UNIVERSITY OF TECHNOLOGY
IN THE EUROPEAN CAPITAL OF CULTURE
CHEMNITZ

Neurocomputing

Linear classification

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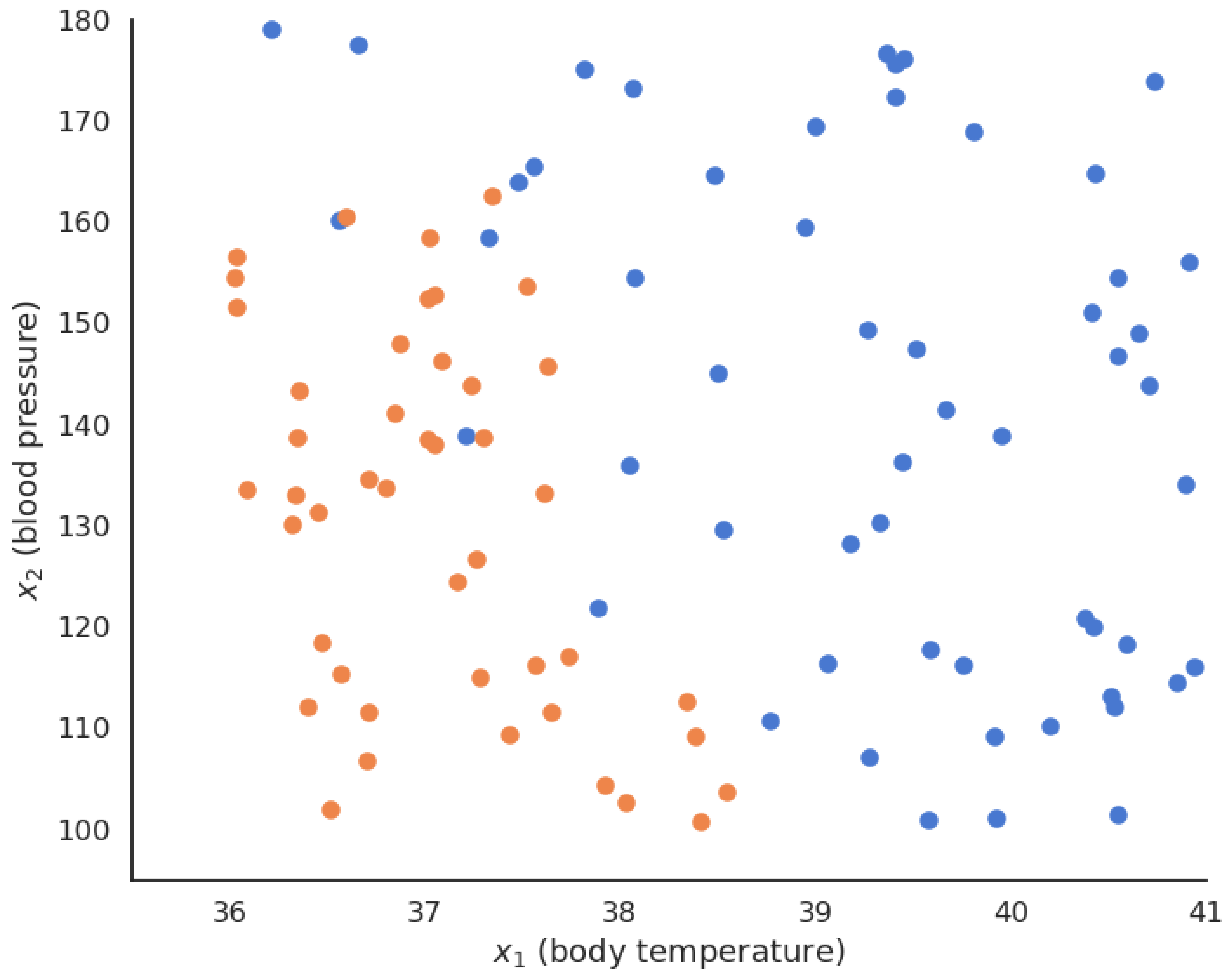
1 - Hard linear classification

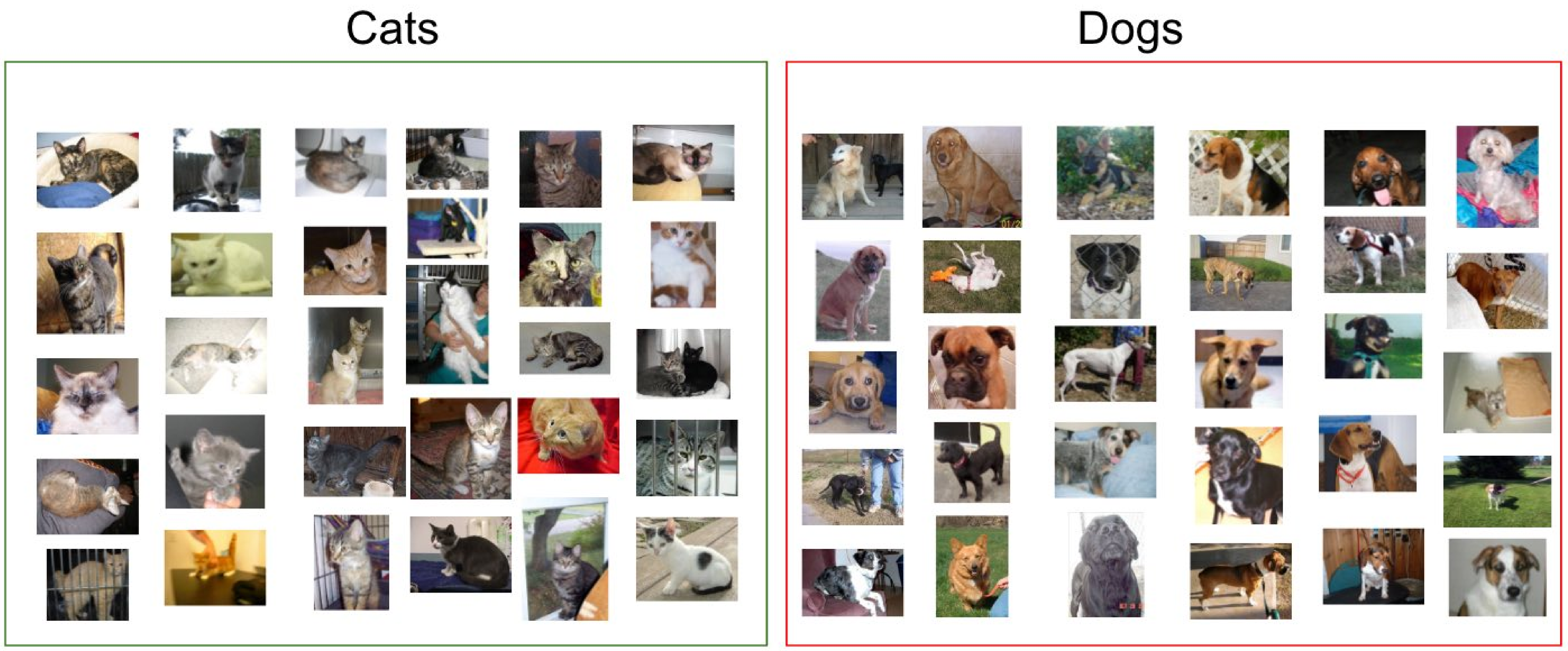
Binary classification

- The training data $\mathcal{D}$ is composed of N examples $(\mathbf{x}_i, t_i)_{i=1..N}$, with a d-dimensional input vector $\mathbf{x}_i \in \Re^d$ and a binary output $t_i \in \{-1, +1\}$
- The data points where $t = +1$ are called the **positive class**, the other the **negative class**.



Binary classification

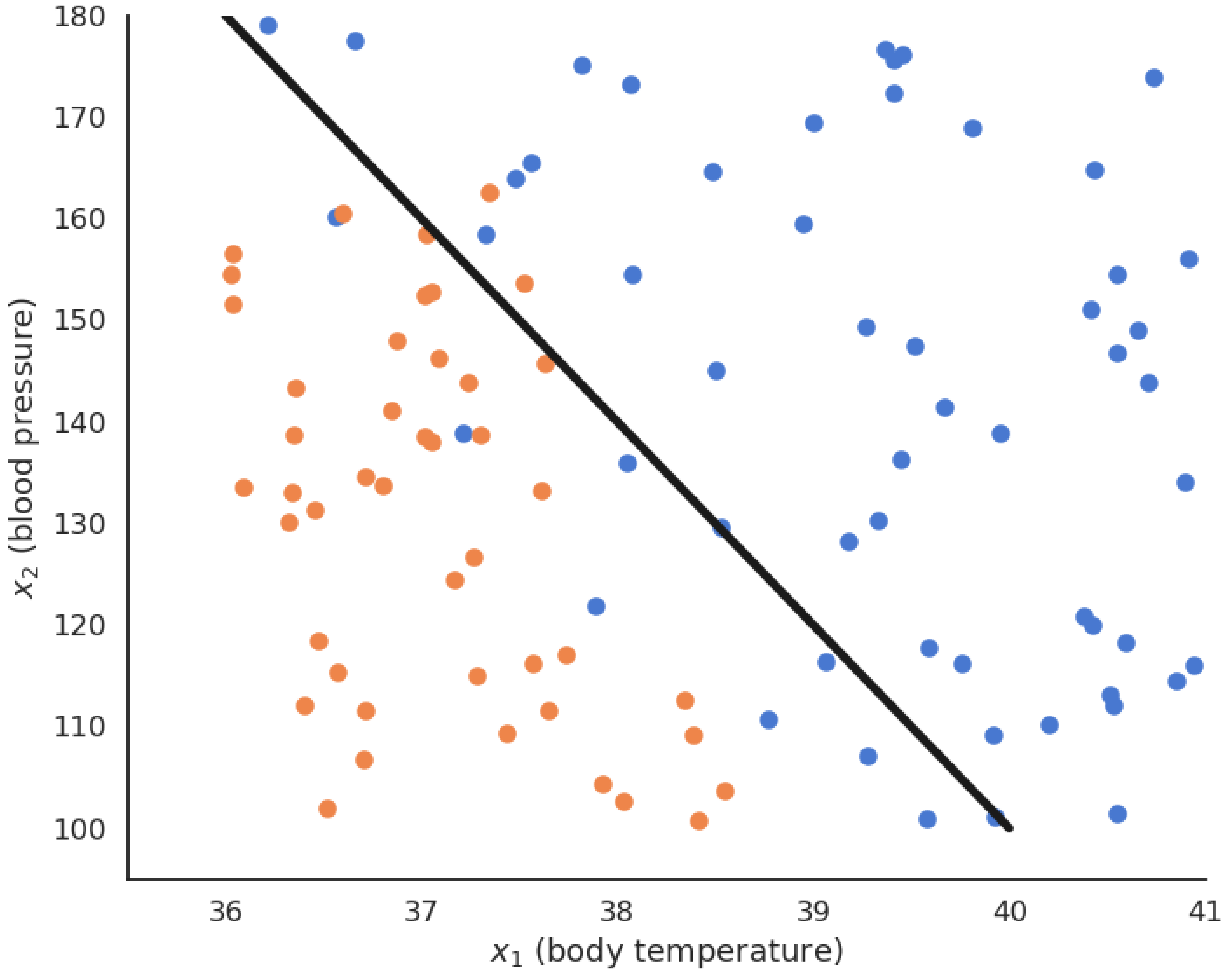
- For example, the inputs $\mathbf{x}_i$ can be images (one dimension per pixel) and the positive class corresponds to cats ($t_i = +1$), the negative class to dogs ($t_i = -1$).



Sample of cats & dogs images from Kaggle Dataset

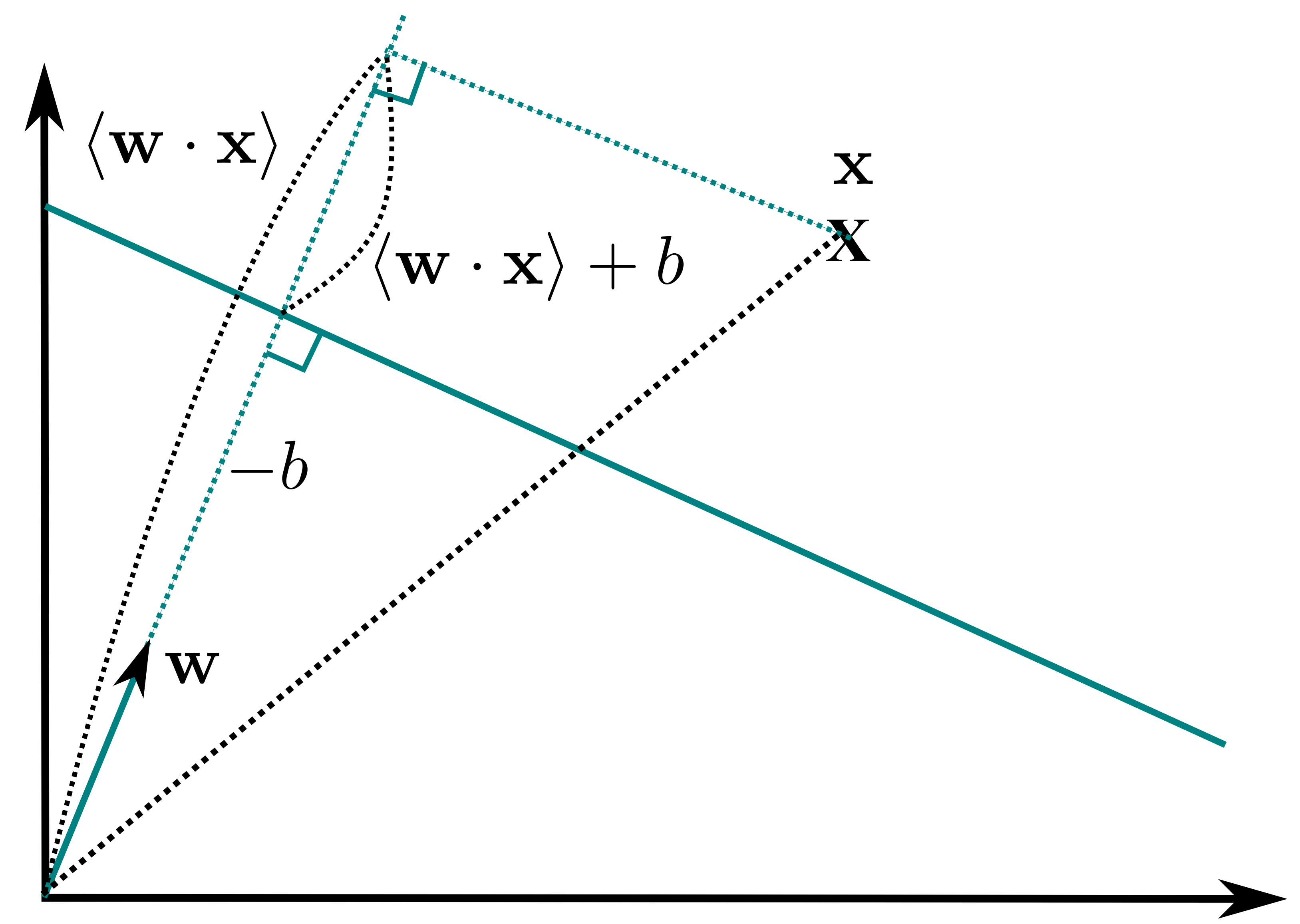
Binary linear classification

- We want to find the hyperplane $(\mathbf{w}, b)$ of $\Re^d$ that correctly separates the two classes.



Binary linear classification

- For a point $\mathbf{x} \in \mathcal{D}$, $\langle \mathbf{w} \cdot \mathbf{x} \rangle + b$ is the projection of $\mathbf{x}$ onto the hyperplane $(\mathbf{w}, b)$.
  - If $\langle \mathbf{w} \cdot \mathbf{x} \rangle + b > 0$, the point is above the hyperplane.
  - If $\langle \mathbf{w} \cdot \mathbf{x} \rangle + b < 0$, the point is below the hyperplane.
  - If $\langle \mathbf{w} \cdot \mathbf{x} \rangle + b = 0$, the point is on the hyperplane.
- By looking at the **sign** of $\langle \mathbf{w} \cdot \mathbf{x} \rangle + b$, we can predict the class of the input:



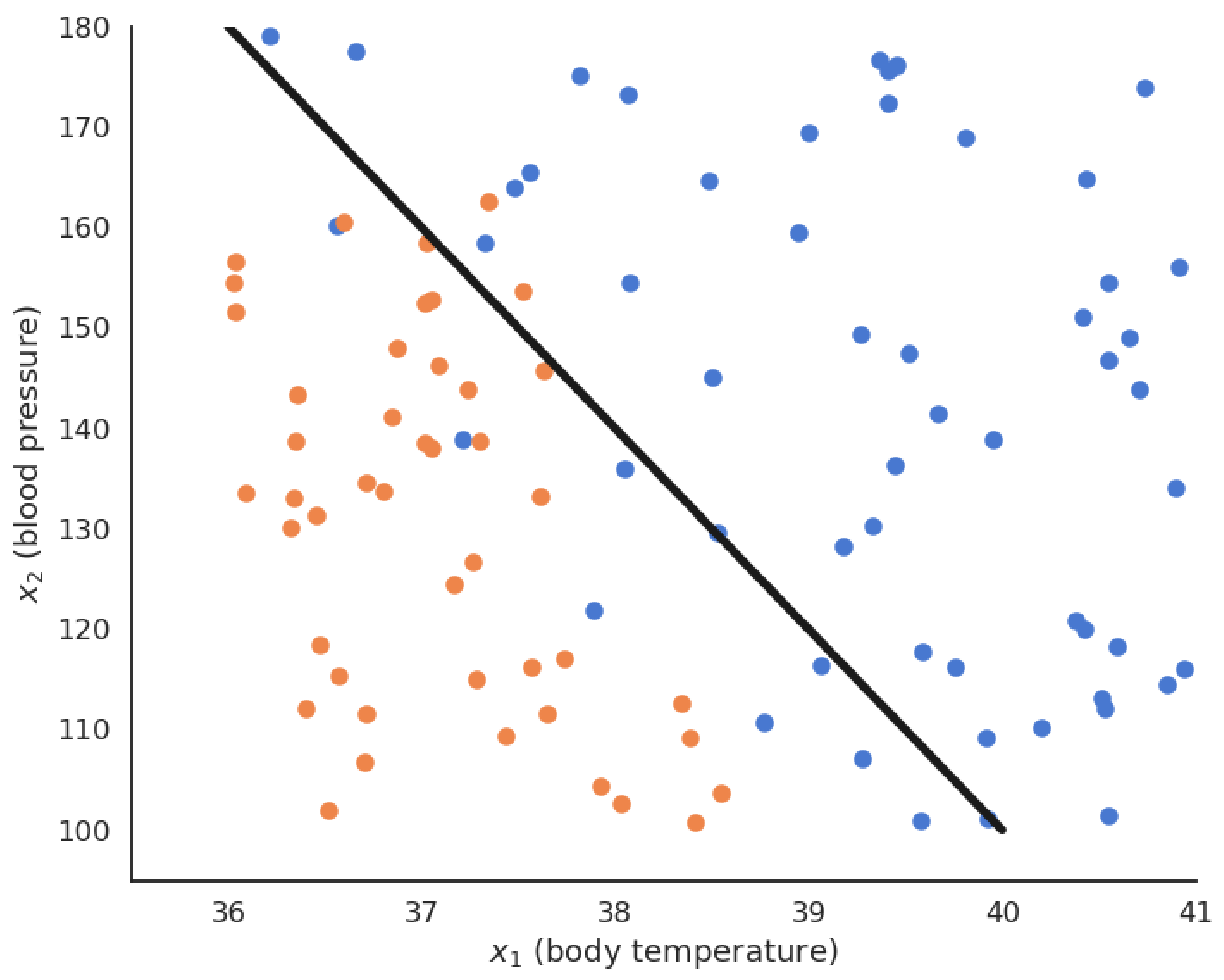
$\langle \mathbf{w} \cdot \mathbf{x} \rangle$
$\mathbf{x}$
$\langle \mathbf{w} \cdot \mathbf{x} \rangle + b$
$-b$
$\mathbf{w}$

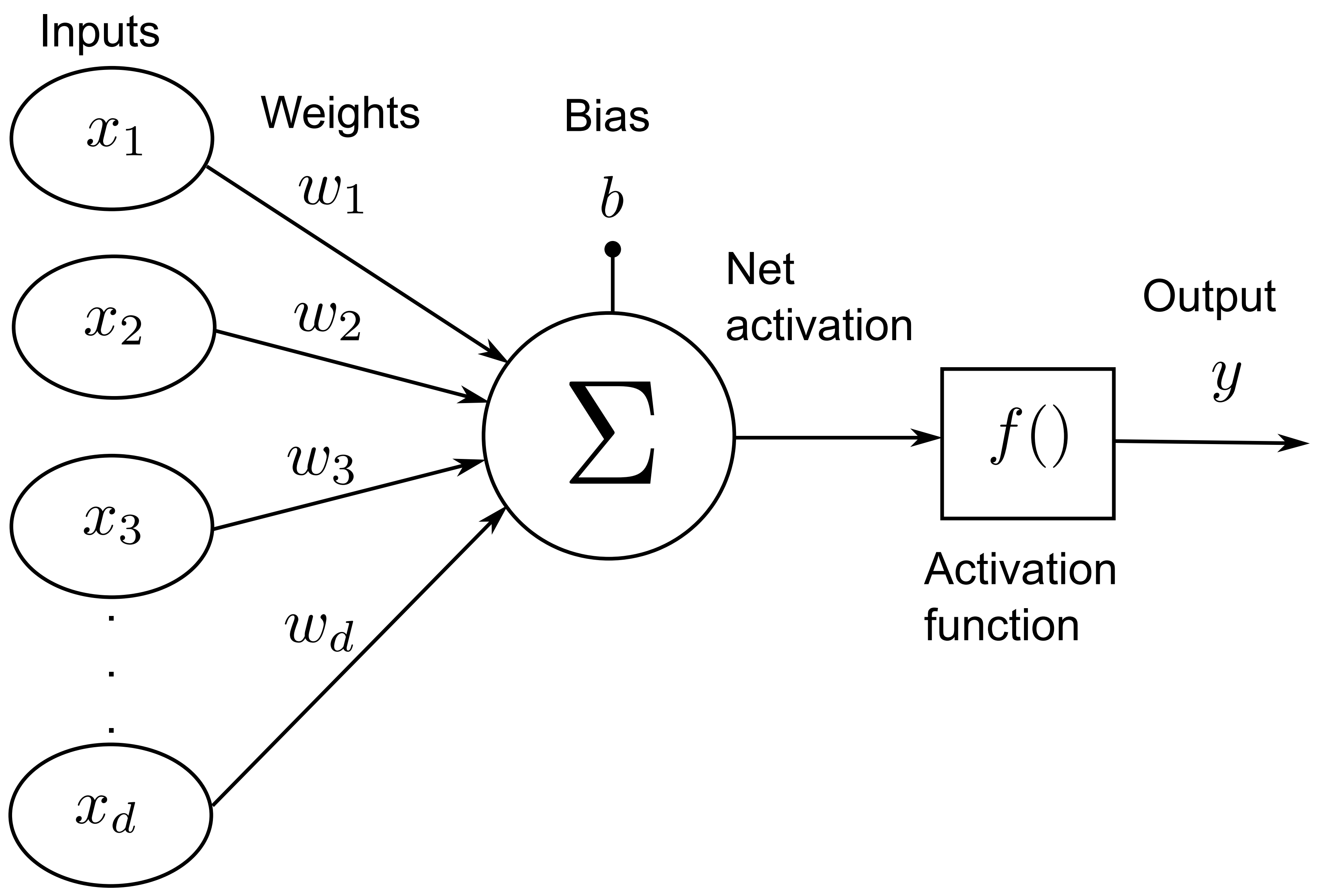
$$\operatorname{sign}(\langle \mathbf{w} \cdot \mathbf{x} \rangle + b) = \begin{cases} +1 \text{ if } \langle \mathbf{w} \cdot \mathbf{x} \rangle + b \geq 0 \\ -1 \text{ if } \langle \mathbf{w} \cdot \mathbf{x} \rangle + b < 0 \end{cases}$$

Binary linear classification

- Binary linear classification can be made by a single **artificial neuron** using the sign transfer function.

