Logistic Regression

Chris Cornwell

Feb 27, 2025

Outline

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Decision boundaries

For model h, made for classification task (with data points $\mathbf{x} \in \mathbb{R}^d$), write $C_y \subset \mathbb{R}^d$ for the set of points with label y, i.e.,

$$C_y = h^{-1}(y) = \{\mathbf{x} \in \mathbb{R}^d \mid h(\mathbf{x}) = y\}.$$

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Say $y \neq y'$ and a point is in the boundary of both C_y and $C_{y'}$. We say that point is on a **decision boundary** of the model. In a half-space model (last lecture), the hyperplane determined by $\mathbf{w}$ and b is the decision boundary.

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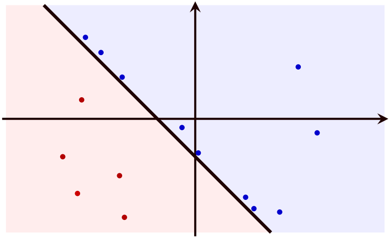

Figure: Many points near the decision boundary

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Also...the immediate change of label across the boundary (a discontinuity in the model) ...perhaps not “natural”?

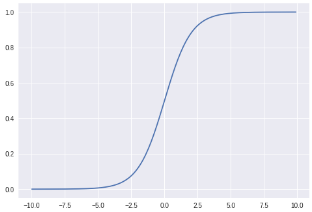
Outline

Incorporating a probability into half-space model

Instead of only capturing the sign of $\mathbf{w} \cdot \mathbf{x} + b$, compose it with the **logistic function**.

$$\sigma(z) = \frac{1}{1 + e^{-z}}.$$

- $0 < \sigma(z) < 1$ for all $z \in \mathbb{R}$;
- $\lim_{z \to \infty} \sigma(z) = 1$ and $\lim_{z \to -\infty} \sigma(z) = 0$;
- $\sigma(0) = 1/2$.



Logistic model, continued

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So, for $\mathbf{x} \in \mathbb{R}^d$, find $\sigma(\mathbf{w} \cdot \mathbf{x} + b)$.

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Given $\mathbf{x} \in \mathbb{R}^d$, the side of the hyperplane H it is on is determined by the sign of $\mathbf{w} \cdot \mathbf{x} + b$. Our half-space model: $h : \mathbb{R}^d \setminus H \longrightarrow \{1, -1\}$.

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- (Positive side) Say that $h(\mathbf{x}) = 1$ if $\mathbf{w} \cdot \mathbf{x} + b > 0$.
- (Negative side) Say that $h(\mathbf{x}) = -1$ if $\mathbf{x} \cdot \mathbf{x} + b < 0$.

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Given data with $\{\pm 1\}$ labels, if there exists a hyperplane H so that $\mathbf{x}$ has label 1 if and only if it is on the positive side, the labeled data are called **linearly separable**.

Linearly separable

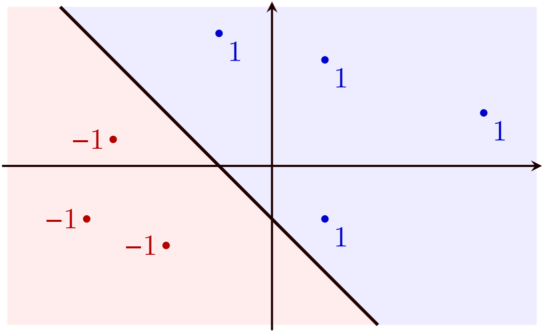

Figure: The hyperplane $H = \{(x_1, x_2) \in \mathbb{R}^2 : x_1 + x_2 + 1 = 0\}$, corresponding positive and negative regions, $\mathbf{w} = (1, 1)$, $b = 1$

Not linearly separable

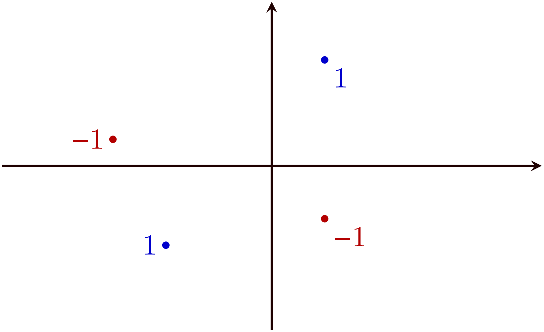

Figure: A data set in $\mathbb{R}^2$ that is not linearly separable.

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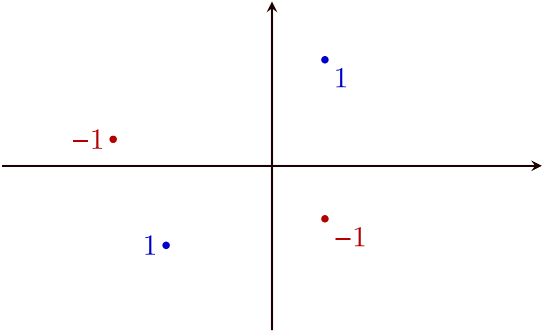

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- A criterion (checkable, in theory) that is equivalent to "not linearly separable"?

