Logistic Regression

Machine Learning Course - CS-433
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Binary classification

We observe some data $S = \{x_n, y_n\}_{n=1}^{N} \in \mathscr{X} \times \{0,1\}$

<u>Goal</u>: given a new observation x, we want to predict its label y

<u>How:</u>

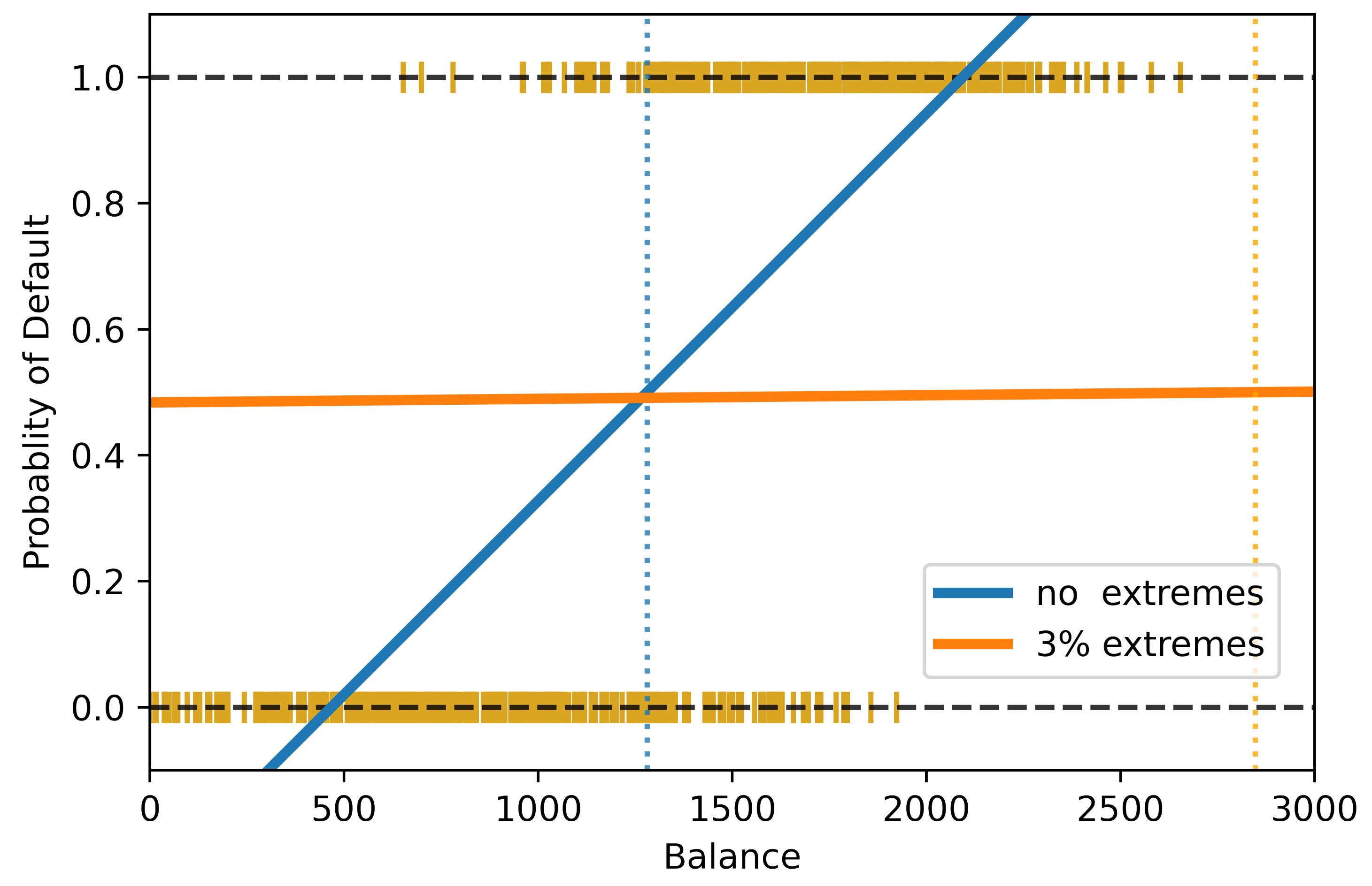
$S = \{x_n, y_n\}_{n=1}^{N}$, $y_n \in \{0,1\}$ $\qquad \mathscr{A} \qquad f_S = \mathscr{A}(S)$

Motivation for logistic regression

Instead of directly modeling the output Y, we can **model the probability** that Y belongs to a specific class. How?

