Introduction to Machine Learning

Linear Classifiers - Perceptrons and Logistic Regression

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Outline

Classification

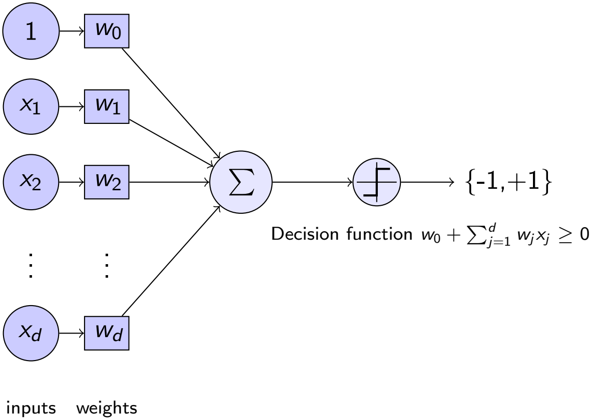
Linear Classifiers
- Linear Classification via Hyperplanes

Logistic Regression
- Using Gradient Descent for Learning Weights
- Using Newton's Method

Supervised Learning - Classification

- Target y is categorical
- e.g., $y \in \{-1, +1\}$ (binary classification)
- A possible problem formulation: Learn f such that $y = f(\mathbf{x})$

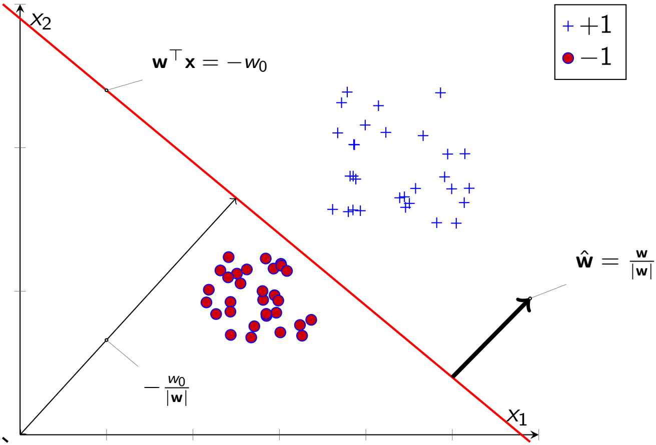
Linear Classifiers



Decision Rule

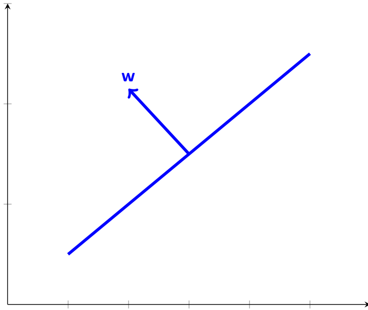
$$y_i = \begin{cases} -1 & \text{if } w_0 + \mathbf{w}^\top \mathbf{x}_i < 0 \\ +1 & \text{if } w_0 + \mathbf{w}^\top \mathbf{x}_i \geq 0 \end{cases}$$

Geometric Interpretation



Linear Hyperplane

- Separates a D-dimensional space into two half-spaces
- Defined by $\mathbf{w} \in \Re^D$
  - *Orthogonal* to the hyperplane
  - This $\mathbf{w}$ goes through the origin
  - How do you check if a point lies "above" or "below" $\mathbf{w}$?
  - What happens for points **on** $\mathbf{w}$?

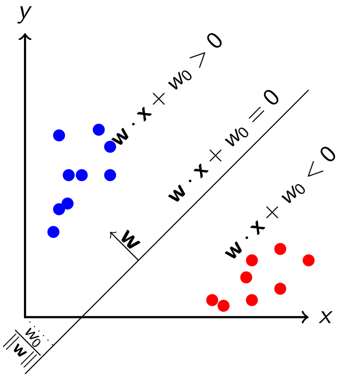


Make hyperplane not go through origin

- Add a bias w_0
  - $w_0 > 0$ - move along $\mathbf{w}$
  - $w_0 < 0$ - move opposite to $\mathbf{w}$
- How to check if point lies above or below $\mathbf{w}$?
  - If $\mathbf{w}^\top \mathbf{x} + w_0 > 0$ then $\mathbf{x}$ is *above*
  - Else, *below*

Line as a Decision Surface

- Decision boundary represented by the hyperplane **w**
- For binary classification, **w** points **towards** the positive class



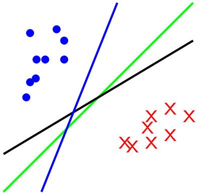
Decision Rule

$$y = sign(\mathbf{w}^\top \mathbf{x} + w_0)$$

- $\mathbf{w}^\top \mathbf{x} + w_0 \geq 0 \Rightarrow y = +1$
- $\mathbf{w}^\top \mathbf{x} + w_0 < 0 \Rightarrow y = -1$

What is Best Hyperplane Separator

- Find a hyperplane that separates the data
  - . . . if the data is linearly separable
- But there can be many choices!
- Find the one with lowest error



Learning w

- What is an appropriate loss function?

