Gradient descent on Logistic model

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Outline

Setup

As usual, sample data $\mathcal{S}$; write $(\mathbf{x}_i, y_i)$ for point in $\mathcal{S}$, with $y_i \in \{1, -1\}$. Parameter space: $\Omega = \mathbb{R}^{d+1} = \{(\mathbf{w}, b) \mid \mathbf{w} \in \mathbb{R}^d, b \in \mathbb{R}\}$. For each $\omega \in \Omega$, we have a function $f_\omega : \mathbb{R}^d \to (0, 1)$ defined as

$$f_\omega(\mathbf{x}) = \sigma(\mathbf{w} \cdot \mathbf{x} + b),$$

where σ is the logistic function. (So, our function output is our probability that the correct label for $\mathbf{x}$ is $+1$.)

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where σ is the logistic function. (So, our function output is our probability that the correct label for $\mathbf{x}$ is $+1$.) What do we use for the empirical loss function? When the "correct" y is $+1$ (and $\mathbf{x}$ is far from the hyperplane), we are in a good situation if is $f_\omega(\mathbf{x})$ very close to 1. Alternatively, if the correct y is -1, then we would like $f_\omega(\mathbf{x})$ to be close to 0.

It will help us to alter the numerical values of our labels: for i with $y_i = 1$, define $\tilde{y}_i = 1$; for i with $y_i = -1$, define $\tilde{y}_i = 0$.[1]

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For these reasons (as well as the rationale for using the logistic function), we use the **log-loss** function (a.k.a. **binary cross-entropy**). It is defined by

$$\mathcal{L}_\mathcal{S}(\omega) = \frac{1}{n} \sum_{i=1}^{n} -\tilde{y}_i \log(f_\omega(\mathbf{x}_i)) - (1 - \tilde{y}_i) \log(1 - f_\omega(\mathbf{x}_i)).$$

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Gradient descent with logistic regression

First, compute the gradient of the log-loss function. Pick some $1 \leq i \leq n$, and write the coordinates of the vector $\mathbf{x}_i \in \mathbb{R}^d$ as $(x_{i,1}, x_{i,2}, \ldots, x_{i,d})$. The term in the log-loss from $\mathbf{x}_i$ is

$$-\tilde{y}_i \log(f_\omega(\mathbf{x}_i)) - (1 - \tilde{y}_i) \log(1 - f_\omega(\mathbf{x}_i)).$$

If $\tilde{y}_i = 1$ then this is simply $-\log(f_\omega(\mathbf{x}_i))$. Recall that $\sigma(z)$ has a derivative satisfying $\frac{d\sigma}{dz} = \sigma(z) * (1 - \sigma(z))$. Using this and the fact that $\frac{d}{dw_j}(\mathbf{w} \cdot \mathbf{x}_i + b) = x_{i,j}$, we get

$$\frac{d}{dw_j}(-\log(f_\omega(\mathbf{x}_i))) = -\frac{x_{i,j} * f_\omega(\mathbf{x}_i) * (1 - f_\omega(\mathbf{x}_i))}{f_\omega(\mathbf{x}_i)} = -x_{i,j} * (1 - f_\omega(\mathbf{x}_i)).$$

The partial with respect to b is simply $-(1 - f_\omega(\mathbf{x}_i))$.

Gradient descent with logistic regression

On the other hand, if $\tilde{y}_i = 0$ then the term in the log-loss function from $\mathbf{x}_i$ is $-\log(1 - f_\omega(\mathbf{x}_i))$. Consequently, we compute

$$\frac{d}{dw_j}\left(-\log(1 - f_\omega(\mathbf{x}_i))\right) = \frac{x_{i,j} * f_\omega(\mathbf{x}_i) * (1 - f_\omega(\mathbf{x}_i))}{1 - f_\omega(\mathbf{x}_i)} = x_{i,j} * f_\omega(\mathbf{x}_i),$$

and the partial with respect to b is $f_\omega(\mathbf{x}_i)$.
Hence, we have, for each $1 \leq j \leq d$,

$$\frac{d}{dw_j}\mathcal{L}_S = \frac{1}{n}\sum_{i=1}^{n} -\tilde{y}_i x_{i,j} * (1 - f_\omega(\mathbf{x}_i)) + (1 - \tilde{y}_i) x_{i,j} f_\omega(\mathbf{x}_i),$$

and

$$\frac{d}{db}\mathcal{L}_S = \frac{1}{n}\sum_{i=1}^{n} -\tilde{y}_i * (1 - f_\omega(\mathbf{x}_i)) + (1 - \tilde{y}_i) f_\omega(\mathbf{x}_i).$$

