Multiclass Logistic Regression, Multilayer Perceptron

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October 24, 2023

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Today's Lecture Objectives

- Implement **muticlass classification** with softmax.
- Reason about linear regression, logistic regression and softmax classification in a **single probablistic framework**: with different target distributions, activation functions and training using maximum likelihood estimate.
- Explain **multi-layer perceptron** as a further generalization of linear models.

Logistic Regression

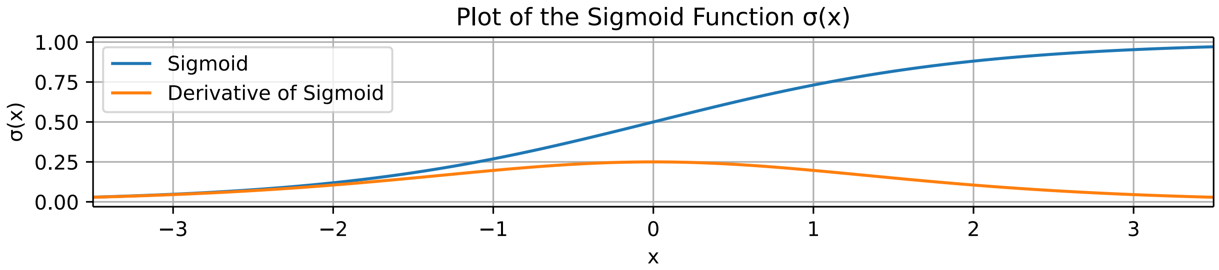
An extension of perceptron, which models the conditional probabilities of $p(C_0|\boldsymbol{x})$ and of $p(C_1|\boldsymbol{x})$. (It can in fact handle also more than two classes, which we will see shortly.)

Logistic regression employs the following parametrization of the conditional class probabilities:

$$p(C_1|\boldsymbol{x}) = \sigma(\boldsymbol{x}^T\boldsymbol{w} + b)$$
$$p(C_0|\boldsymbol{x}) = 1 - p(C_1|\boldsymbol{x}),$$

where σ is the **sigmoid function**

$$\sigma(x) = \frac{1}{1+e^{-x}}.$$



It can be trained using the SGD algorithm.

We denote the output of the "linear part" of the logistic regression as $\bar{y}(\boldsymbol{x}; \boldsymbol{w}) = \boldsymbol{x}^T \boldsymbol{w}$ and the overall prediction as $y(\boldsymbol{x}; \boldsymbol{w}) = \sigma(\bar{y}(\boldsymbol{x}; \boldsymbol{w})) = \sigma(\boldsymbol{x}^T \boldsymbol{w})$.

The logistic regression output $y(\boldsymbol{x}; \boldsymbol{w})$ models the probability of class C_1, $p(C_1|\boldsymbol{x})$.

To give some meaning to the output of the linear part $\bar{y}(\boldsymbol{x}; \boldsymbol{w})$, starting with

$$p(C_1|\boldsymbol{x}) = \sigma(\bar{y}(\boldsymbol{x}; \boldsymbol{w})) = \frac{1}{1 + e^{-\bar{y}(\boldsymbol{x}; \boldsymbol{w})}},$$

we arrive at

$$\bar{y}(\boldsymbol{x}; \boldsymbol{w}) = \log\left(\frac{p(C_1|\boldsymbol{x})}{1 - p(C_1|\boldsymbol{x})}\right) = \log\left(\frac{p(C_1|\boldsymbol{x})}{p(C_0|\boldsymbol{x})}\right),$$

which is called a **logit** and it is a logarithm of odds of the probabilities of the two classes.

Logistic Regression

To train the logistic regression, we use MLE (the maximum likelihood estimation). Its application is straightforward, given that $p(C_1|\boldsymbol{x}; \boldsymbol{w})$ is directly the model output $y(\boldsymbol{x}; \boldsymbol{w})$.

Therefore, the loss for a minibatch $\mathbb{X} = \{(\boldsymbol{x}_1, t_1), (\boldsymbol{x}_2, t_2), \ldots, (\boldsymbol{x}_N, t_N)\}$ is

$$E(\boldsymbol{w}) = \frac{1}{N} \sum_i -\log(p(C_{t_i}|\boldsymbol{x}_i; \boldsymbol{w})).$$

Input: Input dataset ($\boldsymbol{X} \in \mathbb{R}^{N\times D}$, $\boldsymbol{t} \in \{0, +1\}^N$), learning rate $\alpha \in \mathbb{R}^+$.