In the previous lecture, we used a linear regression model $\mathbb{P}(Y = 1 \mid X = x) = x^\top w + w_0$ but

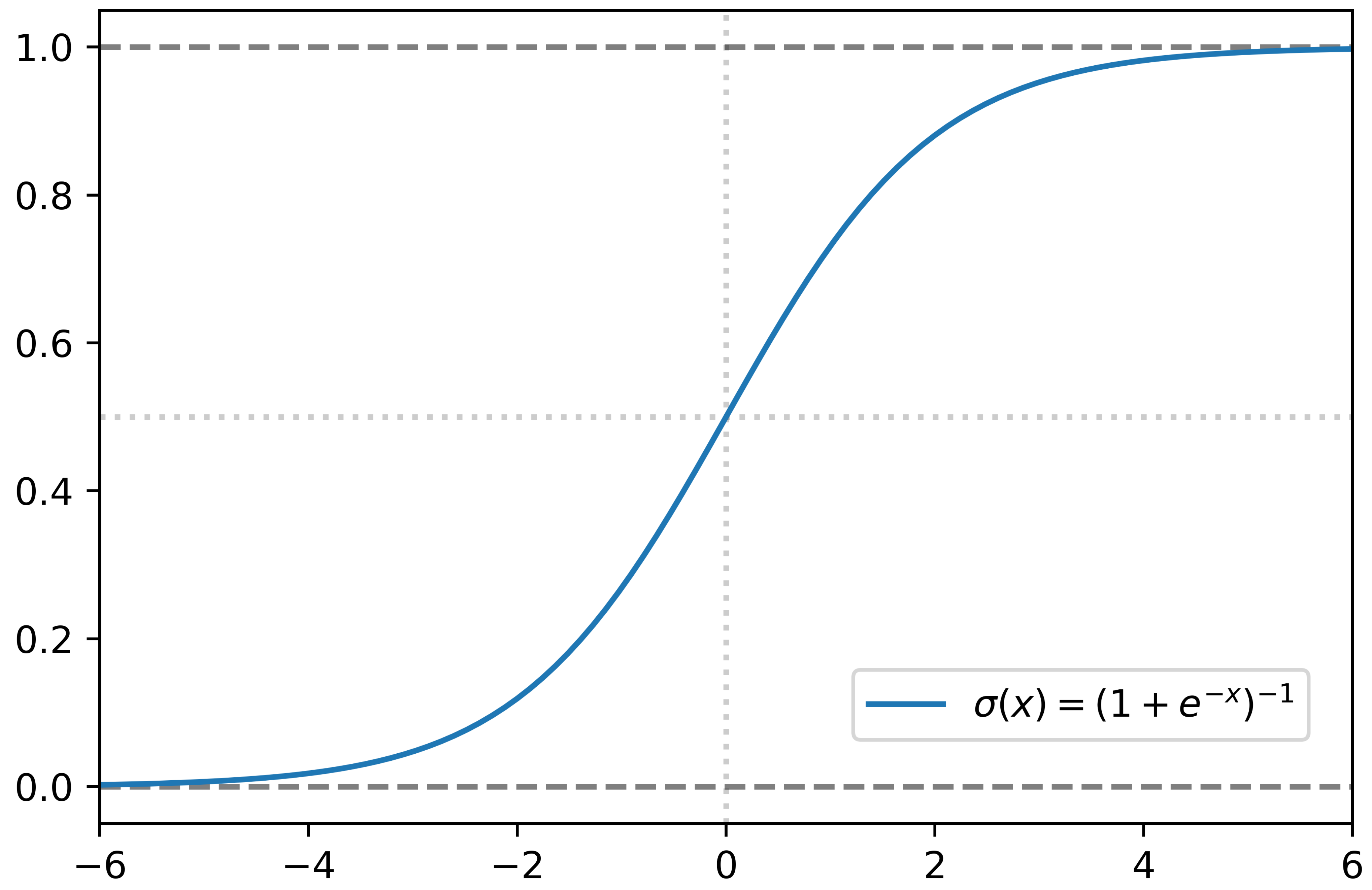
- The predicted value is not in $[0,1]$
- Very large or small prediction values contribute to the error even when they suggest high confidence in the resulting classification



Solution: map the prediction from $(-\infty, +\infty)$ to $[0,1]$

The logistic function

$$\sigma(\eta) := \frac{e^\eta}{1 + e^\eta}$$



Properties of the logistic function:

- $1 - \sigma(\eta) = \dfrac{1 + e^\eta - e^\eta}{1 + e^\eta} = (1 + e^\eta)^{-1}$
- $\sigma'(\eta) = \dfrac{e^\eta(1 + e^\eta) - e^\eta e^\eta}{(1 + e^\eta)^2} = \dfrac{e^\eta}{(1 + e^\eta)^2} = \sigma(\eta)(1 - \sigma(\eta))$

Logistic Regression

$$p(1\,|\,x) := \mathbb{P}(Y=1\,|\,X=x) = \sigma(x^\top w + w_0)$$

$$p(0\,|\,x) := \mathbb{P}(Y=0\,|\,X=x) = 1 - \sigma(x^\top w + w_0)$$

Logistic regression models the **probability that Y belongs to a particular class** using the **logistic function σ**

