CS5489

Lecture 3.2: Support Vector Machines: Part I

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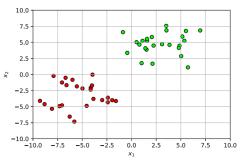
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Overview

- To date we've seen one example of a discriminative linear classifier
 - I.e., logistic regression, which used a maximum likelihood framework to learn the separating hyperplane
- Today we'll introduce a second example, support vector machines (SVMs)
 - A purely geometric approach

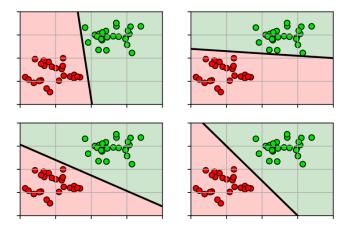
Linearly Separable Data

- For now, assume the training data is **linearly separable**
 - The two classes in the training data can be separated by a line (hyperplane)
 - Example: iris dataset



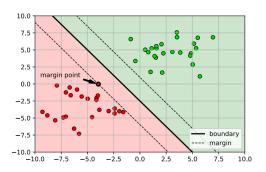
Which is the Best Separating Line?

■ There are many possible solutions



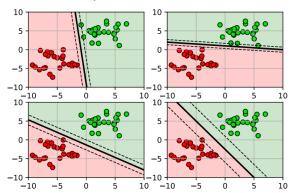
Maximum Margin Principle

- Define the distance between the separating line and the closest point as the margin
 - Think of this space as the "amount of wiggle room" for accommodating errors in estimating w



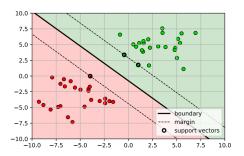
Maximum Margin Principle

- **Idea**: the best separating line is the one that maximizes the margin
 - I.e., puts the most distance between the closest points and the decision boundary



Maximum Margin Principle

- The solution...
 - By symmetry, there should be at least one margin point on each side of the boundary
 - The points on the margins are called the support vectors
 - The points support (define) the margin



Computing the Margin

■ What is the margin (i.e., distance) of $\mathbf{w}^T \mathbf{x} + b = 0$ with respect to a point $(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})$?

$$d^{(i)} = \frac{y^{(i)}(\mathbf{w}^T \mathbf{x}^{(i)} + b)}{\|\mathbf{w}\|_2}$$

- This is called the **geometric** margin
- The numerator $y^{(i)}(\mathbf{w}^T\mathbf{x}^{(i)} + b)$ is called the **functional** margin
- What is the margin of $\mathbf{w}^T \mathbf{x} + b = 0$ with respect to a training set $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)}), i = 1, \dots, M\}$?

$$d = \min\{d^{(i)}\}_{i=1}^{M} = \min_{(\mathbf{x}, y) \in \mathcal{D}} \frac{y(\mathbf{w}^T \mathbf{x} + b)}{\|\mathbf{w}\|_2}$$

Maximizing the Margin

■ The maximum margin solution is found by solving

$$\max_{\mathbf{w},b} \left(\frac{1}{\|\mathbf{w}\|_2} \min_{(\mathbf{x},y) \in \mathcal{D}} y(\mathbf{w}^T \mathbf{x} + b) \right)$$

- Notice that if we make the rescaling $\mathbf{w} \to \gamma \mathbf{w}$ and $b \to \gamma b$, then the objective function is unchanged
- We can use this freedom to set

$$\min_{(\mathbf{x}, y) \in \mathcal{D}} y(\mathbf{w}^T \mathbf{x} + b) = 1$$

Or equivalently,

$$y^{(i)}(\mathbf{w}^T\mathbf{x}^{(i)}+b) \ge 1, \forall i=1,\ldots,M$$

SVM (Primal Form, Hard-Margin)

■ Given a training set $\mathcal{D} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^{M}$, optimize:

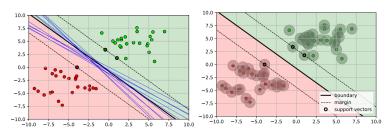
$$\begin{aligned} & \min_{\mathbf{w},b} & & \frac{1}{2} \|\mathbf{w}\|_2^2 \\ & \text{subject to} & & y^{(i)} (\mathbf{w}^T \mathbf{x}^{(i)} + b) \geq 1, \ i = 1, \dots, M \end{aligned}$$

- The objective minimizes the inverse of the margin distance, i.e., maximizes the **geometric** margin
- The inequality constraints ensure that all points are either on or outside of the functional margin
 - The functional margin is set to be distance of 1 from the boundary
- Prediction:
 - Given a new data point x*, use sign of linear function to predict class

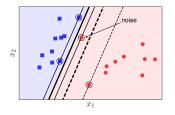
$$y^* = \operatorname{sign}(\mathbf{w}^T \mathbf{x}^* + b)$$

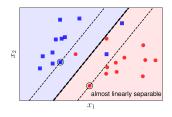
Why is Maximizing the Margin Good?

