Perceptron and Logistic Regression

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Today's Lecture Objectives

After this lecture you should be able to

- Think about binary classification using **geometric intuition** and use the **perceptron algorithm**.
- Define the **main concepts of information theory** (entropy, cross-entropy, KL-divergence) and prove their properties.
- Derive training objectives using the **maximum likelihood principle**.
- Implement and use **logistic regression** for binary classification with SGD.

Perceptron

Binary Classification

Binary classification is a classification in two classes.

The simplest way to evaluate classification is **accuracy**, which is the ratio of input examples that were classified correctly – i.e., where the predicted class and the target class match.

To extend linear regression to binary classification, we might seek a **threshold** and then classify an input as negative/positive depending on whether $y(\boldsymbol{x}; \boldsymbol{w}) = \boldsymbol{x}^T \boldsymbol{w} + b$ is smaller/larger than a given threshold.

Zero value is usually used as the threshold, both because of symmetry and also because the **bias** parameter acts as a trainable threshold anyway.

The set of points with prediction 0 is called a **decision boundary**.

Geometric Intuition

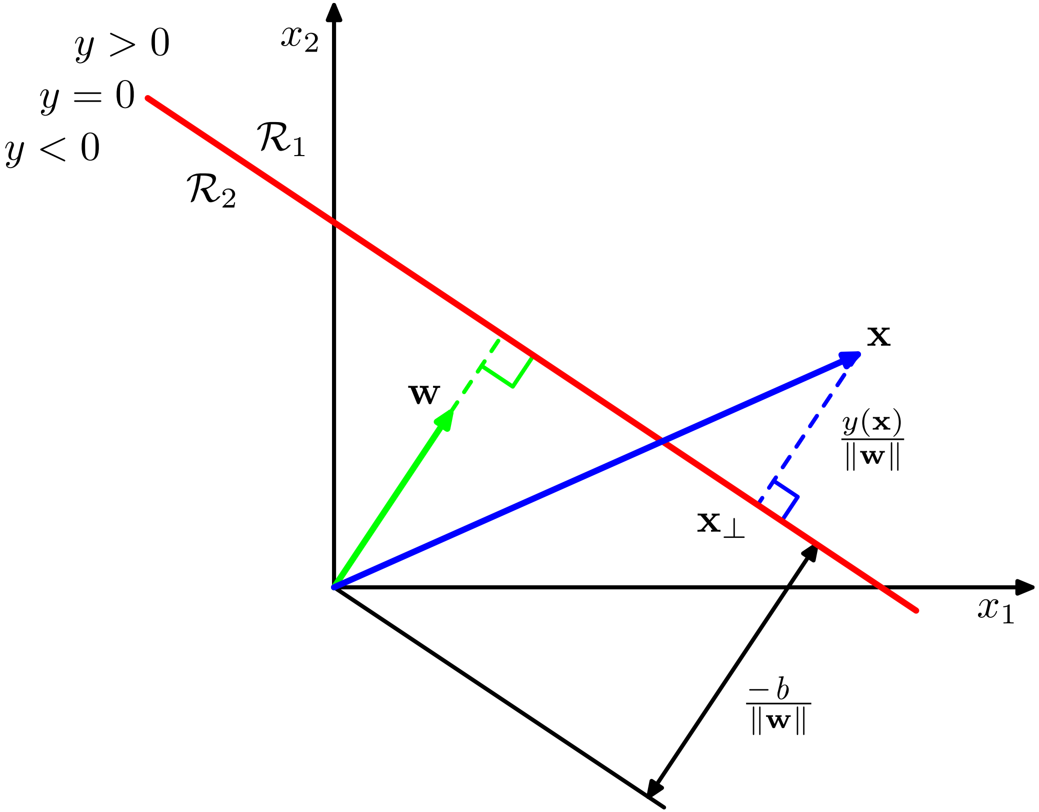


Figure 4.1 of Pattern Recognition and Machine Learning.

