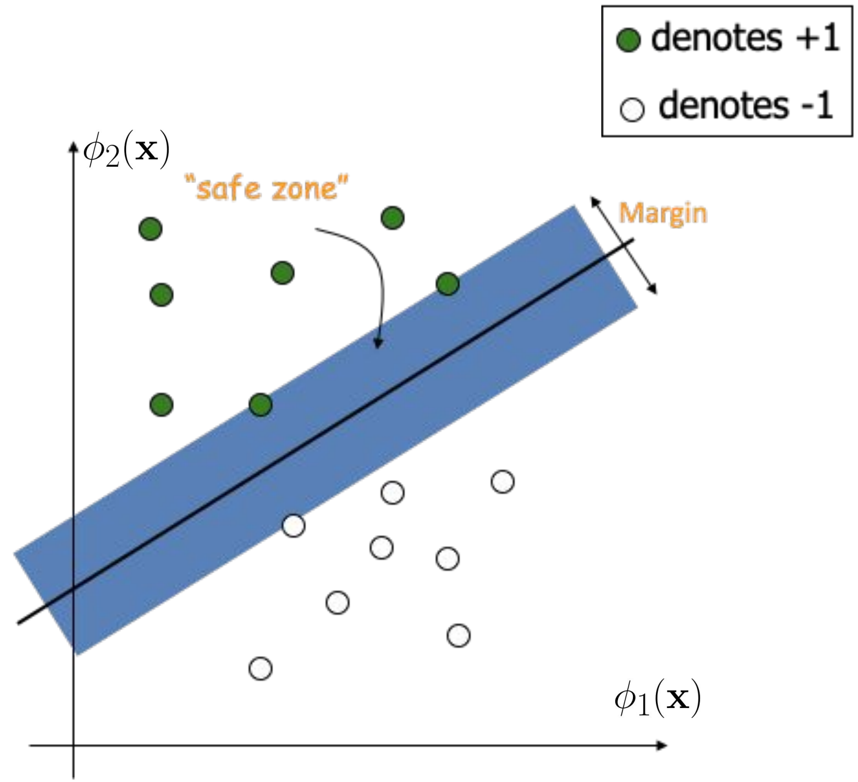
$$= \frac{\mathbf{w}^T\phi(\mathbf{x}) + b}{\|\mathbf{w}\|} \qquad \because \mathbf{w}^T\phi(\mathbf{x}_\perp) + b = 0$$

Maximum Margin Classifier

- 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



Maximum Margin Classifier

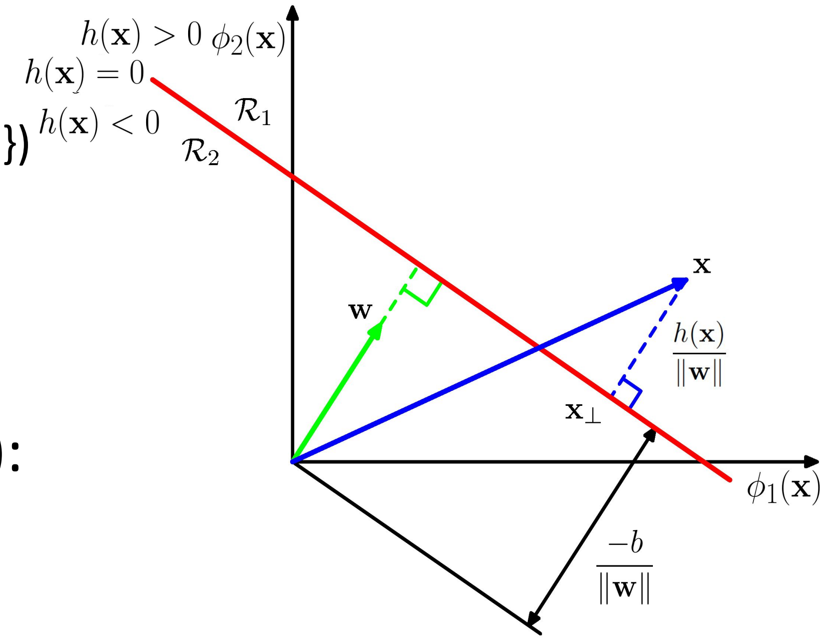
- Distance from $\phi(\mathbf{x})$ to the hyperplane $\mathbf{w}^T\phi(\mathbf{x}) + b = 0$.

