CS5489
Lecture 3.2: Support Vector Machines: Part I

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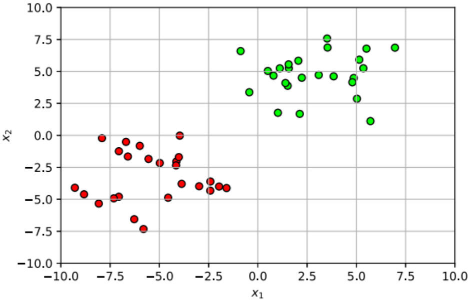
Overview

- 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

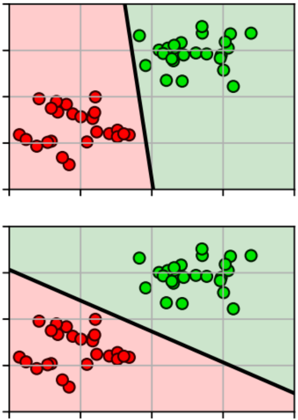
Linearly Separable Data

- 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



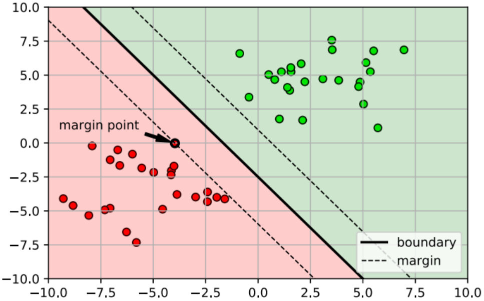
Which is the Best Separating Line?

- There are many possible solutions



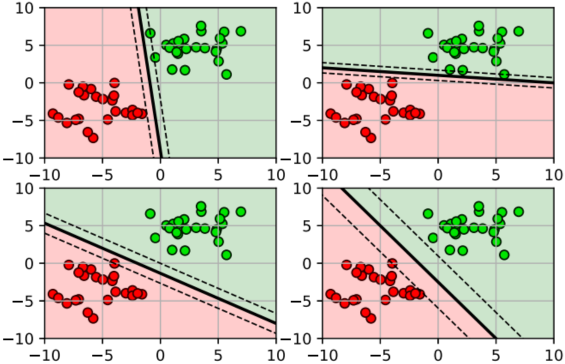
Maximum Margin Principle

- 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 $\mathbf{w}$



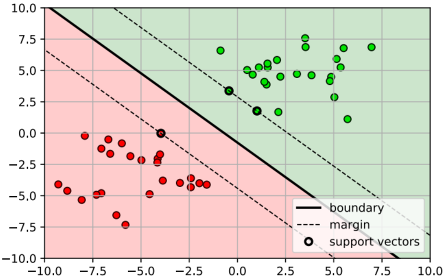
Maximum Margin Principle

- **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 $(\mathbf{x}^{(i)}, y^{(i)})$?

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

  - 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 $\mathcal{D} = \{(\mathbf{x}^{(i)}, y^{(i)}), i = 1, \ldots, M\}$?

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

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,

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

SVM (Primal Form, Hard-Margin)

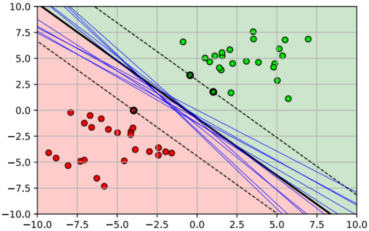
- Given a training set $\mathcal{D} = \{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^{M}$, optimize:

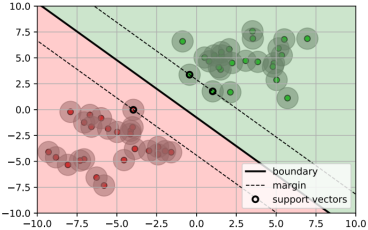
$$\begin{aligned} \min_{\mathbf{w},b} \quad & \frac{1}{2}\|\mathbf{w}\|_2^2 \\ \text{subject to} \quad & y^{(i)}(\mathbf{w}^T\mathbf{x}^{(i)} + b) \geq 1, \ i = 1, \ldots, M \end{aligned}$$

  - 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 $\mathbf{x}^*$, use sign of linear function to predict class
    - $y^* = \text{sign}(\mathbf{w}^T\mathbf{x}^* + b)$

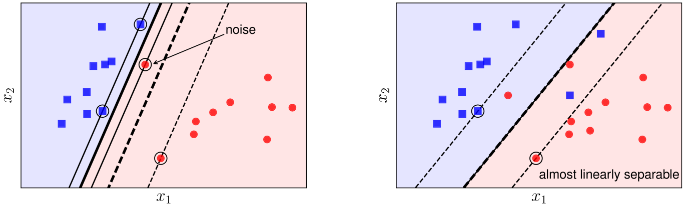
Why is Maximizing the Margin Good?