Perceptron

The perceptron algorithm is probably the oldest one for training weights of a binary classification. Assuming the target value $t \in \{-1, +1\}$, the goal is to find weights $\boldsymbol{w}$ such that for all train data,

$$\operatorname{sign}(y(\boldsymbol{x}_i; \boldsymbol{w})) = \operatorname{sign}(\boldsymbol{x}_i^T \boldsymbol{w}) = t_i,$$

or equivalently,

$$t_i y(\boldsymbol{x}_i; \boldsymbol{w}) = t_i \boldsymbol{x}_i^T \boldsymbol{w} > 0.$$

Note that a set is called **linearly separable**, if there exists a weight vector $\boldsymbol{w}$ such that the above equation holds.

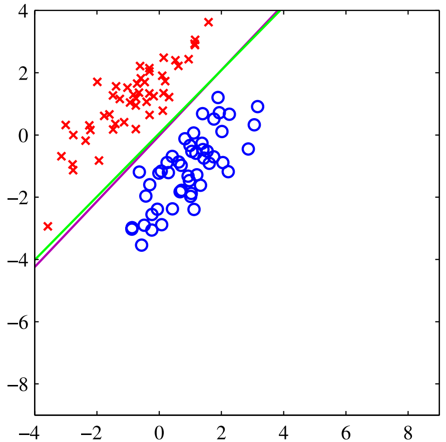


Figure 4.4 of Pattern Recognition and Machine Learning.

Perceptron

The perceptron algorithm was invented by Rosenblatt in 1958.

Input: Linearly separable dataset ($\boldsymbol{X} \in \mathbb{R}^{N \times D}$, $\boldsymbol{t} \in \{-1, +1\}^N$).
Output: Weights $\boldsymbol{w} \in \mathbb{R}^D$ such that $t_i \boldsymbol{x}_i^T \boldsymbol{w} > 0$ for all i.

- $\boldsymbol{w} \leftarrow \mathbf{0}$
- until all examples are classified correctly, process example i:
  - $y \leftarrow \boldsymbol{x}_i^T \boldsymbol{w}$
  - if $t_i y \leq 0$ (incorrectly classified example):
    - $\boldsymbol{w} \leftarrow \boldsymbol{w} + t_i \boldsymbol{x}_i$

We will prove that the algorithm always arrives at some correct set of weights $\boldsymbol{w}$ if the training set is linearly separable.

Proof of Perceptron Convergence

Let $\boldsymbol{w}_*$ be some weights correctly classifying (separating) the training data, and let $\boldsymbol{w}_k$ be the weights after k nontrivial updates of the perceptron algorithm, with $\boldsymbol{w}_0$ being 0.

We will prove that the angle α between $\boldsymbol{w}_*$ and $\boldsymbol{w}_k$ decreases at each step. Note that

$$\cos(\alpha) = \frac{\boldsymbol{w}_*^T \boldsymbol{w}_k}{\|\boldsymbol{w}_*\| \cdot \|\boldsymbol{w}_k\|}.$$

Proof of Perceptron Convergence

Assume that the maximum norm of any training example $\|\boldsymbol{x}\|$ is bounded by R, and that γ is the minimum margin of $\boldsymbol{w}_*$, so for each training example $(\boldsymbol{x}, t)$, $t\boldsymbol{x}^T\boldsymbol{w}_* \geq \gamma$.

First consider the dot product of $\boldsymbol{w}_*$ and $\boldsymbol{w}_k$:

$$\boldsymbol{w}_*^T\boldsymbol{w}_k = \boldsymbol{w}_*^T(\boldsymbol{w}_{k-1} + t_k\boldsymbol{x}_k) \geq \boldsymbol{w}_*^T\boldsymbol{w}_{k-1} + \gamma.$$

By iteratively applying this equation, we get

$$\boldsymbol{w}_*^T\boldsymbol{w}_k \geq k\gamma.$$

Now consider the length of $\boldsymbol{w}_k$:

$$\|\boldsymbol{w}_k\|^2 = \|\boldsymbol{w}_{k-1} + t_k\boldsymbol{x}_k\|^2 = \|\boldsymbol{w}_{k-1}\|^2 + 2t_k\boldsymbol{x}_k^T\boldsymbol{w}_{k-1} + \|\boldsymbol{x}_k\|^2.$$

Because $\boldsymbol{x}_k$ was misclassified, we know that $t_k\boldsymbol{x}_k^T\boldsymbol{w}_{k-1} \leq 0$, so $\|\boldsymbol{w}_k\|^2 \leq \|\boldsymbol{w}_{k-1}\|^2 + R^2$. When applied iteratively, we get $\|\boldsymbol{w}_k\|^2 \leq k \cdot R^2$.

