Gradient descent on Logistic model

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Outline

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Setup

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

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

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What do we use for the empirical loss function?

- *Considering how model should work*: when correct y is $+1$ (and x is far from the hyperplane), good situation is when $f_\omega(\mathrm{x})$ very close to 1. Alternatively, if the correct y is -1, then we would like $f_\omega(\mathrm{x})$ to be close to 0.

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- *From considerations about model*: It helps to alter 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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We then use the log-loss function (a.k.a. binary cross-entropy). It is defined by

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

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Gradient descent with logistic regression

Let's compute the gradient of the log-loss. Pick $1 \leq i \leq n$, and write the coordinates (also called *features*) of the vector $\mathrm{x}_i \in \mathbb{R}^d$ as $(x_{i,1}, x_{i,2}, \ldots, x_{i,d})$.

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$$\frac{\partial}{\partial w_j}(-\log(f_\omega(\mathrm{x}_i))) = -\frac{x_{i,j} * f_\omega(\mathrm{x}_i) * (1 - f_\omega(\mathrm{x}_i))}{f_\omega(\mathrm{x}_i)} = -x_{i,j} * (1 - f_\omega(\mathrm{x}_i)).$$

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

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and the partial with respect to b is $f_\omega(\mathrm{x}_i)$.

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

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

and

$$\frac{\partial}{\partial b}\mathcal{L}_{\mathcal{S}} = \frac{1}{n}\sum_{i=1}^{n} -\tilde{y}_i * (1 - f_\omega(\mathrm{x}_i)) + (1 - \tilde{y}_i) f_\omega(\mathrm{x}_i).$$

Similarity to Perceptron algorithm updates

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

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If $\tilde{y}_i = 1$, but $f_\omega(\mathrm{x}_i)$ is close to 0, then this is *almost* $-x_{i,j} = -y_i x_{i,j}$. Were we to do an update with $\eta = 1$ then we would have $w_j^{(t)} \approx w_j^{(t-1)} + y_i x_{i,j}$. (The Perceptron update in the j^{th} coordinate.)

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Likewise, if $\tilde{y}_i = 0$, but $f_\omega(\mathrm{x}_i)$ is close to 1, then the partial is approximately $x_{i,j}$; so, using $\eta = 1$, we would get $w_j^{(t)} \approx w_j^{(t-1)} - x_{i,j} = w_j^{(t-1)} + y_i x_{i,j}$. (Like the Perceptron algorithm update again.)

Example with Logistic model

Given ± 1-labeled sample data $\mathcal{S} = \{(\mathrm{x}_i, y_i)\}_{i=1}^n$, 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

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

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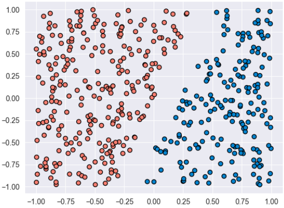
Example: consider simulated sample data below, drawn uniformly from a subset of $[-1,1]^2$, consisting of points at least a fixed distance from $H = \{(x_1, x_2) \in \mathbb{R}^2 \mid 2x_1 - \frac{2}{3}x_2 - \frac{1}{5} = 0\}$. Positively labeled points are in blue.



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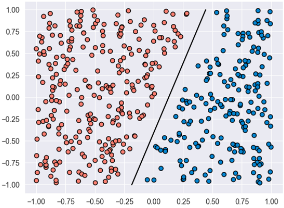
Example (cont'd): Batch gradient descent, with learning rate 0.5, stopping with threshhold 0.0005, gives (approximately) parameters for:

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



Logistic regression on the Iris data

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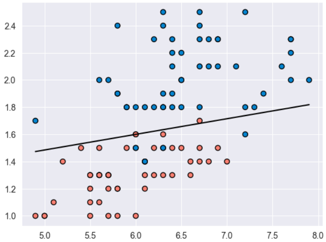
For visualization, I first show just the first and fourth coordinates, and the results for logistic model in 2D.



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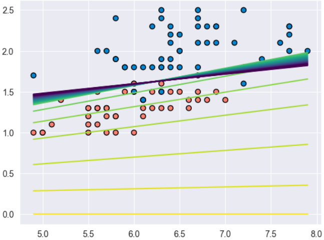
Pictured below are selected lines found during the batch gradient descent.



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

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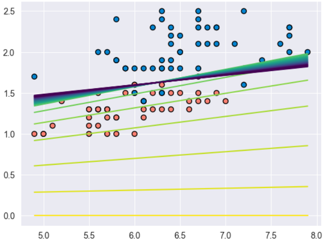
As before, yellow-to-purple is progression through the procedure.
Consecutive lines that are shown have 200 updates between them; ≈ 4000 updates in total.



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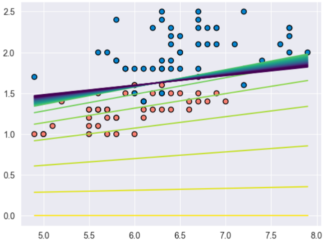

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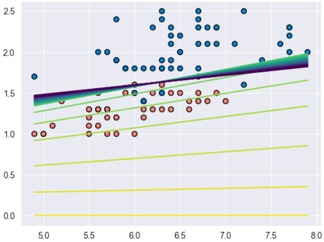
The model on the points in $\mathbb{R}^4$ took less updates (just under 3000). It had 97% accuracy on the data.



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