- 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



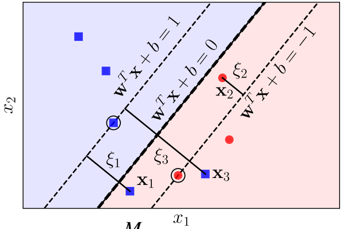


Is Hard-Margin Enough?



- 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 $\xi_i \geq 0$
    - $\xi_i = 0$ means sample is outside of margin area (no slack)
    - $\xi_i > 0$ means sample is inside of margin area (slack)

SVM (Primal Form, Soft-Margin)

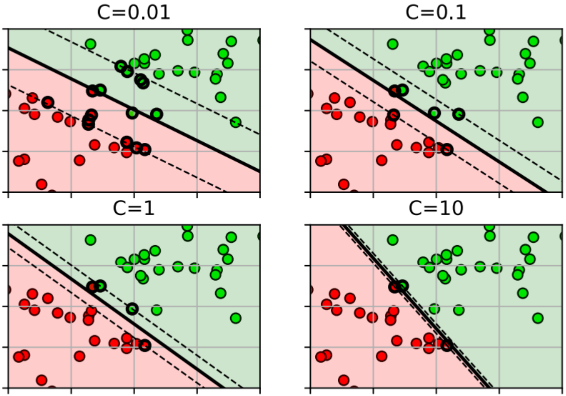


$$\min_{\mathbf{w},b} \quad \frac{1}{2}\|\mathbf{w}\|_2^2 + C\sum_{i=1}^{M}\xi_i$$

$$\text{subject to} \quad y^{(i)}(\mathbf{w}^T\mathbf{x}^{(i)} + b) \geq 1 - \xi_i, \xi_i \geq 0 \ , i = 1, \ldots, M$$

- 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)

The Effect of C



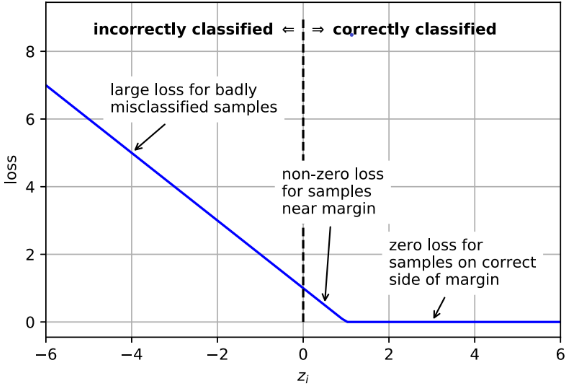
Loss Function

- 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


incorrectly classified ⇐
⇒ correctly classified
large loss for badly misclassified samples
non-zero loss for samples near margin
zero loss for samples on correct side of margin
loss
z_i
8
6
4
2
0
−6
−4
−2
0
2
4
6

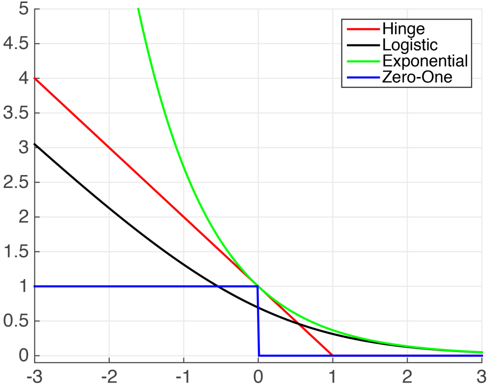
Zero-One Loss

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

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

- 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



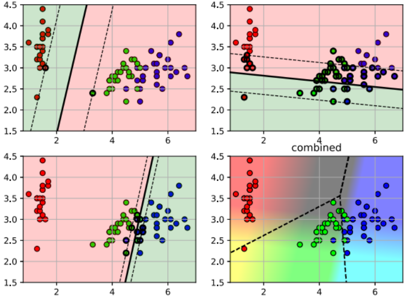
- Exponential loss: $\ell_e(z) = \exp(-z)$
  - Used in the development of other machine learning algorithms, e.g., AdaBoost

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
    - $y^* = \arg\max_{c\in\{1,\ldots,C\}}(\mathbf{w}_c^T\mathbf{x}^* + b_c)/\|\mathbf{w}_c\|_2$

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