  (assuming data is linearly separable, y ∈ {-1, 1})

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

- Margin (defined over training data):

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



Maximum Margin Classifier

- Optimization problem:

$$\arg\max_{w,b} \left\{ \frac{1}{\|\mathbf{w}\|} \min_{n} \left[y^{(n)} \left(\mathbf{w}^T \phi\left(\mathbf{x}^{(n)}\right) + b \right) \right] \right\}$$

- Rescale **w** and b such that:

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

- Optimization is equivalent to:

$$\arg\min_{\mathbf{w},b} \frac{1}{2} \|\mathbf{w}\|^2$$

subject to $y^{(n)} \left(\mathbf{w}^T \phi\left(\mathbf{x}^{(n)}\right) + b \right) \geq 1 \qquad n = 1, \ldots, N.$

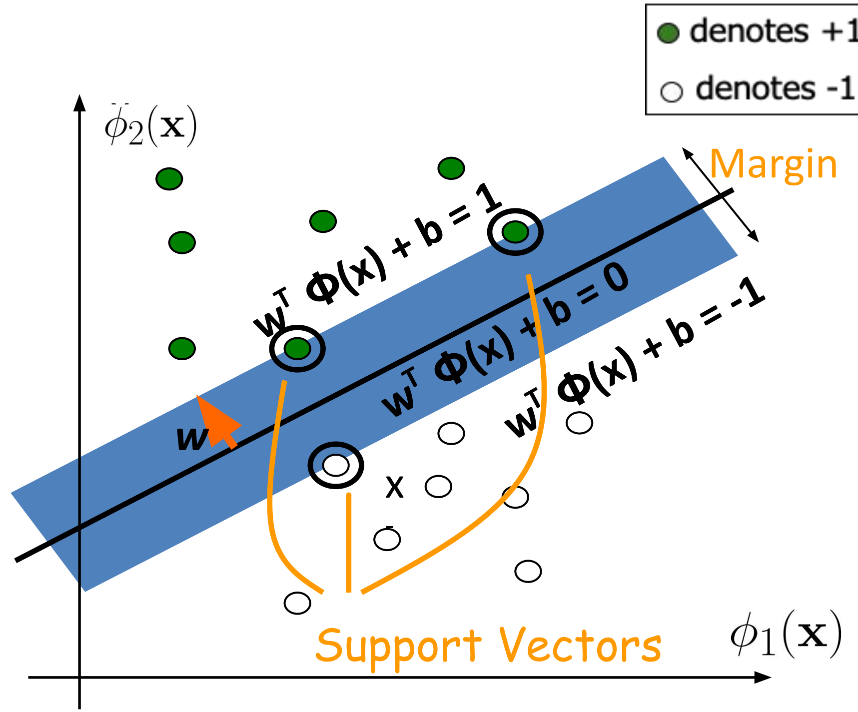
Maximum Margin Classifier

- Optimization problem:

$$\arg\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

subject to

$$\text{For } y^{(n)} = 1, \quad \mathbf{w}^T\phi(\mathbf{x}^{(n)}) + b \geq 1$$
$$\text{For } y^{(n)} = -1, \quad \mathbf{w}^T\phi(\mathbf{x}^{(n)}) + b \leq -1$$



Solving the optimization problem

- Optimization problem:

$$\arg\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

$$\text{subject to } y^{(n)}\left(\mathbf{w}^T\phi\left(\mathbf{x}^{(n)}\right)+b\right) \geq 1, \quad n=1,\ldots,N.$$

- This is a constrained optimization problem.
  - We solve this using Lagrange multipliers (convex optimization).