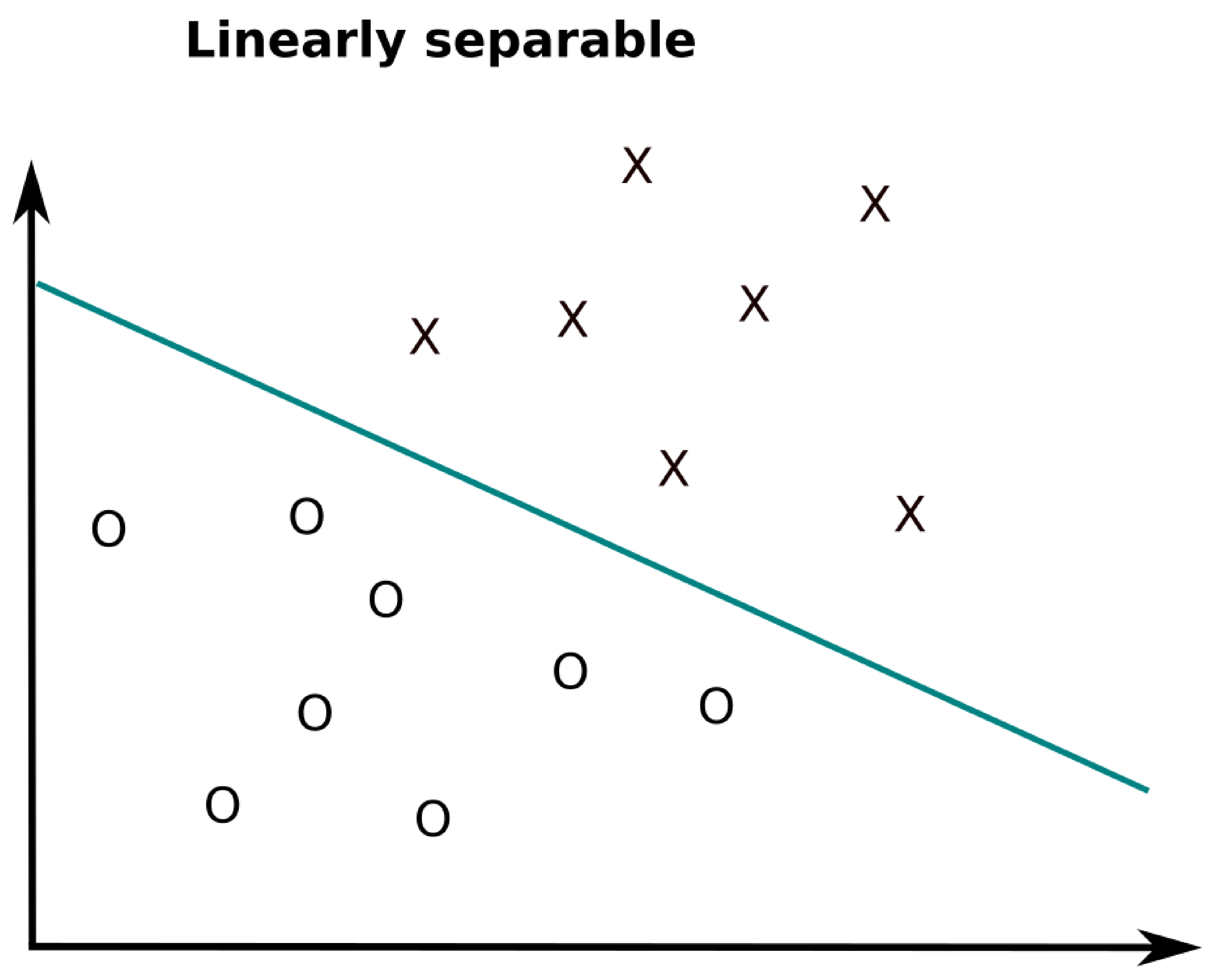
$$y = f_{\mathbf{w},b}(\mathbf{x}) = \text{sign}(\langle \mathbf{w} \cdot \mathbf{x} \rangle + b) = \text{sign}(\sum_{j=1}^{d} w_j \, x_j + b)$$

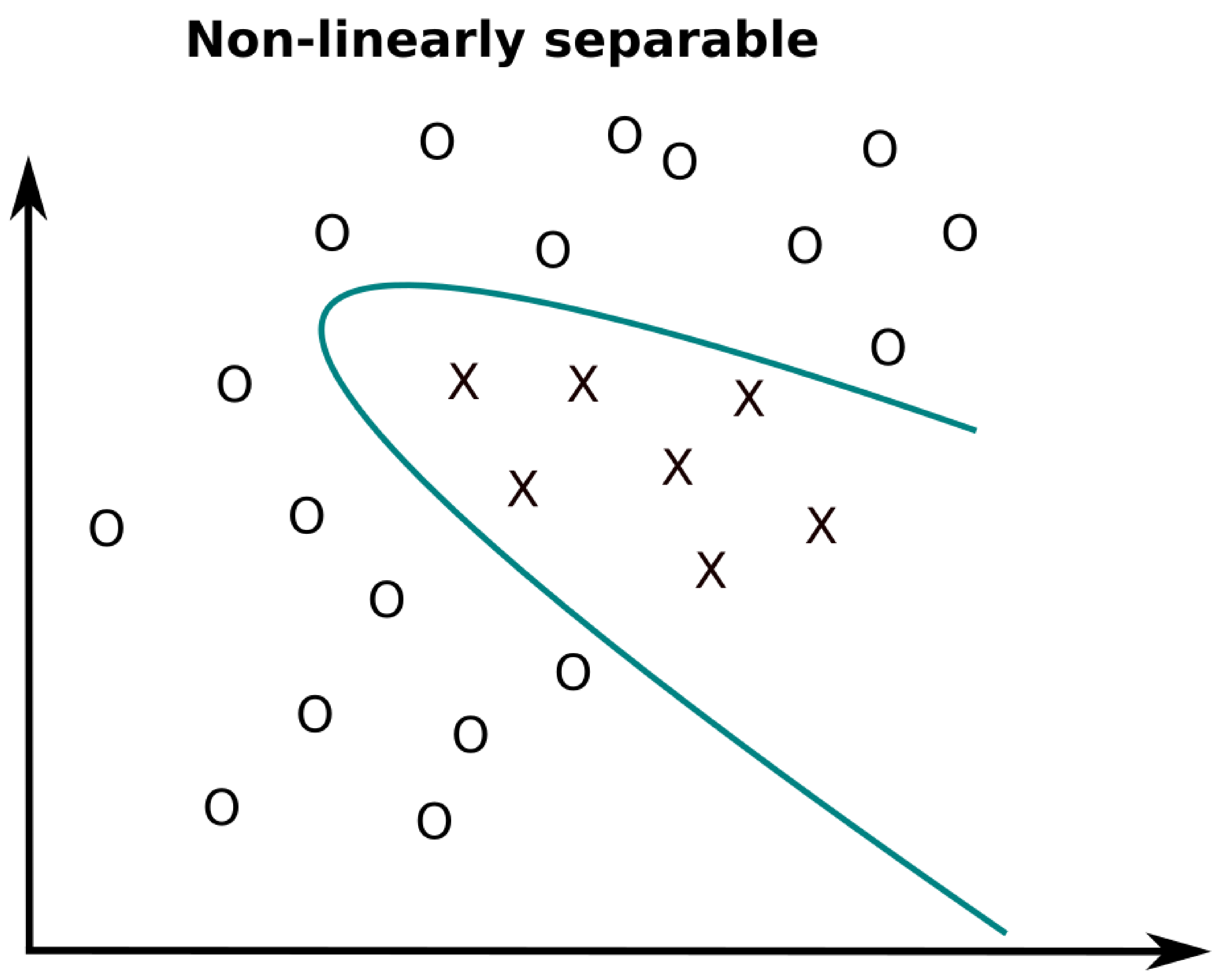




- $\mathbf{w}$ is the weight vector and b is the bias.

Linearly separable datasets





- Linear classification is the process of finding an hyperplane $(\mathbf{w}, b)$ that correctly separates the two classes.
- If such an hyperplane can be found, the training set is said **linearly separable**.
- Otherwise, the problem is **non-linearly separable** and other methods have to be applied (MLP, SVM…).

Linear classification as an optimization problem

- The Perceptron algorithm tries to find the weights and biases minimizing the **mean square error** (*mse*) or **quadratic loss**:

$$\mathcal{L}(\mathbf{w}, b) = \mathbb{E}_\mathcal{D} [(t_i - y_i)^2] \approx \frac{1}{N} \, \sum_{i=1}^{N} (t_i - y_i)^2$$

- When the prediction y_i is the same as the data t_i for all examples in the training set (perfect classification), the mse is minimal and equal to 0.
- We can apply gradient descent to find this minimum.

$$\begin{cases} \Delta \mathbf{w} = - \eta \, \nabla_\mathbf{w} \, \mathcal{L}(\mathbf{w}, b)\\ \\ \Delta b = - \eta \, \nabla_b \, \mathcal{L}(\mathbf{w}, b)\\ \end{cases}$$

Linear classification as an optimization problem

- Let's search for the partial derivative of the quadratic error function with respect to the weight vector:

$$\nabla_{\mathbf{w}} \mathcal{L}(\mathbf{w}, b) = \nabla_{\mathbf{w}} \frac{1}{N} \sum_{i=1}^{N} (t_i - y_i)^2 = \frac{1}{N} \sum_{i=1}^{N} \nabla_{\mathbf{w}} (t_i - y_i)^2 = \frac{1}{N} \sum_{i=1}^{N} \nabla_{\mathbf{w}} l_i(\mathbf{w}, b)$$

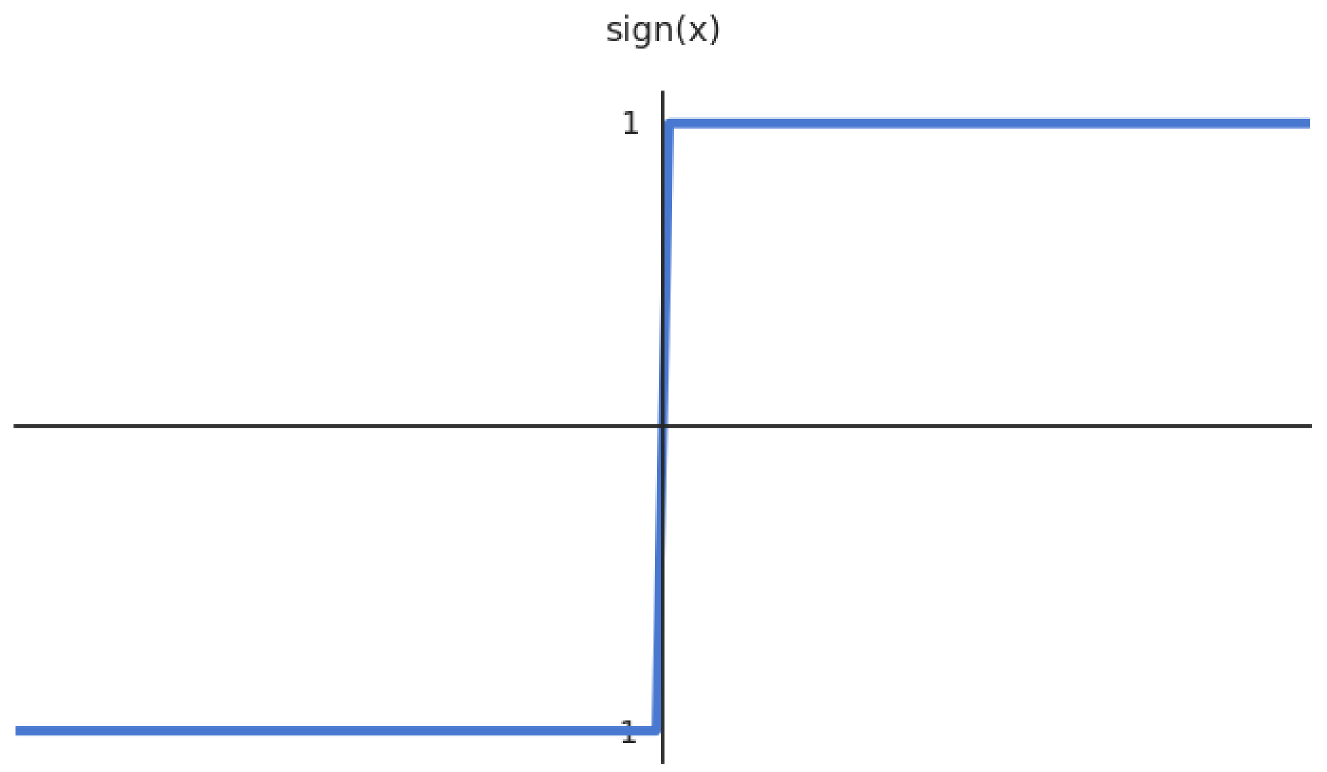
- Everything is similar to linear regression until we get:

$$\nabla_{\mathbf{w}} l_i(\mathbf{w}, b) = -2\,(t_i - y_i)\,\nabla_{\mathbf{w}}\,\text{sign}(\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b)$$

- In order to continue with the chain rule, we would need to differentiate $\text{sign}(x)$.

$$\nabla_{\mathbf{w}} l_i(\mathbf{w}, b) = -2\,(t_i - y_i)\,\text{sign}'(\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b)\,\mathbf{x}_i$$

- But the sign function is **not** differentiable…



Linear classification as an optimization problem

- We will simply pretend that the sign() function is linear, with a derivative of 1:

$$\nabla_\mathbf{w} \, l_i(\mathbf{w}, b) = -2 \, (t_i - y_i) \, \mathbf{x}_i$$

- The update rule for the weight vector $\mathbf{w}$ and the bias b is therefore the same as in linear regression:

$$\begin{cases} \Delta \mathbf{w} = \eta \, \frac{1}{N} \, \sum_{i=1}^{N} (t_i - y_i) \, \mathbf{x}_i \\ \\ \Delta b = \eta \, \frac{1}{N} \, \sum_{i=1}^{N} (t_i - y_i) \\ \end{cases}$$

Batch version of linear classification

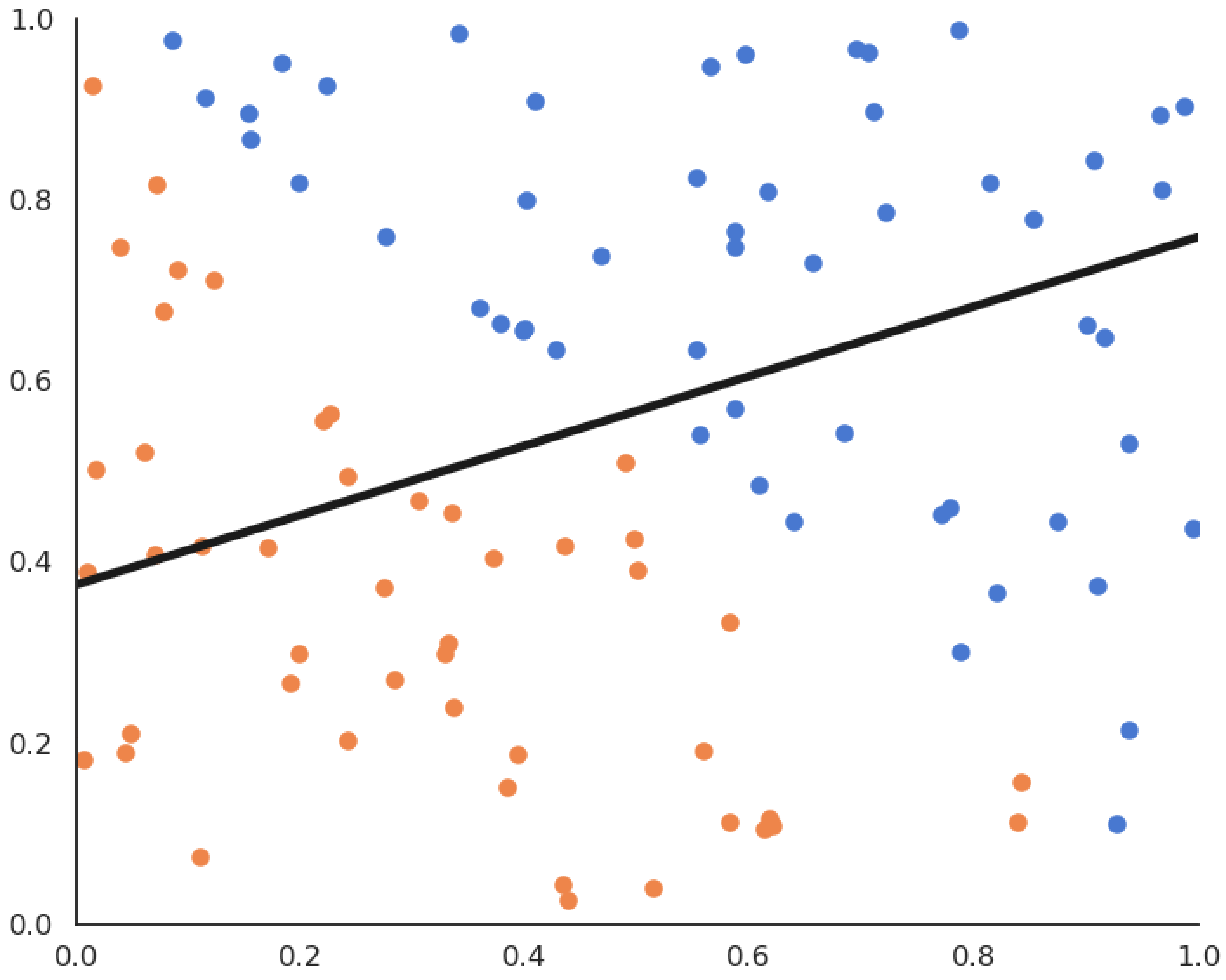
- By applying gradient descent on the quadratic error function, one obtains the following algorithm:

Batch linear classification

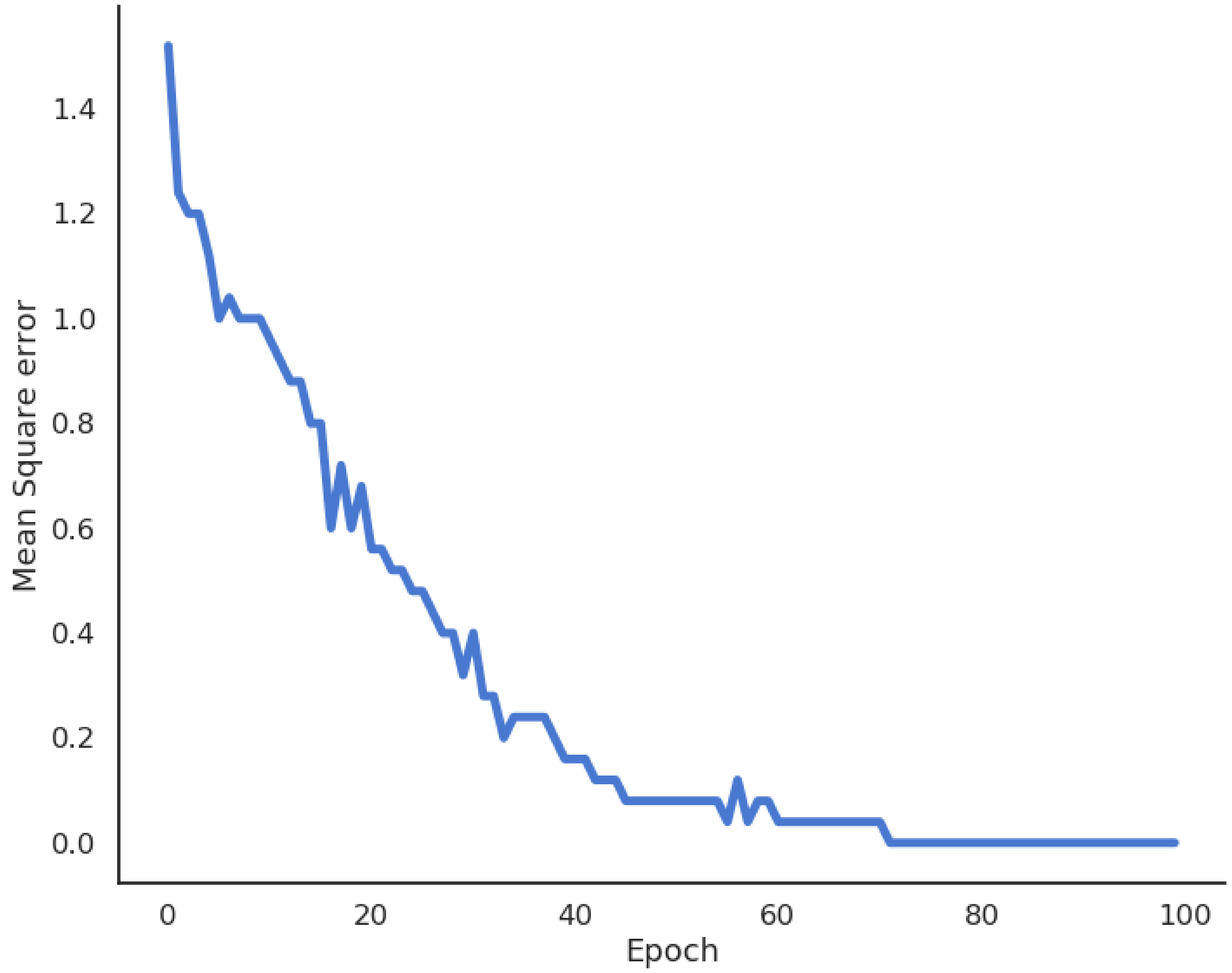
```
• for $M$ epochs:
    ▪ $\mathbf{dw} = 0 \qquad db = 0$
    ▪ for each sample $(\mathbf{x}_i, t_i)$:
        ◦ $y_i = \text{sign}(\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b)$
        ◦ $\mathbf{dw} = \mathbf{dw} + (t_i - y_i) \, \mathbf{x}_i$
        ◦ $db = db + (t_i - y_i)$
    ▪ $\Delta \mathbf{w} = \eta \, \frac{1}{N} \, \mathbf{dw}$
    ▪ $\Delta b = \eta \, \frac{1}{N} \, db$
```

- This is called the **batch** version of the Perceptron algorithm.
- If the data is linearly separable and η is well chosen, it converges to the minimum of the mean square error.