Proof of Perceptron Convergence

Putting everything together, we get

$$\cos(\alpha) = \frac{\boldsymbol{w}_*^T \boldsymbol{w}_k}{\|\boldsymbol{w}_*\| \cdot \|\boldsymbol{w}_k\|} \geq \frac{k\gamma}{\sqrt{kR^2}\|\boldsymbol{w}_*\|}.$$

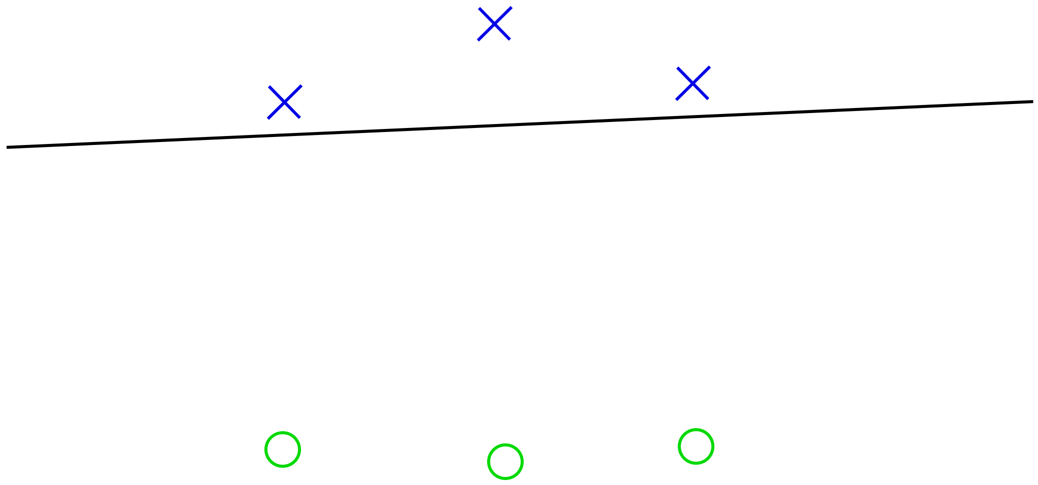
Therefore, the $\cos(\alpha)$ increases during every update. Because the value of $\cos(\alpha)$ is at most one, we can compute the upper bound on the number of steps when the algorithm converges as

$$1 \geq \frac{\sqrt{k}\gamma}{\sqrt{R^2}\|\boldsymbol{w}_*\|} \text{ or } k \leq \frac{R^2\|\boldsymbol{w}_*\|^2}{\gamma^2}.$$

Perceptron Issues

Perceptron has several drawbacks:

- If the input set is not linearly separable, the algorithm never finishes.
- The algorithm performs only prediction, it is not able to return the probabilities of predictions.
- Most importantly, Perceptron algorithm finds *some* solution, not necessarily a good one, because once it finds some, it cannot perform any more updates.