- $\boldsymbol{w} \leftarrow \boldsymbol{0}$ or we initialize $\boldsymbol{w}$ randomly
- until convergence (or patience runs out), process a minibatch of examples $\mathbb{B}$:
  - $\boldsymbol{g} \leftarrow \frac{1}{|\mathbb{B}|} \sum_{i\in\mathbb{B}} \nabla_{\boldsymbol{w}} \Big(-\log\big(p(C_{t_i}|\boldsymbol{x}_i; \boldsymbol{w})\big)\Big)$
  - $\boldsymbol{w} \leftarrow \boldsymbol{w} - \alpha\boldsymbol{g}$

Generalized Linear Models

The logistic regression is in fact an extended linear regression. A linear regression model, which is followed by an **activation function** a, is called **generalized linear model**:

$$p(t|\boldsymbol{x};\boldsymbol{w},b) = y(\boldsymbol{x};\boldsymbol{w},b) = a\big(\bar{y}(\boldsymbol{x};\boldsymbol{w},b)\big) = a(\boldsymbol{x}^T\boldsymbol{w}+b).$$

Name	Activation	Distribution	Loss	Gradient
linear regression	identity	?	$\mathrm{MSE} \propto \mathbb{E}(y(\boldsymbol{x})-t)^2$	$\big(y(\boldsymbol{x})-t\big)\boldsymbol{x}$
logistic regression	$\sigma(\bar{y})$	Bernoulli	$\mathrm{NLL} \propto \mathbb{E}-\log(p(t\vert\boldsymbol{x}))$	?

Logistic Regression Gradient

We start by computing the gradient of the $\sigma(x)$.

$$
\begin{aligned}
\frac{\partial}{\partial x}\sigma(x) &= \frac{\partial}{\partial x}\frac{1}{1+e^{-x}} \\
&= \frac{\frac{\partial}{\partial x} -(1+e^{-x})}{(1+e^{-x})^2} \\
&= \frac{1}{1+e^{-x}} \cdot \frac{e^{-x}}{1+e^{-x}} \\
&= \sigma(x) \cdot \frac{e^{-x}+1-1}{1+e^{-x}} \\
&= \sigma(x) \cdot \big(1-\sigma(x)\big)
\end{aligned}
$$

$$\frac{\partial}{\partial x}\frac{1}{g(x)} = -\frac{\frac{\partial}{\partial x}g(x)}{g(x)^2}$$

$$\frac{\partial}{\partial x}e^{g(x)} = e^{g(x)} \cdot \frac{\partial}{\partial x}g(x)$$

Logistic Regression Gradient

Consider the log-likelihood of logistic regression $\log p(t|\boldsymbol{x};\boldsymbol{w})$. For brevity, we denote $\bar{y}(\boldsymbol{x};\boldsymbol{w}) = \boldsymbol{x}^T\boldsymbol{w}$ just as $\bar{y}$ in the following computation.

Remembering that for $t \sim \mathrm{Ber}(\varphi)$ we have $p(t) = \varphi^t(1-\varphi)^{1-t}$, we can rewrite the log-likelihood to:

$$\begin{aligned}\log p(t|\boldsymbol{x};\boldsymbol{w}) &= \log \sigma(\bar{y})^t\big(1-\sigma(\bar{y})\big)^{1-t} \\ &= t\cdot\log\big(\sigma(\bar{y})\big) + (1-t)\cdot\log\big(1-\sigma(\bar{y})\big)\end{aligned}$$

Logistic Regression Gradient

$$\nabla_{\boldsymbol w} - \log p(t|\boldsymbol x; \boldsymbol w) =$$

$$= \nabla_{\boldsymbol w}\Big(- t \cdot \log\big(\sigma(\bar y)\big) - (1-t) \cdot \log\big(1 - \sigma(\bar y)\big)\Big)$$

$$\frac{\partial}{\partial x}\log g(x) = \frac{1}{g(x)} \cdot \frac{\partial}{\partial x} g(x)$$

$$= -t \cdot \frac{1}{\sigma(\bar y)} \cdot \nabla_{\boldsymbol w}\sigma(\bar y) - (1-t) \cdot \frac{1}{1-\sigma(\bar y)} \cdot \nabla_{\boldsymbol w}\big(1 - \sigma(\bar y)\big)$$

$$\frac{\partial}{\partial x} f\big(g(x)\big) = \frac{\partial}{\partial g(x)} f\big(g(x)\big) \cdot \frac{\partial}{\partial x} g(x) = \frac{\partial}{\partial z} f(z) \cdot \frac{\partial}{\partial x} g(x)$$

$$\nabla_{\boldsymbol w}\sigma(\bar y) = \tfrac{\partial}{\partial \bar y}\sigma(\bar y) \cdot \nabla_{\boldsymbol w}\bar y$$

$$= -t \cdot \frac{1}{\sigma(\bar y)} \cdot \sigma(\bar y) \cdot \big(1 - \sigma(\bar y)\big) \cdot \nabla_{\boldsymbol w}\bar y + (1-t) \cdot \frac{1}{1-\sigma(\bar y)} \cdot \sigma(\bar y) \cdot \big(1 - \sigma(\bar y)\big) \cdot \nabla_{\boldsymbol w}\bar y$$

$$= \Big(- t + t\sigma(\bar y) + \sigma(\bar y) - t\sigma(\bar y)\Big)\boldsymbol x$$