- The true w is uncertain
 - Maximizing the margin allows the most uncertainty (wiggle room) for w, while keeping all the points correctly classified
- The data points are uncertain
 - Maximizing the margin allows the most wiggle of the points, while keeping all the points correctly classified



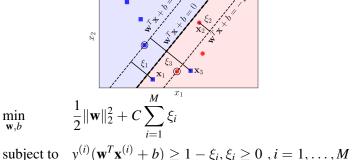
Is Hard-Margin Enough?





- Solution: use the same linear classifier
 - Allow some training samples to violate margin
 - I.e., are inside the margin (or even mis-classified)
 - Define "slack" variable $\xi_i \ge 0$
 - $\xi_i = 0$ means sample is outside of margin area (no slack)
 - \bullet $\xi_i > 0$ means sample is inside of margin area (slack)

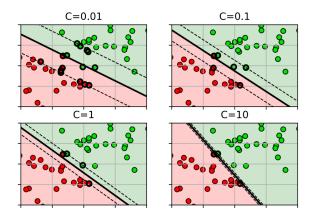
SVM (Primal Form, Soft-Margin)



- Introduces a parameter C as penalty for violating the margin
 - Smaller value means allow more violations (less penalty)
 - Larger value means don't allow violations (more penalty)

min $\mathbf{w}.b$

The Effect of C



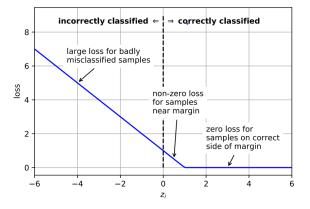
Loss Function

■ In the case of primal-form SVM with soft-margin, it is equivalent to minimizing the function:

$$\sum_{i=1}^{M} \max(0, 1 - y^{(i)}(\mathbf{w}^{T}\mathbf{x}^{(i)} + b)) + \frac{1}{C}||\mathbf{w}||_{2}^{2},$$

- Hinge loss function $\ell_h(z) = \max(0, 1-z)$
 - Note: max(a, b) returns whichever value (a or b) is larger
- It takes tens of years from hinge loss to SVM

Hinge Loss



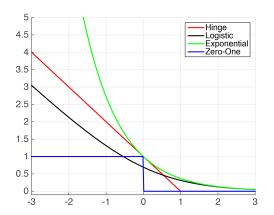
Zero-One Loss

Both the logistic loss and the hinge loss are convex relaxations of the zero-one loss:

$$\ell_{01}(z) = \mathbb{I}[z \le 0]$$

- The average zero-one loss over a data set is exactly the classification error rate
- This is the loss function we'd like to minimize, but this generally isn't computationally feasible, thus the need for surrogate loss functions

Loss Function Comparison



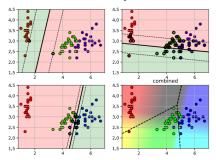
- Exponential loss: $\ell_e(z) = \exp(-z)$
 - Used in the development of other machine learning algorithms, e.g., AdaBoost

Multiclass SVM

- "1-vs-1" multiclass classification
 - Train binary classifiers on all pairs of classes
 - 3-class example: 1 vs 2, 1 vs 3, 2 vs 3
 - To label a sample, pick the class with the most votes among the binary classifiers
 - Problem: 1v1 classification is very slow when there are a large number of classes
 - If there are C classes, need to train C(C-1)/2 binary classifiers!
- "1-vs-rest" multiclass classification
 - Train 1-vs-rest binary classifiers
 - 3-class example: 1 vs {2,3}, 2 vs {1,3}, 3 vs {1,2}
 - To label a sample, pick the class with the largest geometric margin
 - $\mathbf{v}^* = \arg\max_{c \in \{1,...,C\}} (\mathbf{w}_c^T \mathbf{x}^* + b_c) / \|\mathbf{w}_c\|_2$

Example: 3-Class Iris Dataset

Decision boundaries for each binary classifier



SVM Summary

Classifier:

- Linear function $f(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b$
- Given new sample \mathbf{x}^* , predict $y^* = \operatorname{sign}(\mathbf{w}^T \mathbf{x}^* + b)$

■ Training:

- Maximize the margin of the training data
 - I.e., maximize the separation between the points and the decision boundary
- Allow some training samples to violate the margin
 - Use cross-validation to pick the hyperparameter *C*

Summary

■ Linear classifiers:

- Separate the data using a linear surface (hyperplane)
- $y = \operatorname{sign}(\mathbf{w}^T \mathbf{x} + b)$

■ Two formulations:

- Logistic regression maximize the probability of the data
- Support vector machine maximize the margin of the hyperplane

Loss functions:

- Logistic regression push the classification boundary as far as possible from all points
- Support vector machine ensure a margin of 1 between boundary and the closest point

Summary

Advantages:

- SVM works well on high-dimensional features (N large), and has low generalization error
- LR has well-defined probabilities

■ Disadvantages:

- Decision surface can only be linear!
 - Next lecture we will see how to deal with non-linear decision surfaces