Multi-class classification with Softmax function

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Outline

- Repeat logistic function
- Softmax function
- Derivative of the softmax function

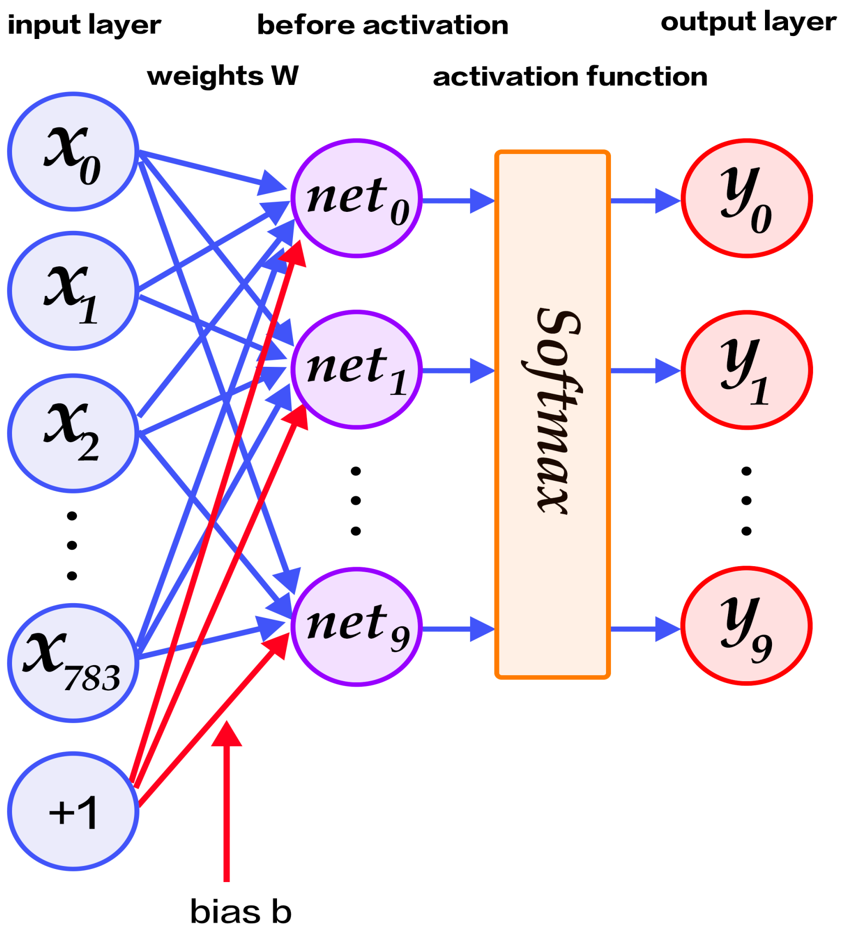
Logistic function

$$\boldsymbol{\sigma(z) = \frac{1}{1 + e^{-z}}}$$

$$h_\theta(x) = P(y = 1|x;\theta) \quad = \quad \frac{\mathbf{1}}{\mathbf{1} + \boldsymbol{e^{-\theta^T x}}}$$