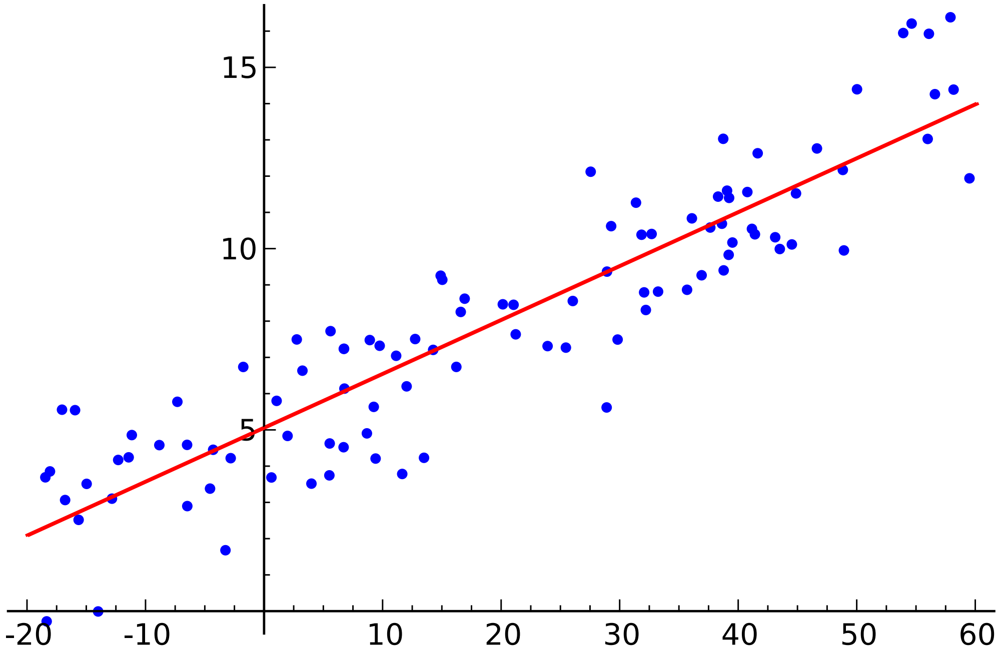
$$= \big(y(\boldsymbol x; \boldsymbol w) - t\big)\boldsymbol x$$

The logistic regression is in fact an extended linear regression. A linear regression model, which is followed by some **activation function** a, is called **generalized linear model**:

$$p(t|\boldsymbol{x};\boldsymbol{w},b) = y(\boldsymbol{x};\boldsymbol{w},b) = a\big(\bar{y}(\boldsymbol{x};\boldsymbol{w},b)\big) = a(\boldsymbol{x}^T\boldsymbol{w}+b).$$

Name	Activation	Distribution	Loss	Gradient
linear regression	identity	?	$\mathrm{MSE} \propto \mathbb{E}(y(\boldsymbol{x})-t)^2$	$\big(y(\boldsymbol{x})-t\big)\boldsymbol{x}$
logistic regression	$\sigma(\bar{y})$	Bernoulli	$\mathrm{NLL} \propto \mathbb{E} -\log(p(t\vert\boldsymbol{x}))$	$\big(y(\boldsymbol{x})-t\big)\boldsymbol{x}$

Mean Square Error as MLE



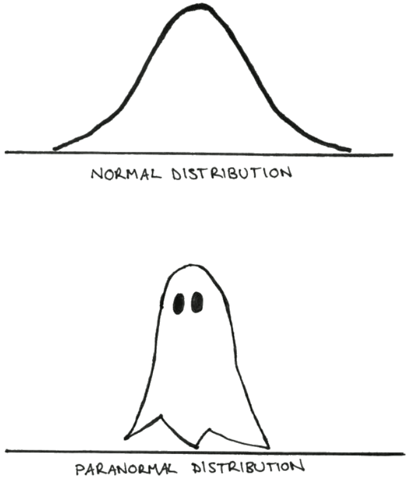
https://upload.wikimedia.org/wikipedia/commons/3/3a/Linear_regression.svg

During regression, we predict a number, not a probability distribution. To generate a distribution, we might consider a distribution with the mean of the predicted value and a fixed variance σ^2 – the most general such a distribution is the normal distribution.

Mean Square Error as MLE

Therefore, assume our model generates a distribution $p(t|\boldsymbol{x};\boldsymbol{w}) = \mathcal{N}(t; y(\boldsymbol{x};\boldsymbol{w}), \sigma^2)$.

Now we can apply the maximum likelihood estimation and get



https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2465539/

$$\begin{aligned}
\arg\max_{\boldsymbol{w}} p(\boldsymbol{t}|\boldsymbol{X};\boldsymbol{w}) &= \arg\min_{\boldsymbol{w}} \sum_{i=1}^N -\log p(t_i|\boldsymbol{x}_i;\boldsymbol{w}) \\
&= \arg\min_{\boldsymbol{w}} -\sum_{i=1}^N \log \sqrt{\frac{1}{2\pi\sigma^2}} e^{-\frac{(t_i - y(\boldsymbol{x}_i;\boldsymbol{w}))^2}{2\sigma^2}} \\
&= \arg\min_{\boldsymbol{w}} -N\log(2\pi\sigma^2)^{-1/2} - \sum_{i=1}^N -\frac{\big(t_i - y(\boldsymbol{x}_i;\boldsymbol{w})\big)^2}{2\sigma^2} \\
&= \arg\min_{\boldsymbol{w}} \sum_{i=1}^N \frac{\big(t_i - y(\boldsymbol{x}_i;\boldsymbol{w})\big)^2}{2\sigma^2} = \arg\min_{\boldsymbol{w}} \frac{1}{N}\sum_{i=1}^N \big(y(\boldsymbol{x}_i;\boldsymbol{w}) - t_i\big)^2.
\end{aligned}$$

