50.039 – Theory and Practice of Deep Learning

Alex

Week 03: Classification by logistic regression

1 Logistic regression

Key takeaways:

- logistic regression is a classification algorithm
- output are scores in $[0, 1]$ which can be used as a probability for a label class
- logistic regression is linear mapping with the logistic sigmoid on top
- it is an exemplary model for a single neuron
- the cross entropy loss
- crossentropy loss can be derived by maximum likelihood on top of probabilities for a predicted class

Classification goal: Given an input space $\mathcal{X}$, the goal is to predict for every sample $x \in \mathcal{X}$ to which class it belongs. For 2 class classification, the goal is: to predict in the output space $\mathcal{Y} = \{-1, +1\}$ or $\mathcal{Y} = \{0, 1\}$.

Can be generalized to C classes, then $\mathcal{Y} = \{0, 1, 2, 3, \ldots, C-1\}$. We focus on 2 classes here. So much to the question of input and output spaces. Lets go over to the question of model.

How to use a linear model ? Linear model has unbounded values, we need values in $\{-1, +1\}$

$$f(x) = w \cdot x + b$$

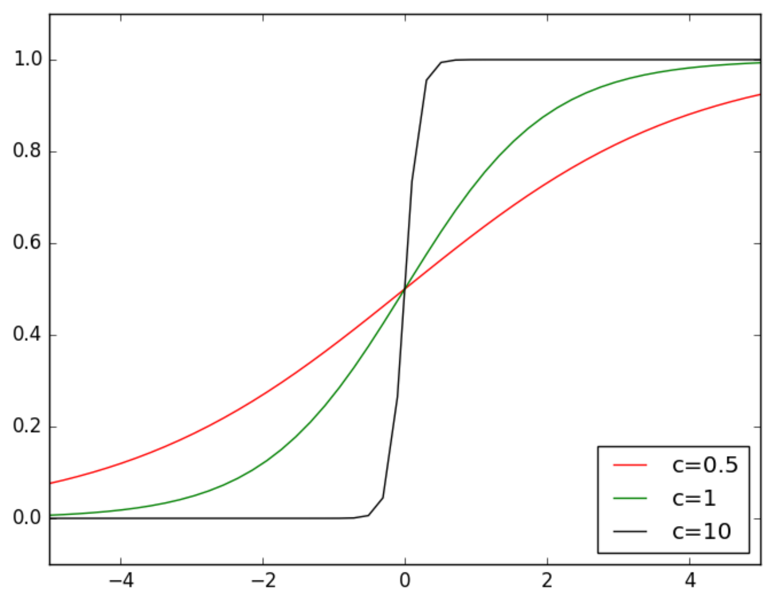
We had before the following idea for a classification mapping $f(x) = sign(g(x))$. So if $f(x) > 0$, then we predict the label $+1$, otherwise we predict -1 ($f(x) = 0$ is a tie case).

- The classification switches at the set of points x such that $f(x) = 0$.
- Intuition: for points x with $f(x) \approx 0$, we are not sure about the prediction.
  the larger $|f(x)|$, the more confident one should be to predict a class label.
- $f(x) >> 0$ large positive, we should be confident about the prediction $+1$
- $f(x) << 0$ large negative, we should be confident about the prediction -1

Can we encode this confidence as a probability?

- Lets map $(-\infty, +\infty)$ onto $(0, 1)$ such that 0 gets mapped onto 0.5.
- $+\infty$ should be mapped in the limit to 1
- $-\infty$ should be mapped in the limit to 0

$$\begin{aligned}
s(a) &= \frac{\exp(a)}{1+\exp(a)} = \frac{1}{\exp(-a)+1}\frac{\exp(a)}{\exp(a)} = \frac{1}{\exp(-a)+1} \\
\lim_{a\to-\infty} s(a) &= \frac{\exp(-\infty)}{1+\exp(-\infty)} = \frac{0}{1+0} = 0 \\
\lim_{a\to+\infty} s(a) &= \frac{1}{\exp(-\infty)+1} = \frac{1}{0+1} = 1
\end{aligned}$$



$s(ca) = \frac{\exp(ca)}{1+\exp(ca)} = \frac{1}{\exp(-ca)+1}$ for different values of c.