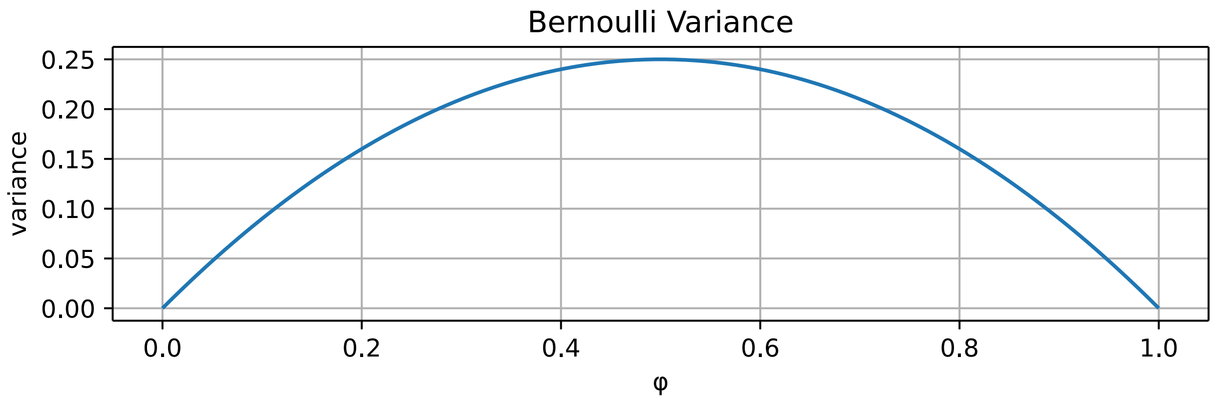


Basics of Probability

Bernoulli Distribution

The Bernoulli distribution is a distribution over a binary random variable. It has a single parameter $\varphi \in [0, 1]$, which specifies the probability that the random variable is equal to 1.

$$P(x) = \varphi^x (1 - \varphi)^{1-x}$$
$$\mathbb{E}[x] = \varphi$$
$$\mathrm{Var}(x) = \varphi(1 - \varphi)$$



Categorical Distribution

Extension of the Bernoulli distribution to random variables taking one of K different discrete outcomes. It is parametrized by $\boldsymbol{p} \in [0,1]^K$ such that $\sum_{i=0}^{K-1} p_i = 1$.

We represent outcomes as vectors $\in \{0,1\}^K$ in **one-hot encoding**. Therefore, an outcome $x \in \{0, 1, \ldots, K-1\}$ is represented as a vector

$$\mathbf{1}_x \stackrel{\text{def}}{=} \big([i = x]\big)_{i=0}^{K-1} = \big(\underbrace{0, \ldots, 0}_{x}, 1, \underbrace{0, \ldots, 0}_{K-x-1}\big).$$

The outcome probability, mean, and variance are very similar to the Bernoulli distribution.

$$P(\boldsymbol{x}) = \prod\nolimits_{i=0}^{K-1} p_i^{x_i}$$

$$\mathbb{E}[x_i] = p_i$$

$$\mathrm{Var}(x_i) = p_i(1 - p_i)$$

Information Theory

Self Information

Amount of **surprise** when a random variable is sampled.

- Should be zero for events with probability 1.
- Less likely events are more surprising.
- Independent events should have **additive** information.

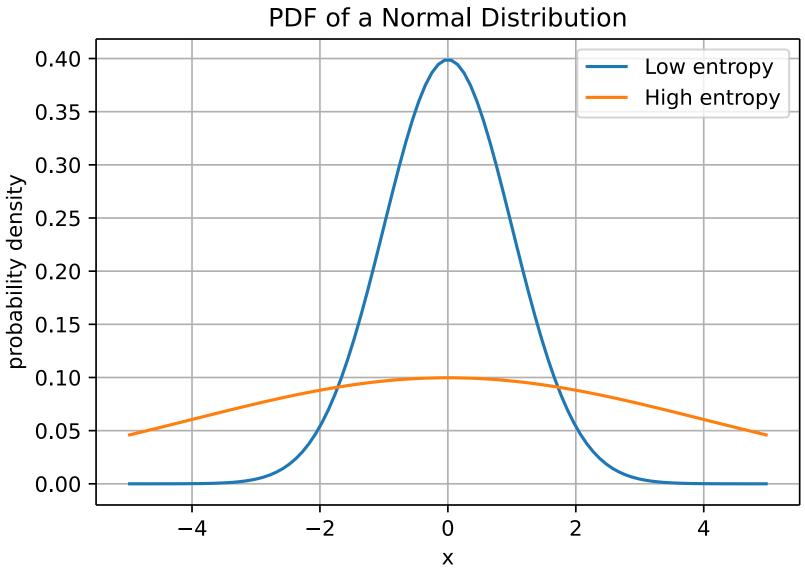
$$I(x) \stackrel{\text{def}}{=} -\log P(x) = \log \frac{1}{P(x)}$$

Entropy

Amount of **surprise** in the whole distribution.

$$H(P) \stackrel{\text{def}}{=} \mathbb{E}_{\mathrm{x}\sim P}[I(x)] = -\mathbb{E}_{\mathrm{x}\sim P}[\log P(x)]$$

- for discrete P: $H(P) = -\sum_x P(x) \log P(x)$
- for continuous P: $H(P) = -\int P(x) \log P(x)\,\mathrm{d}x$



Because $\lim_{x\to 0} x \log x = 0$, for $P(x) = 0$ we consider $P(x) \log P(x)$ to be zero.