Linear classification: batch version



Linear classification: batch version



Online version of linear classification : the Perceptron algorithm

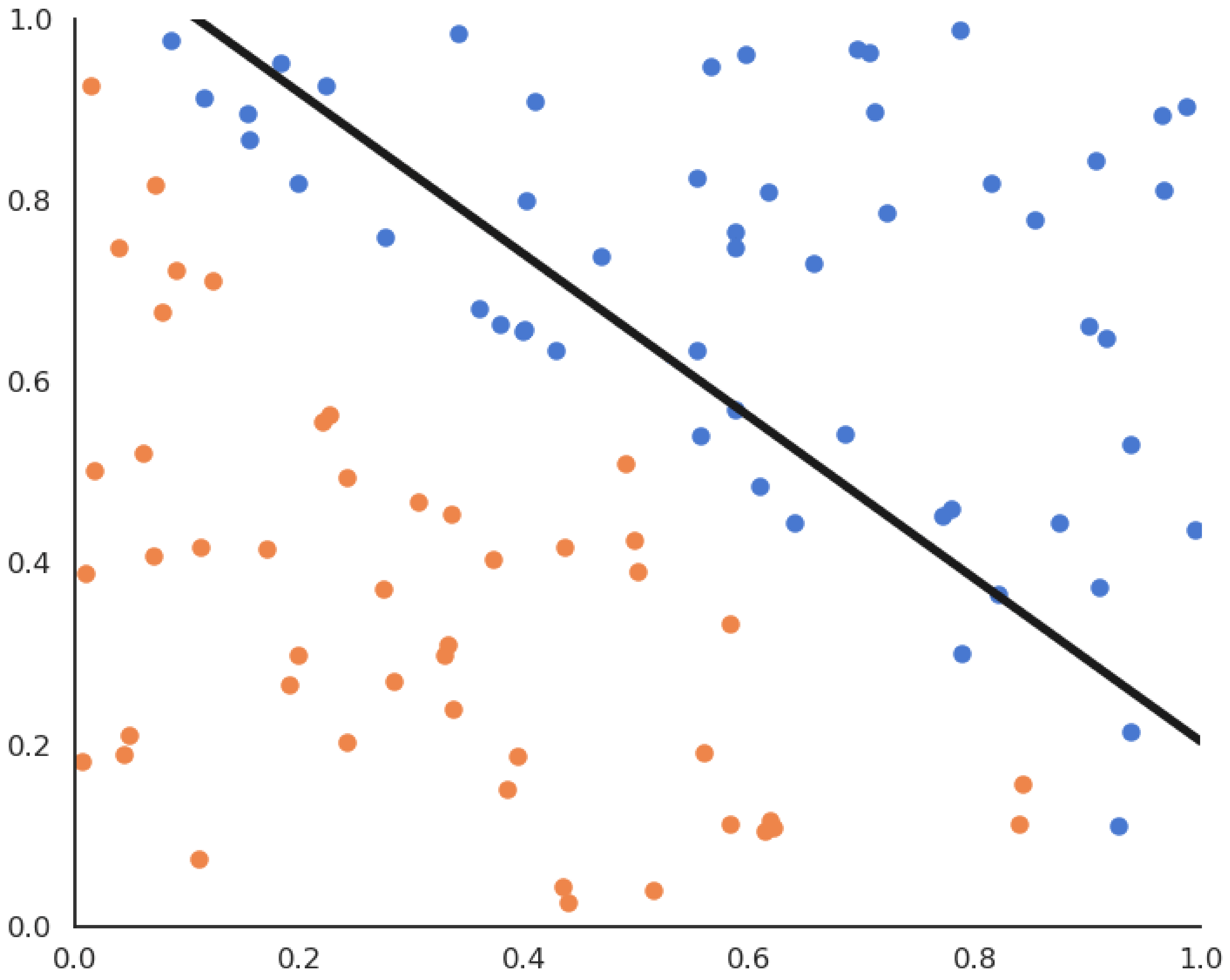
- The **Perceptron algorithm** was invented by the psychologist Frank Rosenblatt in 1958. It was the first algorithmic neural network able to learn linear classification.

Perceptron algorithm

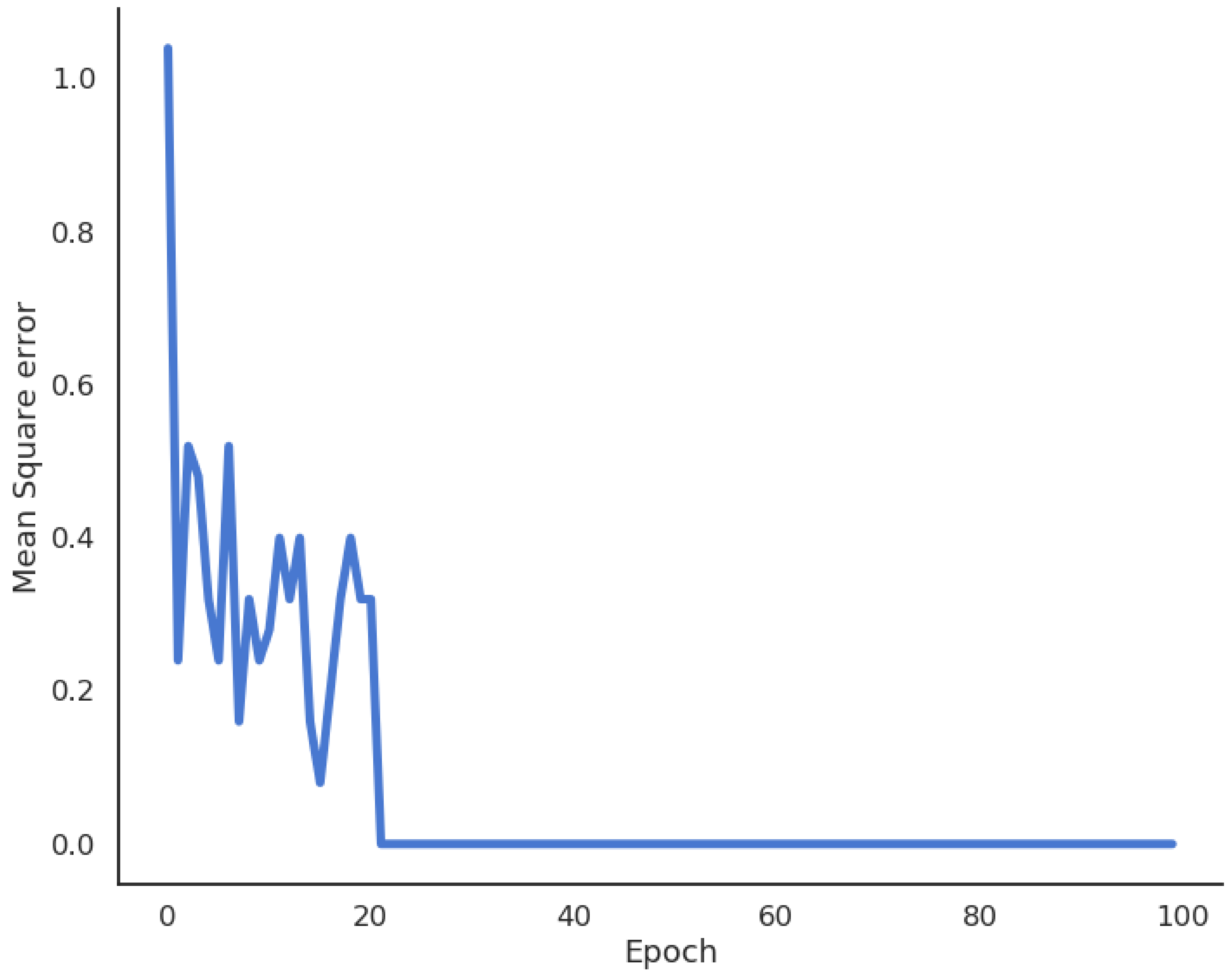
```
- for $M$ epochs:
    - for each sample $(\mathbf{x}_i, t_i)$:
        - $y_i = \text{sign}( \langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b)$
        - $\Delta \mathbf{w} = \eta \, (t_i - y_i) \, \mathbf{x}_i$
        - $\Delta b = \eta \, (t_i - y_i)$
```

- This algorithm iterates over all examples of the training set and applies the **delta learning rule** to each of them immediately, not at the end on the whole training set.
- One could check whether there are still classification errors on the training set at the end of each epoch and stop the algorithm.
- The delta learning rule depends on the learning rate η, the error made by the prediction $(t_i - y_i)$ and the input $\mathbf{x}_i$.

Linear classification: online version



Linear classification: online version



Batch vs. Online learning

- The mean square error is defined as the **expectation** over the data:

$$\mathcal{L}(\mathbf{w}, b) = \mathbb{E}_\mathcal{D}[(t_i - y_i)^2]$$

- **Batch learning** uses the whole training set as samples to estimate the mse:

$$\mathcal{L}(\mathbf{w}, b) \approx \frac{1}{N} \sum_{i=1}^N (t_i - y_i)^2$$

$$\Delta \mathbf{w} = \eta \, \frac{1}{N} \sum_{i=1}^N (t_i - y_i) \, \mathbf{x_i}$$

- **Online learning** uses a single sample to estimate the mse:

$$\mathcal{L}(\mathbf{w}, b) \approx (t_i - y_i)^2$$

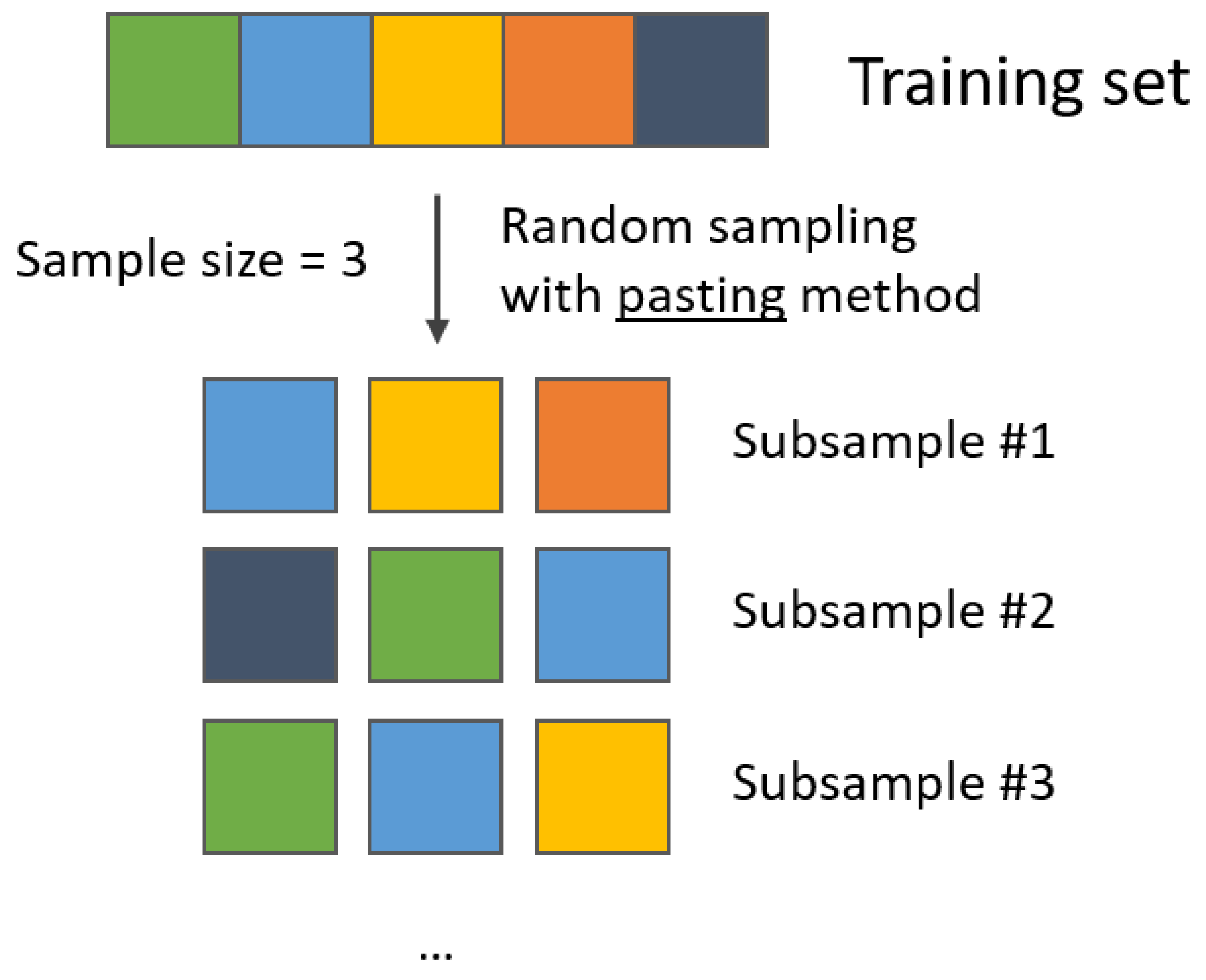
$$\Delta \mathbf{w} = \eta \, (t_i - y_i) \, \mathbf{x_i}$$

- Batch learning has less bias (central limit theorem) and is less sensible to noise in the data, but is very slow.
- Online learning converges faster, but can be instable and overfits (high variance).

Stochastic Gradient Descent - SGD

- In practice, we use a trade-off between batch and online learning called **Stochastic Gradient Descent (SGD)** or **Minibatch Gradient Descent**.

- The training set is randomly split at each epoch into small chunks of data (a **minibatch**, usually 32 or 64 examples) and the batch learning rule is applied on each chunk.



$$\Delta \mathbf{w} = \eta \, \frac{1}{K} \sum_{i=1}^{K} (t_i - y_i) \, \mathbf{x_i}$$

- If the **batch size** is well chosen, SGD is as stable as batch learning and as fast as online learning.
- The minibatches are randomly selected at each epoch (i.i.d).

- Online learning is a stochastic gradient descent with a batch size of 1.

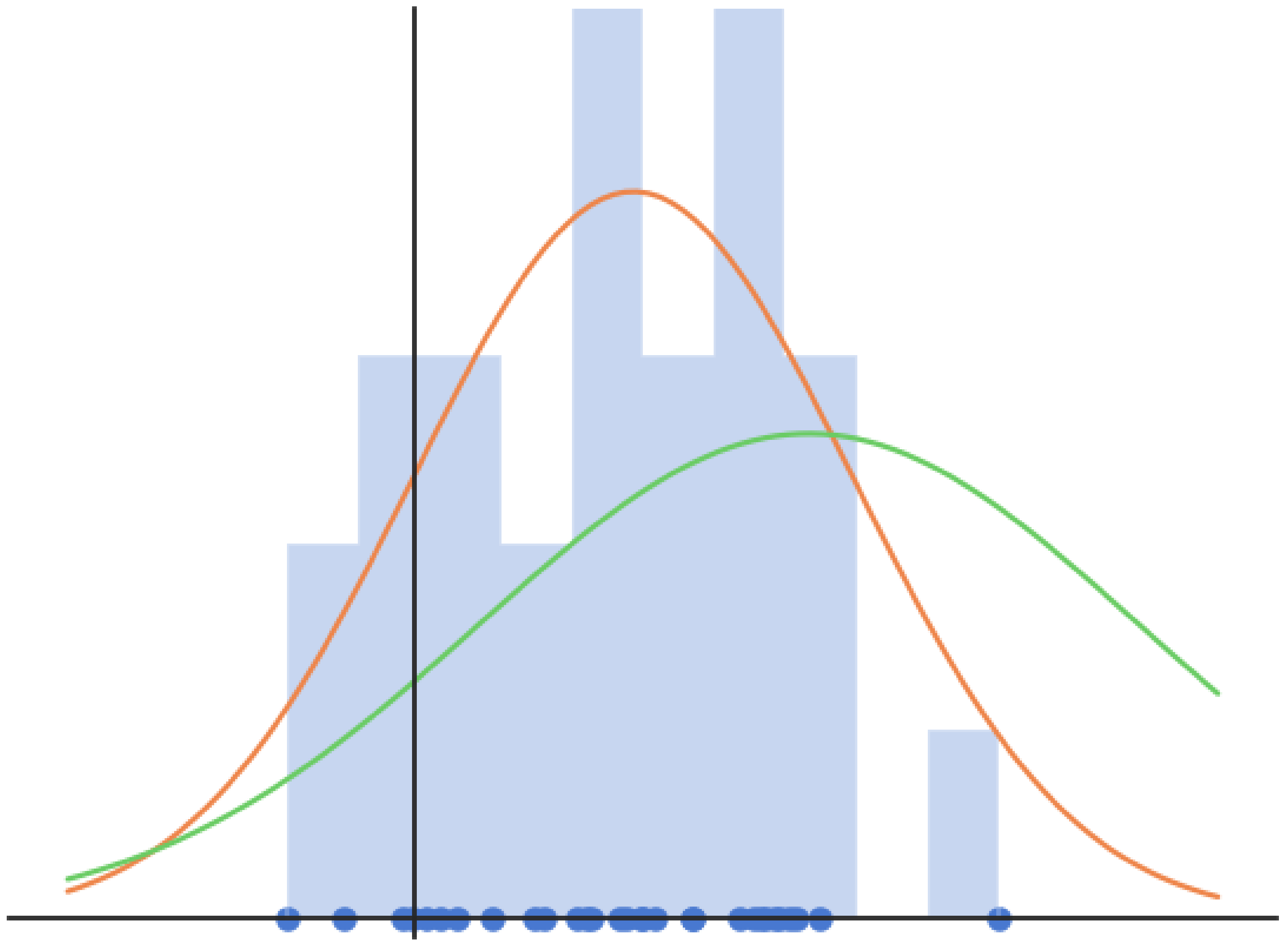
2 - Maximum Likelihood Estimation

Maximum Likelihood Estimation

- Let's consider N **samples** $\{x_i\}_{i=1}^N$ independently taken from a **normal distribution** X.
- The probability density function (pdf) of a normal distribution is:

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

where μ is the mean of the distribution and σ its standard deviation.



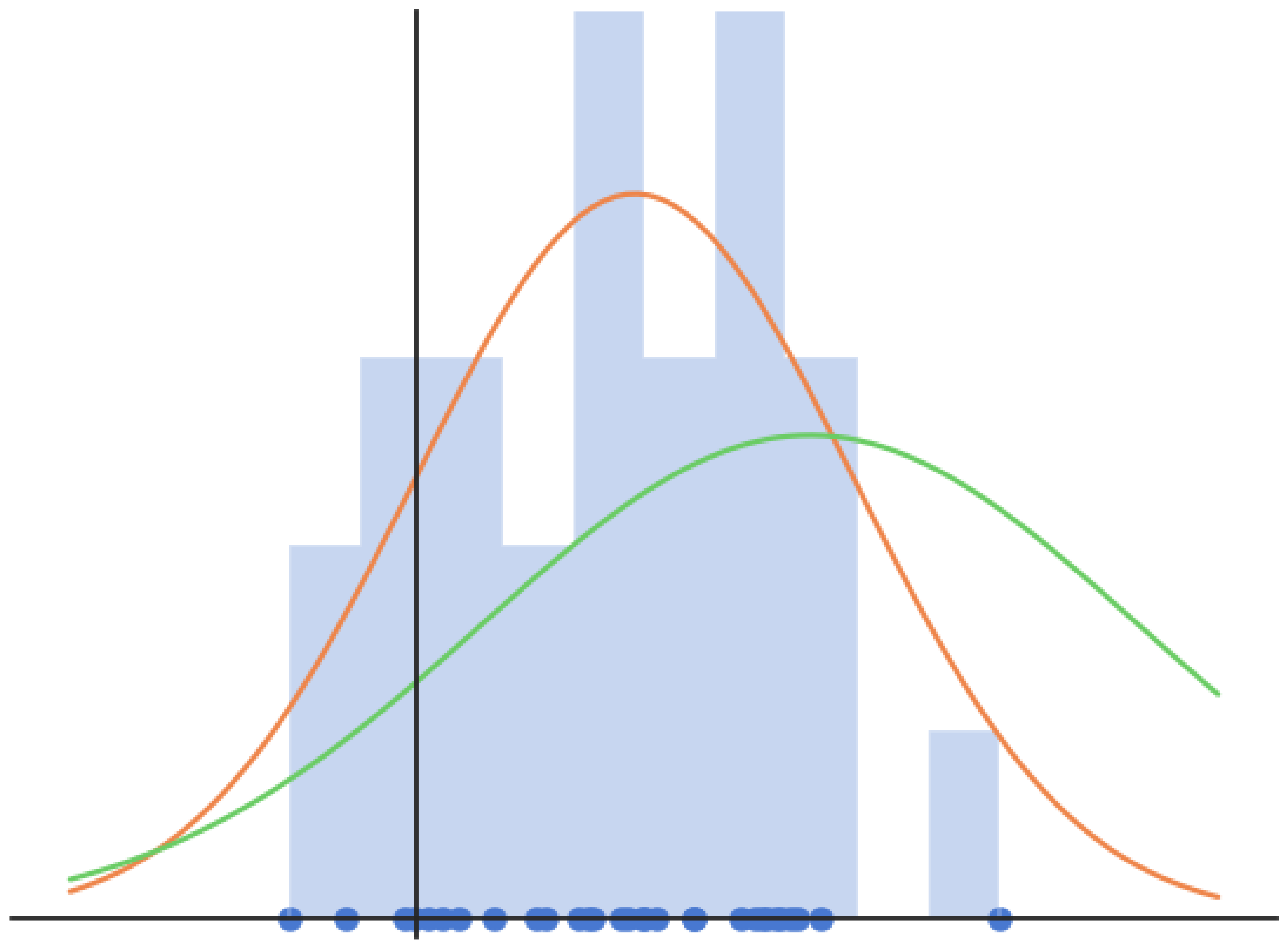
- The problem is to find the values of μ and σ which explain best the observations $\{x_i\}_{i=1}^N$.