We have therefore extended the GLM table to

Name	Activation	Distribution	Loss	Gradient
linear regression	identity	Normal	$\mathrm{NLL} \propto \mathrm{MSE}$	$\big(y(\boldsymbol x) - t\big)\boldsymbol x$
logistic regression	$\sigma(\bar y)$	Bernoulli	$\mathrm{NLL} \propto \mathbb{E} - \log(p(t\vert\boldsymbol x))$	$\big(y(\boldsymbol x) - t\big)\boldsymbol x$

To extend the binary logistic regression to a multiclass case with K classes, we:

- generate K outputs, each with its own set of weights, so that for $\boldsymbol W \in \mathbb{R}^{D\times K}$,

$$\bar{\boldsymbol y}(\boldsymbol x; \boldsymbol W) = \boldsymbol x^T \boldsymbol W, \quad \text{or in other words,} \quad \bar{\boldsymbol y}(\boldsymbol x; \boldsymbol W)_i = \boldsymbol x^T (\boldsymbol W_{*,i})$$

- generalize the sigmoid function to a $\operatorname{softmax}$ function, such that

$$\operatorname{softmax}(\boldsymbol z)_i = \frac{e^{z_i}}{\sum_j e^{z_j}}.$$

  Note that the original sigmoid function can be written as

$$\sigma(x) = \operatorname{softmax}\left([x \;\; 0]\right)_0 = \frac{e^x}{e^x + e^0} = \frac{1}{1 + e^{-x}}.$$

The resulting classifier is also known as **multinomial logistic regression**, **maximum entropy classifier** or **softmax regression**.

Multiclass Logistic Regression

Using the $\operatorname{softmax}$ function, we naturally define that

$$p(C_i|\boldsymbol{x};\boldsymbol{W}) = \boldsymbol{y}(\boldsymbol{x};\boldsymbol{W})_i = \operatorname{softmax}\big(\bar{\boldsymbol{y}}(\boldsymbol{x};\boldsymbol{W})\big)_i = \operatorname{softmax}(\boldsymbol{x}^T\boldsymbol{W})_i = \frac{e^{(\boldsymbol{x}^T\boldsymbol{W})_i}}{\sum_j e^{(\boldsymbol{x}^T\boldsymbol{W})_j}}.$$

Considering the definition of the $\operatorname{softmax}$ function, it is natural to obtain the interpretation of the linear part of the model $\bar{\boldsymbol{y}}(\boldsymbol{x};\boldsymbol{W})$ as **logits** by computing a logarithm of the above:

$$\bar{\boldsymbol{y}}(\boldsymbol{x};\boldsymbol{W})_i = \log(p(C_i|\boldsymbol{x};\boldsymbol{W})) + c.$$

The constant c is present, because the output of the model is *overparametrized* (for example, the probability of the last class could be computed from the remaining ones). This is connected to the fact that softmax is invariant to addition of a constant:

$$\operatorname{softmax}(\boldsymbol{z}+c)_i = \frac{e^{z_i+c}}{\sum_j e^{z_j+c}} = \frac{e^{z_i}}{\sum_j e^{z_j}} \cdot \frac{e^c}{e^c} = \operatorname{softmax}(\boldsymbol{z})_i.$$

Multiclass Logistic Regression

To train K-class classification, analogously to the binary logistic regression we can use MLE and train the model using minibatch stochastic gradient descent:

Input: Input dataset ($\boldsymbol{X} \in \mathbb{R}^{N\times D}$, $\boldsymbol{t} \in \{0, 1, \ldots, K-1\}^N$), learning rate $\alpha \in \mathbb{R}^+$.
Model: Let $\boldsymbol{w}$ denote all parameters of the model (in our case, the parameters are a weight matrix $\boldsymbol{W}$ and maybe a bias vector $\boldsymbol{b}$).

- $\boldsymbol{w} \leftarrow \mathbf{0}$ or we initialize $\boldsymbol{w}$ randomly
- until convergence (or patience runs out), process a minibatch of examples $\mathbb{B}$:
  - $\boldsymbol{g} \leftarrow \frac{1}{|\mathbb{B}|}\sum_{i\in\mathbb{B}} \nabla_{\boldsymbol{w}}\Big(-\log\big(p(C_{t_i}|\boldsymbol{x}_i;\boldsymbol{w})\big)\Big)$
  - $\boldsymbol{w} \leftarrow \boldsymbol{w} - \alpha\boldsymbol{g}$

Multiclass Logistic Regression

Note that the decision regions of the binary/multiclass logistic regression are convex (and therefore connected).

To see this, consider $\boldsymbol{x}_A$ and $\boldsymbol{x}_B$ in the same decision region R_k.