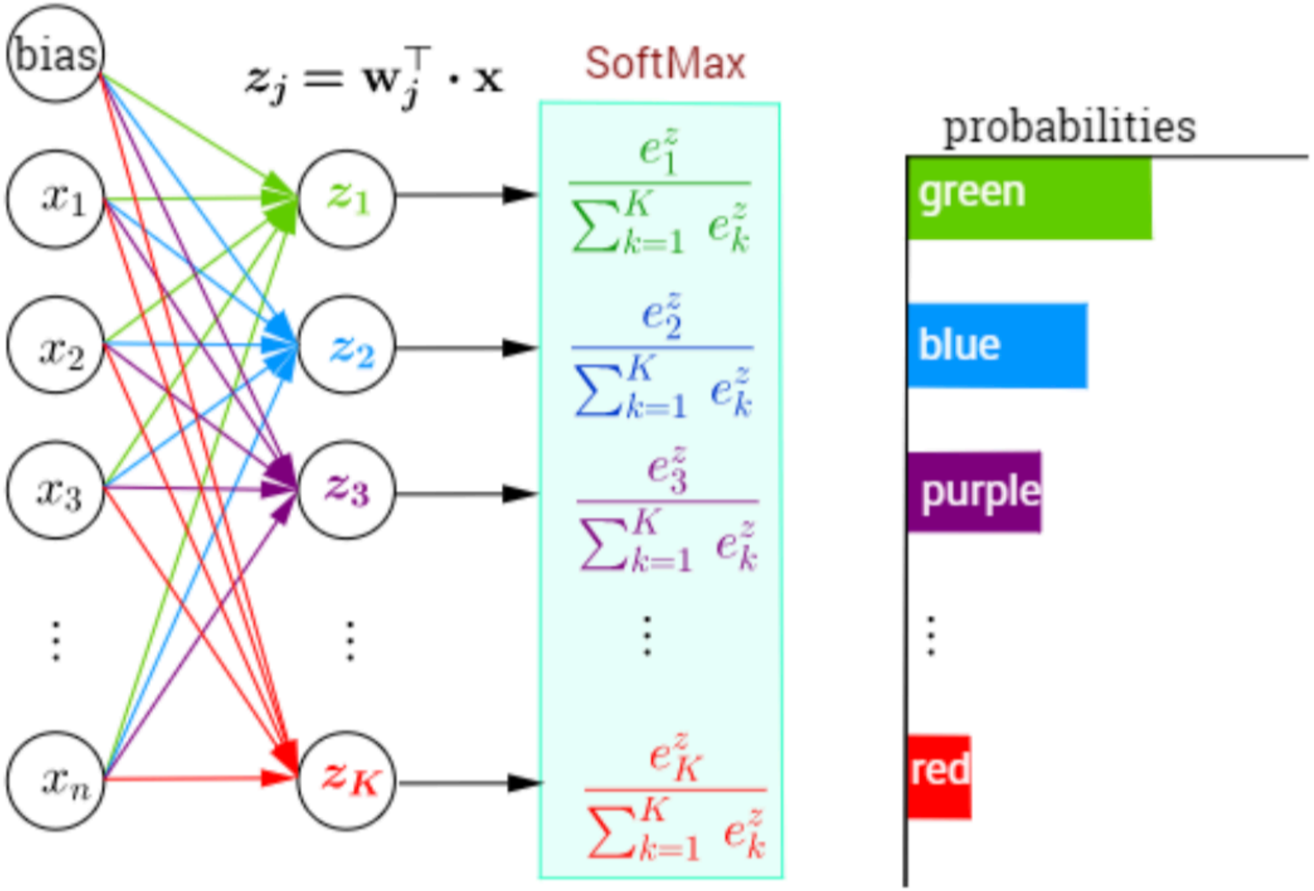
$$P(y = 0|x;\theta) = 1 - P(y = 1|x;\theta) \quad = \quad \frac{\boldsymbol{e^{-\theta^T x}}}{\mathbf{1} + \boldsymbol{e^{-\theta^T x}}}$$

NN with Softmax layer



NN with Softmax layer

$$\mathbf{z} = \begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ \vdots \\ z_K \end{bmatrix} = \begin{bmatrix} \mathbf{w}_1^\top \\ \mathbf{w}_2^\top \\ \mathbf{w}_3^\top \\ \vdots \\ \mathbf{w}_K^\top \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix}$$



Softmax function

The denominator $\sum_{d=1}^{C} e^{z_d}$ acts as a regularizer to make sure that $\sum_{c=1}^{C} y_c = 1$. As the output layer of a neural network, the softmax function can be represented graphically as a layer with C neurons.

We can write the probabilities that the class is $t = c$ for $c = 1 \dots C$ given input $\mathbf{z}$ as:

$$\begin{bmatrix} P(t=1|\mathbf{z}) \\ \vdots \\ P(t=C|\mathbf{z}) \end{bmatrix} = \begin{bmatrix} \varsigma(\mathbf{z})_1 \\ \vdots \\ \varsigma(\mathbf{z})_C \end{bmatrix} = \frac{1}{\sum_{d=1}^{C} e^{z_d}} \begin{bmatrix} e^{z_1} \\ \vdots \\ e^{z_C} \end{bmatrix}$$

Where $P(t = c|\mathbf{z})$ is thus the probability that that the class is c given the input $\mathbf{z}$.

$$y_c = \varsigma(\mathbf{z})_c = \frac{e^{z_c}}{\sum_{d=1}^{C} e^{z_d}} \quad \text{for } c = 1 \cdots C$$