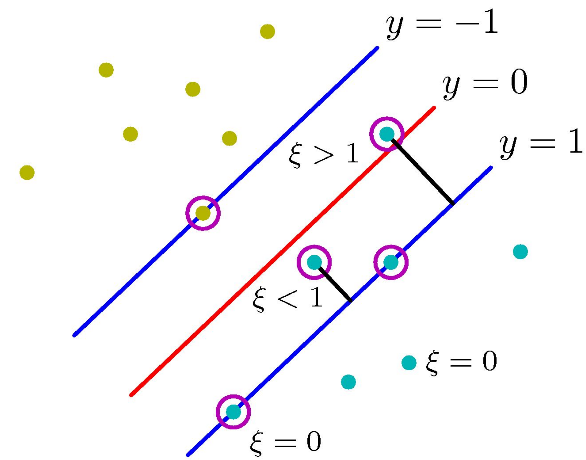
Support Vector Machines

- Hard SVM requires separable sets

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

- Soft SVM introduces *slack variables* for each data point

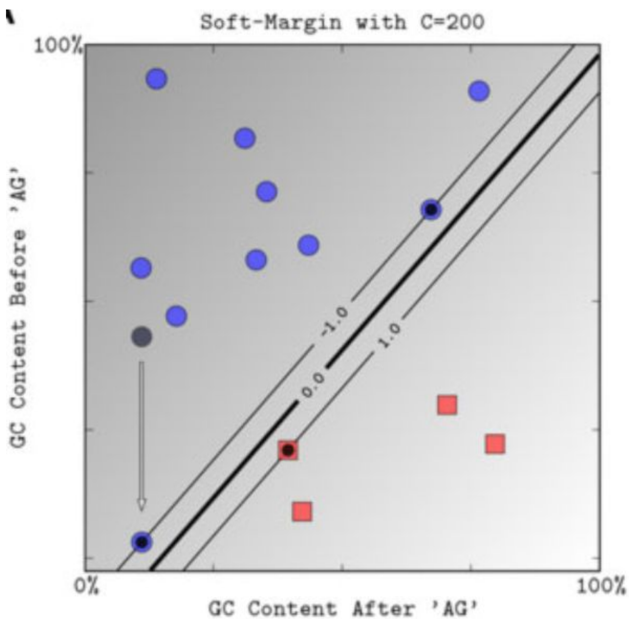
$$y^{(n)} h\left(\mathbf{x}^{(n)}\right) \geq 1 - \xi^{(n)}$$

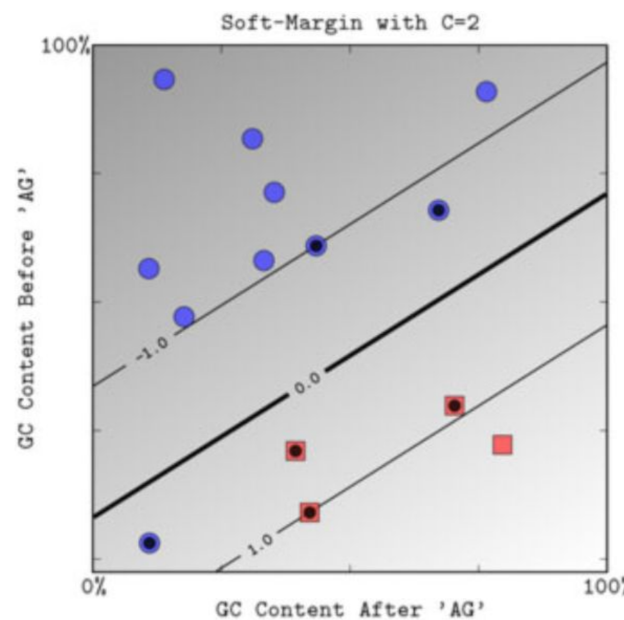


Recall: $$h\left(\mathbf{x}\right) = \mathbf{w}^T \phi\left(\mathbf{x}\right) + b$$

Soft SVM

- A little slack can give much better margin.