Any point $\boldsymbol{x}$ lying on the line connecting them is their convex combination, $\boldsymbol{x} = \lambda\boldsymbol{x}_A + (1-\lambda)\boldsymbol{x}_B$, and from the linearity of $\bar{\boldsymbol{y}}(\boldsymbol{x}) = \boldsymbol{x}^T\boldsymbol{W}$ it follows that

$$\bar{\boldsymbol{y}}(\boldsymbol{x}) = \lambda\bar{\boldsymbol{y}}(\boldsymbol{x}_A) + (1-\lambda)\bar{\boldsymbol{y}}(\boldsymbol{x}_B).$$

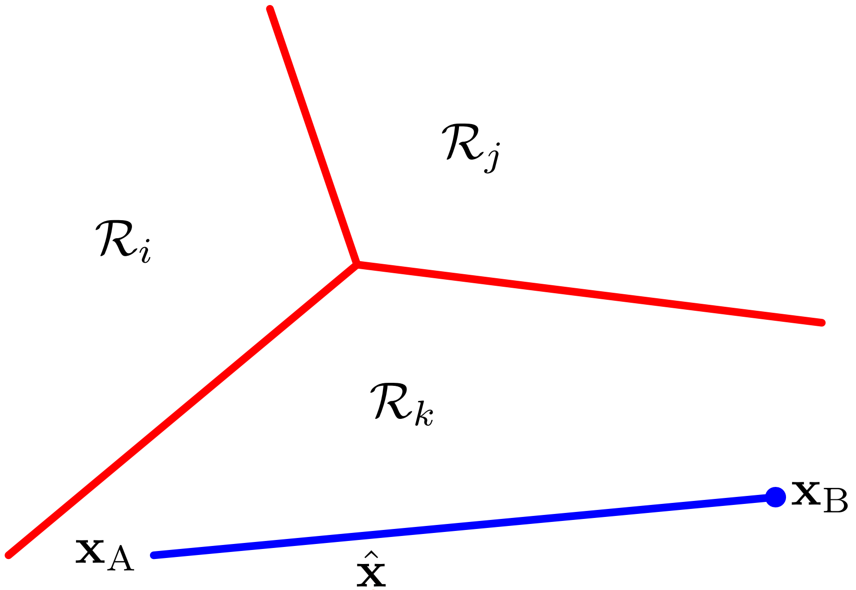
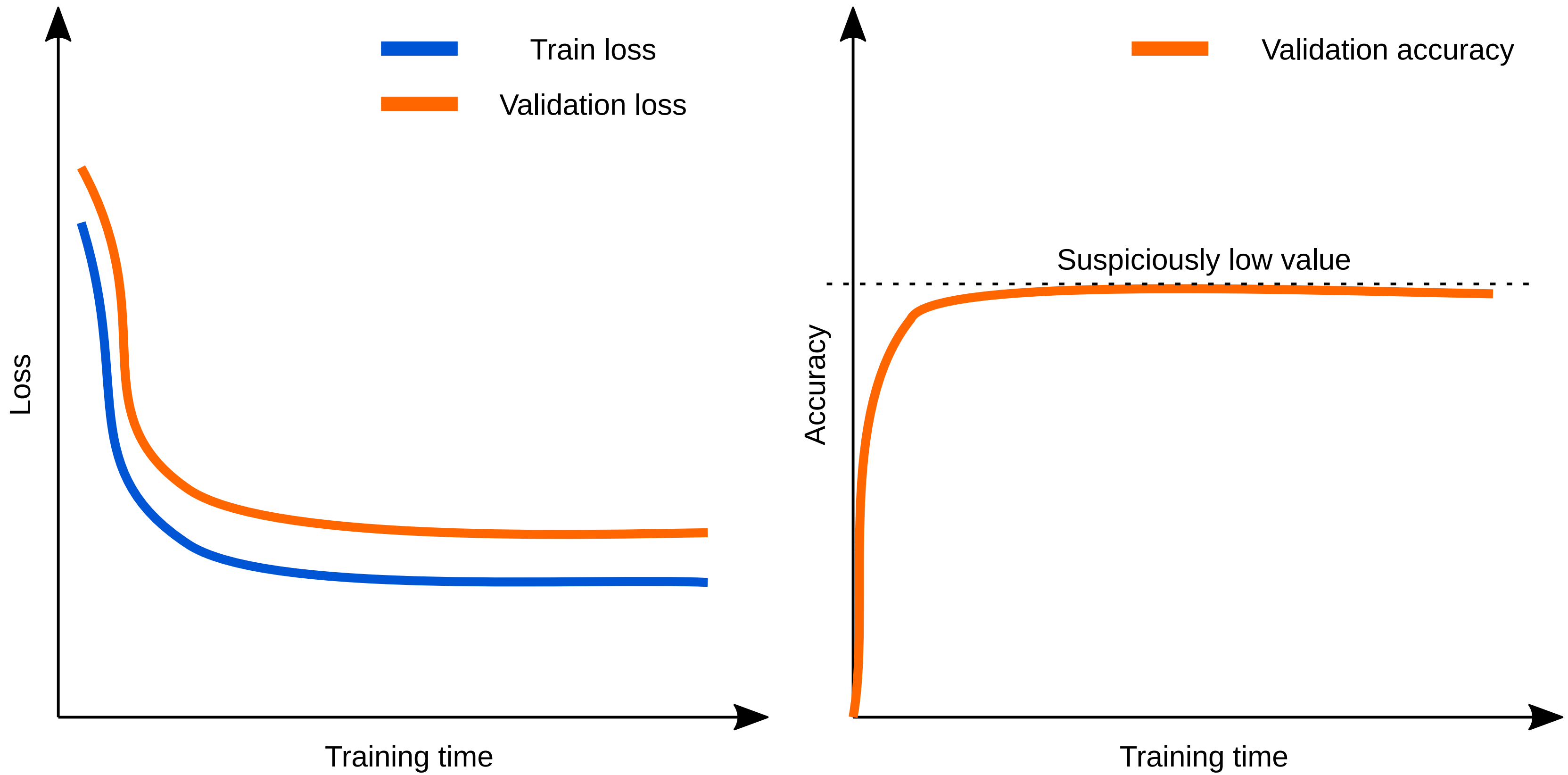