Note that in the continuous case, the continuous entropy (also called *differential entropy*) has slightly different semantics, for example, it can be negative.

For binary logarithms, the entropy is measured in **bits**.
However, from now on, all logarithms are *natural logarithms* with base *e* (and then the entropy is measured in units called **nats**).

Cross-Entropy

$$H(P, Q) \stackrel{\text{def}}{=} -\mathbb{E}_{\mathrm{x} \sim P}[\log Q(x)]$$

Gibbs Inequality

- $H(P, Q) \geq H(P)$
- $H(P) = H(P, Q) \Leftrightarrow P = Q$

Proof: Consider $H(P) - H(P, Q) = \sum_x P(x) \log \frac{Q(x)}{P(x)}$.

Using the fact that $\log x \leq (x - 1)$ with equality only for $x = 1$, we get

$$\sum_x P(x) \log \frac{Q(x)}{P(x)} \leq \sum_x P(x) \left(\frac{Q(x)}{P(x)} - 1\right) = \sum_x Q(x) - \sum_x P(x) = 0.$$

For the equality to hold, $\frac{Q(x)}{P(x)}$ must be 1 for all x, i.e., $P = Q$.

Kullback-Leibler Divergence (KL Divergence)

Sometimes also called **relative entropy**.

$$D_{\mathrm{KL}}(P\|Q) \stackrel{\text{def}}{=} H(P,Q) - H(P) = \mathbb{E}_{\mathrm{x}\sim P}[\log P(x) - \log Q(x)]$$

- consequence of Gibbs inequality: $D_{\mathrm{KL}}(P\|Q) \geq 0$, $D_{\mathrm{KL}}(P\|Q) = 0$ iff $P = Q$
- generally $D_{\mathrm{KL}}(P\|Q) \neq D_{\mathrm{KL}}(Q\|P)$

Normal (or Gaussian) Distribution

A distribution over real numbers, parametrized by mean μ and variance σ^2:

$$\mathcal{N}(x;\mu,\sigma^2) = \sqrt{\frac{1}{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

For standard values $\mu = 0$ and $\sigma^2 = 1$ we get $\mathcal{N}(x;0,1) = \sqrt{\frac{1}{2\pi}} e^{-\frac{x^2}{2}}$.

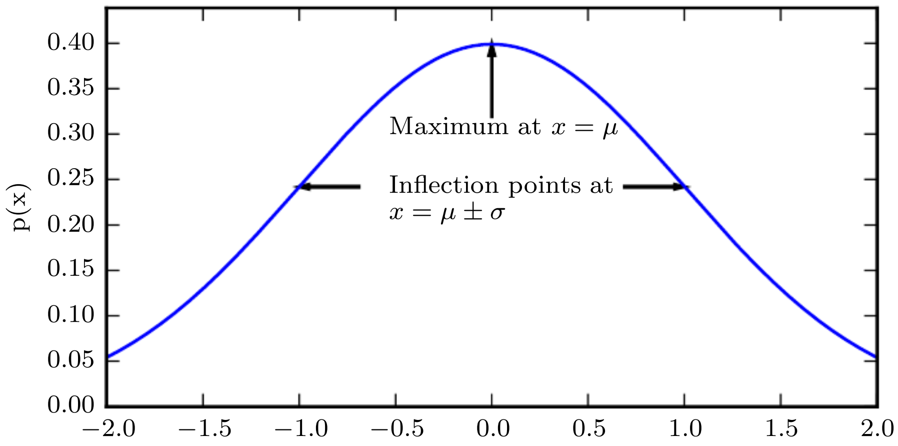


Figure 3.1 of "Deep Learning" book, https://www.deeplearningbook.org.

Central Limit Theorem

The sum of independent identically distributed random variables with finite non-zero variance converges to normal distribution.

Principle of Maximum Entropy

Given a set of constraints, a distribution with maximal entropy fulfilling the constraints can be considered the most general one, containing as little additional assumptions as possible.

Considering distributions with a **given mean and variance**, it can be proven (using variational inference) that such a distribution with **maximum entropy** is exactly the normal distribution.

