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IN3050 Mathgroup, Derivatives

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Loss Functions
Motivation

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Understanding what the function with are optimizing actually means, and why we are chosing it over other functions, is an important part to understand what we can expect of the model when it is trained.

We will look at *Mean Square Error (MSE)*, *binary cross entropy loss* and *multi-class cross entropy loss*. This also includes looking at the *sigmoid-* and *softmax-function* to make sense of the loss.

Loss Functions 2

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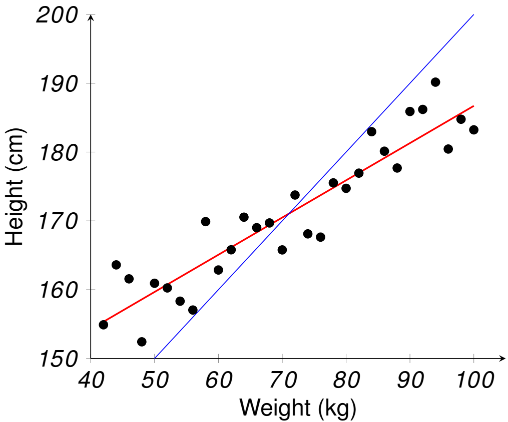
- At any point during or after training, we can meassure the models performance by putting the *outputs* (predicted values) and the true labels into a loss function.
- The higher the loss function, the worse our model fits adapts to our data, so we want to minimize the loss-function.
- Interpreting the loss from *training* and *testing* can be very different, but for now, let us focus on the function itself.

Arriving at our first loss function

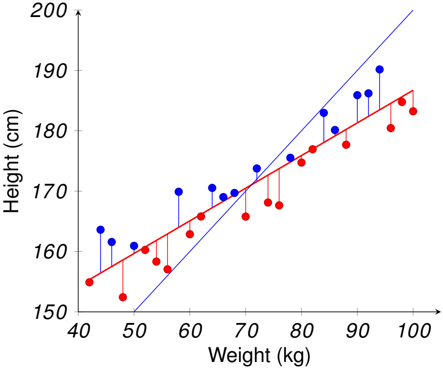
We want to determine how good a linear model fits our data.



Which line fits the data the best, and how do we measure it?

Arriving at our first loss function2

We can sum the distance from the points onto the line.



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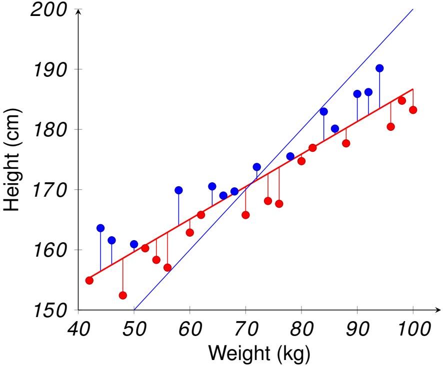

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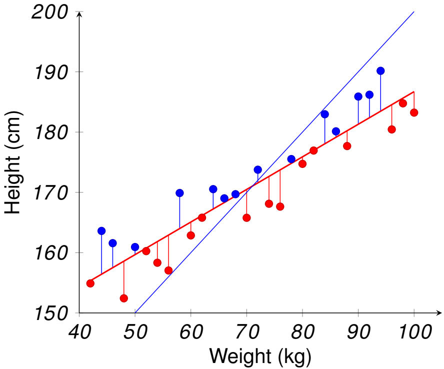

One important point is that we do not want *negative* and *positive* values to cancel each other.
We can therefore *square* the distance, to make everything positive. We then take the mean over all the errors (residuals).

Mean Squared Error

Definition and Breakdown

One of the most widely used loss functions is the *Mean Squared Error* (MSE).
It is defined as

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(t_i - \hat{y}_i)^2$$

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- One term of the sum becomes $(t_i - \hat{y}_i)^2$. This is the difference between the true label t_i and the predicted value $\hat{y}$, squared. We squared it to make it positive (so positive and negative values do not cancel each other).
- We then sum over the N amount of inputs, $\sum_{i=1}^{N}(t_i - \hat{y}_i)^2 = (t_1 - \hat{y}_1)^2 + (t_2 - \hat{y}_2)^2 + \ldots + (t_N - \hat{y}_N)^2$

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- Lastly, we divide by N, to average over the amount of inputs. If we did not do this, then smaller amount of training data would give smaller error.

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- It is easy to differentiate, which is very important when optimizing it.
- Some models can be optimized *analytically*, without the use of iterativly updating the weights.

Classification

What about classification? We can use MSE, but it does not make so much intuitively sense, and performs poorly mathematically.

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- We can interpret $\hat{y}_i = 0.8$ as the model guessing that observation $\mathbf{x}_i$ has *probability* 0.8 to be 1, and probability 0.2 to be 0.

Sigmoid function

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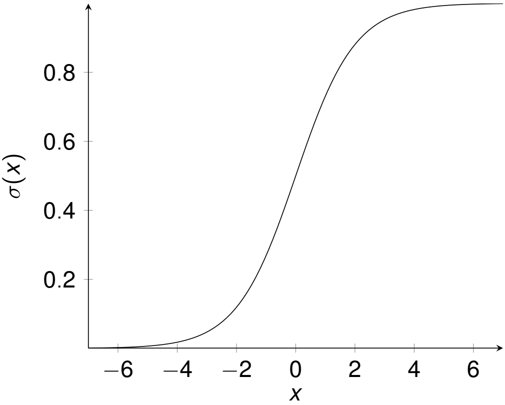
It looks like this:



Sigmoid function 2

We can now put the values we get from our model, say h, into the sigmoid function, to convert it to probabilities.