Figure 4.3 of Pattern Recognition and Machine Learning.

Given that $\bar{\boldsymbol{y}}(\boldsymbol{x}_A)_k$ was the largest among $\bar{\boldsymbol{y}}(\boldsymbol{x}_A)$ and also given that $\bar{\boldsymbol{y}}(\boldsymbol{x}_B)_k$ was the largest among $\bar{\boldsymbol{y}}(\boldsymbol{x}_B)$, it must be the case that $\bar{\boldsymbol{y}}(\boldsymbol{x})_k$ is the largest among all $\bar{\boldsymbol{y}}(\boldsymbol{x})$.

What went wrong?



The model only predicts the majority class. Insufficient features, too high learning rate.

The multiclass logistic regression can now be added to the GLM table:

Name	Activation	Distribution	Loss	Gradient
linear regression	identity	Normal	$\mathrm{NLL} \propto \mathrm{MSE}$	$\big(y(\boldsymbol x) - t\big)\boldsymbol x$
logistic regression	$\sigma(\bar y)$	Bernoulli	$\mathrm{NLL} \propto \mathbb{E} - \log(p(t\vert\boldsymbol x))$	$\big(y(\boldsymbol x) - t\big)\boldsymbol x$
multiclass logistic regression	$\operatorname{softmax}(\bar{\boldsymbol y})$	categorical	$\mathrm{NLL} \propto \mathbb{E} - \log(p(t\vert\boldsymbol x))$	$\big((\boldsymbol y(\boldsymbol x) - \mathbf{1}_t)\boldsymbol x^T\big)^T$

Recall that $\mathbf{1}_t = \big([i = t]\big)_{i=0}^{K-1}$ is one-hot representation of target $t \in \{0, 1, \ldots, K-1\}$.

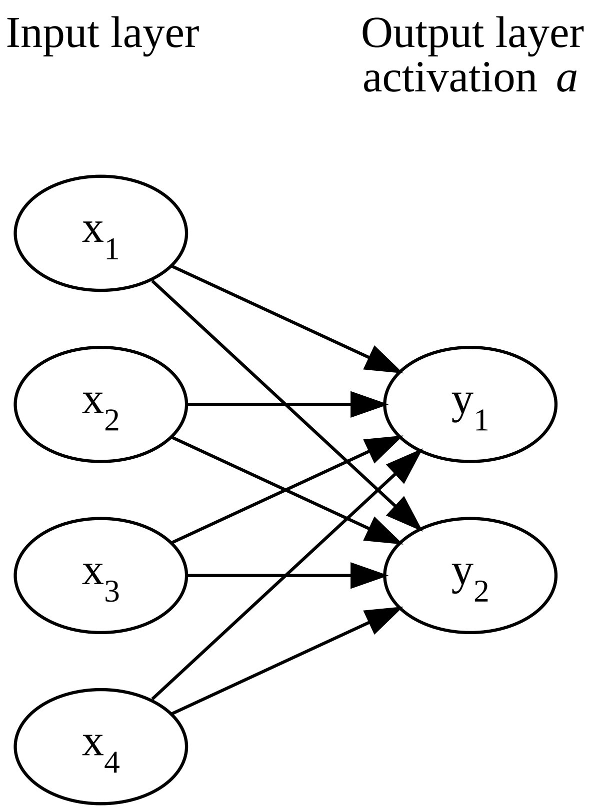
The gradient $\big((\boldsymbol y(\boldsymbol x) - \mathbf{1}_t)\boldsymbol x^T\big)^T$ can be of course also computed as $\boldsymbol x\big(\boldsymbol y(\boldsymbol x) - \mathbf{1}_t\big)^T$.

Multilayer Perceptron

We can reformulate the generalized linear models in the following framework.