Maximum Likelihood Estimation

Maximum Likelihood Estimation

Let $\boldsymbol{X} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\}$ be training data drawn independently from the data-generating distribution p_{data}.

We denote the **empirical data distribution** as $\hat{p}_{\text{data}}$, where

$$\hat{p}_{\text{data}}(\boldsymbol{x}) \stackrel{\text{def}}{=} \frac{\big|\{i : \boldsymbol{x}_i = \boldsymbol{x}\}\big|}{N}.$$

Let $p_{\text{model}}(\mathbf{x}; \boldsymbol{w})$ be a family of distributions.

- If the weights are fixed, $p_{\text{model}}(\mathbf{x}; \boldsymbol{w})$ is a probability distribution.
- If we instead consider the fixed training data $\boldsymbol{X}$, then

$$L(\boldsymbol{w}) = p_{\text{model}}(\boldsymbol{X}; \boldsymbol{w}) = \prod\nolimits_{i=1}^{N} p_{\text{model}}(\boldsymbol{x}_i; \boldsymbol{w})$$

is called the **likelihood**. Note that even if the value of the likelihood is in range $[0, 1]$, it is not a probability, because the likelihood is not a probability distribution.

Maximum Likelihood Estimation

Let $\boldsymbol{X} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\}$ be training data drawn independently from the data-generating distribution $p_\textrm{data}$. We denote the empirical data distribution as $\hat p_\textrm{data}$ and let $p_\textrm{model}(\mathbf{x}; \boldsymbol{w})$ be a family of distributions.

The **maximum likelihood estimation** of $\boldsymbol{w}$ is:

$$\begin{aligned}
\boldsymbol{w}_\textrm{MLE} &= \arg\max_{\boldsymbol{w}} p_\textrm{model}(\boldsymbol{X}; \boldsymbol{w}) = \arg\max_{\boldsymbol{w}} \prod\nolimits_{i=1}^N p_\textrm{model}(\boldsymbol{x}_i; \boldsymbol{w}) \\
&= \arg\min_{\boldsymbol{w}} \sum\nolimits_{i=1}^N -\log p_\textrm{model}(\boldsymbol{x}_i; \boldsymbol{w}) \\
&= \arg\min_{\boldsymbol{w}} \mathbb{E}_{\mathbf{x} \sim \hat p_\textrm{data}} [-\log p_\textrm{model}(\boldsymbol{x}; \boldsymbol{w})] \\
&= \arg\min_{\boldsymbol{w}} H(\hat p_\textrm{data}(\mathbf{x}), p_\textrm{model}(\mathbf{x}; \boldsymbol{w})) \\
&= \arg\min_{\boldsymbol{w}} D_\textrm{KL}(\hat p_\textrm{data}(\mathbf{x}) \| p_\textrm{model}(\mathbf{x}; \boldsymbol{w})) + H(\hat p_\textrm{data}(\mathbf{x}))
\end{aligned}$$

MLE can be easily generalized to the conditional case, where our goal is to predict t given $\boldsymbol{x}$:

$$\begin{aligned}
\boldsymbol{w}_{\text{MLE}} &= \arg\max_{\boldsymbol{w}} p_{\text{model}}(\boldsymbol{t}|\boldsymbol{X};\boldsymbol{w}) = \arg\max_{\boldsymbol{w}} \prod\nolimits_{i=1}^{N} p_{\text{model}}(t_i|\boldsymbol{x}_i;\boldsymbol{w}) \\
&= \arg\min_{\boldsymbol{w}} \sum\nolimits_{i=1}^{N} -\log p_{\text{model}}(t_i|\boldsymbol{x}_i;\boldsymbol{w}) \\
&= \arg\min_{\boldsymbol{w}} \mathbb{E}_{(\mathbf{x},\mathrm{t})\sim\hat{p}_{\text{data}}}[-\log p_{\text{model}}(t|\boldsymbol{x};\boldsymbol{w})] \\
&= \arg\min_{\boldsymbol{w}} H(\hat{p}_{\text{data}}(\mathrm{t}|\mathbf{x}), p_{\text{model}}(\mathrm{t}|\mathbf{x};\boldsymbol{w})) \\
&= \arg\min_{\boldsymbol{w}} D_{\text{KL}}(\hat{p}_{\text{data}}(\mathrm{t}|\mathbf{x})\|p_{\text{model}}(\mathrm{t}|\mathbf{x};\boldsymbol{w})) + H(\hat{p}_{\text{data}}(\mathrm{t}|\mathbf{x}))
\end{aligned}$$