Likelihood

The likelihood $\mathcal{L}(\theta|\mathbf{t},\mathbf{z})$ can be rewritten as the joint probability of generating $\mathbf{t}$ and $\mathbf{z}$ given the parameters θ: $P(\mathbf{t},\mathbf{z}|\theta)$. Which can be written as a conditional distribution:

$$P(\mathbf{t},\mathbf{z}|\theta) = P(\mathbf{t}|\mathbf{z},\theta)P(\mathbf{z}|\theta)$$

Since we are not interested in the probability of $\mathbf{z}$ we can reduce this to: $\mathcal{L}(\theta|\mathbf{t},\mathbf{z}) = P(\mathbf{t}|\mathbf{z},\theta)$. Which can be written as $P(\mathbf{t}|\mathbf{z})$ for fixed θ. Since each t_c is dependent on the full $\mathbf{z}$, and only 1 class can be activated in the $\mathbf{t}$ we can write

$$P(\mathbf{t}|\mathbf{z}) = \prod_{i=c}^{C} P(t_c|\mathbf{z})^{t_c} = \prod_{c=1}^{C} \varsigma(\mathbf{z})_c^{t_c} = \prod_{c=1}^{C} y_c^{t_c}$$

Likelihood

$$P(\mathbf{t}|\mathbf{z}) = \prod_{i=c}^{C} P(t_c|\mathbf{z})^{t_c} = \prod_{c=1}^{C} \varsigma(\mathbf{z})_c^{t_c} = \prod_{c=1}^{C} y_c^{t_c}$$

As was noted during the derivation of the loss function of the logistic function, maximizing this likelihood can also be done by minimizing the negative log-likelihood:

$$-\log \mathcal{L}(\theta|\mathbf{t},\mathbf{z}) = \xi(\mathbf{t},\mathbf{z}) = -\log \prod_{c=1}^{C} y_c^{t_c} = \sum_{c=1}^{C} t_c \cdot \log(y_c)$$

Cross-entropy loss function

$$H(p,q) = -\sum_{\forall x} p(x)\log(q(x))$$

$$H(p,q) \;=\; -\sum_i p_i \log q_i$$

The cross-entropy error function over a batch of multiple samples of size n can be calculated as:

$$\xi(T,Y) = \sum_{i=1}^{n} \xi(\mathbf{t}_i, \mathbf{y}_i) = -\sum_{i=1}^{n}\sum_{c=1}^{C} t_{ic} \cdot \log(y_{ic})$$

Where t_{ic} is 1 if and only if sample i belongs to class c, and y_{ic} is the output probability that sample i belongs to class c.

Derivative of the softmax function

To use the softmax function in neural networks, we need to compute its derivative. If we define $\Sigma_C = \sum_{d=1}^{C} e^{z_d} \text{ for } c = 1 \cdots C$ so that $y_c = e^{z_c}/\Sigma_C$, then this derivative $\partial y_i / \partial z_j$ of the output $\mathbf{y}$ of the softmax function with respect to its input $\mathbf{z}$ can be calculated as:

$$\text{if } i = j : \frac{\partial y_i}{\partial z_i} = \frac{\partial \frac{e^{z_i}}{\Sigma_C}}{\partial z_i} = \frac{e^{z_i}\Sigma_C - e^{z_i}e^{z_i}}{\Sigma_C^2} = \frac{e^{z_i}}{\Sigma_C}\frac{\Sigma_C - e^{z_i}}{\Sigma_C} = \frac{e^{z_i}}{\Sigma_C}(1 - \frac{e^{z_i}}{\Sigma_C}) = y_i(1 - y_i)$$

$$\text{if } i \neq j : \frac{\partial y_i}{\partial z_j} = \frac{\partial \frac{e^{z_i}}{\Sigma_C}}{\partial z_j} = \frac{0 - e^{z_i}e^{z_j}}{\Sigma_C^2} = -\frac{e^{z_i}}{\Sigma_C}\frac{e^{z_j}}{\Sigma_C} = -y_i y_j$$

Note that if $i = j$ this derivative is similar to the derivative of the logistic function.