The convergence of $s(a \to -\infty) \to 0, s(a \to +\infty) \to 1$ shows that: $s(a)$ can be interpreted as a probability, expressing confidence for $P(Y = +1|X = x)$

Definition: Logistic sigmoid function

$$s(a) = \frac{\exp(a)}{1+\exp(a)} = \frac{1}{\exp(-a)+1} \frac{\exp(a)}{\exp(a)} = \frac{1}{\exp(-a)+1}$$

Definition: Logistic regression model

The logistic regression model consists of plugging in the output of the linear/affine mapping $f_{w,b}(x) = w \cdot x + b$ into the logistic sigmoid function $s(a)$.

$$h(x) = s(f_{w,b}(x)) = \frac{\exp(w \cdot x + b)}{1 + \exp(w \cdot x + b)} = \frac{1}{\exp(-w \cdot x - b) + 1}$$

Its output $h(x) \in (0, 1)$ can be interpreted for 2 classes as $P(Y = +1|X = x)$ – the confidence/belief expressed as a probability that sample x has classification label $y = +1$.

Above establishes the logistic regression model. What we need is loss function and a way to optimize it.[1]
We need to define a loss function for this model. Model outputs a probability, so one can use maximum likelihood principle.

1.1 The cross-entropy loss for 2-class classification

Definition: cross-entropy loss for 2-class classification

Suppose we have for every sample x_i a function $p(x_i) = (p_1(x_i), p_2(x_i))$ which provides a probability $p_1(x_i) = P(Y = +1|X = x_i)$ for the positive class and $p_2(x_i) = P(Y = -1|X = x_i)$ for the negative class.
Furthermore let $\bar{y}_i = (y_i + 1)/2$ be the mapping of the labels $y_i \in \{-1, +1\}$ onto $\{-1, +1\}$.
Then the crossentropy loss for a sample (x_i, y_i) is given as

$$\begin{aligned} L(p(x_i), y_i) &= \begin{cases} -\log(p_1(x_i)) & \text{if } y_i = +1 \\ -\log(p_2(x_i)) & \text{if } y_i = -1 \end{cases} \\ &= -\bar{y}_i \log(p_1(x_i)) - (1 - \bar{y}_i)\log(1 - p_1(x_i)) \end{aligned}$$

- Why these two definitions are equivalent?
- Does such a log-probability make sense as a loss?

Side note: the cross-entropy is actually defined between two probability distribution and related to the KL-divergence, which is a divergence measure between two probability distributions.

Therefore the loss averaged over a dataset is

$$\frac{1}{n}\sum_i -\bar{y}_i \log(p_1(x_i)) - (1 - \bar{y}_i)\log(1 - p_1(x_i))$$

plugged in with out model we have $p_1(x_i) = h(x_i) = \frac{1}{\exp(-w \cdot x - b) + 1}$. Therefore the optimization problem to be solved is (it is ajust an expression for finding the best parameters minimizing the loss)

$$(w^*, b^*) = \text{argmin}_{w,b} \frac{1}{n}\sum_i -\bar{y}_i \log(h(x_i)) - (1 - \bar{y}_i)\log(1 - h(x_i))$$

[1] Why $s(a)$ encodes a conditional probability $P(Y = +1|X = x)$ and not a joint probability $P(Y = +1, X = x)$? – bcs the latter would have $P(Y = +1, X = x) + P(Y = -1, X = x) =$????

1.2 Derivation of the cross entropy loss

The roadmap of steps for the derivation:

1. the maximum likelihood principle
2. $h(x) = P(Y = +1|X = x)$, that is the logistic output $h(x)$ encodes $P(Y = +1|X = x)$
3. from there can obtain as an expression for both labels:
   $P(Y = \bar{y}|X = x) = h(x)^{\bar{y}}(1 - h(x))^{1-\bar{y}}$ given that $\bar{y} \in \{0, +1\}$
   This holds because of
   $$h(x)^{\bar{y}}(1 - h(x))^{1-\bar{y}} = \begin{cases} h(x) = P(Y = +1|X = x) & \text{if } \bar{y} = 1 \\ 1 - h(x) = P(Y = -1|X = x) & \text{if } \bar{y} = 0 \end{cases}$$
4. conditional independence:
   $P(Y_1 = y_1, Y_2 = y_2, \dots, Y_n = y_n|x_1, x_2, ..., x_n) =$
   $P(Y_1 = y_1|x_1) \cdot P(Y_2 = y_2|x_2) \cdot \dots \cdot P(Y_n = y_n|x_n)$
5. plugging in above independence into the likelihood term $L(w) = P(Y_1 = y_1, Y_2 = y_2, \dots, Y_n = y_n|x_1, x_2, ..., x_n) = \prod_{i=1}^{n} P(Y_i = y_i|x_i)$
6. understanding the goal: want to maximize the probability of observing all labels y_i for given data points x_i, so maximize $L(w)$: $w^* = \text{argmax}_w L(w)$
7. applying neglog-transform: $w^* = \text{argmin} - log(L(w))$

Recap: maximum likelihood:

Suppose one has a dataset $D_n = (z_1, \dots, z_n)$ and wants to fit *the parameter* w of a probability model P. P takes $(z_1, \dots, z_n)$ as input and produces a probability $P(z_1, \dots, z_n|w) \in (0, 1)$ for observing the dataset $(z_1, \dots, z_n)$.