- Assume we have an input node for every input feature.
- Additionally, we have an output node for every model output (one for linear regression or binary classification, K for classification in K classes).
- Every input node and output node are connected with a directed edge, and every edge has an associated weight.
- Value of every (output) node is computed by summing the values of predecessors multiplied by the corresponding weights, added to a bias of this node, and finally passed through an activation function a:

$$y_i = a\left(\sum\nolimits_j x_j w_{j,i} + b_i\right)$$



or in matrix form $\boldsymbol{y} = a(\boldsymbol{x}^T \boldsymbol{W} + \boldsymbol{b})$, or for a batch of examples $\boldsymbol{X}$, $\boldsymbol{Y} = a(\boldsymbol{X}\boldsymbol{W} + \boldsymbol{b})$.

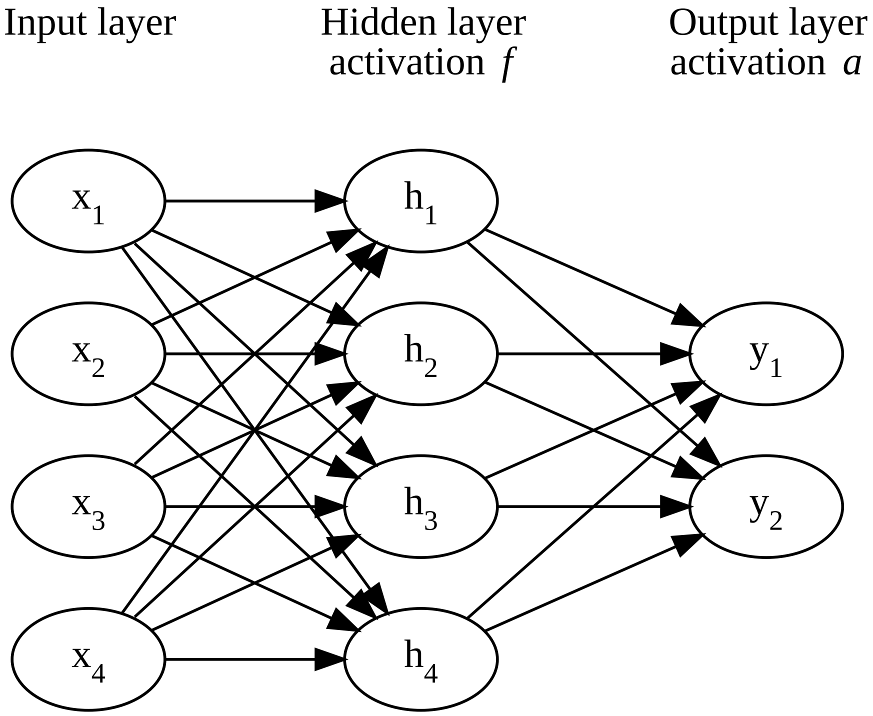
We now extend the model by adding a **hidden layer** with activation f.

- The computation is performed analogously:

$$h_i = f\left(\sum\nolimits_j x_j w_{j,i}^{(h)} + b_i^{(h)}\right),$$
$$y_i = a\left(\sum\nolimits_j h_j w_{j,i}^{(y)} + b_i^{(y)}\right),$$

or in matrix form

$$\boldsymbol h = f\left(\boldsymbol x^T \boldsymbol W^{(h)} + \boldsymbol b^{(h)}\right),$$
$$\boldsymbol y = a\left(\boldsymbol h^T \boldsymbol W^{(y)} + \boldsymbol b^{(y)}\right),$$



and for batch of inputs $\boldsymbol H = f\left(\boldsymbol X \boldsymbol W^{(h)} + \boldsymbol b^{(h)}\right)$ and $\boldsymbol Y = a\left(\boldsymbol H \boldsymbol W^{(y)} + \boldsymbol b^{(y)}\right)$.

Note that:

- the structure of the *input* layer depends on the input features;
- the structure and the *activation* function of the *output* layer depends on the target data;
- however, the *hidden* layer has no pre-image in the data and is completely arbitrary – which is the reason why it is called a *hidden* layer.

Also note that we can absorb biases into weights analogously to the generalized linear models.

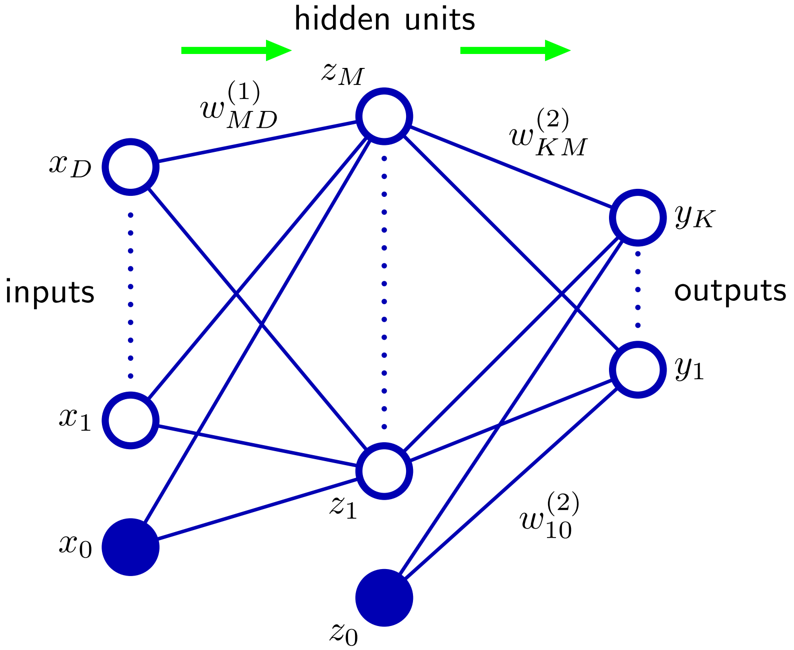


Figure 5.1 of Pattern Recognition and Machine Learning.