Outline

Setup for Perceptron algorithm

Labeled data: $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)$, with $\mathbf{x}_i \in \mathbb{R}^d$ and $y_i \in \{\pm 1\}$ for all i.
Assuming labeled data is linearly separable, the Perceptron algorithm is a procedure that is guaranteed to find a hyperplane that separates the data.[1]

[1] Introduced in *The perceptron: A probabilistic model for information storage and organization in the brain*, F. Rosenblatt, Psychological Review **65** (1958), 386–407.

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To describe it: for each $\mathbf{x}_i$, use X_i to denote the $(d+1)$-vector consisting of $\mathbf{x}_i$ with 1 appended at the end;
Additionally, use W to denote the vector $\mathbf{w}$ with b appended at the end.

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Additionally, use W to denote the vector $\mathbf{w}$ with b appended at the end.
Note that $W \cdot X_i = \mathbf{w} \cdot \mathbf{x}_i + b$.
For linearly separable data, our goal is to find $W \in \mathbb{R}^{d+1}$ so that $W \cdot X_i$ and y_i have the same sign (both positive or both negative), for all $1 \leq i \leq n$.

- Equivalently, we need $y_i W \cdot X_i > 0$ for all $1 \leq i \leq n$.

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Perceptron algorithm

Suppose the data is linearly separable. Also, `x` is an $n \times d$ array of points, with ith row equal to $\mathtt{x}_i$, and `y` is array of the labels. The Perceptron algorithm finds `W` iteratively as follows.[2]

[2] Recall, in pseudo-code block, left-facing arrow means *assign* to variable on left.

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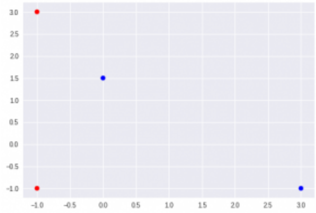
```
input: x, y   ## x is n by d, y is 1d array
X ← append 1 to each row of x
W ← (0,0,...,0)   ## Initial W
while (exists i with y[i]*dot(W, X[i]) ≤ 0){
    W ← W + y[i]*X[i]
}
return W
```

[2]Recall, in pseudo-code block, left-facing arrow means *assign* to variable on left.

Example

A simple example in $\mathbb{R}^2$, with $n = 4$ points.

$$\text{x: } \begin{bmatrix} -1 & 3 \\ -1 & -1 \\ 3 & -1 \\ 0 & 1.5 \end{bmatrix} \qquad \text{y: } \begin{bmatrix} -1 \\ -1 \\ 1 \\ 1 \end{bmatrix}$$



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Use $W^{(t)}$ for value of W on step t. Start: $W^{(1)} = (0, 0, 0)$.
Next step: $W^{(2)} = \vec{0} + y_1 X_1 = -1 * (-1, 3, 1) = (1, -3, -1)$.

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Next: since $y_1 W^{(2)} \cdot X_1 > 0$, check
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$$W^{(3)} = W^{(2)} + y_2 X_2 = (2, -2, -2).$$

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Continue in this way – on each step check dot products (in order) with $y_1 X_1, y_2 X_2, y_3 X_3, y_4 X_4$. Eventually you return the vector $W^{(10)} = (4,-0.5,1)$.

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i.e., $H = \{(x_1, x_2) \in \mathbb{R}^2 : \; 4x_1 - 0.5x_2 + 1 = 0\}$ separates the points.

Perceptron algorithm, stopping time

Under our assumptions for Perceptron algorithm, a guarantee on eventually stopping.

Theorem

Define $R = \max_i |X_i|$ *and* $B = \min_i\{|V| : \forall i, y_i V \cdot X_i \geq 1\}$. *Then, the Perceptron algorithm stops after at most* $(RB)^2$ *iterations and, when it stops with output* W*, then* $y_i W \cdot X_i > 0$ *for all* $1 \leq i \leq n$.

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Idea of proof: Write W^* for vector that realizes the minimum B. Also, write $W^{(t)}$ for the vector W on the t^{th} step, with $W^{(1)} = (0, 0, \ldots, 0)$.

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Now, by Cauchy-Schwarz inequality, $T \leq BR\sqrt{T}$, which we can rearrange to $T \leq (BR)^2$.

Another example, the Iris data set

First discussed by R.A. Fisher in a 1936 paper, Iris data set commonly used in explanations. It contains 150 points in $\mathbb{R}^4$, each for an individual iris flower from one of 3 species: Iris setosa, Iris virginica, and Iris versicolor.

Figure: Images by G. Robertson, E. Hunt, Radomil ©CC BY-SA 3.0

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Iris setosa points are linearly separable from the other two.

Labels: *Iris setosa* $\longleftarrow$ 1; *Other species* $\longleftarrow$ -1.

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Begin by opening the notebook `'perceptron-iris-notebook.ipynb'` ...After completing the algorithm, should get final $W = (\mathbf{w}, b)$, where $\mathbf{w} = (1.3, 4.1, -5.2, -2.2)$ and $b = 1$.

Figure: Images by G. Robertson, E. Hunt, Radomil ©CC BY-SA 3.0