The maximum likelihood principle states: Given D_n, choose the parameter w such that the probability of drawing/observing the data under $P = P_w$ is maximized, that is:

$$w^* = \text{argmax}_w P(z_1, \dots, z_n|w)$$

SideNote: maximum a-posteriori, fully bayesian methods offer often better ways to fit models.

Derivation of the loss function:

How to apply this idea? We want to maximize the joint probability of observing all the labels y_i given all the data points x_i:

$$w^* = \text{argmax}_w P(Y_1 = y_1, Y_2 = y_2, \dots, Y_n = y_n | x_1, x_2, ..., x_n)$$

How to arrive at this ?We have

- a dataset $D_n = ((x_1, y_1), \dots, (x_n, y_n))$.
- $h(x) = P(Y = +1|X = x)$
- For likelihood we need an expression of type $P(Y = y|X = x)$. **From now on we will assume** $y_i \in \{0, 1\}$

$$h(x)^y(1 - h(x))^{1-y} = \begin{cases} h(x) = P(Y = +1|X = x) & \text{if } y = 1 \\ 1 - h(x) = P(Y = -1|X = x) & \text{if } y = 0 \end{cases}$$

so we have:

$$\begin{aligned} P(Y = y|X = x) &= P(Y = +1|X = x)^y \cdot P(Y = 0|X = x)^{1-y} \\ &= h(x)^y(1 - h(x))^{1-y} \quad \text{for } y \in \{0, 1\} \end{aligned}$$

We assume here a conditional likelihood, that is we fix our datapoints x_i, and optimize the parameter w such that the distribution over the labels y_i gets high probability. So we want to optimize:

$$P(Y_1 = y_1, Y_2 = y_2, \dots, Y_n = y_n | x_1, x_2, ..., x_n)$$

if we **assume that all samples are statistically independent**, that is $P((x_1, y_1), \dots, (x_n, y_n)) = P(x_1, y_1) \cdot P(x_2, y_2) \cdot \dots \cdot P(x_n, y_n)$, then we can get:

$$\begin{aligned} L(w) =& P(Y_1 = y_1, Y_2 = y_2, \dots, Y_n = y_n | x_1, x_2, ..., x_n) \\ =& \frac{P(Y_1 = y_1, Y_2 = y_2, \dots, Y_n = y_n, x_1, x_2, ..., x_n)}{P(x_1, x_2, ..., x_n)} \\ =& \frac{P(Y_1 = y_1, x_1)P(Y_2 = y_2, x_2) \cdot \dots \cdot P(Y_n = y_n, x_n)}{P(x_1, x_2, ..., x_n)} \\ =& \frac{P(Y_1 = y_1, x_1)P(Y_2 = y_2, x_2) \cdot \dots \cdot P(Y_n = y_n, x_n)}{P(x_1)P(x_2) \cdot \dots \cdot P(x_n)} \\ =& P(Y_1 = y_1|x_1) \cdot P(Y_2 = y_2|x_2) \cdot \dots \cdot P(Y_n = y_n|x_n) \\ =& h(x_1)^{y_1}(1 - h(x_1))^{1-y_1} \cdot h(x_2)^{y_2}(1 - h(x_2))^{1-y_2} \cdot \dots \cdot h(x_n)^{y_n}(1 - h(x_n))^{1-y_n} \\ =& \prod_{i=1}^{n} h(x_i)^{y_i}(1 - h(x_i))^{1-y_i} \end{aligned}$$

Result: applying maximum likelihood, to find the parameter w, such that the probability $P(Y_1 = y_1, Y_2 = y_2, \ldots, Y_n = y_n | x_1, x_2, ..., x_n)$ is maximized is the same as maximizing the term

$$L(w) = \prod_{i=1}^{n} h(x_i)^{y_i} (1 - h(x_i))^{1-y_i}$$

with respect to parameter w.

This is a product –difficult to optimize using gradients (product rule), instead we can maximize the logarithm of this term.