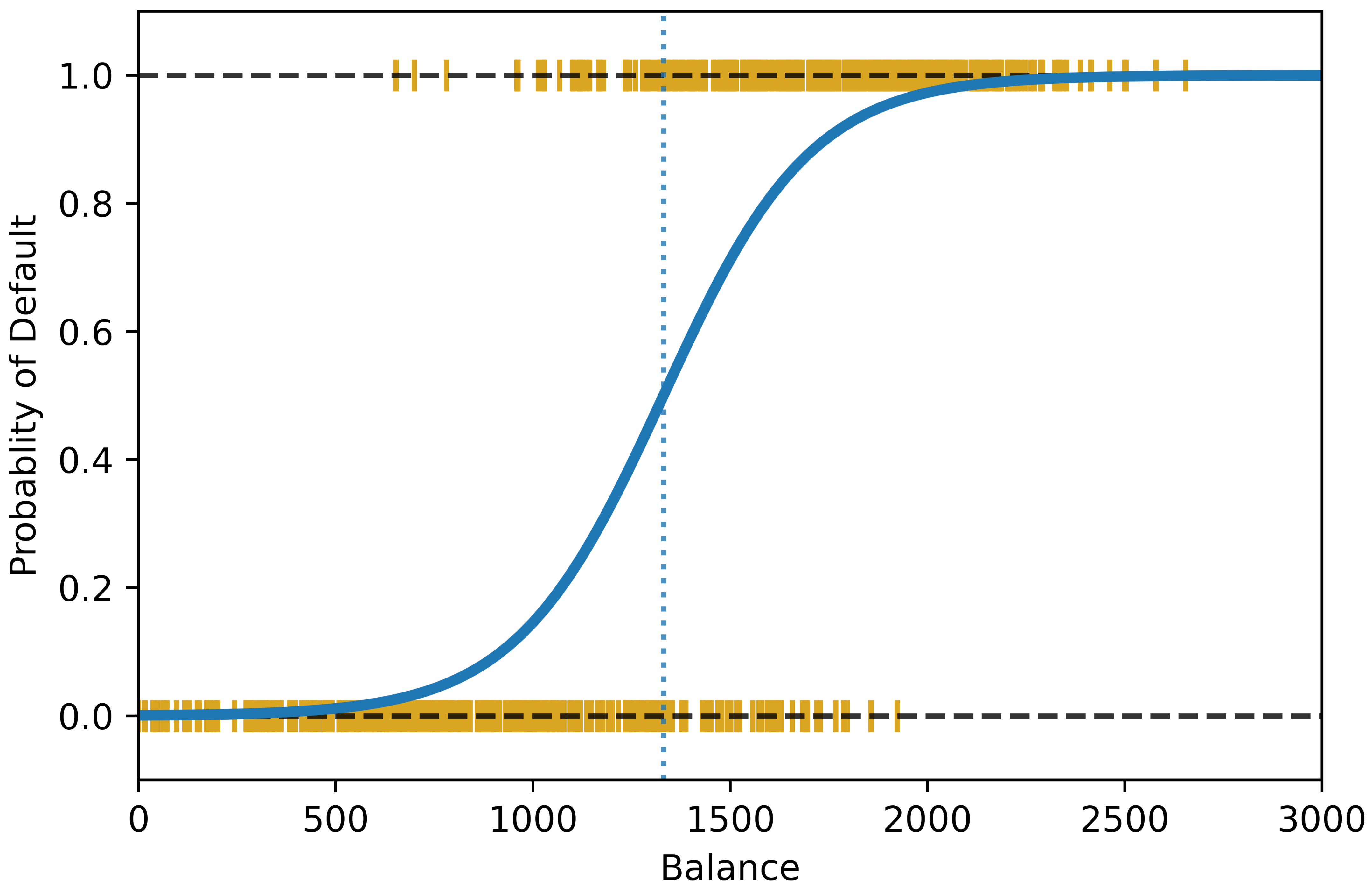
<u>Label prediction:</u> **quantize** the probability:

If $p(1\,|\,x) \geq 1/2$, you predict the class 1
If $p(1\,|\,x) < 1/2$, you predict the class 0