Similarity to Perceptron algorithm updates

Consider the **per-example loss**: given one "example" $(\mathbf{x}_i, y_i) \in \mathcal{S}$, have the term $-\tilde{y}_i \log(f_\omega(\mathbf{x}_i)) - (1 - \tilde{y}_i) \log(1 - f_\omega(\mathbf{x}))$.
Its partial w.r.t. w_j is

$$-\tilde{y}_i x_{i,j} * (1 - f_\omega(\mathbf{x}_i)) + (1 - \tilde{y}_i) x_{i,j} f_\omega(\mathbf{x}_i).$$

If $\tilde{y}_i = 1$, but $f_\omega(\mathbf{x}_i)$ is close to o, then this is *almost* $-y_i x_{i,j}$. Were we to do an update with $\eta = 1$ then we would have $w_j^{(t)} \approx w_j^{(t-1)} + y_i x_{i,j}$. This is almost the Perceptron update (in the j^{th} coordinate).
Likewise, if $\tilde{y}_i = 0$, but $f_\omega(\mathbf{x}_i)$ is close to 1, then the partial is approximately $x_{i,j}$; so, using $\eta = 1$, we would get $w_j^{(t)} \approx w_j^{(t-1)} - x_{i,j} = w_j^{(t-1)} + y_i x_{i,j}$. Again, this is almost the Perceptron algorithm update.

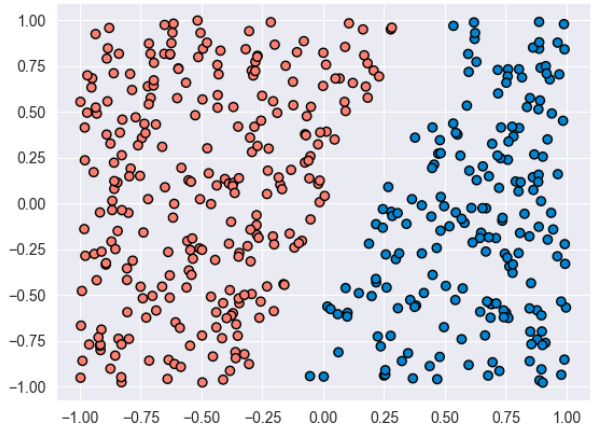
Example with Logistic model

Given ± 1-labeled sample data $\mathcal{S} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$, we found an expression for each partial derivative of $\mathcal{L}_\mathcal{S}$. In fact, if we call $w_{d+1} = b$ and $x_{i,d+1} = 1$ for every $1 \leq i \leq n$, then

$$\frac{d}{dw_j}\mathcal{L}_\mathcal{S} = \frac{1}{n}\sum_{i=1}^{n} -\tilde{y}_i x_{i,j}(1 - f_\omega(\mathbf{x}_i)) + (1 - \tilde{y}_i)x_{i,j} f_\omega(\mathbf{x}_i)$$

for every $1 \leq j \leq d + 1$.

Example: consider simulated sample data below, drawn uniformly from subset of $[-1, 1]^2$ that is at least a fixed distance from $H = \{(x_1, x_2) \in \mathbb{R}^2 \mid 2x_1 - \frac{2}{3}x_2 - \frac{1}{5} = 0\}$. Positively labeled points are in blue.