Soft SVM

- Maximize the margin, and also penalize for the slack variables

$$\min_{\mathbf{w},b,\xi} \quad C\sum_{n=1}^{N}\xi^{(n)} + \frac{1}{2}\|\mathbf{w}\|^2$$

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

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

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

Formulation of soft-margin SVM

- Maximize the margin, and also penalize for the slack variables

- Primal optimization
  - Optimization w.r.t

$$
\begin{aligned}
\min_{\mathbf{w},b,\xi} \quad & C\sum_{n=1}^{N}\xi^{(n)} + \frac{1}{2}\|\mathbf{w}\|^2 \\
\text{Subject to} \quad & y^{(n)}h\left(\mathbf{x}^{(n)}\right) \geq 1-\xi^{(n)}\ \forall n \\
& \xi^{(n)} \geq 0, \forall n
\end{aligned}
$$

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

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

$$\min_{\mathbf{w},b,\xi} \quad C\sum_{n=1}^{N}\xi^{(n)} + \frac{1}{2}\|\mathbf{w}\|^2$$

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

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

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

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

Converting constraints into penalty

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

$$\min_{\mathbf{w},b,\xi} \quad C\sum_{n=1}^{N}\xi^{(n)} + \frac{1}{2}\|\mathbf{w}\|^2$$
$$\text{Subject to} \quad y^{(n)}h\left(\mathbf{x}^{(n)}\right) \geq 1 - \xi^{(n)} \quad \forall n$$
$$\xi^{(n)} \geq 0, \forall n$$

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

- Rewriting the constraints: for each n,

$$\xi^{(n)} \geq 1 - y^{(n)}h\left(\mathbf{x}^{(n)}\right)$$
$$\xi^{(n)} \geq 0$$
$$\Rightarrow \quad \xi^{(n)} \geq \max\left(0, 1 - y^{(n)}h\left(\mathbf{x}^{(n)}\right)\right)$$

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

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

Converting constraints into penalty

- Original optimization problem

$$\begin{aligned} \min_{\mathbf{w},b,\xi} \quad & C\sum_{n=1}^{N}\xi^{(n)} + \tfrac{1}{2}\|\mathbf{w}\|^2 \\ \text{Subject to} \quad & y^{(n)}h\left(\mathbf{x}^{(n)}\right) \geq 1-\xi^{(n)} \ \forall n \\ & \xi^{(n)} \geq 0, \forall n \end{aligned}$$

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

- An equivalent optimization problem

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

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

Gradients

- Computing the (sub) gradient with respect w and b:
  - Recall: $h(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) + b$

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

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

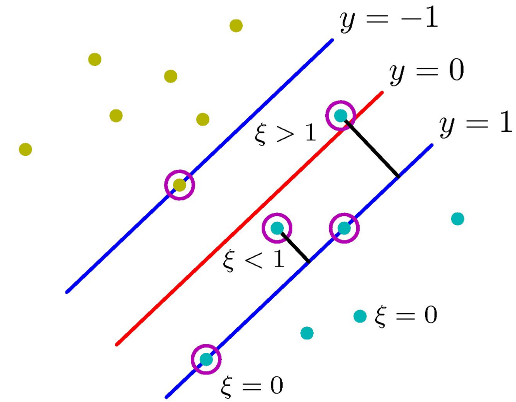
$$\nabla_{b} \mathcal{L} = -C \sum^{N} y^{(n)} I\left(1 - y^{(n)} h\left(\mathbf{x}^{(n)}\right) \geq 0\right)$$

- 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

$$\arg\max_{w,b}\left\{\frac{1}{\|\mathbf{w}\|}\min_n\left[y^{(n)}\left(\mathbf{w}^T\phi\left(\mathbf{x}^{(n)}\right)+b\right)\right]\right\} \Leftrightarrow \arg\min_{\mathbf{w},b}\frac{1}{2}\|\mathbf{w}\|^2$$

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

Need to use constrained convex optimization to solve this problem

$\Downarrow$ Relax the constraints

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

$$\min_{\mathbf{w},b,\xi} \quad C\sum_{n=1}^{N}\xi^{(n)}+\tfrac{1}{2}\|\mathbf{w}\|^2$$

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

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

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

Primal problem can be solved using gradient methods.

Thank you!

Click here to take the quiz!

Next class: *Dual view* of Soft SVM