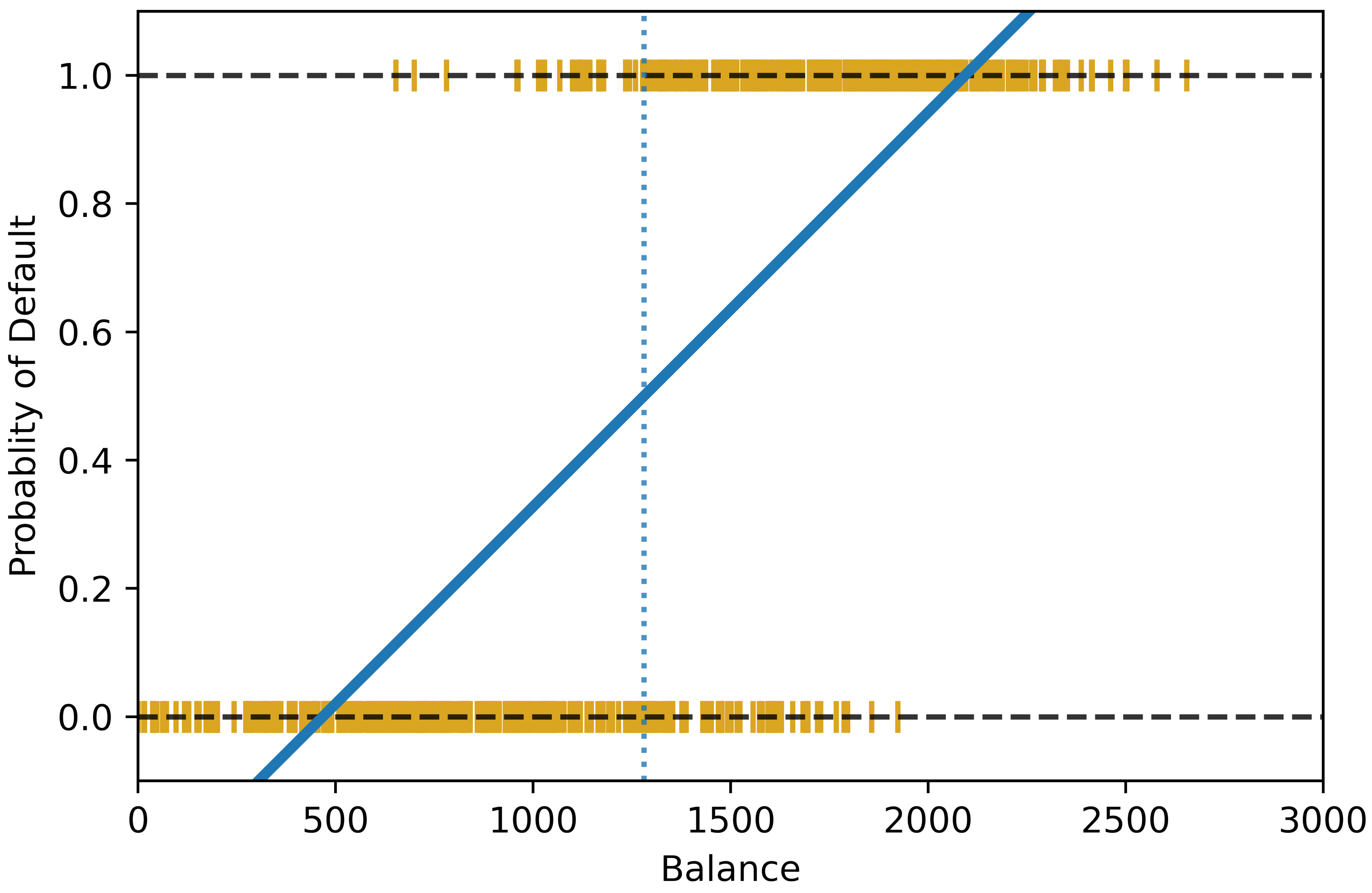
<u>Interpretation:</u>

- Very large $|x^\top w + w_0|$ corresponds to $p(1\,|\,x)$ very close to 0 or 1 (high confidence)
- Small $|x^\top w + w_0|$ corresponds to $p(1\,|\,x)$ very close to .5 (low confidence)