Maximum Likelihood Estimation

- The idea of MLE is to maximize the joint density function for all observations. This function is expressed by the **likelihood function**:

$$L(\mu,\sigma) = P(\mathbf{x};\mu,\sigma) = \prod_{i=1}^{N} f(x_i;\mu,\sigma)$$

- When the pdf takes high values for all samples, it is quite likely that the samples come from this particular distribution.



- The likelihood function reflects how well the parameters μ and σ explain the observations $\{x_i\}_{i=1}^{N}$.
- Note: the samples must be i.i.d. so that the likelihood is a product.

Maximum Likelihood Estimation

- We therefore search for the values μ and σ which **maximize** the likelihood function.

$$\max_{\mu, \sigma} \quad L(\mu, \sigma) = \prod_{i=1}^{N} f(x_i; \mu, \sigma)$$

- For the normal distribution, the likelihood function is:

$$\begin{aligned}
L(\mu, \sigma) &= \prod_{i=1}^{N} f(x_i; \mu, \sigma) \\
&= \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi\sigma^2}} \, \exp{- \frac{(x_i - \mu)^2}{2\sigma^2}} \\
&= (\frac{1}{\sqrt{2\pi\sigma^2}})^N \, \prod_{i=1}^{N} \exp{- \frac{(x_i - \mu)^2}{2\sigma^2}} \\
&= (\frac{1}{\sqrt{2\pi\sigma^2}})^N \, \exp{- \frac{\sum_{i=1}^{N}(x_i - \mu)^2}{2\sigma^2}}
\end{aligned}$$

Maximum Likelihood Estimation

- To find the maximum of $L(\mu, \sigma)$, we need to search where the gradient is equal to zero:

$$\begin{cases} \frac{\partial L(\mu, \sigma)}{\partial \mu} = 0 \\ \frac{\partial L(\mu, \sigma)}{\partial \sigma} = 0 \end{cases}$$

- The likelihood function is complex to differentiate, so we consider its logarithm $l(\mu, \sigma) = \log(L(\mu, \sigma))$ which has a maximum for the same value of (μ, σ) as the log function is monotonic.

$$\begin{aligned} l(\mu, \sigma) &= \log(L(\mu, \sigma)) \\ &= \log \left((\frac{1}{\sqrt{2\pi\sigma^2}})^N \ \exp - \frac{\sum_{i=1}^N (x_i - \mu)^2}{2\sigma^2} \right) \\ &= - \frac{N}{2} \log(2\pi\sigma^2) - \frac{\sum_{i=1}^N (x_i - \mu)^2}{2\sigma^2} \end{aligned}$$

- $l(\mu, \sigma)$ is called the **log-likelihood** function.

Maximum Likelihood Estimation

$$l(\mu, \sigma) = -\frac{N}{2}\log(2\pi\sigma^2) - \frac{\sum_{i=1}^{N}(x_i - \mu)^2}{2\sigma^2}$$

- The maximum of the log-likelihood function respects:

$$\begin{aligned}
\frac{\partial l(\mu, \sigma)}{\partial \mu} &= \frac{\sum_{i=1}^{N}(x_i - \mu)}{\sigma^2} = 0 \\
\frac{\partial l(\mu, \sigma)}{\partial \sigma} &= -\frac{N}{2}\frac{4\pi\sigma}{2\pi\sigma^2} + \frac{\sum_{i=1}^{N}(x_i - \mu)^2}{\sigma^3} \\
&= -\frac{N}{\sigma} + \frac{\sum_{i=1}^{N}(x_i - \mu)^2}{\sigma^3} = 0
\end{aligned}$$

- We obtain:

$$\mu = \frac{1}{N}\sum_{i=1}^{N} x_i \qquad \sigma^2 = \frac{1}{N}\sum_{i=1}^{N}(x_i - \mu)^2$$

Maximum Likelihood Estimation

- Unsurprisingly, the mean and variance of the normal distribution which best explains the data are the mean and variance of the data…

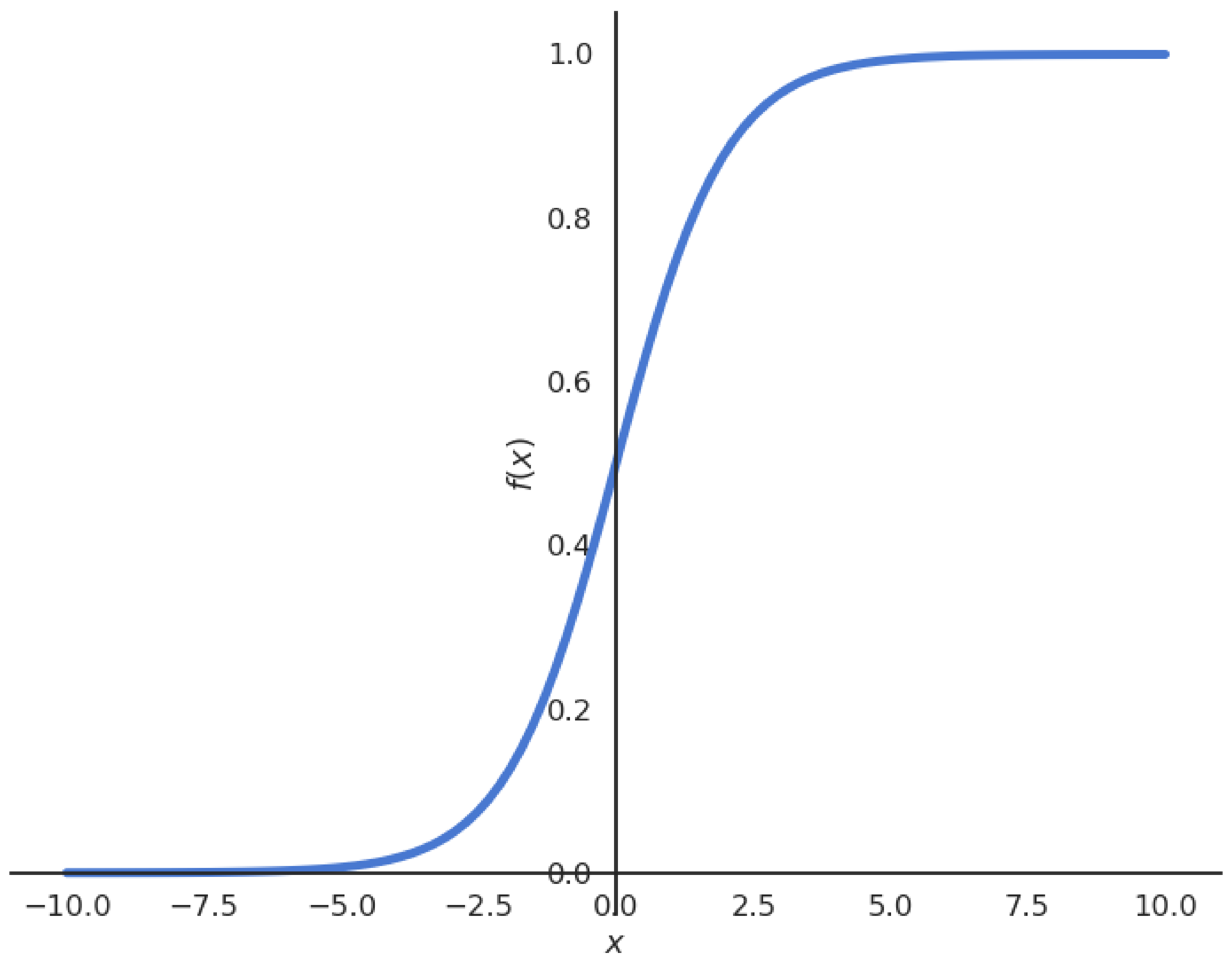
$$\mu = \frac{1}{N} \sum_{i=1}^{N} x_i \qquad \sigma^2 = \frac{1}{N} \sum_{i=1}^{N} (x_i - \mu)^2$$

- The same principle can be applied to estimate the parameters of any distribution: normal, exponential, Bernouilli, Poisson, etc…
- When a machine learning method has an probabilistic interpretation (i.e. it outputs probabilities), MLE can be used to find its parameters.
- One can use global optimization like here, or gradient descent to estimate the parameters iteratively.

3 - Soft linear classification : Logistic regression

Reminder: Logistic regression

- We want to perform a regression, but where the targets t_i are bounded betwen 0 and 1.



- We can use a logistic function instead of a linear function in order to transform the net activation into an output:

$$y = \sigma(w \, x + b) = \frac{1}{1 + \exp(-w \, x - b)}$$

Use of logistic regression for soft classification

- Logistic regression can be used in binary classification if we consider $y = \sigma(w \, x + b)$ as the probability that the example belongs to the positive class ($t = 1$).

$$P(t = 1 | x; w, b) = y; \qquad P(t = 0 | x; w, b) = 1 - y$$

- The output t therefore comes from a Bernouilli distribution $\mathcal{B}$ of parameter $p = y = f_{w,b}(x)$. The probability mass function (pmf) is:

$$f(t | x; w, b) = y^t \, (1 - y)^{1-t}$$

- If we consider our training samples (x_i, t_i) as independently taken from this distribution, our task is:
  - to find the parameterized distribution that best explains the data, which means:
  - to find the parameters w and b maximizing the **likelihood** that the samples t come from a Bernouilli distribution when x, w and b are given.
- We only need to apply **Maximum Likelihood Estimation** (MLE) on this Bernouilli distribution!

MLE for logistic regression

- The likelihood function for logistic regression is :

$$
\begin{aligned}
L(w, b) = P(t|x; w, b) = \prod_{i=1}^{N} f(t_i|x_i; w, b) \\
= \prod_{i=1}^{N} y_i^{t_i} \, (1 - y_i)^{1-t_i}
\end{aligned}
$$

- The likelihood function is quite hard to differentiate, so we take the **log-likelihood** function:

$$
\begin{aligned}
l(w, b) = \log L(w, b) \\
= \sum_{i=1}^{N} [t_i \, \log y_i + (1 - t_i) \, \log(1 - y_i)]
\end{aligned}
$$

- or even better: the **negative log-likelihood** which will be minimized using gradient descent:

$$
\mathcal{L}(w, b) = - \sum_{i=1}^{N} [t_i \, \log y_i + (1 - t_i) \, \log(1 - y_i)]
$$

MLE for logistic regression

- We then search for the minimum of the negative log-likelihood function by computing its gradient (here for a single sample):

$$
\begin{aligned}
\frac{\partial l_i(w, b)}{\partial w} & = - \frac{\partial}{\partial w} [t_i \, \log y_i + (1 - t_i) \, \log(1 - y_i)] \\
& = - t_i \, \frac{\partial}{\partial w} \log y_i - (1 - t_i) \, \frac{\partial}{\partial w} \log(1 - y_i) \\
& = - t_i \, \frac{\frac{\partial}{\partial w} y_i}{y_i} - (1 - t_i) \, \frac{\frac{\partial}{\partial w} (1 - y_i)}{1 - y_i} \\
& = - t_i \, \frac{y_i \, (1 - y_i) \, x_i}{y_i} + (1 - t_i) \, \frac{y_i \, (1 - y_i) \, x_i}{1 - y_i} \\
& = - (t_i - y_i) \, x_i
\end{aligned}
$$

- Same gradient as the linear perceptron, but with a non-linear output function!

Logistic regression for soft classification

- Logistic regression is a regression method used for classification. It uses a non-linear transfer function $\sigma(x) = \frac{1}{1+\exp(-x)}$ applied on the net activation:

$$y_i = \sigma(\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b)$$

- The continuous output y is interpreted as the probability of belonging to the positive class.

$$P(t_i = 1 | \mathbf{x}_i; \mathbf{w}, b) = y_i; \qquad P(t_i = 0 | \mathbf{x}_i; \mathbf{w}, b) = 1 - y_i$$

- We minimize the **negative log-likelihood** loss function using gradient descent:

$$\mathcal{L}(\mathbf{w}, b) = - \sum_{i=1}^{N} [t_i \, \log y_i + (1 - t_i) \, \log(1 - y_i)]$$

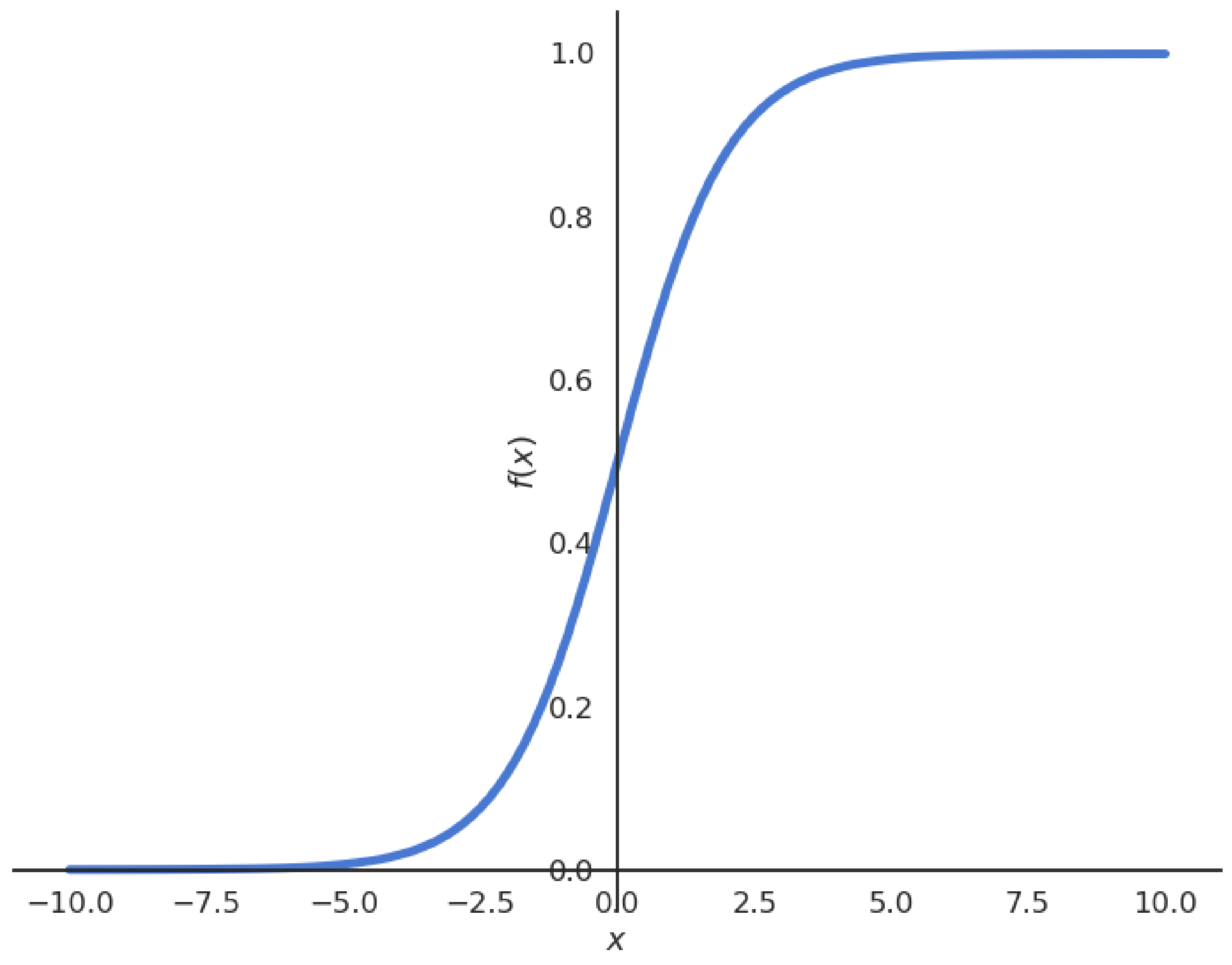
- We obtain the delta learning rule, using the class as a target and the probability as a prediction:

$$\begin{cases} \Delta \mathbf{w} = \eta \, (t_i - y_i) \, \mathbf{x}_i \\ \\ \Delta b = \eta \, (t_i - y_i) \end{cases}$$

Logistic regression

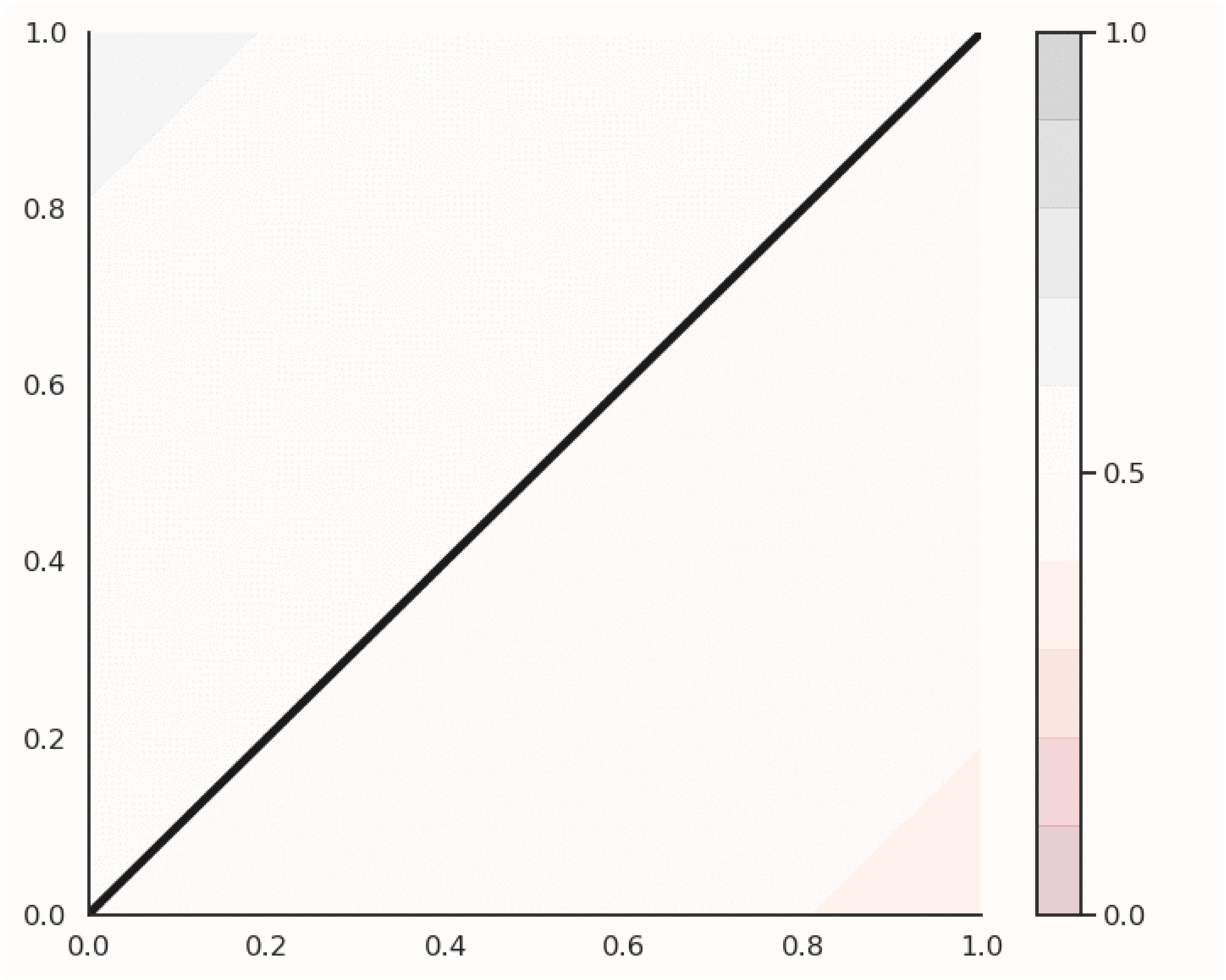
Logistic regression

```
• $\mathbf{w} = 0 \qquad b = 0$
• for $M$ epochs:
    ▪ for each sample $(\mathbf{x}_i, t_i)$:
        ∘ $y_i = \sigma(\langle \mathbf{w} \cdot \mathbf{x}_i \rangle + b)$
        ∘ $\Delta \mathbf{w} = \eta \, (t_i - y_i) \, \mathbf{x}_i$
        ∘ $\Delta b = \eta \, (t_i - y_i)$
```

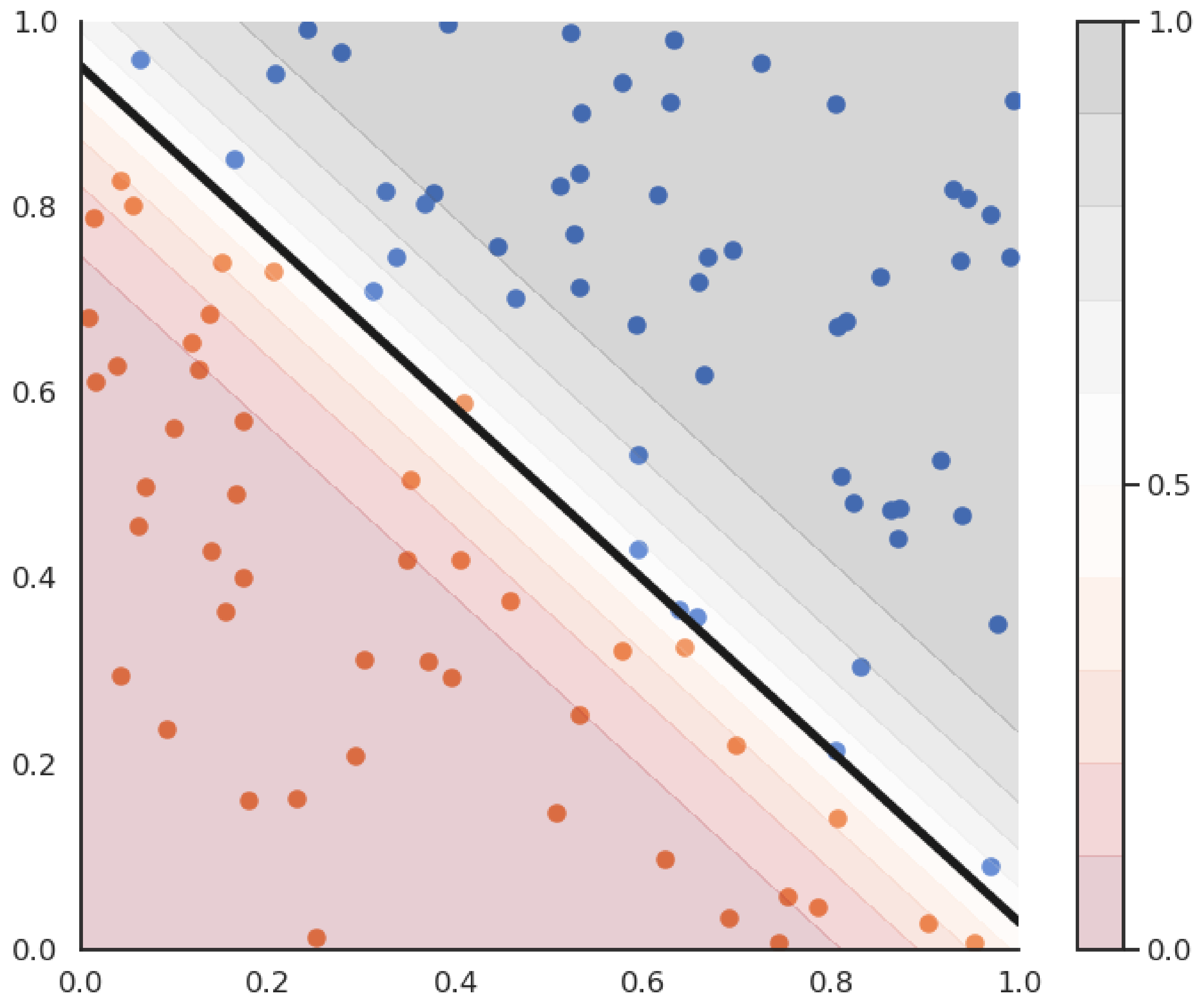


- Logistic regression works just like linear classification, except in the way the prediction is done.
- To know to which class $\mathbf{x}_i$ belongs, simply draw a random number between 0 and 1:
    - if it is smaller than y_i (probability y_i), it belongs to the positive class.
    - if it is bigger than y_i (probability $1 - y_i$), it belongs to the negative class.
- Alternatively, you can put a **hard limit** at 0.5:
    - if $y_i > 0.5$ then the class is positive.
    - if $y_i < 0.5$ then the class is negative.