0-1 Loss

- Number of mistakes in training data

$$J(\mathbf{w}) = \min_{\mathbf{w}, w_0} \sum_{i=1}^{n} \mathbb{I}(y_i(\mathbf{w}^\top \mathbf{x}_i + w_0) < 0)$$

- Hard to optimize
- Solution - replace it with a mathematically manageable loss

Different Loss Functions

Note

From now on, assuming that intercept and constant terms are included in $\mathbf{w}$ and $\mathbf{x}_i$, respectively.

- **Squared Loss** - Perceptron

$$J(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}(y_i - \mathbf{w}^\top \mathbf{x}_i)^2 \tag{1}$$

- **Logistic Loss** - Logistic Regression

$$J(\mathbf{w}) = \frac{1}{n}\sum_{i=1}^{n}\log\left(1 + \exp\left(-y_i \mathbf{w}^\top \mathbf{x}_i\right)\right) \tag{2}$$

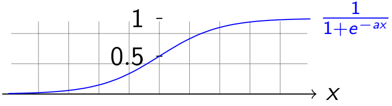
- **Hinge Loss** - Support Vector Machine

$$J(\mathbf{w}) = \sum_{i=1}^{n}\max\left(0, 1 - y_i \mathbf{w}^\top \mathbf{x}_i\right) \tag{3}$$

Logistic Regression

Geometric Interpretation

- Use regression to predict discrete values
- *Squash* output to $[0, 1]$ using sigmoid function
- Output less than 0.5 is one class and greater than 0.5 is the other



Probabilistic Interpretation

- Probability of $\mathbf{x}$ to belong to class $+1$

Logistic Loss Function

- For one training observation,
  - if $y_i = +1$, the probability of the predicted value to be $+1$
$$p_i = \frac{1}{1 + \exp\left(-\mathbf{w}^\top \mathbf{x}_i\right)}$$
  - if $y_i = -1$, the probability of the predicted value to be -1
$$p_i = 1 - \frac{1}{1 + \exp\left(-\mathbf{w}^\top \mathbf{x}_i\right)} = \frac{1}{1 + \exp\left(\mathbf{w}^\top \mathbf{x}_i\right)}$$
  - In general
$$p_i = \frac{1}{1 + \exp\left(-y_i \mathbf{w}^\top \mathbf{x}_i\right)}$$
- For logistic regression, the objective is to minimize the negative of the log probability:
$$J(\mathbf{w}) = -\sum_{i=1}^{n} \log\left(p_i\right) = \sum_{i=1}^{n} \log\left(1 + \exp\left(-y_i \mathbf{w}^\top \mathbf{x}_i\right)\right)$$

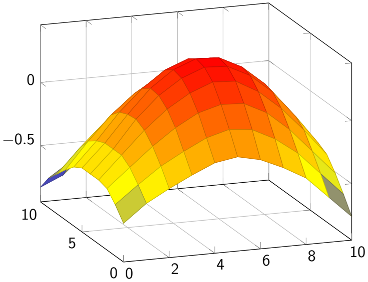
Learning Logistic Regression Model

- Direct minimization??
  - No closed form solution for minimizing error
- Gradient Descent
- Newton's Method

Using Gradient Descent for Learning Weights

- Compute gradient of $J(\mathbf{w})$ with respect to $\mathbf{w}$
- A convex function of $\mathbf{w}$ with a unique global minima

$$\nabla J(\mathbf{w}) = -\frac{1}{n}\sum_{i=1}^{n}\frac{y_i}{1+\exp\left(y_i\mathbf{w}^\top\mathbf{x}_i\right)}\mathbf{x}_i$$



- Update rule:

$$\mathbf{w}_{k+1} = \mathbf{w}_k - \eta\frac{d}{d\mathbf{w}_k}LL(\mathbf{w}_k)$$

Using Newton's Method

- Setting η is sometimes *tricky*
- Too large – incorrect results
- Too small – slow convergence
- Another way to speed up convergence:

Newton's Method

$$\mathbf{w}_{k+1} = \mathbf{w}_k - \eta \mathbf{H}_k^{-1} \nabla J(\mathbf{w}_k)$$

Hessian

$$\mathbf{H}(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^{n} \frac{\exp\left(y_i \mathbf{w}^\top \mathbf{x}_i\right)}{\left(1 + \exp\left(y_i \mathbf{w}^\top \mathbf{x}_i\right)\right)^2} \mathbf{x}_i \mathbf{x}_i^\top$$

References