where the conditional entropy is defined as $H(\hat{p}_{\text{data}}) = \mathbb{E}_{(\mathbf{x},\mathrm{t})\sim\hat{p}_{\text{data}}}[-\log(\hat{p}_{\text{data}}(t|\boldsymbol{x};\boldsymbol{w}))]$ and the conditional cross-entropy as $H(\hat{p}_{\text{data}}, p_{\text{model}}) = \mathbb{E}_{(\mathbf{x},\mathrm{t})\sim\hat{p}_{\text{data}}}[-\log(p_{\text{model}}(t|\boldsymbol{x};\boldsymbol{w}))]$.

The resulting *loss function* is called **negative log-likelihood** (**NLL**), or **cross-entropy**, or **Kullback-Leibler divergence**.

Logistic Regression

Logistic Regression

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

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 a **sigmoid function**

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

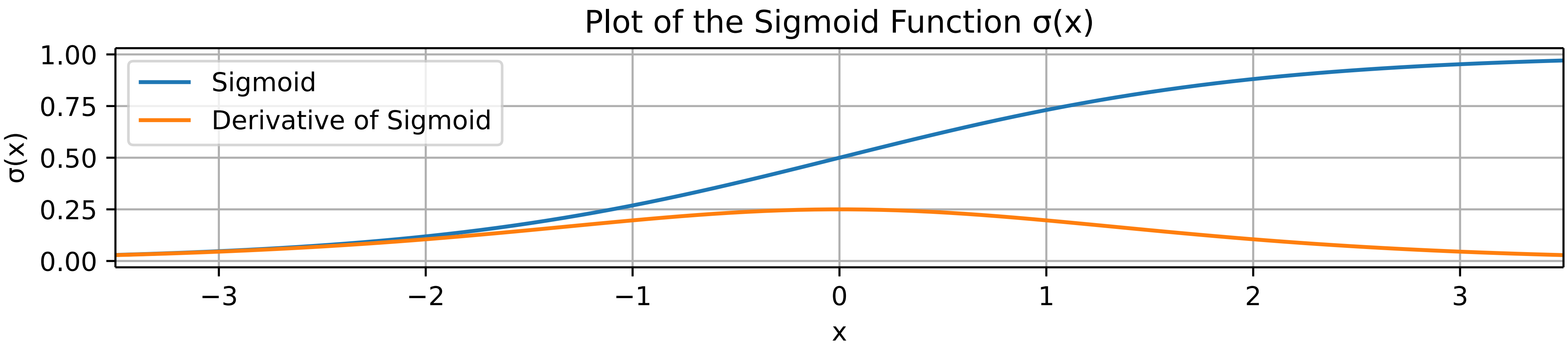
It can be trained using the SGD algorithm.

Sigmoid Function

The sigmoid function has values in range $(0, 1)$, is monotonically increasing and it has a derivative of $\frac{1}{4}$ at $x = 0$.

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

$$\sigma'(x) = \sigma(x)\big(1 - \sigma(x)\big)$$



We denote the output of the "linear part" of logistic regression as

$$\bar{y}(\boldsymbol{x}; \boldsymbol{w}) = \boldsymbol{x}^T \boldsymbol{w},$$

and the overall prediction as

$$y(\boldsymbol{x}; \boldsymbol{w}) = \sigma(\bar{y}(\boldsymbol{x}; \boldsymbol{w})) = \sigma(\boldsymbol{x}^T \boldsymbol{w}).$$

To train 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 $\mathbb{B}$:
  - $\boldsymbol{g} \leftarrow \frac{1}{|\mathbb{B}|} \sum_{i \in \mathbb{B}} \nabla_{\boldsymbol{w}} \Big(-\log \big(p(C_{t_i}|\boldsymbol{x}_i; \boldsymbol{w})\big)\Big)$
  - $\boldsymbol{w} \leftarrow \boldsymbol{w} - \alpha \boldsymbol{g}$

Practical note

Everything we learned about **features** and L^2 **regularization** holds for logistic regression too.

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