Logistic regression



Logistic regression and confidence score

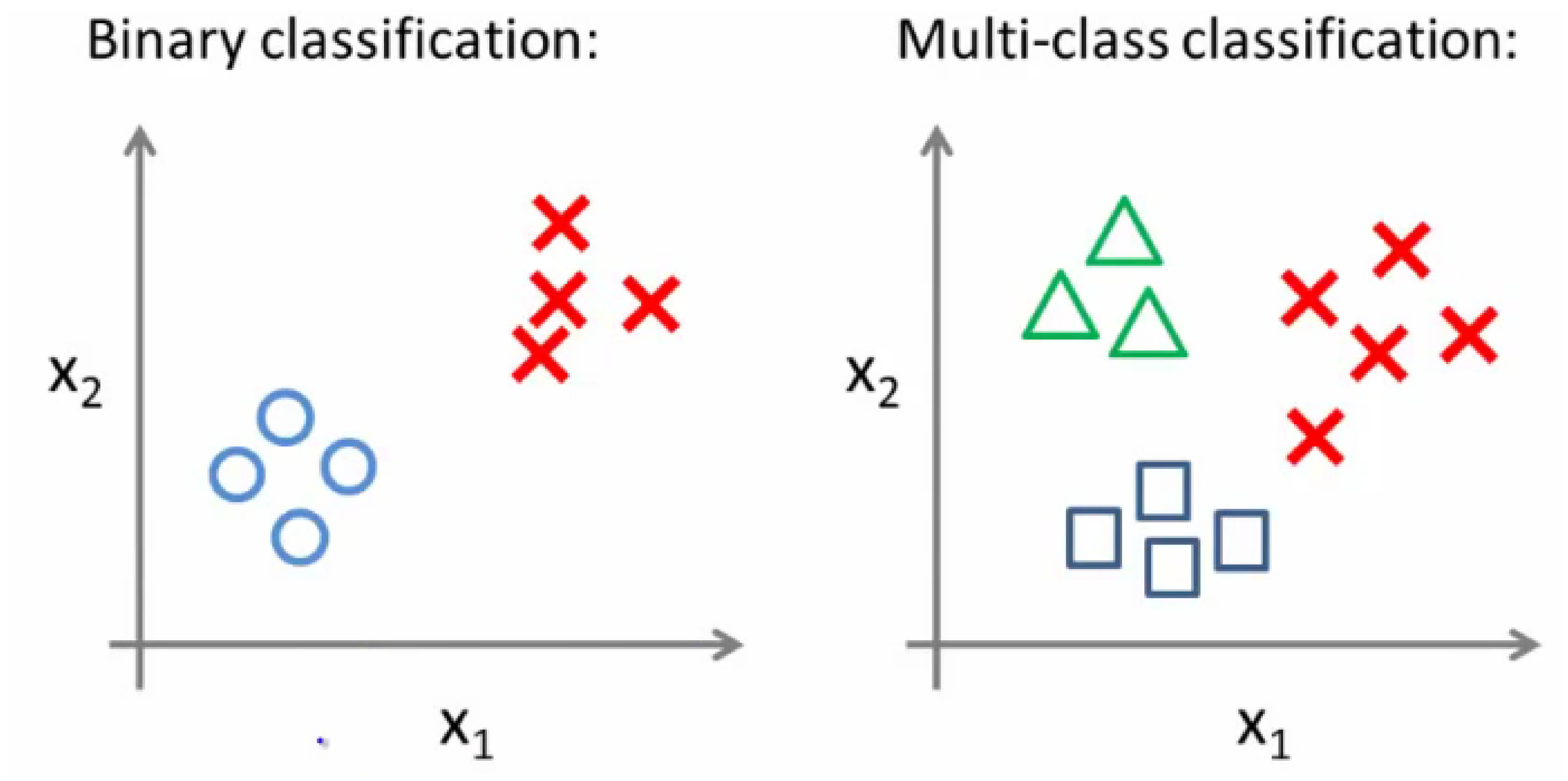


- Logistic regression also provides a **confidence score**:
  - the closer y is from 0 or 1, the more confident we can be that the classification is correct.
- This is particularly important in **safety critical** applications:
  - If you detect the positive class but with a confidence of 0.51, you should perhaps not trust the prediction.
  - If the confidence score is 0.99, you can probably trust the prediction.

4 - Multi-class classification

Multi-class classification

- Can we perform multi-class classification using the previous methods when $t \in \{A, B, C\}$ instead of $t = +1$ or -1?



Multi-class classification

Two main solutions:

- **One-vs-All** (or One-vs-the-rest): one trains simultaneously a binary (linear) classifier for each class. The examples belonging to this class form the positive class, all others are the negative class:
    - A vs. B and C
    - B vs. A and C
    - C vs. A and B

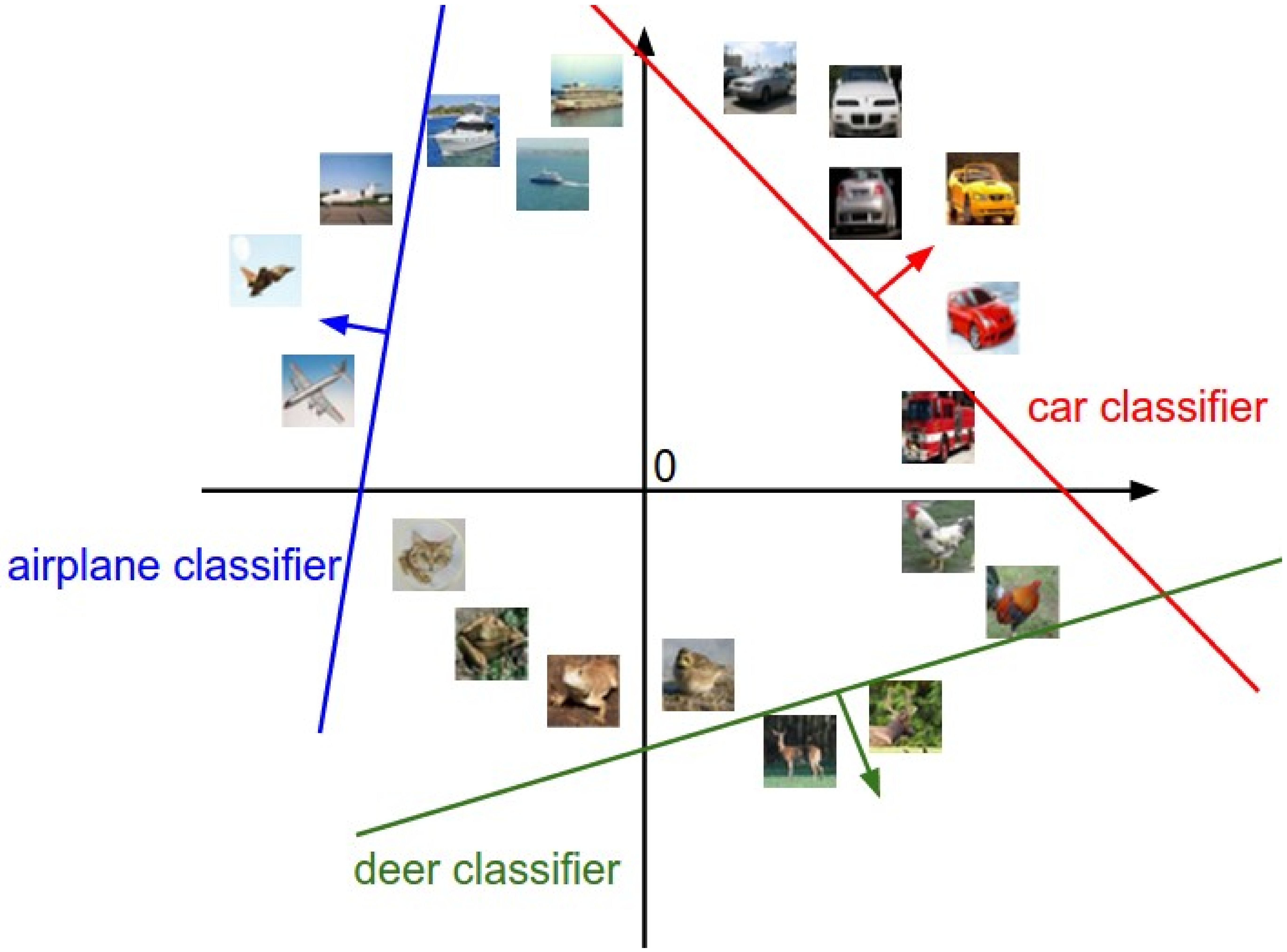
If multiple classes are predicted for a single example, ones needs a confidence level for each classifier saying how sure it is of its prediction.

- **One-vs-One**: one trains a classifier for each pair of class:
    - A vs. B
    - B vs. C
    - C vs. A

A majority vote is then performed to find the correct class.

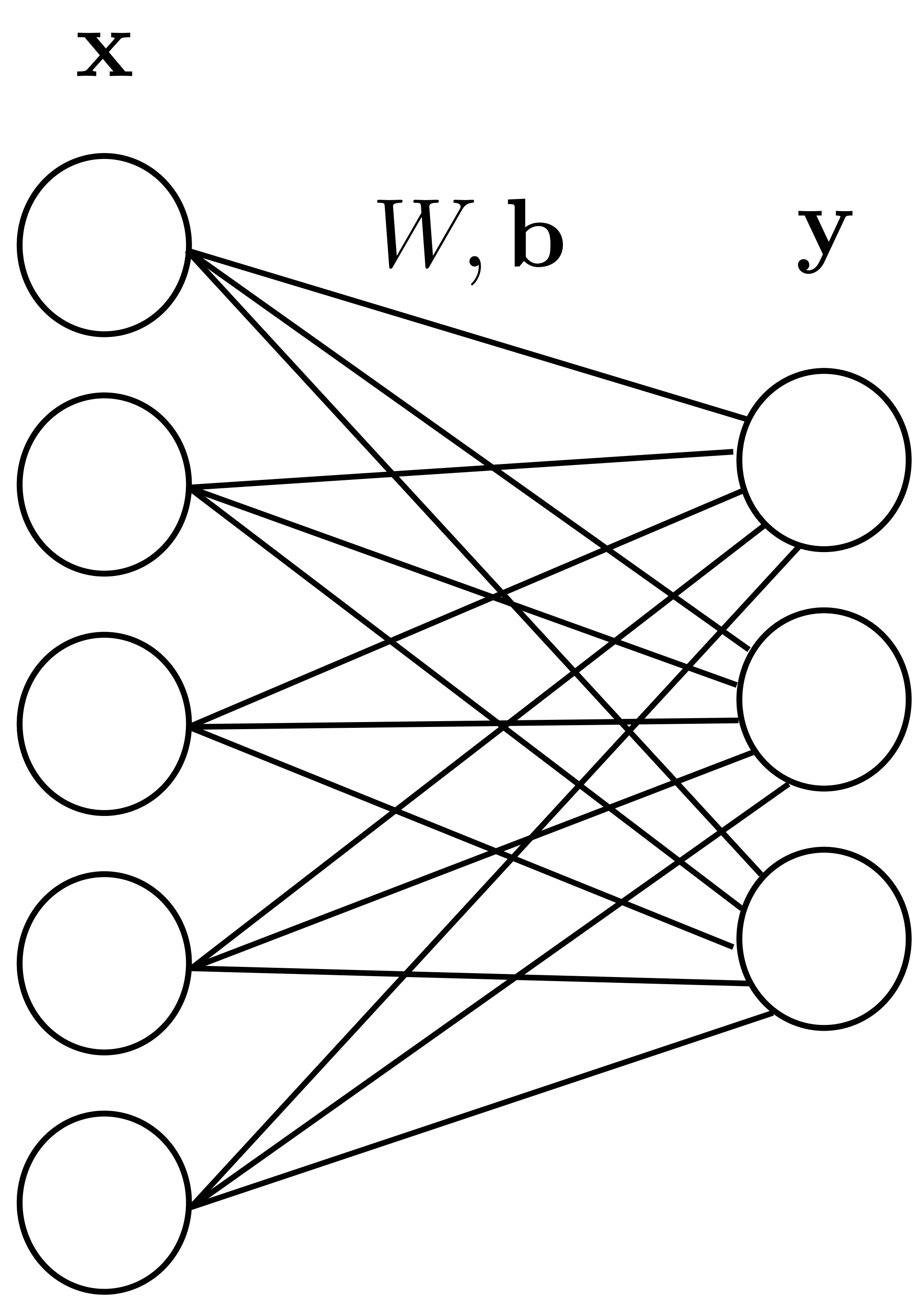
Multi-class classification

- Example of **One-vs-All** classification: one binary classifier per class.



Source http://cs231n.github.io/linear-classify

Softmax linear classifier



- Suppose we have C classes (dog vs. cat vs. ship vs...).
- The One-vs-All scheme involves C binary classifiers $(\mathbf{w}_i, b_i)$, each with a weight vector and a bias, working on the same input $\mathbf{x}$.

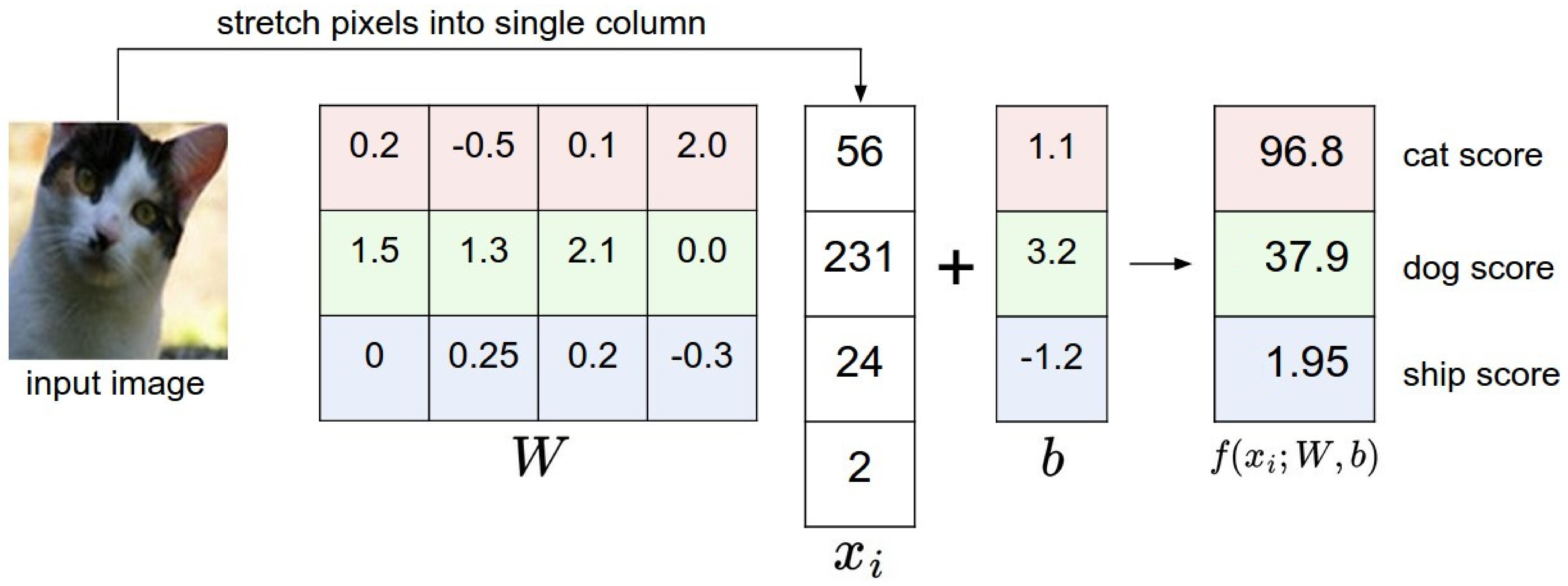
$$y_i = f(\langle \mathbf{w}_i \cdot \mathbf{x} \rangle + b_i)$$

- Putting all neurons together, we obtain a **linear perceptron** similar to multiple linear regression:

$$\mathbf{y} = f(W \times \mathbf{x} + \mathbf{b})$$

- The C weight vectors form a $C \times d$ **weight matrix** W, the biases form a vector $\mathbf{b}$.

Softmax linear classifier



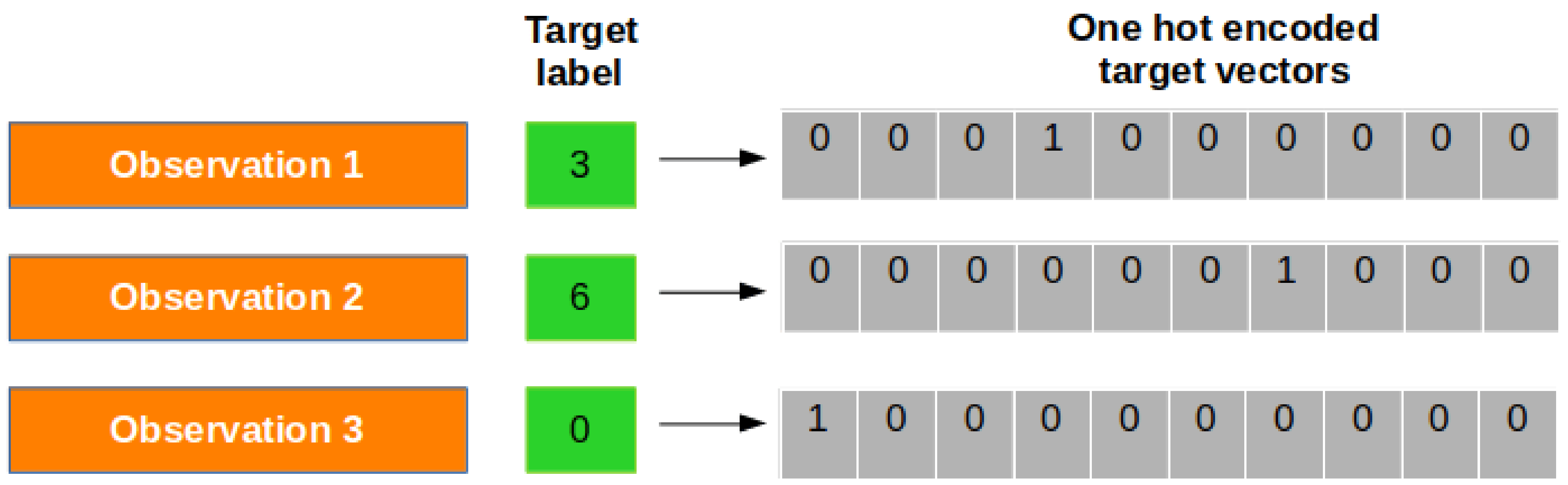
- The net activations form a vector $\mathbf{z}$:

$$\mathbf{z} = f_{W,\mathbf{b}}(\mathbf{x}) = W \times \mathbf{x} + \mathbf{b}$$

- Each element z_j of the vector $\mathbf{z}$ is called the **logit score** of the class:
  - the higher the score, the more likely the input belongs to this class.
- The logit scores are not probabilities, as they can be negative and do not sum to 1.

One-hot encoding

- How do we represent the ground truth $\mathbf{t}$ for each neuron?
- The target vector $\mathbf{t}$ is represented using **one-hot encoding**.