This is what we do with *logistic regression*. We have linear weights, as with linear regression: $h = \beta_0 + \beta_1 x_1 + \ldots + \beta_m x_m$, and then get our probability with $\hat{y} = \sigma(h)$.

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Note that the sigmoid function can be used with other models as well, for example some kinds of neural networks.

Binary Cross Entropy Loss

Let us now slowly get to the loss function. Let us first look at when the true label is 1, $t_i = 1$. We want to have a low loss for when $\hat{y}_i$ is close to 1, and a high loss when it is close to 0.

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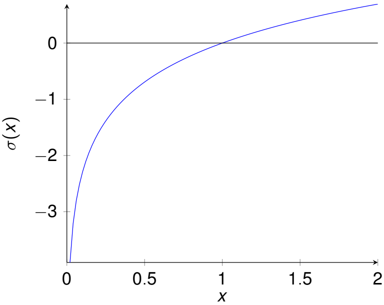

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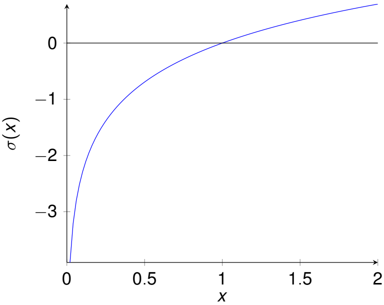

Note that we will only be using x-values between 0 and 1. We get that $\log(x)$ is close to 0 when x is close to 1, and $\log(x)$ goes to $-\inf$ when x goes to 0.

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Repeat: We get that $\log(x)$ is close to 0 when x is close to 1, and $\log(x)$ goes to $-\inf$ when x goes to 0.

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This is almost all the intuition behind the loss function, There is a couple of ways to write this in one line.

Binary Cross Entropy Loss 2

The complete formula can be written ass

$$L(\hat{\mathbf{y}}, \mathbf{t}) = -\frac{1}{N}\sum_{i=1}^{N}(t_i \log(\hat{y}_i) + (1 - t_i)\log(1 - \hat{y}_i))$$

- Notice that only one of the term is non-zero! Since every t_i is either 0 or 1, either t_i or $(1 - t_i)$ will be 0, and cancel out the term.

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- We then sum over all the predictions and true labels and divide by N, the amount of observations. Notice that we have also moved the minus-sign outside the sum.
- The terms can be equivalently written as $\log(\hat{y}_i)^{t_i} \cdot \log(1 - \hat{y}_i)^{1-t_i}$ (look at what happens when t_i equals 0 and 1).

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- This is often call just ”Cross Entropy Loss” or ”Log Loss”. The name comes from *information theory*.
- Two reason that it works well in practice is that it 1) makes a convex function for logistic regression and 2) the derivative is very easy to compute.

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In the binary situation, we made $\hat{y}_i$ be between 0 and 1. **Question:** What should we do we the C-dimensional vector $\hat{\mathbf{y}}_i$?
Answer: We can let the inputs in $\hat{\mathbf{y}}_\mathbf{i}$ *sum* to 1. One way of doing this is with the *softmax*-function

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- The denominator is the sum of the numerators, making the sum of the $s(h_i)$'s sum to 1, $\sum_{i=1}^{C} s(h_i) = 1$.
- Due to the positive and summming to 1 properties, we can interpret the outputs of the softmax for class i as the *probability of the input to belong in class i*.

Multiclass Cross Entropy Loss

We are now ready to define Multiclass Cross Entropy Loss, which may be the most used loss function for multiclass classification. For one input, is defined as:

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- For the input k that represent the true class (assume $t_k = 1$), the loss will be determined by $-\log \hat{y}_k$. This works, since if $\hat{y}_k$ is close to 1, we get close to 0 loss, and if it is close to 0, the loss goes to infinity.

Multiclass Cross Entropy Loss 2

$$-\sum_{j=1}^{C} t_j \log(s(h_j)) = -\sum_{i=j}^{C} t_j \log(\hat{y}_j)$$

It is important that we use something like the softmax function to make the outputs sum to 1.

Question: What happens if we would not use the softmax function, but just use for example a sigmoid activation function in each output node?

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Answer: We might get every node to output 1 and get 0 loss for every input.

Multiclass Cross Entropy Loss 3

Note that this was only for *one* ovservation, so to get the full loss we have to sum over all of the observations.

$$-\frac{1}{N}\sum_{i=1}^{N}\sum_{j=1}^{C} t_{i,j}\log(\hat{y}_{i,j})$$

where $t_{i,j}$ marks the j'th input to the label of the i'th observation.

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- We can also use other loss functions.
- One reason this works well is that the derivative is very quick to compute.
- The binary cross entropy loss can also be written at this form, but then we would have to one-hot-encode the labels and outputs, instead of just using 0 and 1.

Summary

We have (hopefully) looked at:

- What loss functions are and represent.
- Mean Squared Error for regression.
- Sigmoid function and binary cross entropy loss.
- Softmax function and multiclass cross entropy loss.