Logistic Regression and Gradient Descent

Pattern Recognition and Machine Learning

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Supervised learning setting



We are given a training set $\{X_i, Y_i\}_{i=1}^N$, with $X_i \in \mathbb{R}^m$ and $Y_i \in \{0, 1\}$ for each i = 1, ..., N.

- N is the number of training examples;
- each example $X_i = \{x_i^{(1)}, \dots, x_i^{(m)}\}$ is a vector of m features;
- each label Y_i is either 0 or 1.

Logistic regression



We need to learn a function that maps X to Y such that "it works well on the training set".

Logistic regression



We need to learn the parameters \mathbf{w} of a parametric function that maps X to Y such that "it works well on the training set".

Logistic regression



We need to learn the parameters w of a parametric function that maps X to Y such that some error is as low as possible on the training set.



The function for classification has the following form:

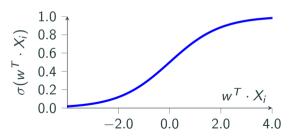
$$F(X_i, w) = \sigma(w^T \cdot X_i), \quad \text{where} \quad \sigma(x) = \frac{1}{1 + e^{-x}} = \frac{e^x}{1 + e^x}$$



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• $\sigma(x)$ is called **sigmoid function**;

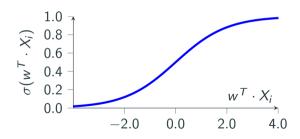




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- $\sigma(x)$ is called **sigmoid function**;
- w is a vector in R^m, and is called weight vector;

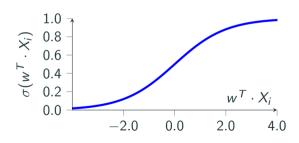




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- $\sigma(x)$ is called **sigmoid function**;
- w is a vector in R^m, and is called weight vector;
- w is initialized randomly, but will improve as training goes.



Binary crossentropy loss



During training, we want to minimize the following function:

$$\mathcal{L}(w) = -\frac{1}{N} \sum_{i=1}^{N} [Y_i \log(F(X_i, w)) + (1 - Y_i) \log(1 - F(X_i, w))]$$

Gradient Descent¹



Gradient descent is an iterative optimization algorithm for finding the minimum of a function. How? Take step proportional to the negative of the gradient of the function at the current point.

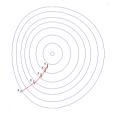


Figure 1: Gradient descent on a series of level sets

¹Credits for this slide: Andrea Palazzi https://github.com/ndrplz/deep_learning_lectures

Gradient Descent Update¹



If we consider a function $f(\theta)$, the gradient descent update can be expressed as:

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} f(\boldsymbol{\theta}) \tag{1}$$

for each parameter θ_i .

The size of the step is controlled by **learning rate** α .

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Visualizing Gradient Descent¹



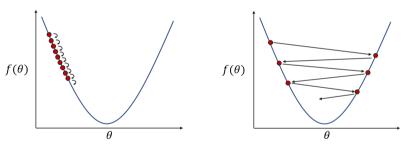
Gradient Descent for 1-d function $f(\theta)$.

¹Credits for this slide: Andrea Palazzi https://github.com/ndrplz/deep_learning_lectures

Learning Rate¹



Choosing the the right **learning rate** α is essential to correctly proceed towards the minimum. A step *too small* could lead to an extremely *slow* convergence. If the step is *too big* the optimizer could *overshoot* the minimum or even *diverge*.



Learning Rate too small

Learning Rate too big

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Simplify our loss



Back to our problem. We need to take the derivative of this function w.r.t. w:

$$\mathcal{L}(w) = -\frac{1}{N} \sum_{i=1}^{N} [Y_i \log(F(X_i, w)) + (1 - Y_i) \log(1 - F(X_i, w))]$$

$$= -\frac{1}{N} \sum_{i=1}^{N} \left[Y_i \log\left(\frac{e^{w^T \cdot X_i}}{1 + e^{w^T \cdot X_i}}\right) + (1 - Y_i) \log\left(\frac{1}{1 + e^{w^T \cdot X_i}}\right) \right]$$

$$= -\frac{1}{N} \sum_{i=1}^{N} \left[Y_i(w^T \cdot X_i) - Y_i \log\left(1 + e^{w^T \cdot X_i}\right) + (Y_i - 1) \log\left(1 + e^{w^T \cdot X_i}\right) \right]$$

$$= -\frac{1}{N} \sum_{i=1}^{N} \left[Y_i(w^T \cdot X_i) - \log\left(1 + e^{w^T \cdot X_i}\right) \right]$$

Derive the loss function



Back to our problem. We need to take the derivative of this function w.r.t. w:

$$\mathcal{L}(w) = -\frac{1}{N} \sum_{i=1}^{N} \left[Y_i(w^T \cdot X_i) - \log\left(1 + e^{w^T \cdot X_i}\right) \right]$$

$$\frac{\delta \mathcal{L}(w)}{\delta w_j} = -\frac{1}{N} \sum_{i=1}^{N} \left[Y_i x_i^{(j)} - \frac{e^{w^T \cdot X_i}}{1 + e^{w^T \cdot X_i}} x_i^{(j)} \right]$$

$$= -\frac{1}{N} \sum_{i=1}^{N} \left[Y_i - \frac{e^{w^T \cdot X_i}}{1 + e^{w^T \cdot X_i}} \right] x_i^{(j)}$$

$$= -\frac{1}{N} \sum_{i=1}^{N} \left[Y_i - F(X_i, w) \right] x_i^{(j)}$$

Final gradient and update



Back to our problem. We need to take the derivative of this function w.r.t. w:

$$\frac{\delta \mathcal{L}(w)}{\delta w} = \begin{bmatrix} \frac{\delta \mathcal{L}(w)}{\delta w_1} \\ \frac{\delta \mathcal{L}(w)}{\delta w_2} \\ \vdots \\ \frac{\delta \mathcal{L}(w)}{\delta w_m} \end{bmatrix} = \begin{bmatrix} -\frac{1}{N} \sum_{i=1}^{N} (Y_i - F(X_i, w)) x_i^{(1)} \\ -\frac{1}{N} \sum_{i=1}^{N} (Y_i - F(X_i, w)) x_i^{(2)} \\ \vdots \\ -\frac{1}{N} \sum_{i=1}^{N} (Y_i - F(X_i, w)) x_i^{(m)} \end{bmatrix} = -\frac{X^T \cdot (Y - F(X, w))}{N}$$

We will update the vector w accordingly:

$$w \leftarrow w - \alpha \frac{\delta \mathcal{L}(w)}{\delta w}$$

Wrap up: algorithm



Algorithm 1 pseudocode for training

- 1: $X, Y \leftarrow load_training_data()$
- 2: set learning rate α
- 3: initialize w randomly
- 4: for e = 1 to $number_of_training_steps$ do
- 5: compute the prediction according to the current weights F(X, w)
- 6: compute the loss function $\mathcal{L}(w)$
- 7: compute the derivative of the loss function w.r.t. weights $\frac{\delta \mathcal{L}(w)}{\delta w}$
- 8: update the weight vector $\mathbf{w} \leftarrow \mathbf{w} \alpha \frac{\delta \mathcal{L}(\mathbf{w})}{\delta \mathbf{w}}$
- 9: end for

Today's case study





- We want to predict if a character is alive or dead;
- (Some) of our features are:
 - male or female;
 - married or not;
 - number of deaths witnessed;
 - number of dead relatives;
 - ... and many more.