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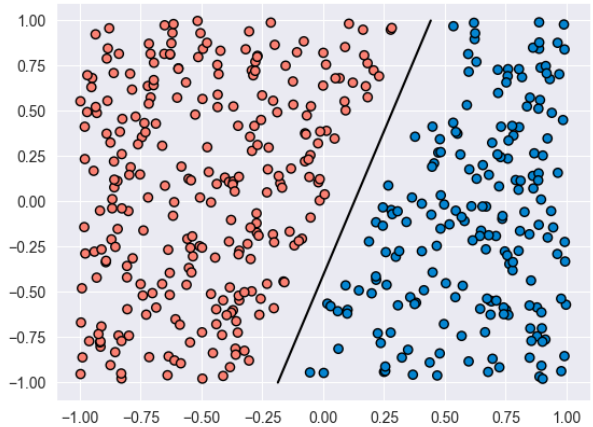
for every $1 \leq j \leq d + 1$.

Example (cont'd): Batch gradient descent, with learning rate 0.5, stopping with threshhold 0.0005, gives (approximately) parameters for:

$$\hat{H} = \{(x_1, x_2) \in \mathbb{R}^2 \mid 2.01x_1 - 0.63x_2 - 0.26 = 0\}.$$

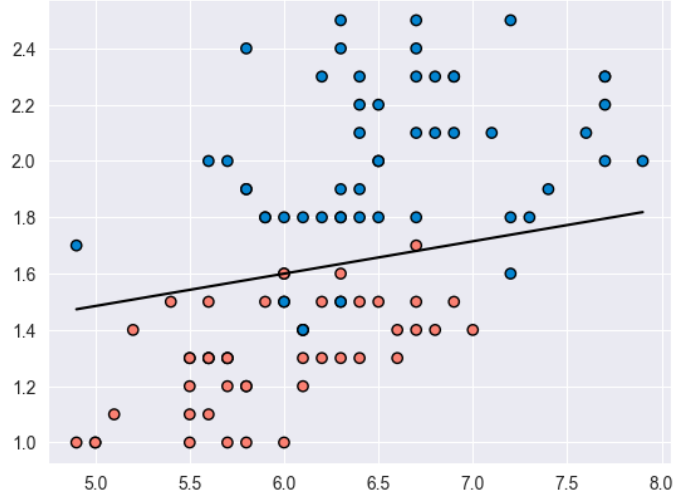


Logistic regression on the Iris data

Recall the Iris data set: 150 points, 50 from each of three species of Iris flower. Two of the species in the data set, Iris versicolor and Iris virginica, are not linearly separable.

We can use gradient descent on the logistic model to find a hyperplane that does *well* in classifying the versicolor versus virginica – it correctly classifies 97 out of the 100 points.

For visualization, I first show just the first and fourth coordinates, and the results for logistic model in 2D.



Logistic regression on the Iris data

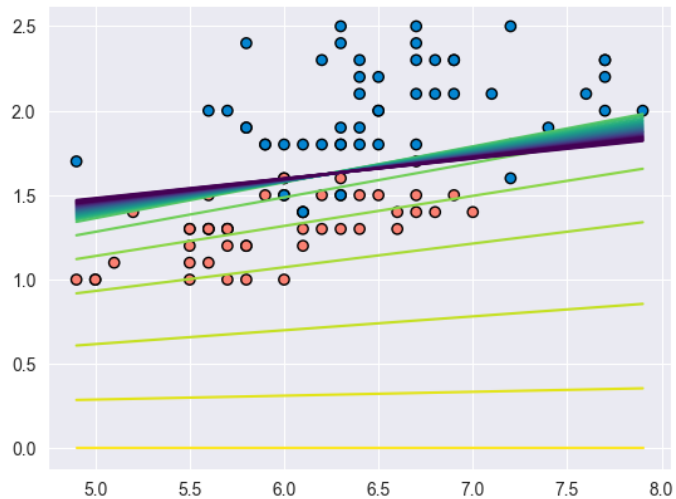
Pictured below are selected lines found during the batch gradient descent.

As before, yellow-to-purple is progression through the procedure.

Consecutive lines that are shown have 200 updates between them; ≈ 4000 updates in total.

The accuracy in this 2D projection is 92% (the final hyperplane correctly labeled 92 out of 100).[2]

The model on the points in $\mathbb{R}^4$ took less updates (just under 3000). It had 97% accuracy on the data.



[2] Recall, the model labels the point with $+1$ when $f_\omega(\mathbf{x}) \geq 0.5$.