Derivative of the cross-entropy loss function for the softmax function

$$\xi(T,Y) = \sum_{i=1}^{n} \xi(\mathbf{t}_i, \mathbf{y}_i) = -\sum_{i=1}^{n}\sum_{c=1}^{C} t_{ic} \cdot \log(y_{ic})$$

$$\frac{\partial \xi}{\partial \theta_j} = \frac{\partial \xi}{\partial y_c} \cdot \frac{\partial y_c}{\partial z_c} \cdot \frac{\partial z_c}{\partial \theta_j}$$

$$y_c = \varsigma(\mathbf{z})_c = \frac{e^{z_c}}{\sum_{d=1}^{C} e^{z_d}} \quad \text{for } c = 1 \cdots C$$

Derivative of the cross-entropy loss function for the softmax function

$$\xi(T,Y)=\sum_{i=1}^{n}\xi(\mathbf{t}_i,\mathbf{y}_i)=-\sum_{i=1}^{n}\sum_{c=1}^{C}t_{ic}\cdot\log(y_{ic})$$

$$\frac{\partial \log(y_c)}{\partial y_c}=\frac{1}{y_c}$$

$$(\ln x)'=\frac{1}{x}$$

$$\frac{\partial\xi}{\partial\theta_j}=\frac{\partial\xi}{\partial y_c}\cdot\frac{\partial y_c}{\partial z_c}\cdot\frac{\partial z_c}{\partial\theta_j}$$

$$y_c=\varsigma(\mathbf{z})_c=\frac{e^{z_c}}{\sum_{d=1}^{C}e^{z_d}}\quad\text{for } c=1\cdots C$$

$$\text{if } i=j:\frac{\partial y_i}{\partial z_i}=\frac{\partial\frac{e^{z_i}}{\Sigma_C}}{\partial z_i}=\frac{e^{z_i}\Sigma_C-e^{z_i}e^{z_i}}{\Sigma_C^2}=\frac{e^{z_i}}{\Sigma_C}\frac{\Sigma_C-e^{z_i}}{\Sigma_C}=\frac{e^{z_i}}{\Sigma_C}(1-\frac{e^{z_i}}{\Sigma_C})=y_i(1-y_i)$$

$$\text{if } i\neq j:\frac{\partial y_i}{\partial z_j}=\frac{\partial\frac{e^{z_i}}{\Sigma_C}}{\partial z_j}=\frac{0-e^{z_i}e^{z_j}}{\Sigma_C^2}=-\frac{e^{z_i}}{\Sigma_C}\frac{e^{z_j}}{\Sigma_C}=-y_iy_j$$

$$\left(\frac{u}{v}\right)'=\frac{u'v-uv'}{v^2}$$

Derivative of the cross-entropy loss function for the softmax function

$$\frac{\partial \xi}{\partial z_i} = ?$$

Derivative of the cross-entropy loss function for the softmax function

The derivative $\partial\xi/\partial z_i$ of the loss function with respect to the softmax input z_i can be calculated as:

$$
\begin{aligned}
\frac{\partial \xi}{\partial z_i} &= -\sum_{j=1}^{C} \frac{\partial t_j \log(y_j)}{\partial z_i} = -\sum_{j=1}^{C} t_j \frac{\partial \log(y_j)}{\partial z_i} = -\sum_{j=1}^{C} t_j \frac{1}{y_j} \frac{\partial y_j}{\partial z_i} \\
&= -\frac{t_i}{y_i} \frac{\partial y_i}{\partial z_i} - \sum_{j \neq i}^{C} \frac{t_j}{y_j} \frac{\partial y_j}{\partial z_i} = -\frac{t_i}{y_i} y_i (1 - y_i) - \sum_{j \neq i}^{C} \frac{t_j}{y_j} (-y_j y_i) \\
&= -t_i + t_i y_i + \sum_{j \neq i}^{C} t_j y_i = -t_i + \sum_{j=1}^{C} t_j y_i = -t_i + y_i \sum_{j=1}^{C} t_j \\
&= y_i - t_i
\end{aligned}
$$

Gradient Descent?

$$J(\theta) = -\frac{1}{m}[\sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1 - y^{(i)}) \log (1 - h_\theta(x^{(i)}))]$$

Want $\min_\theta J(\theta)$:

Repeat $\{$

$$\theta_j := \theta_j - \alpha \sum_{i=1}^{m} (h_\theta(x^{(i)}) - y^{(i)}) x_j^{(i)}$$

(simultaneously update all θ_j)

$\}$

Example of Softmax and classification

- https://medium.com/@awjuliani/simple-softmax-in-python-tutorial-d6b4c4ed5c16
- https://www.kaggle.com/saksham219/softmax-regression-for-iris-classification
- https://scikit-learn.org/stable/auto_examples/linear_model/plot_iris_logistic.html