Comparison of logistic and linear regression for balanced data

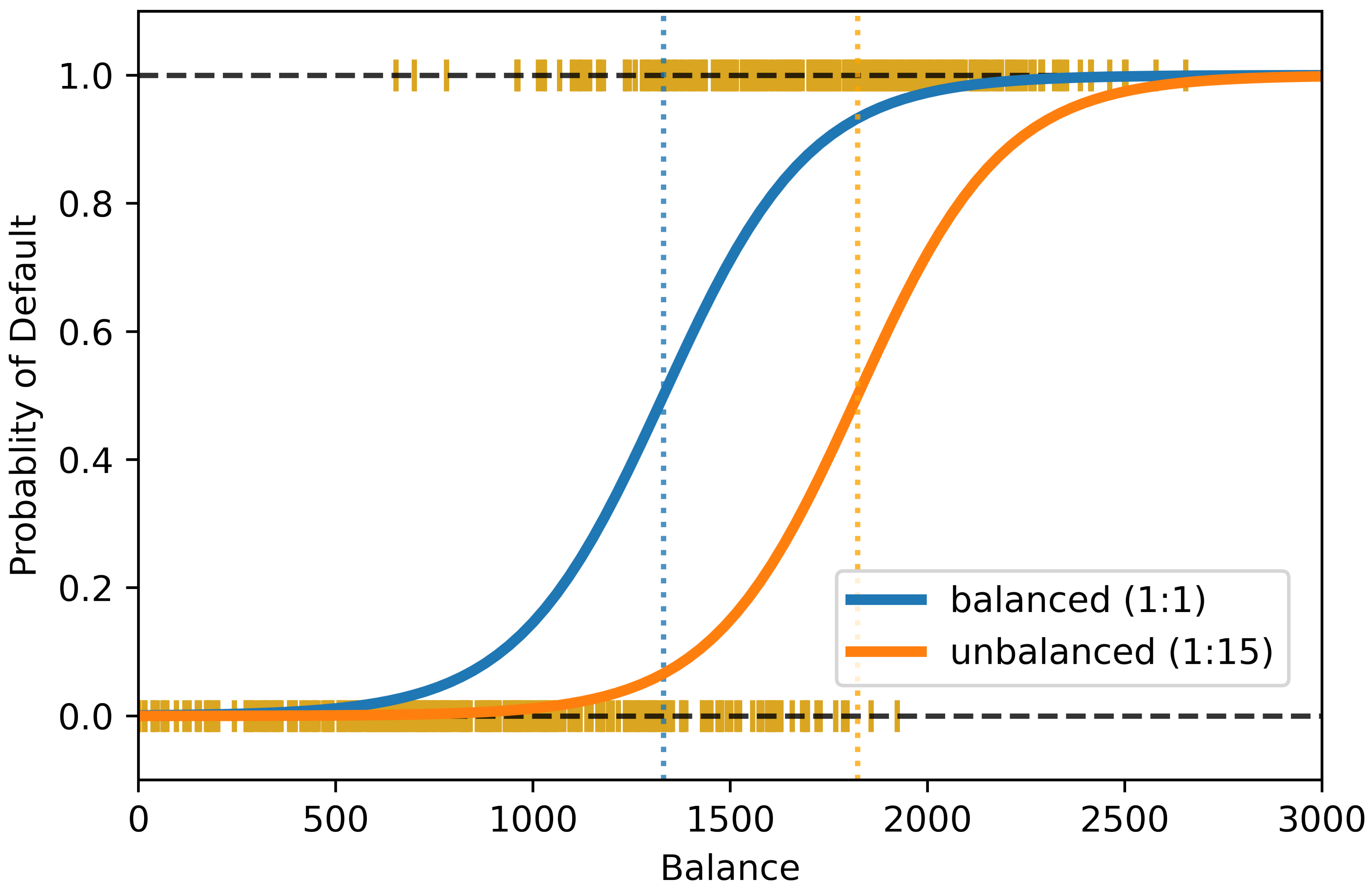


Logistic regression

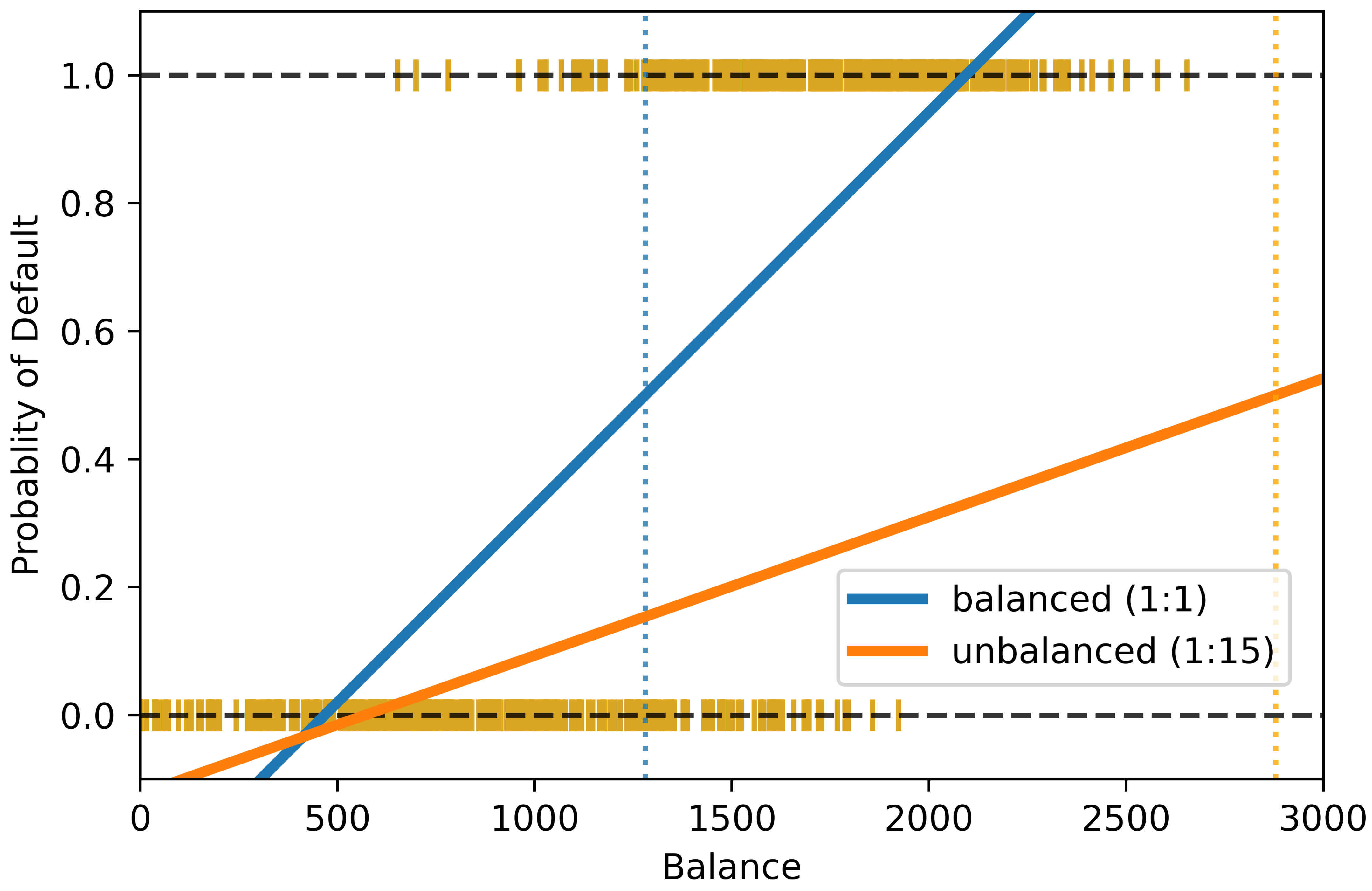