- Logarithms turns products into sums.

$$log(\prod_i a_i) = \sum_i log(a_i)$$

- Logarithms preserve points minizing or maximizing a function: If a point w is a maximizer of a $L(w)$, then it is also a maximizer of $\log L(w)$, because a logarithm is a strictly monotonically growing function . That is:

$$w^* = \text{argmax} L(w)$$
$$\text{so: } L(w^*) > L(w) \Leftrightarrow \log L(w^*) > \log L(w)$$

The final step: Maximizing a function f is same as minimizing -1 times this function f, so in the end: we can minimize the negative logarithm of above likelihood, in short: neg-log-likelihood. Thus our **loss function** will be the negative logarithm of the likelihood.
Goal:

$$\begin{aligned}
w^* &= \text{argmin}_w - \log\left(L(w)\right) \\
&= \text{argmin}_w - \log\left(\prod_{i=1}^{n} h(x_i)^{y_i}(1-h(x_i))^{1-y_i}\right) \\
&= \text{argmin}_w (-1) \cdot \sum_{i=1}^{n} \log\left(h(x_i)^{y_i}(1-h(x_i))^{1-y_i}\right) \\
&= \text{argmin}_w (-1) \cdot \sum_{i=1}^{n} \log\left(h(x_i)^{y_i}\right) + \log\left((1-h(x_i))^{1-y_i}\right) \\
&= \text{argmin}_w (-1) \cdot \sum_{i=1}^{n} y_i \log\left(h(x_i)\right) + (1-y_i)\log\left(1-h(x_i)\right)
\end{aligned}$$

This is exactly the sum of cross-entropy losses over our data. We only need to add an averaging term $\frac{1}{n}$ to be done. Note that this derivation shows another insight: the sum of losses over data samples is motivated by a conditional independence assumption.

1.3 Using the gradient of the loss

The gradient of the loss function is simple. We will use

$$\frac{\partial log(s(a))}{\partial a} = 1 - s(a)$$
$$\frac{\partial log(1 - s(a))}{\partial a} = -s(a)$$

and we know $h(x) = s(w \cdot x)$

The gradient with respect to w will be:

$$\nabla_w L = \nabla_w \left((-1) \cdot \sum_{i=1}^{n} y_i \log(s(w \cdot x_i)) + (1 - y_i) \log(1 - s(w \cdot x_i)) \right)$$
$$\nabla_w L = \sum_{i=1}^{n} x_i (s(w \cdot x_i) - y_i) = \sum_{i=1}^{n} x_i (h(x_i) - y_i)$$

Observation 1:

The gradient has a nice interpretation: it is the sum of data points x_i weighted by differences between the predicted value $h(x_i) = s(w \cdot x_i)$ and the true value $y_i \in \{0, 1\}$.

Observation 2:
There is another effect that is important in the context of neural networks: the gradient does not suffer from saturation of the logistic sigmoid. To understand this, consider the derivative of $s(a)$.

$$s'(a) = \frac{e^{-a}}{(1 + e^{-a})^2} \leq \begin{cases} e^{-a} & a \geq 0 \\ \frac{1}{(1+e^{-a})^2} & a < 0 \end{cases}$$

Observation 3:
If both classes in the data can be perfectly separated by a linear mapping, then optimization will try to make the weights w to go to infinity. This is a source of instability during optimization time. Why?

$\log h(x_i) = 0$ if $h(x_i) = 1$. So trying to make the loss to zero for $y_i = 1$ means that one tries to make $h(x_i) = 1$

$h(x) = s(wx)$ converges to $0, +1$ for very large values of wx. so making $P(Y = y|X = x)$ to 1 for all data points – requires to push $f(x) = wx$ to very large values for all data points. This can be done by upscaling w to huge values such as $w \mapsto 10^{10}w$.

Observation 4:
What is missing here? A bias term.

$$f_{w,b}(x) = s(wx + b)$$

Can be approximately included by augmenting all your datapoints by adding an extra dimension which is constant :

$$x_i = (x_i^{(1)}, \ldots, x_i^{(d)}) \mapsto \hat{x_i} = (x_i^{(1)}, \ldots, x_i^{(d)}, 1)$$
$$(w, w^{(d+1)}) \cdot \hat{x_i} = w \cdot x_i + w^{(d+1)} \cdot 1 \sim wx + b$$

The only caveat here: any regularization term on w now has effect on the bias term, too. Zero-meaning the features makes this effect less harmful.

1.4 Solving the optimization problem

Apply the gradient descent algorithm from last lecture! Gradient is given.

Side question: why we did not exercise this for the case of linear model and hinge-loss?
Demo:

One can observe oscillations for too high learning rates, even for a simple 2 by 2 point dataset.

Can use again polynomial features.