Output Layer Activation Functions

- regression:
  - identity activation: we model normal distribution on output (linear regression)
- binary classification:
  - $\sigma(x)$: we model the Bernoulli distribution (the model predicts a probability)

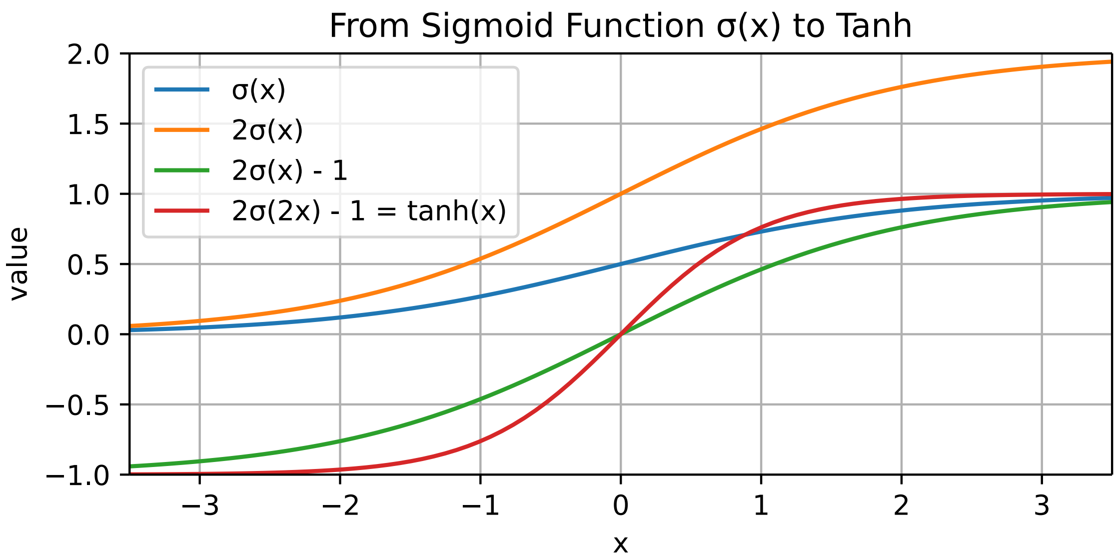
$$\sigma(x) \stackrel{\text{def}}{=} \frac{1}{1 + e^{-x}}$$

- K-class classification:
  - $\operatorname{softmax}(\boldsymbol{x})$: we model the (usually overparametrized) categorical distribution

$$\operatorname{softmax}(\boldsymbol{x}) \propto e^{\boldsymbol{x}}, \quad \operatorname{softmax}(\boldsymbol{x})_i \stackrel{\text{def}}{=} \frac{e^{\boldsymbol{x}_i}}{\sum_j e^{\boldsymbol{x}_j}}$$

Hidden Layer Activation Functions

- no activation (identity): does not help, composition of linear mapping is a linear mapping
- σ (but works suboptimally – nonsymmetrical, $\frac{d\sigma}{dx}(0) = 1/4$)
- $\tanh$
  - result of making σ symmetrical and making derivation in zero 1
  - $\tanh(x) = 2\sigma(2x) - 1$
- ReLU
  - $\max(0, x)$
  - the most common nonlinear activation used nowadays



Training MLP

The multilayer perceptron can be trained using again a minibatch SGD algorithm:

Input: Input dataset ($\boldsymbol{X} \in \mathbb{R}^{N\times D}$, $\boldsymbol{t}$ targets), learning rate $\alpha \in \mathbb{R}^+$.
Model: Let $\boldsymbol{w}$ denote all parameters of the model (all weight matrices and bias vectors).

- initialize $\boldsymbol{w}$
  - set weights randomly
    - for a weight matrix processing a layer of size M to a layer of size O, we can sample its elements uniformly for example from the $\left[-\frac{1}{\sqrt{M}}, \frac{1}{\sqrt{M}}\right]$ range
    - the exact range becomes more important for networks with many hidden layers
  - set biases to 0
- until convergence (or patience runs out), process a minibatch of examples $\mathbb{B}$:
  - $\boldsymbol{g} \leftarrow \frac{1}{|\mathbb{B}|} \sum_{i\in\mathbb{B}} \nabla_{\boldsymbol{w}} \Big(-\log \big(p(t_i|\boldsymbol{x}_i; \boldsymbol{w})\big)\Big)$
  - $\boldsymbol{w} \leftarrow \boldsymbol{w} - \alpha \boldsymbol{g}$