Linear regression

Comparison of logistic and linear regression for unbalanced data

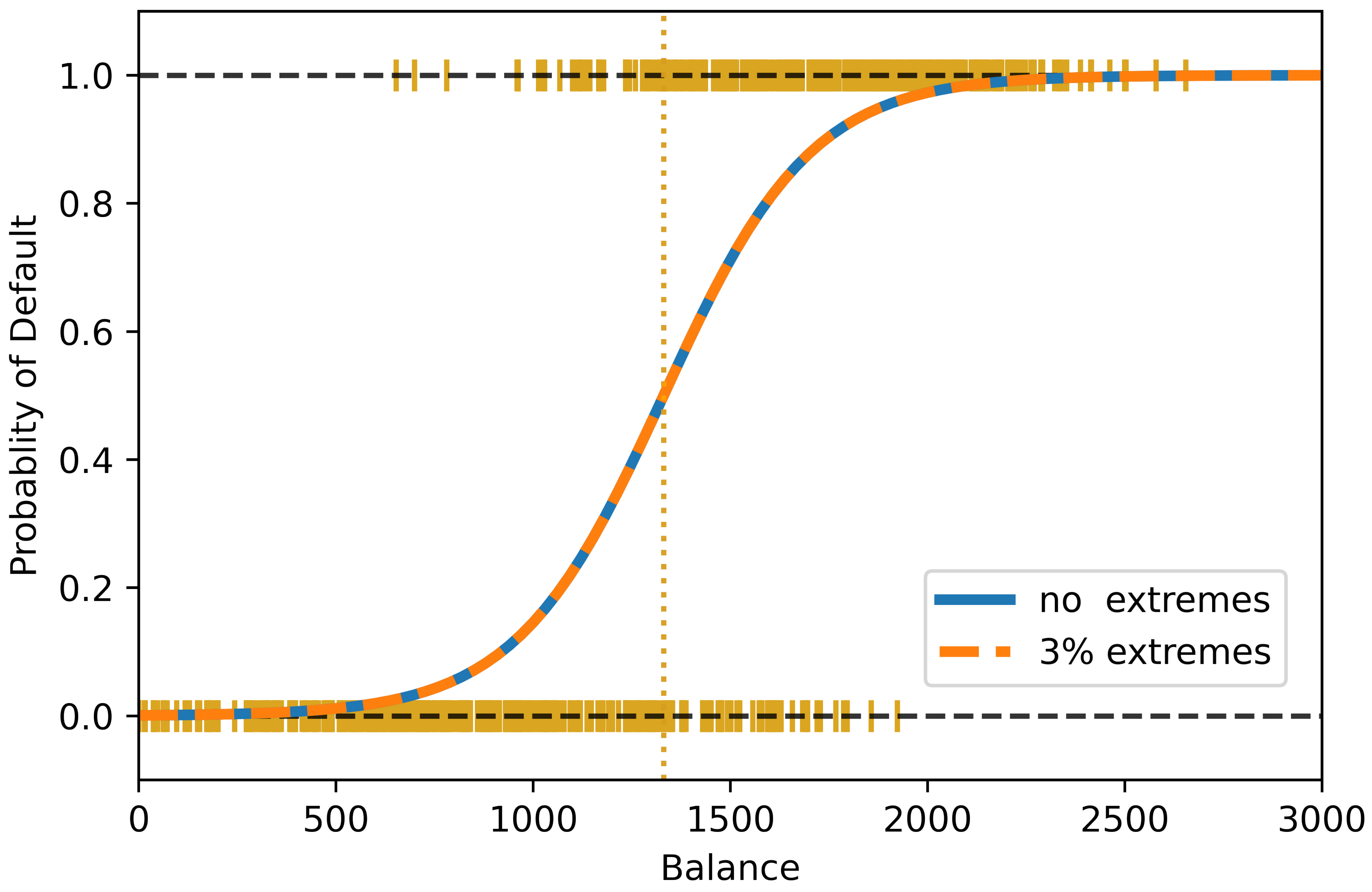


Logistic regression