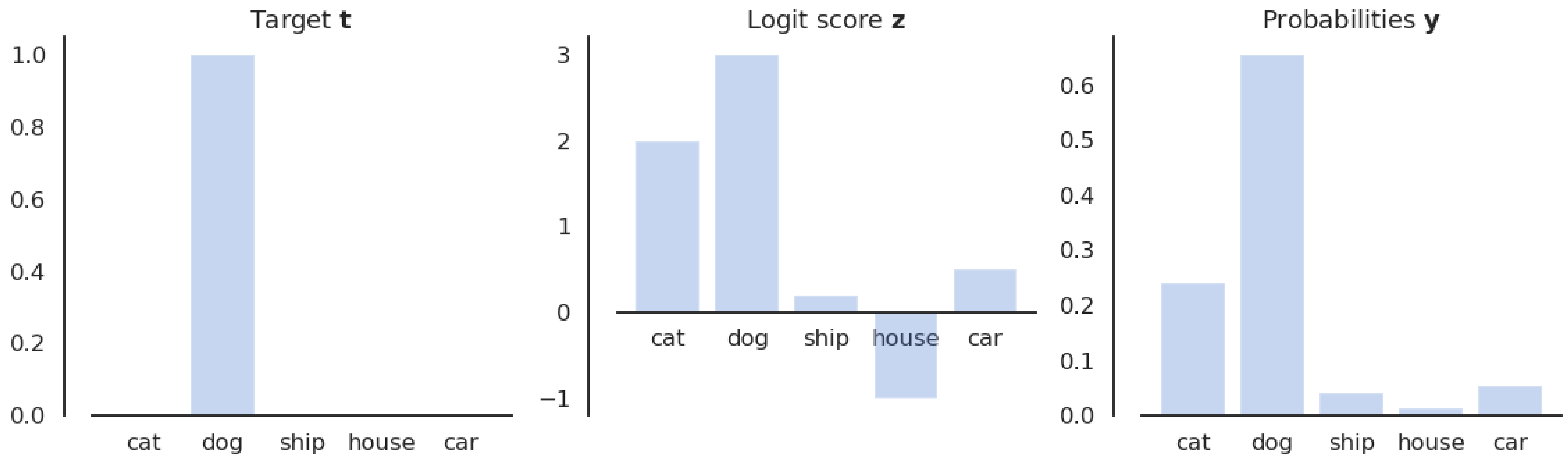
- The binary vector has one element per class: only one element is 1, the others are 0.
- Example:

$$\mathbf{t} = [\text{cat}, \text{dog}, \text{ship}, \text{house}, \text{car}] = [0, 1, 0, 0, 0]$$

One-hot encoding

- The labels can be seen as a **probability distribution** over the training set, in this case a **multinomial** distribution (a dice with C sides).
- For a given image $\mathbf{x}$ (e.g. a picture of a dog), the conditional pmf is defined by the one-hot encoded vector $\mathbf{t}$:

$$P(\mathbf{t}|\mathbf{x}) = [P(\text{cat}|\mathbf{x}), P(\text{dog}|\mathbf{x}), P(\text{ship}|\mathbf{x}), P(\text{house}|\mathbf{x}), P(\text{car}|\mathbf{x})] = [0, 1, 0, 0, 0]$$

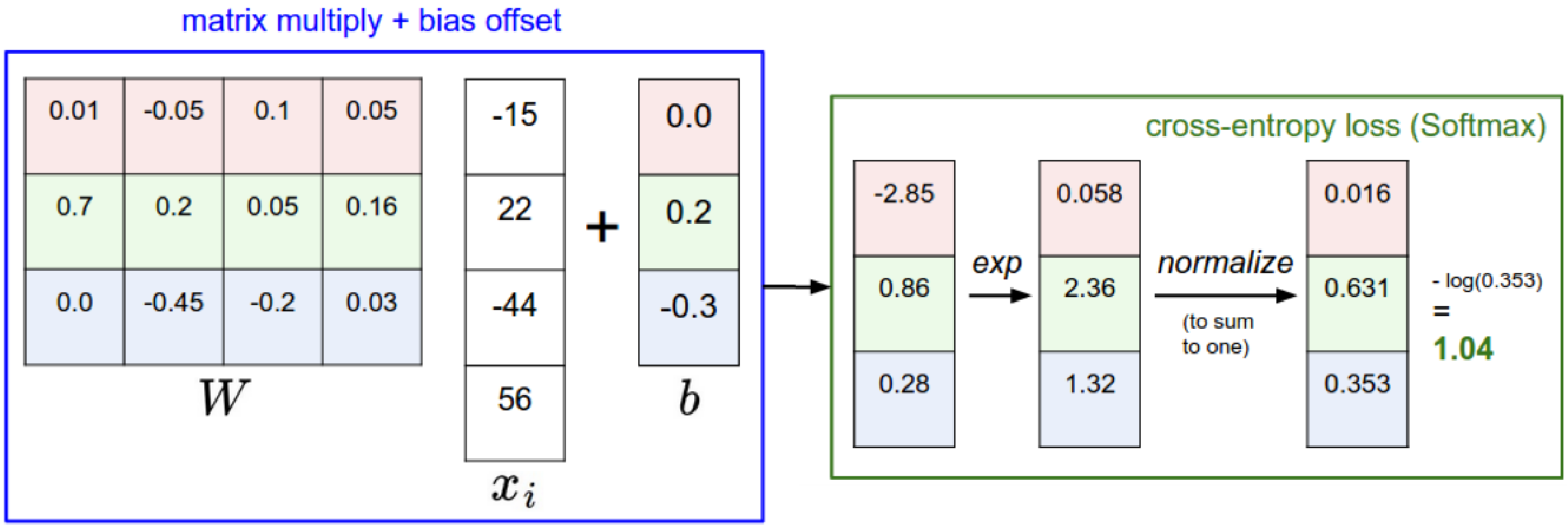


- We need to transform the logit score $\mathbf{z}$ into a **probability distribution** $P(\mathbf{y}|\mathbf{x})$ that should be as close as possible from $P(\mathbf{t}|\mathbf{x})$.

Softmax linear classifier

- The **softmax** operator makes sure that the sum of the outputs $\mathbf{y} = \{y_i\}$ over all classes is 1.

$$y_j = P(\text{class} = \text{j}|\mathbf{x}) = \mathcal{S}(z_j) = \frac{\exp(z_j)}{\sum_k \exp(z_k)}$$

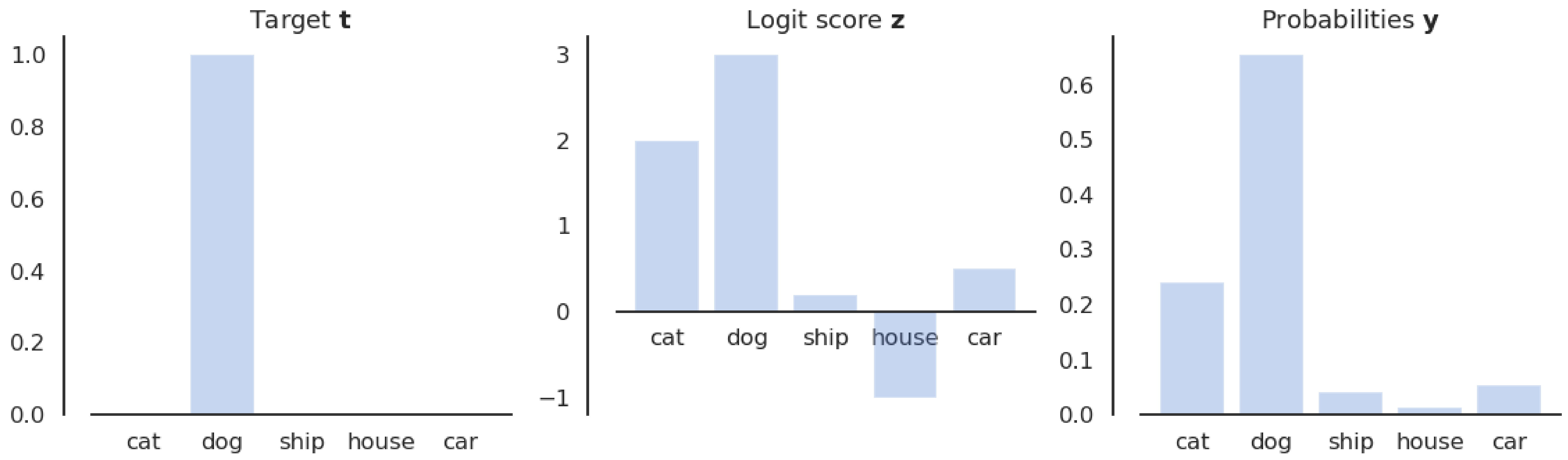


- The higher z_j, the higher the probability that the example belongs to class j.
- This is very similar to logistic regression for soft classification, except that we have multiple classes.

Cross-entropy loss function

- We cannot use the mse as a loss function, as the softmax function would be hard to differentiate:

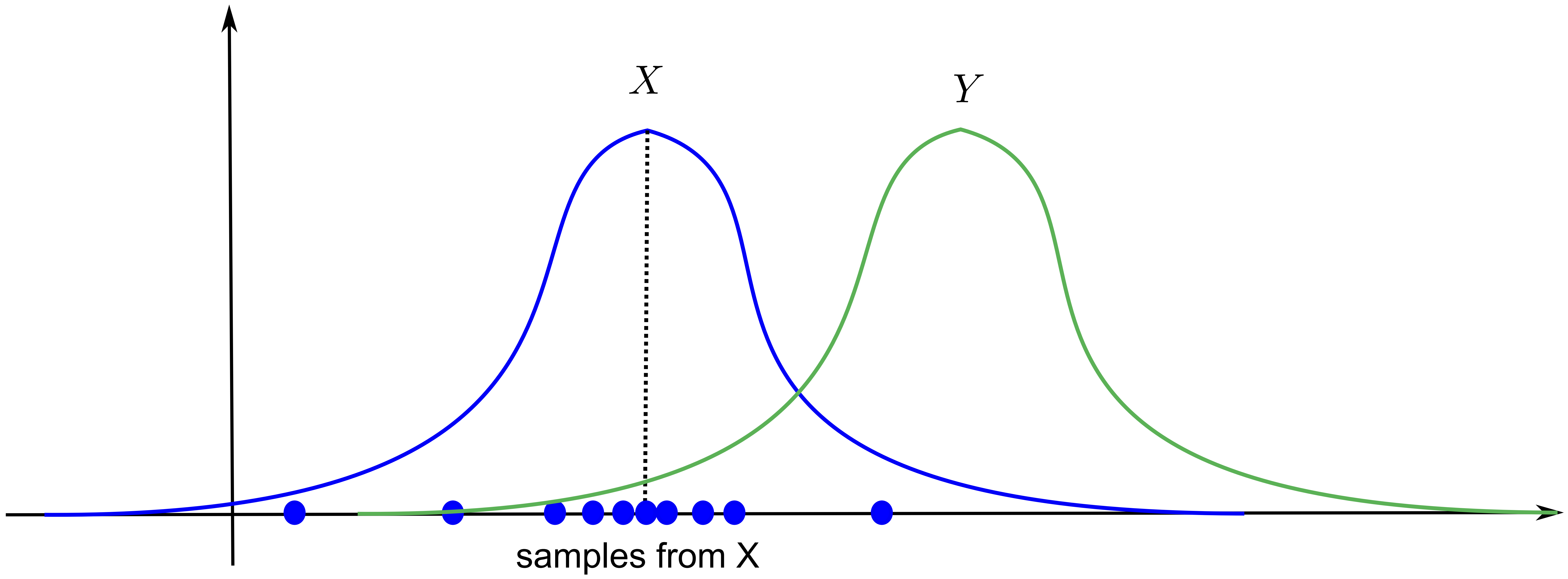
$$\text{mse}(W, \mathbf{b}) = \sum_j (t_j - \frac{\exp(z_j)}{\sum_k \exp(z_k)})^2$$



- We actually want to minimize the statistical distance netween two distributions:
  - The model outputs a multinomial probability distribution $\mathbf{y}$ for an input $\mathbf{x}$: $P(\mathbf{y} | \mathbf{x}; W, \mathbf{b})$.
  - The one-hot encoded classes also come from a multinomial probability distribution $P(\mathbf{t} | \mathbf{x})$.
- We search which parameters $(W, \mathbf{b})$ make the two distributions $P(\mathbf{y} | \mathbf{x}; W, \mathbf{b})$ and $P(\mathbf{t} | \mathbf{x})$ close.

Cross-entropy loss function

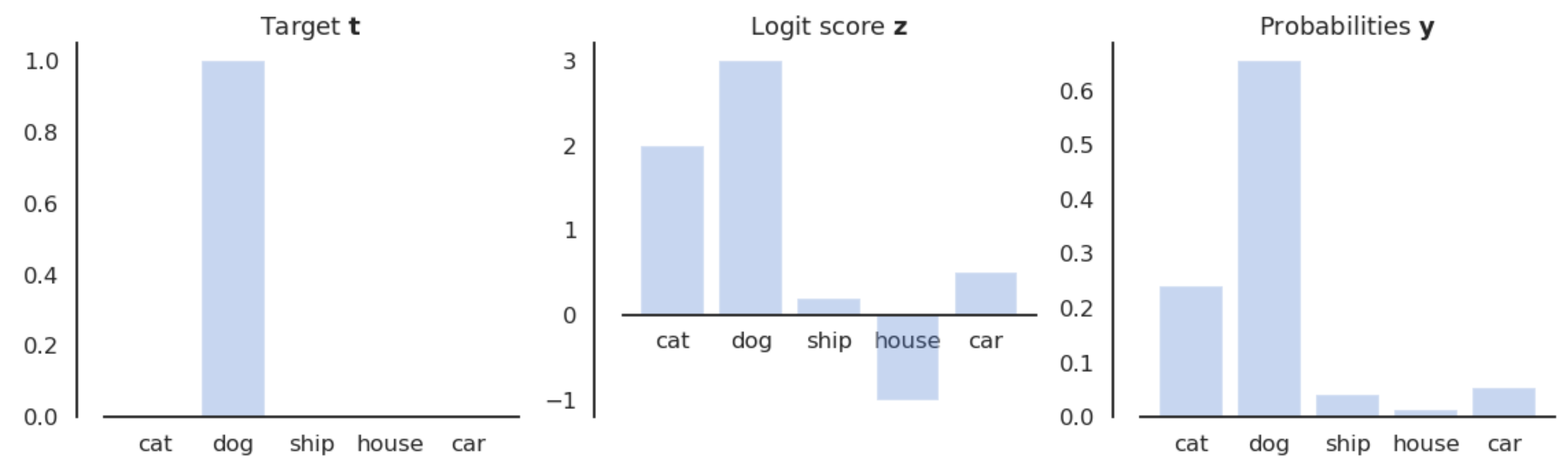
- The training data $\{\mathbf{x}_i, \mathbf{t}_i\}$ represents samples from $P(\mathbf{t}|\mathbf{x})$.
- $P(\mathbf{y}|\mathbf{x}; W, \mathbf{b})$ is a good model of the data when the two distributions are close, i.e. when the **negative log-likelihood** of each sample under the model is small.



- For an input $\mathbf{x}$, we minimize the **cross-entropy** between the target distribution and the predicted outputs:

$$l(W, \mathbf{b}) = \mathcal{H}(\mathbf{t}|\mathbf{x}, \mathbf{y}|\mathbf{x}) = \mathbb{E}_{t \sim P(\mathbf{t}|\mathbf{x})}[- \log P(\mathbf{y} = t|\mathbf{x})]$$

Cross-entropy and negative log-likelihood



- The cross-entropy samples from $\mathbf{t} | \mathbf{x}$:

$$l(W, \mathbf{b}) = \mathcal{H}(\mathbf{t}|\mathbf{x}, \mathbf{y}|\mathbf{x}) = \mathbb{E}_{t \sim P(\mathbf{t}|\mathbf{x})} [- \log P(\mathbf{y} = t | \mathbf{x})] = - \sum_{j=1}^{C} P(t_j | \mathbf{x}) \, \log P(y_j = t_j | \mathbf{x})$$

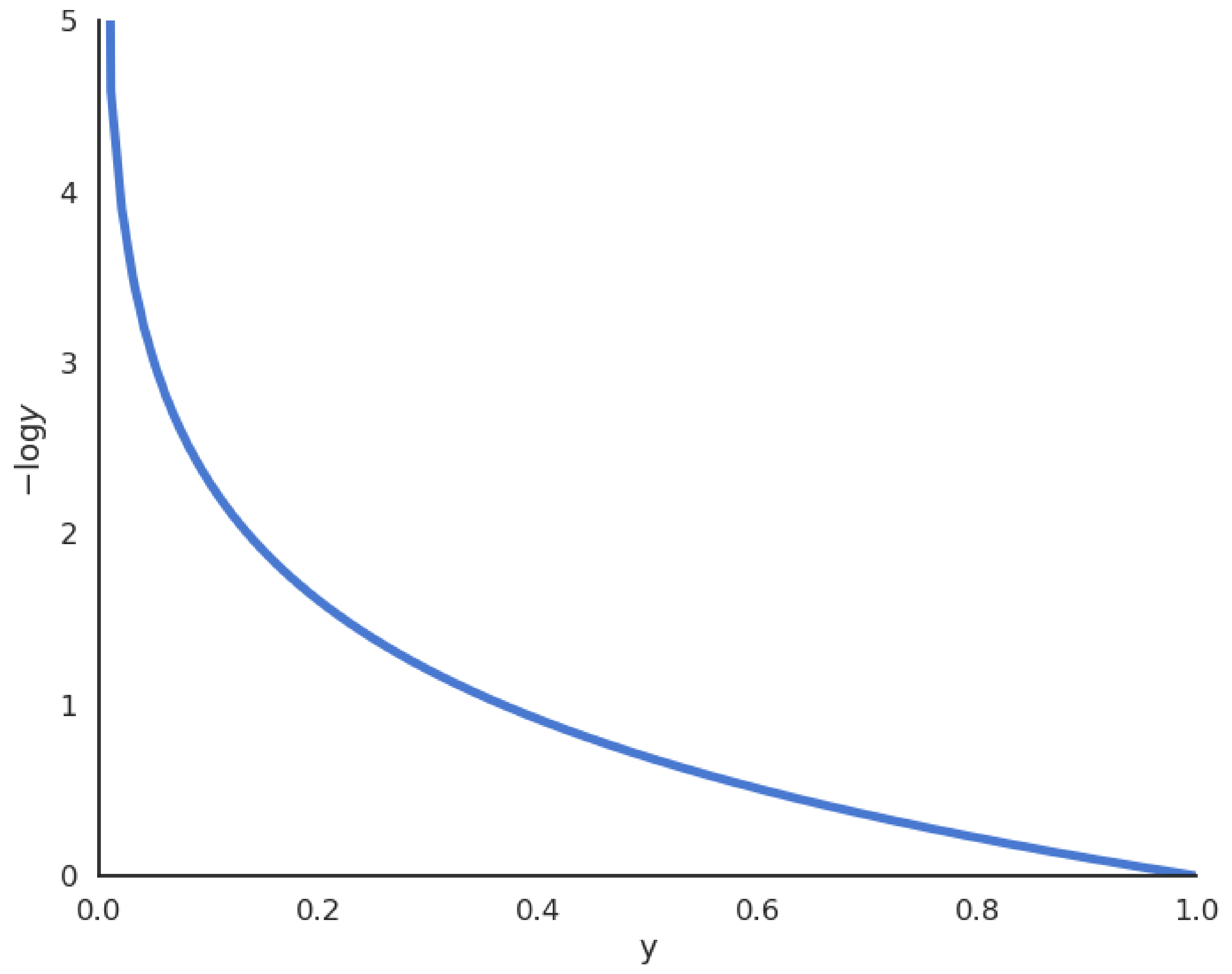
- For a given input $\mathbf{x}$, $\mathbf{t}$ is non-zero only for the correct class t^*, as $\mathbf{t}$ is a one-hot encoded vector $[0, 1, 0, 0, 0]$:

$$l(W, \mathbf{b}) = - \log P(\mathbf{y} = t^* | \mathbf{x})$$

- If we note j^* the index of the correct class t^*, the cross entropy is simply:

$$l(W, \mathbf{b}) = - \log y_{j^*}$$

Cross-entropy and negative log-likelihood



- As only one element of $\mathbf{t}$ is non-zero, the cross-entropy is the same as the **negative log-likelihood** of the prediction for the true label:

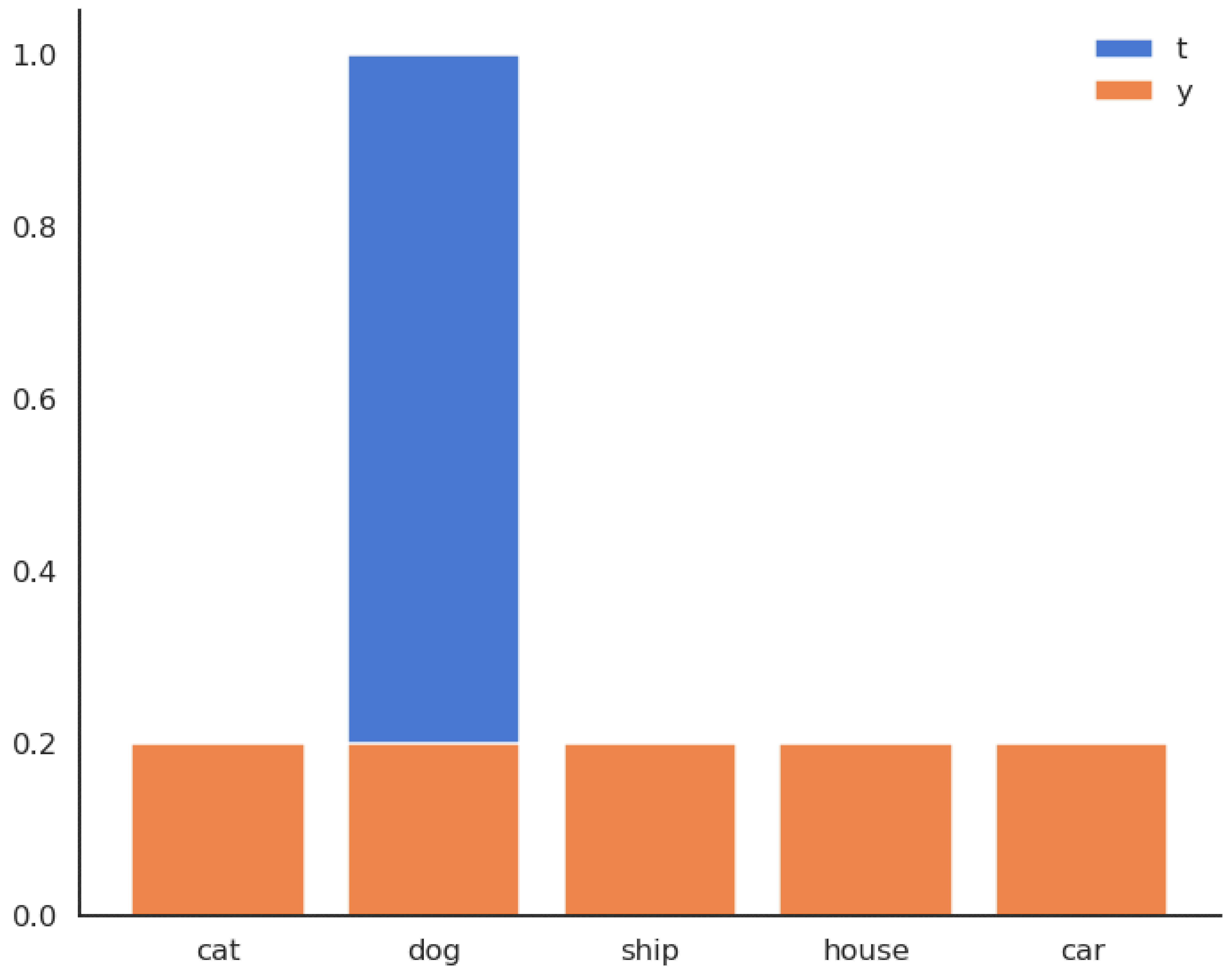
$$l(W, \mathbf{b}) = - \log y_{j^*}$$

- The minimum of $- \log y$ is obtained when $y = 1$:
    - We want to classifier to output a probability 1 for the true label.
- Because of the softmax activation function, the probability for the other classes should become closer from 0.

$$y_j = P(\text{class = j}) = \frac{\exp(z_j)}{\sum_k \exp(z_k)}$$

- Minimizing the cross-entropy / negative log-likelihood pushes the output distribution $\mathbf{y} | \mathbf{x}$ to be as close as possible to the target distribution $\mathbf{t} | \mathbf{x}$.

