Logistic Regression and Gradient Descent

Pattern Recognition and Machine Learning

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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 $i = 1, \dots, N$.

- 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.

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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".

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

Logistic regression classification rule

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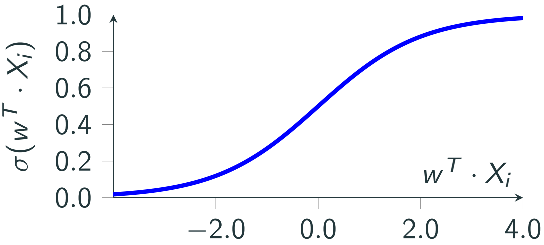
- $\sigma(x)$ is called **sigmoid function**;



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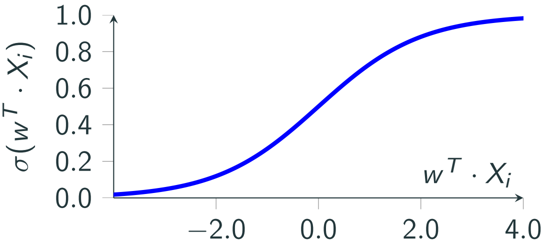
- $\sigma(x)$ is called **sigmoid function**;
- w is a vector in $\mathbb{R}^m$, and is called **weight vector**;



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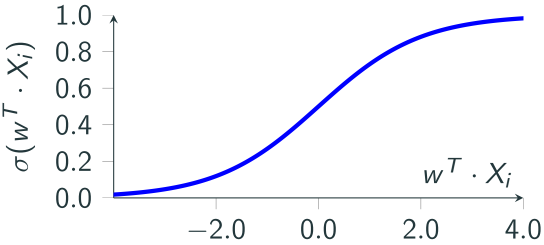
- $\sigma(x)$ is called **sigmoid function**;
- w is a vector in $\mathbb{R}^m$, and is called **weight vector**;
- w is initialized randomly, but will improve as training goes.



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 Descent[1]

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.

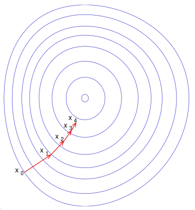


Figure 1: Gradient descent on a series of level sets

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

Gradient Descent Update[1]

If we consider a function $f(\boldsymbol{\theta})$, 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_j.

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

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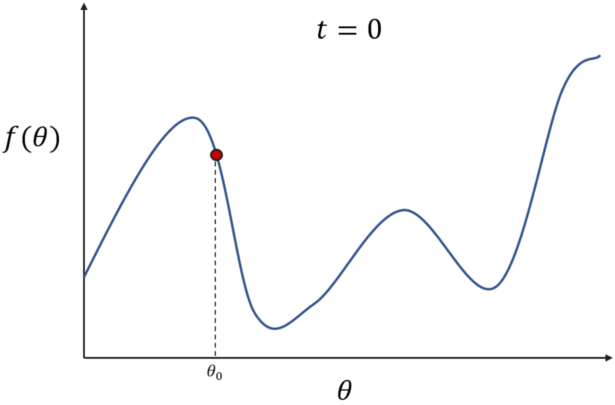
Visualizing Gradient Descent[1]

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



$$\frac{df}{d\theta} < 0$$

$$\theta_{new} = \theta_{old} - \alpha \frac{df}{d\theta}$$

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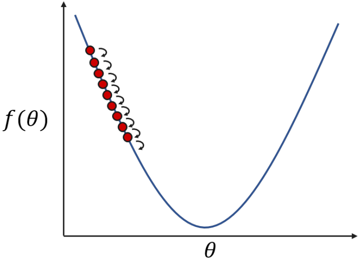
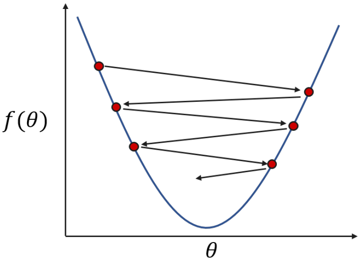
Learning Rate[1]

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

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

Derive the loss function

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

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

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

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:

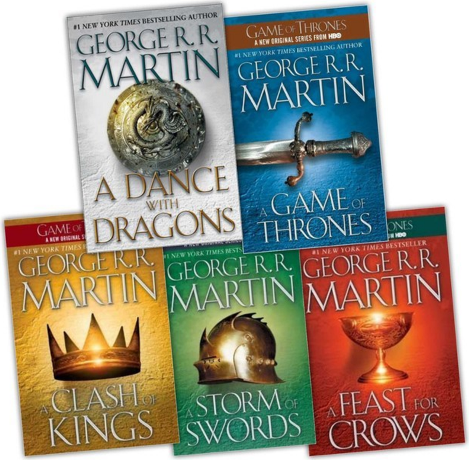
$$w \leftarrow w - \alpha \frac{\delta \mathcal{L}(w)}{\delta w}$$

Wrap up: algorithm

Algorithm 1 pseudocode for training

$X, Y \leftarrow \mathit{load\_training\_data}()$
set learning rate α
initialize w randomly
for $e = 1$ to $\mathit{number\_of\_training\_steps}$ **do**
    compute the prediction according to the current weights $F(X, w)$
    compute the loss function $\mathcal{L}(w)$
    compute the derivative of the loss function w.r.t. weights $\frac{\delta \mathcal{L}(w)}{\delta w}$
    update the weight vector $w \leftarrow w - \alpha \frac{\delta \mathcal{L}(w)}{\delta w}$
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.