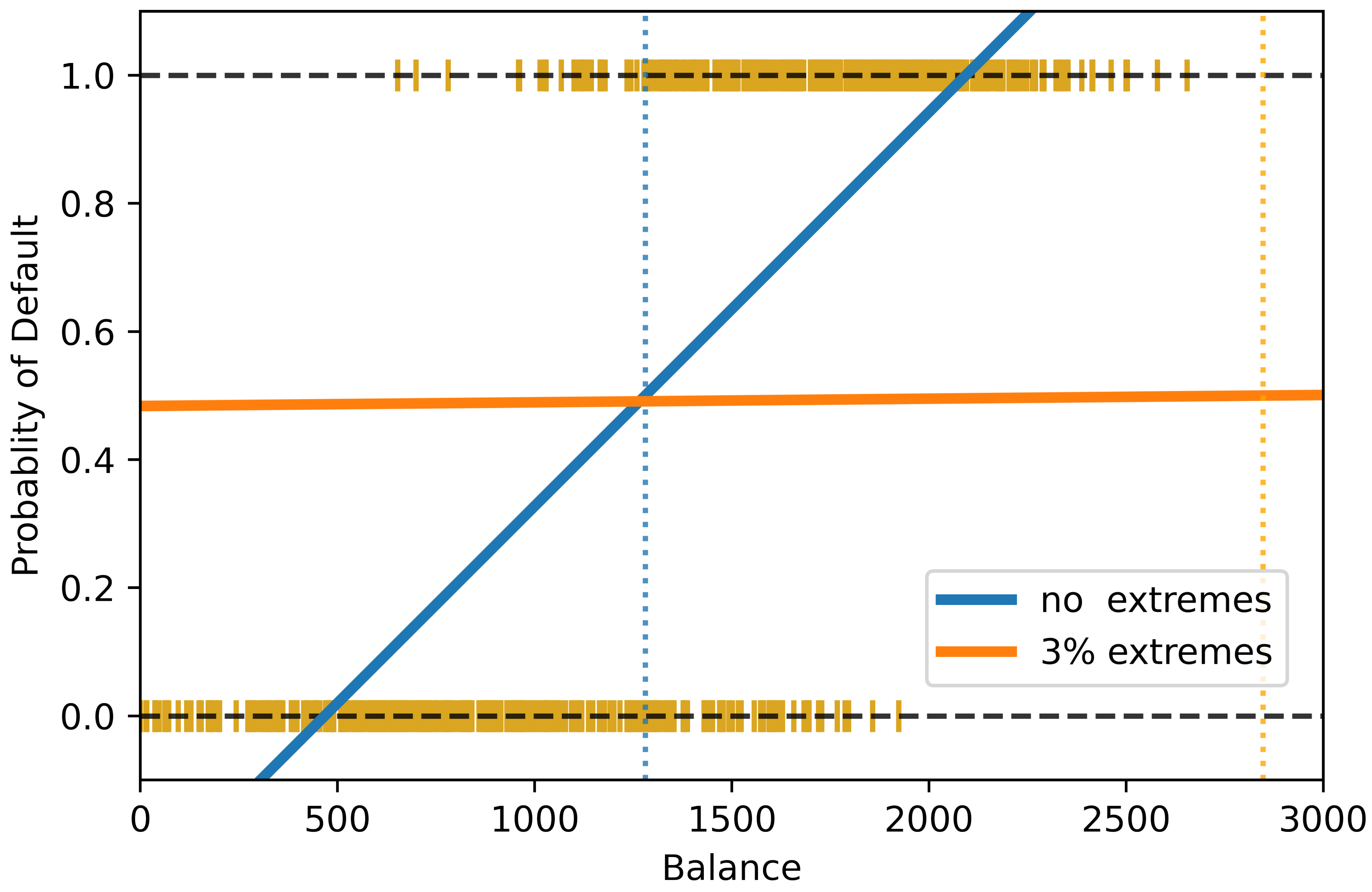


Linear regression

Comparison of logistic and linear regression for data with extreme values

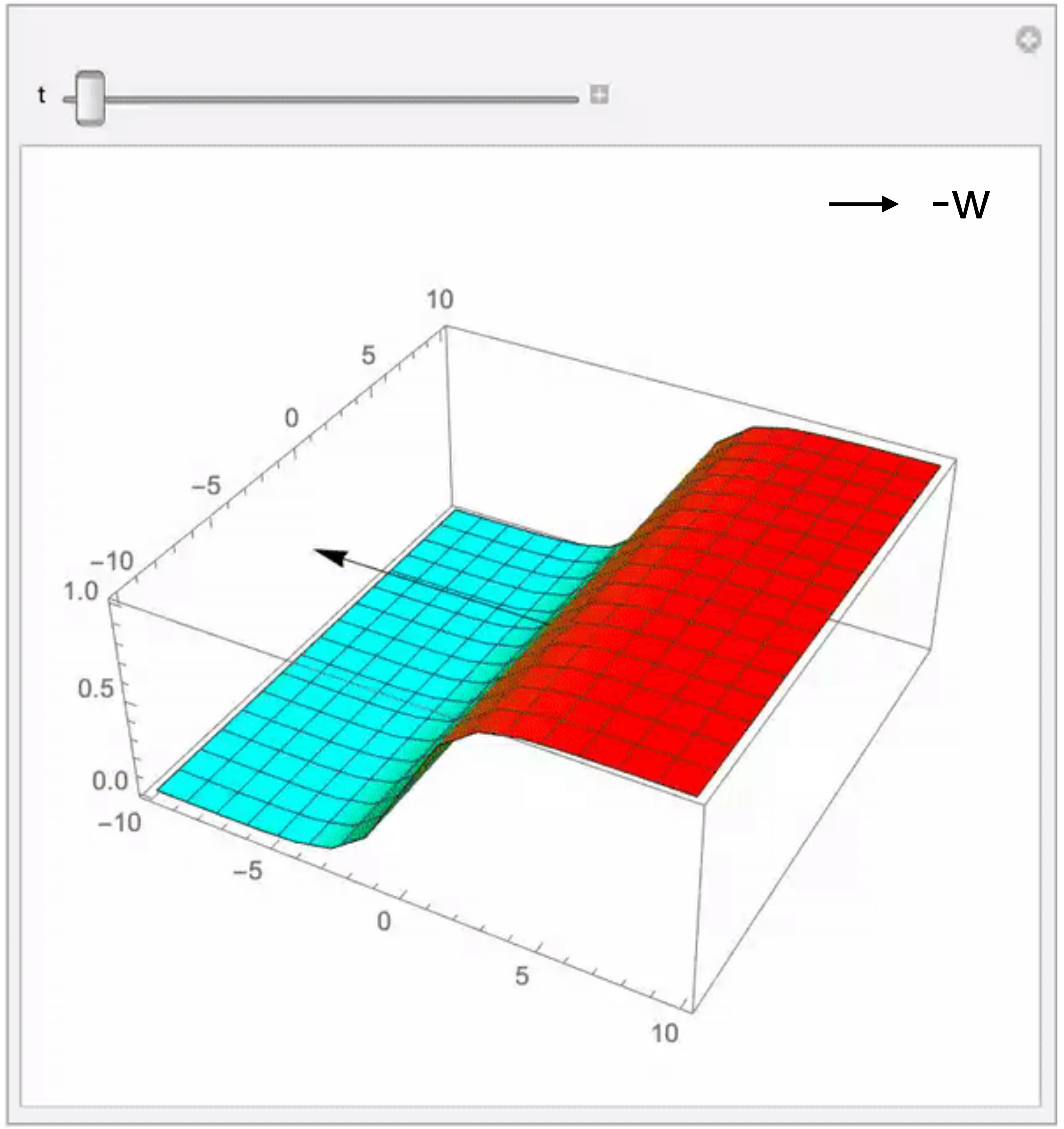