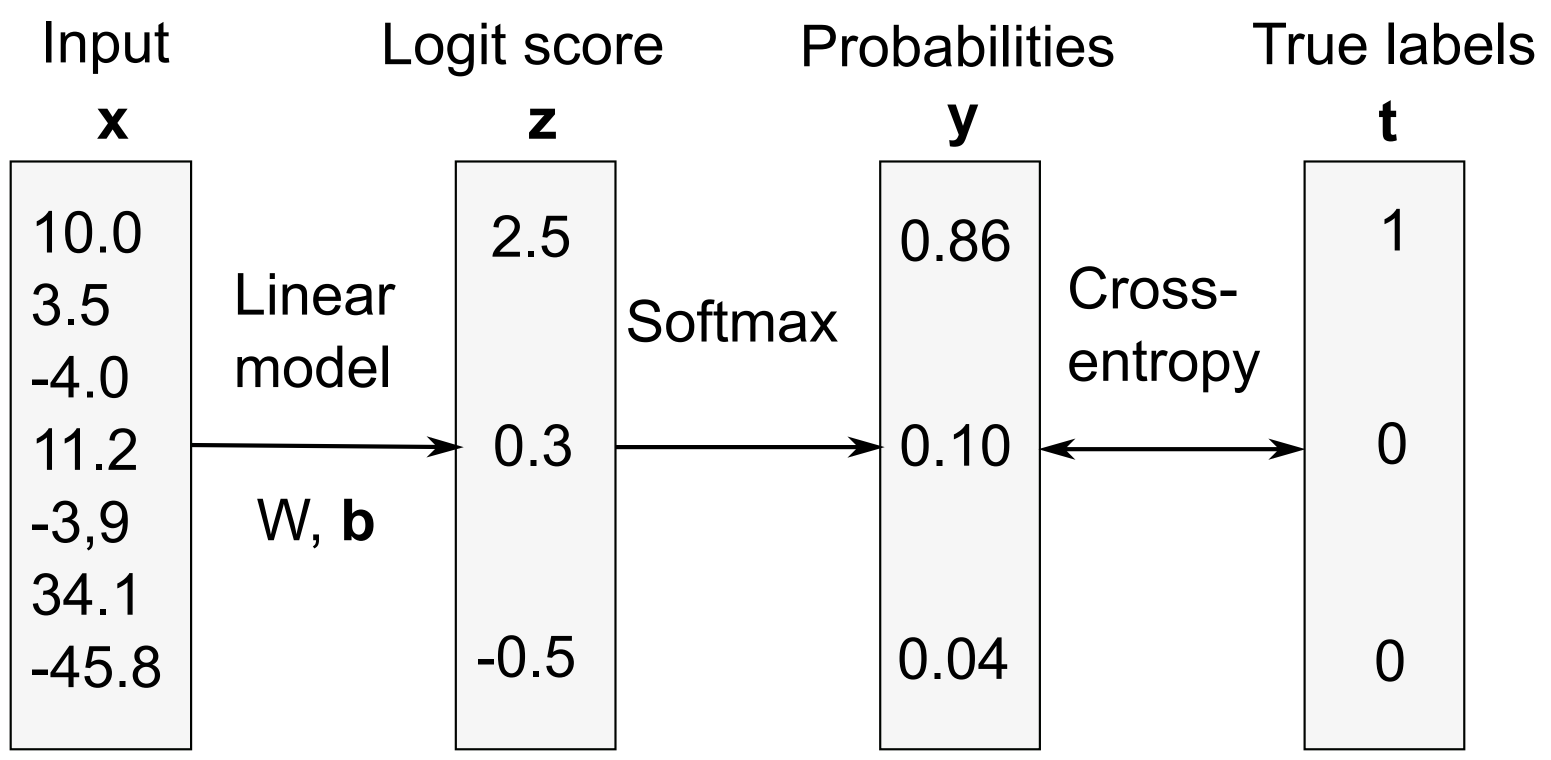
Cross-entropy loss function



Cross-entropy loss function

- As $\mathbf{t}$ is a binary vector $[0, 1, 0, 0, 0]$, the cross-entropy / negative log-likelihood can also be noted as the dot product between $\mathbf{t}$ and $\log \mathbf{y}$:

$$l(W, \mathbf{b}) = - \langle \mathbf{t} \cdot \log \mathbf{y} \rangle = - \sum_{j=1}^{C} t_j \, \log y_j = - \log y_{j^*}$$



- The **cross-entropy loss function** is then the expectation over the training set of the individual cross-entropies:

$$\mathcal{L}(W, \mathbf{b}) = \mathbb{E}_{\mathbf{x}, \mathbf{t} \sim \mathcal{D}}[- \langle \mathbf{t} \cdot \log \mathbf{y} \rangle] \approx \frac{1}{N} \sum_{i=1}^{N} - \langle \mathbf{t}_i \cdot \log \mathbf{y}_i \rangle$$

Cross-entropy loss function

- The nice thing with the **cross-entropy** loss function, when used on a softmax activation function, is that the partial derivative w.r.t the logit score $\mathbf{z}$ is simple:

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

i.e. the same as with the mse in linear regression!

- Vector notation:

$$
\frac{\partial l(W, \mathbf{b})}{\partial \mathbf{z}} = - (\mathbf{t} - \mathbf{y})
$$

See https://peterroelants.github.io/posts/cross-entropy-softmax/ for more explanations on the differentiation.

Cross-entropy loss function

- As:

$$\mathbf{z} = W \times \mathbf{x} + \mathbf{b}$$

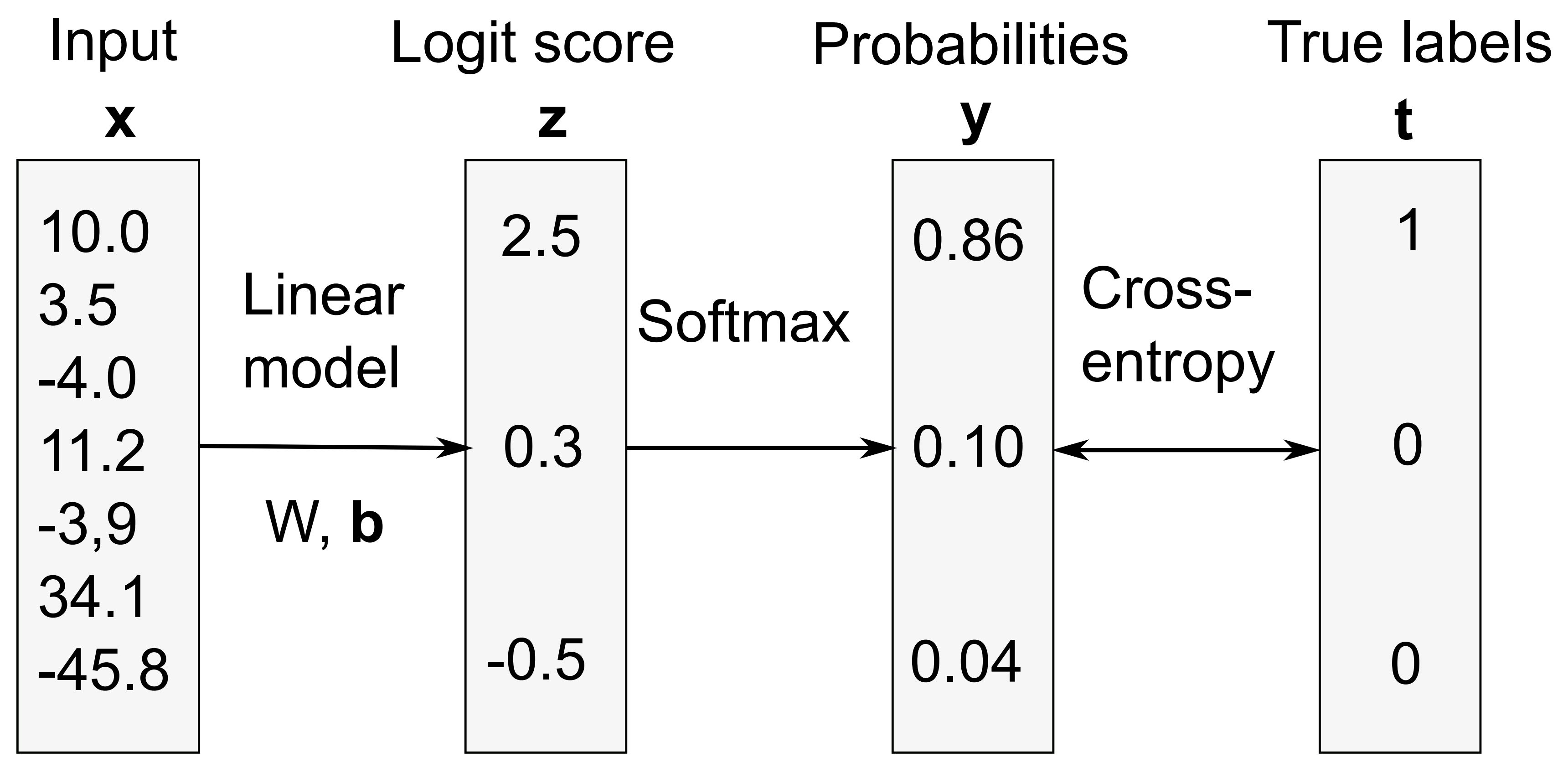
we can obtain the partial derivatives:

$$\begin{cases} \dfrac{\partial l(W, \mathbf{b})}{\partial W} = \dfrac{\partial l(W, \mathbf{b})}{\partial \mathbf{z}} \times \dfrac{\partial \mathbf{z}}{\partial W} = -(\mathbf{t} - \mathbf{y}) \times \mathbf{x}^T \\ \\ \dfrac{\partial l(W, \mathbf{b})}{\partial \mathbf{b}} = \dfrac{\partial l(W, \mathbf{b})}{\partial \mathbf{z}} \times \dfrac{\partial \mathbf{z}}{\partial \mathbf{b}} = -(\mathbf{t} - \mathbf{y}) \end{cases}$$

- So gradient descent leads to the **delta learning rule**:

$$\begin{cases} \Delta W = \eta \, (\mathbf{t} - \mathbf{y}) \times \mathbf{x}^T \\ \\ \Delta \mathbf{b} = \eta \, (\mathbf{t} - \mathbf{y}) \end{cases}$$

Softmax linear classifier



- We first compute the **logit scores $\mathbf{z}$** using a linear layer:

$$\mathbf{z} = W \times \mathbf{x} + \mathbf{b}$$

- We turn them into probabilities $\mathbf{y}$ using the **softmax activation function**:

$$y_j = \frac{\exp(z_j)}{\sum_k \exp(z_k)}$$

- We minimize the **cross-entropy** / **negative log-likelihood** on the training set:

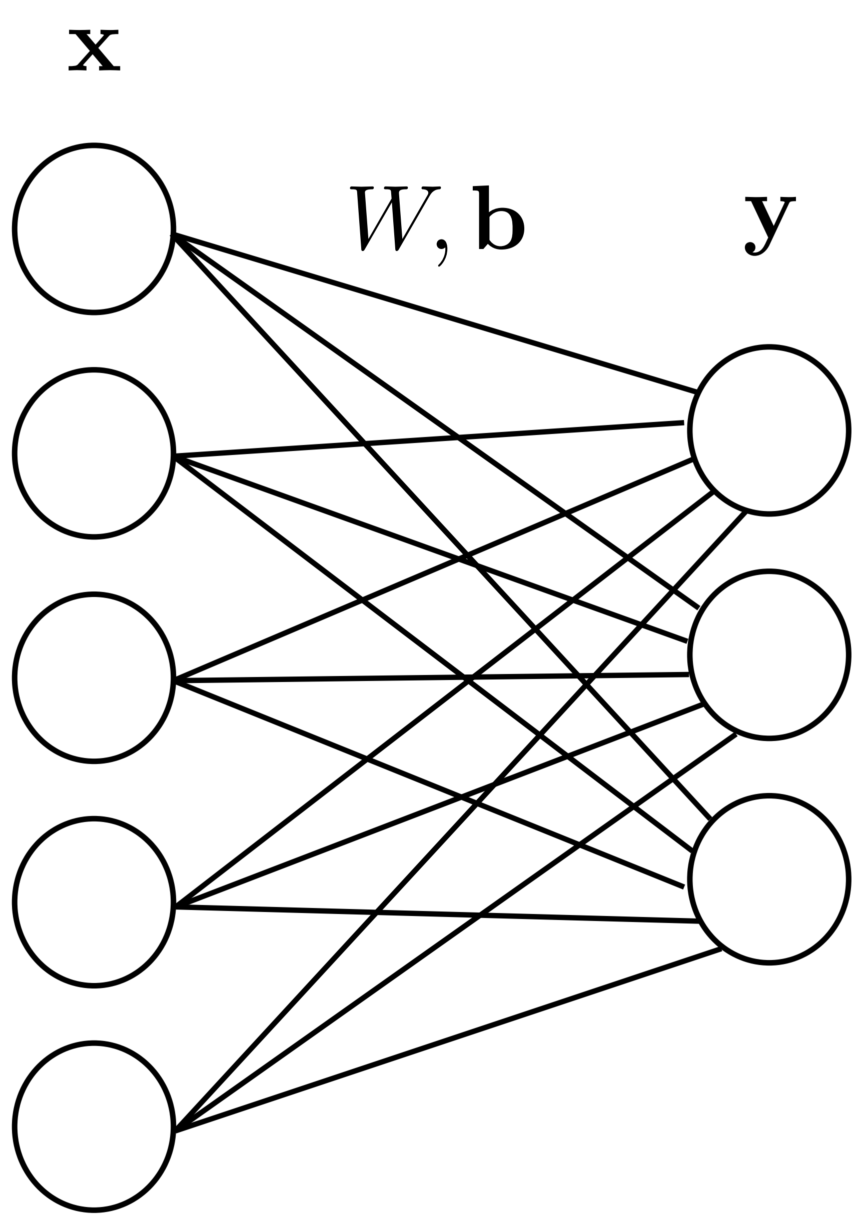
$$\mathcal{L}(W, \mathbf{b}) = \mathbb{E}_{\mathbf{x}, \mathbf{t} \sim \mathcal{D}}[- \langle \mathbf{t} \cdot \log \mathbf{y} \rangle]$$

which simplifies into the **delta learning rule**:

$$\begin{cases} \Delta W = \eta \, (\mathbf{t} - \mathbf{y}) \times \mathbf{x}^T \\ \\ \Delta \mathbf{b} = \eta \, (\mathbf{t} - \mathbf{y}) \end{cases}$$

Comparison of linear classification and regression

- Classification and regression differ in the nature of their outputs: in classification they are discrete, in regression they are continuous values.



- However, when trying to minimize the mismatch between a model $\mathbf{y}$ and the real data $\mathbf{t}$, we have found the same **delta learning rule**:

$$\begin{cases} \Delta W = \eta \, (\mathbf{t} - \mathbf{y}) \times \mathbf{x}^T \\ \\ \Delta \mathbf{b} = \eta \, (\mathbf{t} - \mathbf{y}) \end{cases}$$

- Regression and classification are in the end the same problem for us. The only things that needs to be adapted is the **activation function** of the output and the **loss function**.

- For regression, we use linear activation functions and the **mean square error** (mse):

$$\mathcal{L}(W, \mathbf{b}) = \mathbb{E}_{\mathbf{x}, \mathbf{t} \sim \mathcal{D}}[||\mathbf{t} - \mathbf{y}||^2]$$

- For classification, we use the softmax activation function and the **cross-entropy** (negative log-likelihood) loss function.

$$\mathcal{L}(W, \mathbf{b}) = \mathbb{E}_{\mathbf{x}, \mathbf{t} \sim \mathcal{D}}[- \langle \mathbf{t} \cdot \log \mathbf{y} \rangle]$$

5 - Multi-label classification

Multi-label classification

GK Hart/Vikki Hart/Getty Images

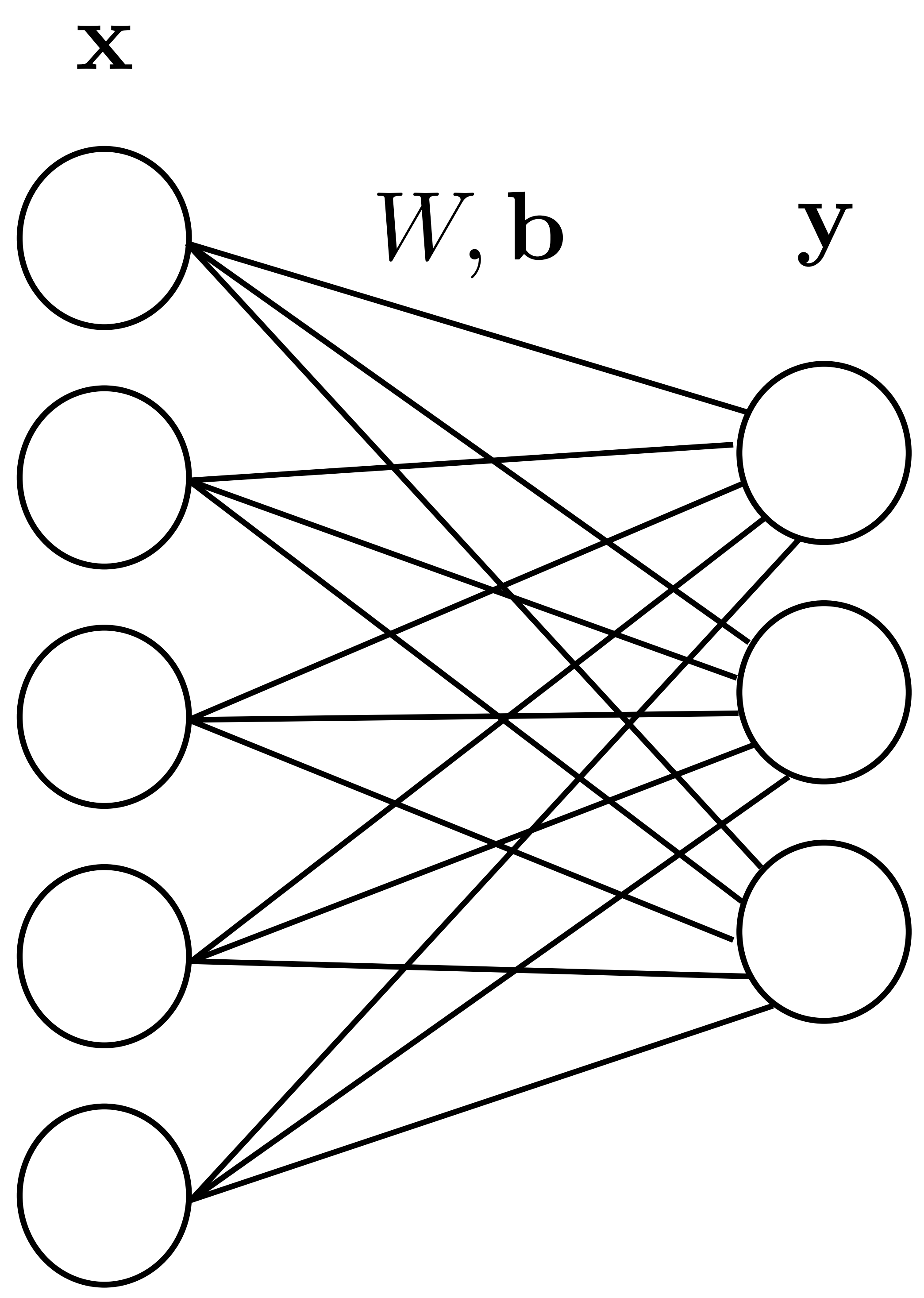
- What if there is more than one label on the image?
- The target vector $\mathbf{t}$ does not represent a probability distribution anymore:

$$\mathbf{t} = [\text{cat}, \text{dog}, \text{ship}, \text{house}, \text{car}] = [1, 1, 0, 0, 0]$$

- Normalizing the vector does not help: it is not a dog **or** a cat, it is a dog **and** a cat.

$$\mathbf{t} = [\text{cat}, \text{dog}, \text{ship}, \text{house}, \text{car}] = [0.5, 0.5, 0, 0, 0]$$

Multi-label classification



- For multi-label classification, we can simply use the **logistic** activation function for the output neurons:

$$\mathbf{y} = \sigma(W \times \mathbf{x} + \mathbf{b})$$

- The outputs are between 0 and 1, but they do not sum to one. Each output neuron performs **logistic regression for soft classification** on their class:

$$y_j = P(\text{class} = j | \mathbf{x})$$

- Each output neuron y_j has a binary target t_j (one-vs-the-rest) and has to minimize the negative log-likelihood:

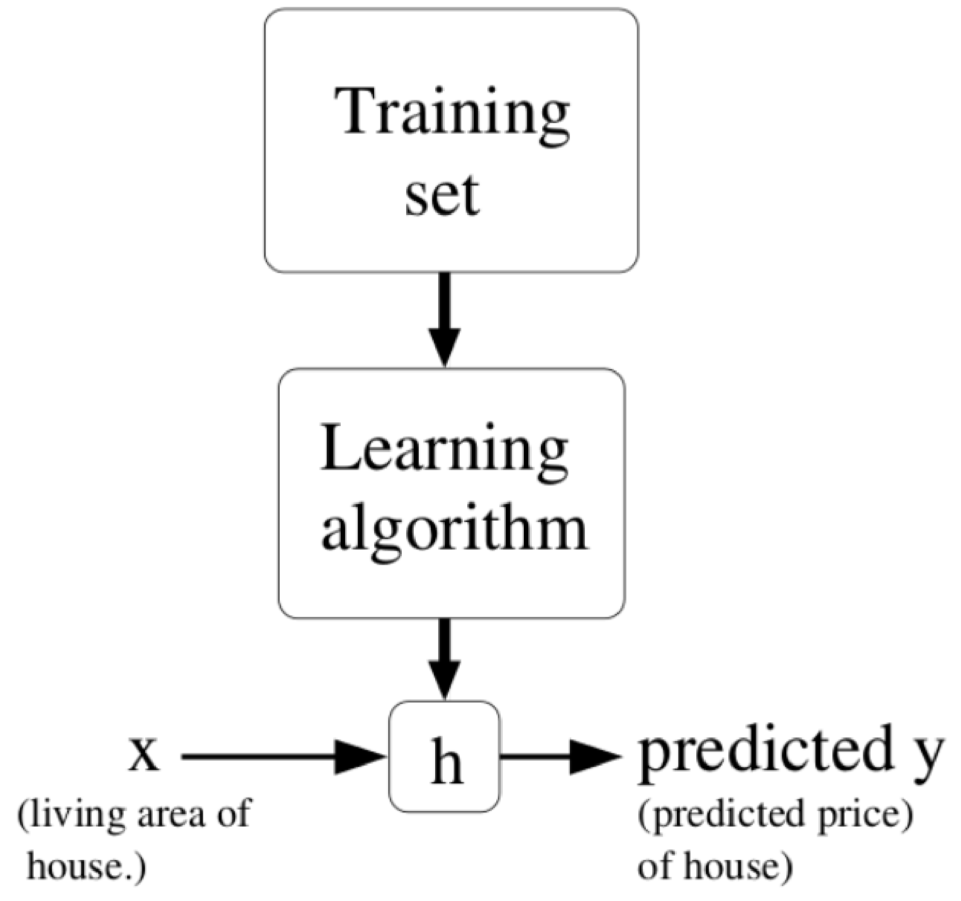
$$l_j(W, \mathbf{b}) = - t_j \, \log y_j + (1 - t_j) \, \log(1 - y_j)$$

- The **binary cross-entropy** loss is the sum of the negative log-likelihood for each class:

$$\mathcal{L}(W, \mathbf{b}) = \mathbb{E}_{\mathcal{D}}[- \sum_{j=1}^C t_j \, \log y_j + (1 - t_j) \, \log(1 - y_j)]$$

6 - Metrics

Training vs. Generalization error



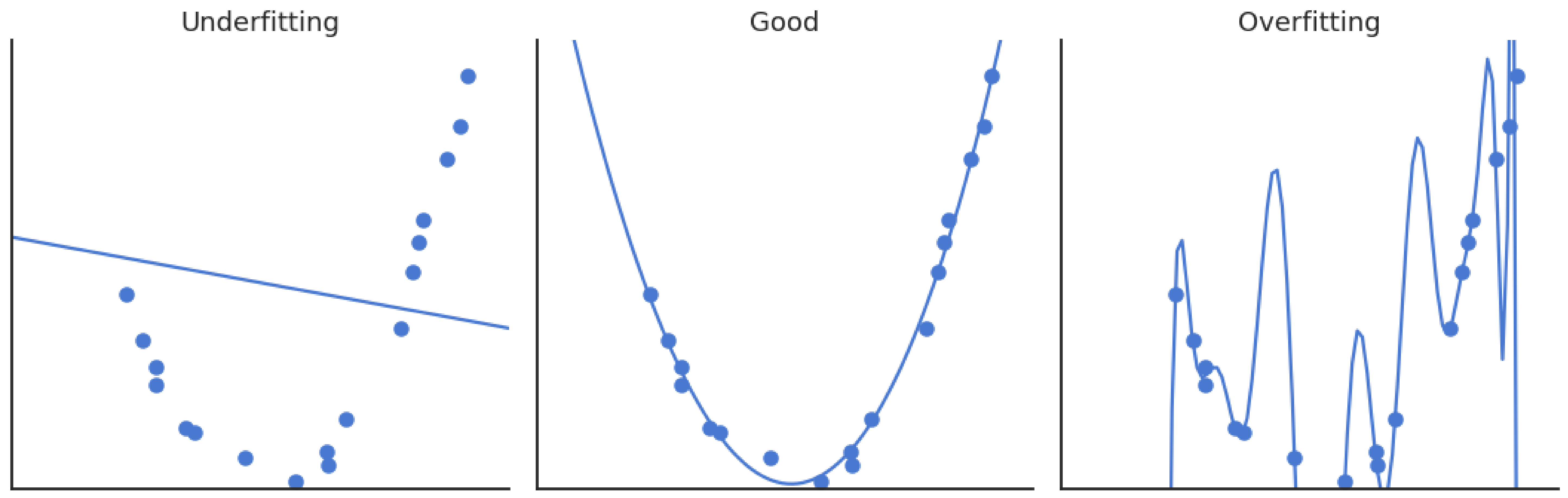
- The **training error** is the error made on the training set.
  - Easy to measure for classification: number of misclassified examples divided by the total number.

$$\epsilon_{\mathcal{D}} = \frac{\text{number of misclassifications}}{\text{number of examples}}$$

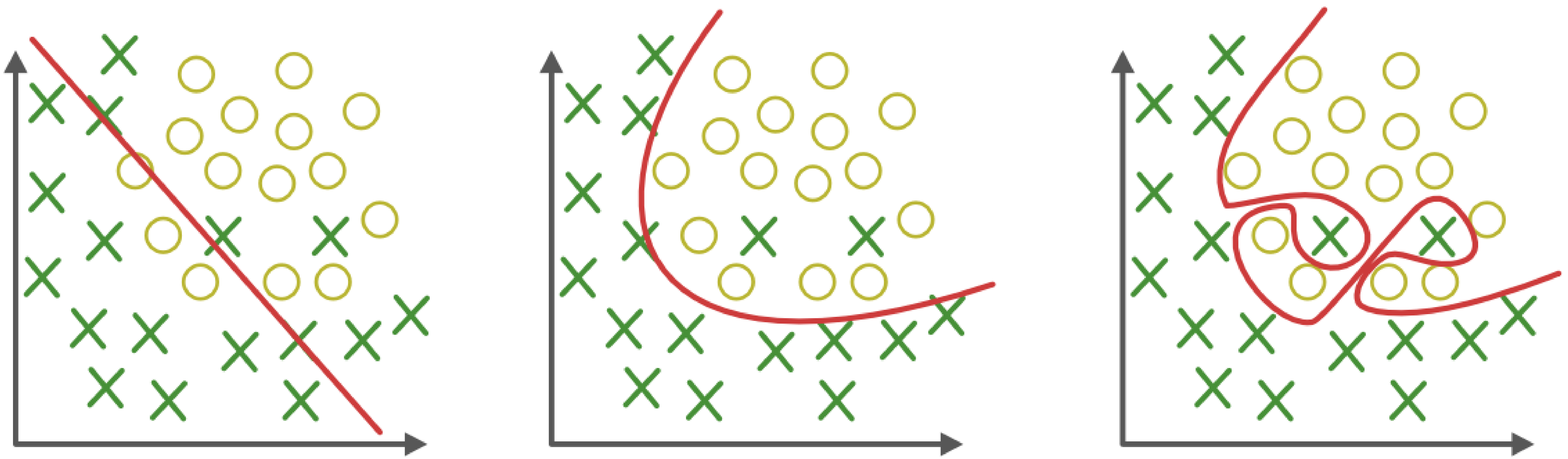
  - Totally irrelevant on usage: reading the training set has a training error of 0%.

- What matters is the **generalization error**, which is the error that will be made on new examples (not used during learning).
  - Much harder to measure (potentially infinite number of new examples, what is the correct answer?).
  - Often approximated by the **empirical error on the test set**: one keeps a number of training examples out of the learning phase and one tests the performance on them.
  - Need for **cross-validation** to detect **overfitting**.

Overfitting in regression

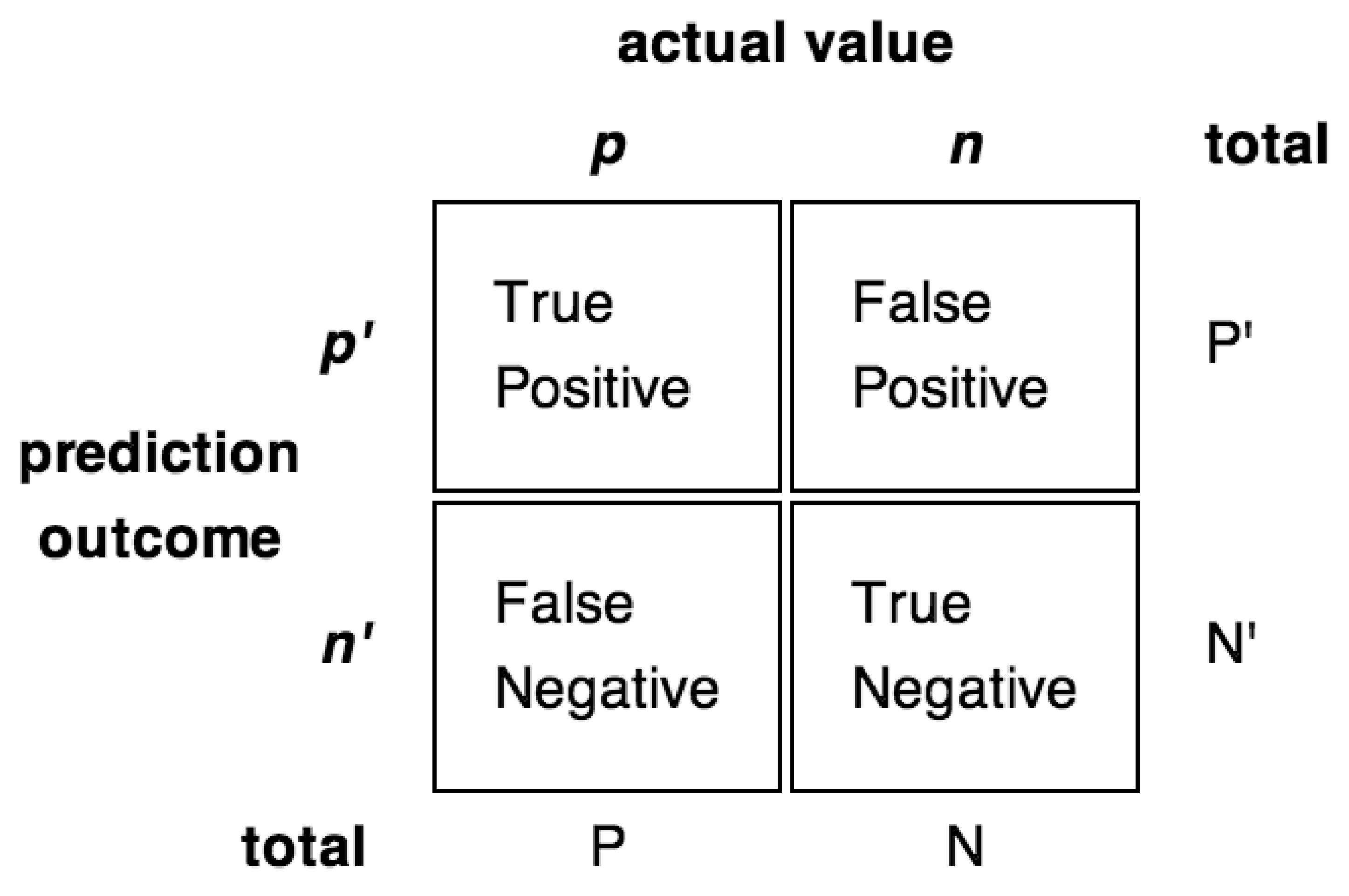


Overfitting in classification



Classification errors

Confusion matrix

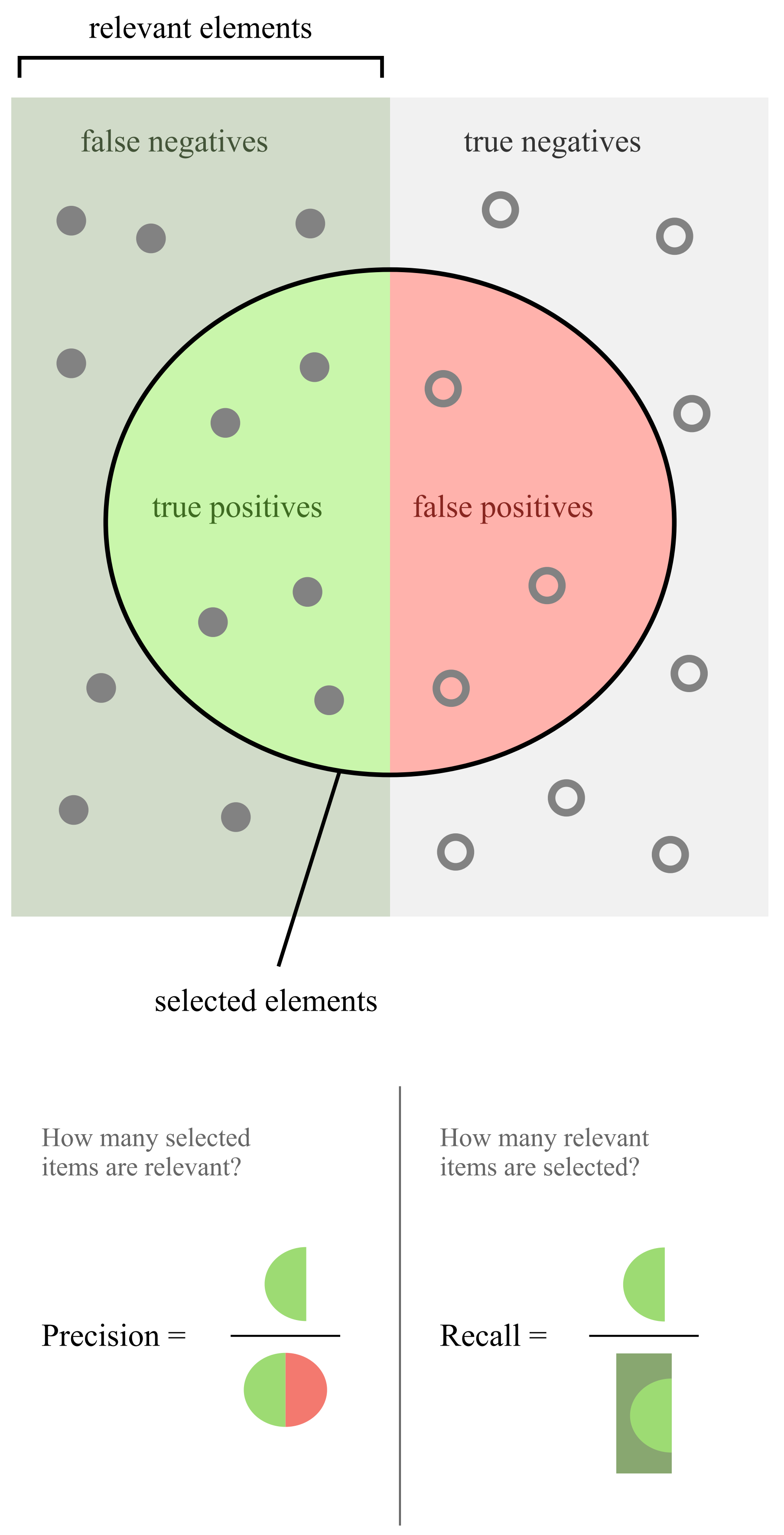


		actual value		
		p	***n***	**total**
prediction outcome	***p'***	True Positive	False Positive	P'
	n'	False Negative	True Negative	N'
	total	P	N	

Source:
https://alliance.seas.upenn.edu/~cis520/dynamic/2017/wiki/index.php?n=Lectures.PrecisionRecall

- Classification errors can also depend on the class:
  - **False Positive** errors (FP, false alarm, type I) is when the classifier predicts a positive class for a negative example.
  - **False Negative** errors (FN, miss, type II) is when the classifier predicts a negative class for a positive example.
- **True Positive** (TP) and **True Negative** (TN) are correctly classified examples.
- Is it better to fail to detect a cancer (FN) or to incorrectly predict one (FP)?

Classification errors



- Error

$$\epsilon = \frac{\mathrm{FP} + \mathrm{FN}}{\mathrm{TP} + \mathrm{FP} + \mathrm{TN} + \mathrm{FN}}$$

- Accuracy (1 - error)

$$\mathrm{acc} = \frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \mathrm{FP} + \mathrm{TN} + \mathrm{FN}}$$

- Recall (hit rate, sensitivity) and Precision (specificity)

$$R = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}} \quad P = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}}$$

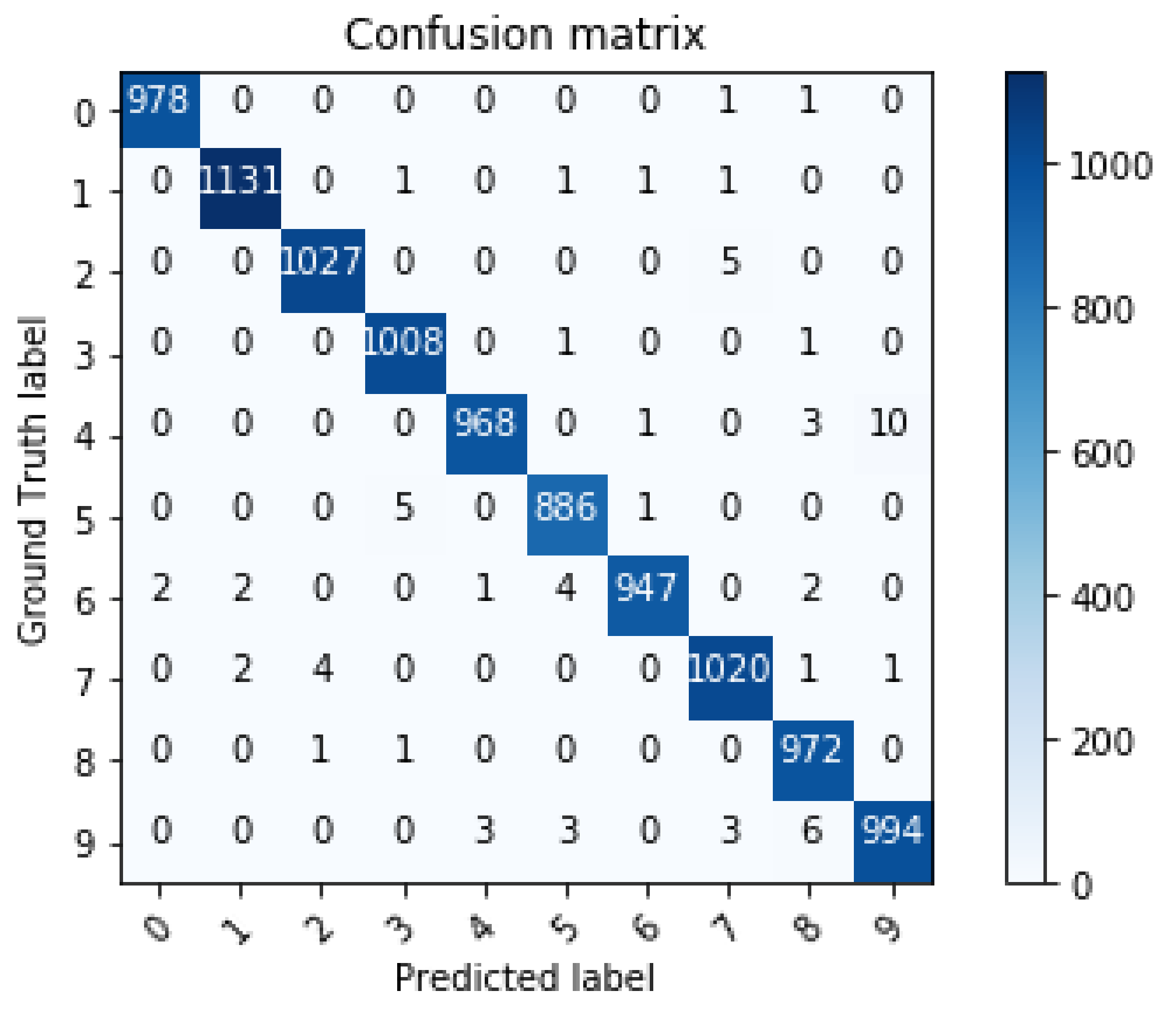
- F1 score = harmonic mean of precision and recall

$$\mathrm{F1} = \frac{2\,P\,R}{P + R}$$

Source:
https://upload.wikimedia.org/wikipedia/commons/2/26/Precisionrecall.svg

Confusion matrix

- For multiclass classification problems, the **confusion matrix** tells how many examples are correctly classified and where confusion happens.
- One axis is the predicted class, the other is the target class.
- Each element of the matrix tells how many examples are classified or misclassified.
- The matrix should be as diagonal as possible.



Ground Truth label \ Predicted label	0	1	2	3	4	5	6	7	8	9
0	978	0	0	0	0	0	0	1	1	0
1	0	1131	0	1	0	1	1	1	0	0
2	0	0	1027	0	0	0	0	5	0	0
3	0	0	0	1008	0	1	0	0	1	0
4	0	0	0	0	968	0	1	0	3	10
5	0	0	0	5	0	886	1	0	0	0
6	2	2	0	0	1	4	947	0	2	0
7	0	2	4	0	0	0	0	1020	1	1
8	0	0	1	1	0	0	0	0	972	0
9	0	0	0	0	3	3	0	3	6	994

- Using `scikit-learn`:

```python
from sklearn.metrics import confusion_matrix

m = confusion_matrix(t, y)
```