Logistic regression



Linear regression

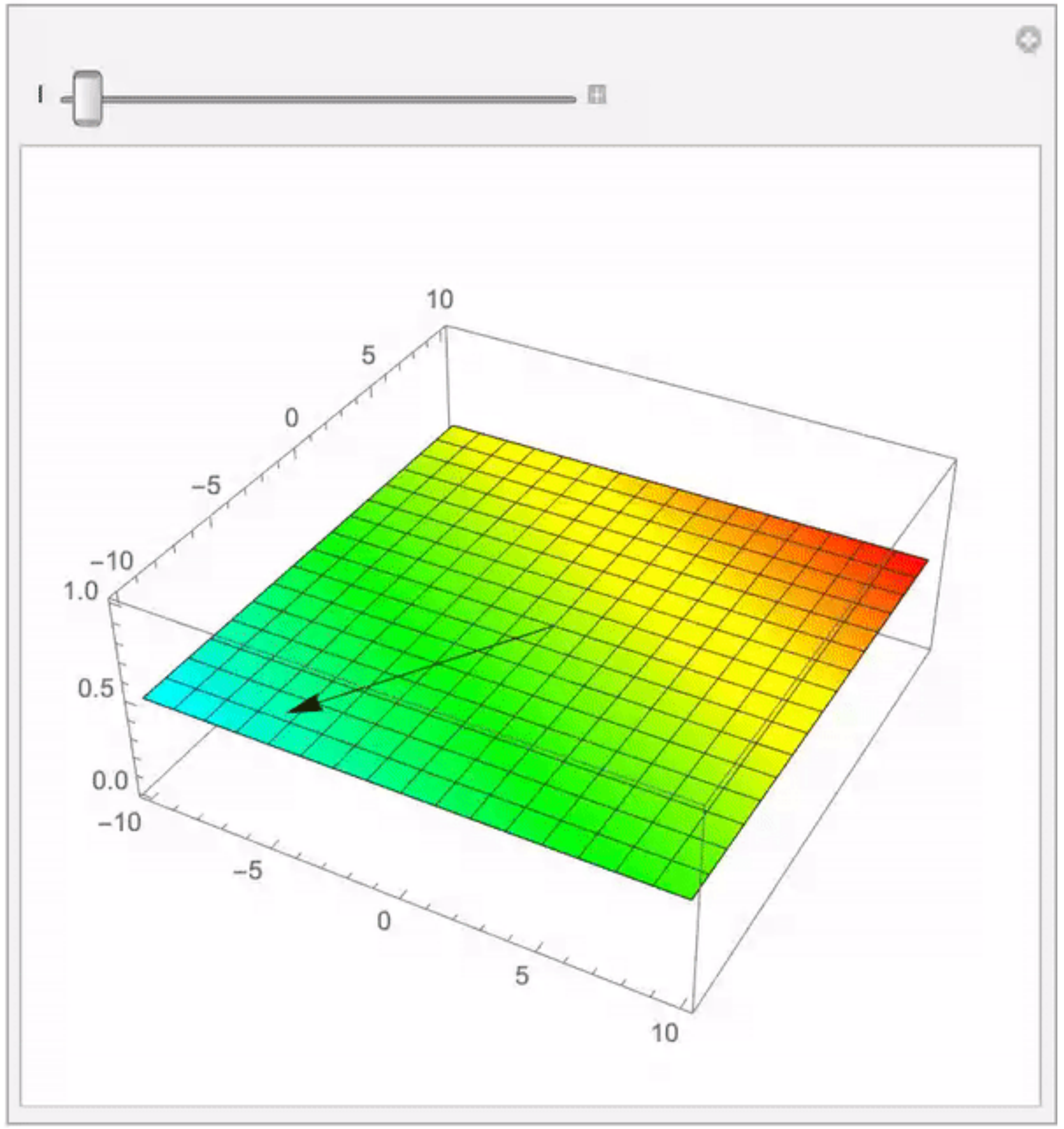
The vector w is orthogonal to the "surface of transition"



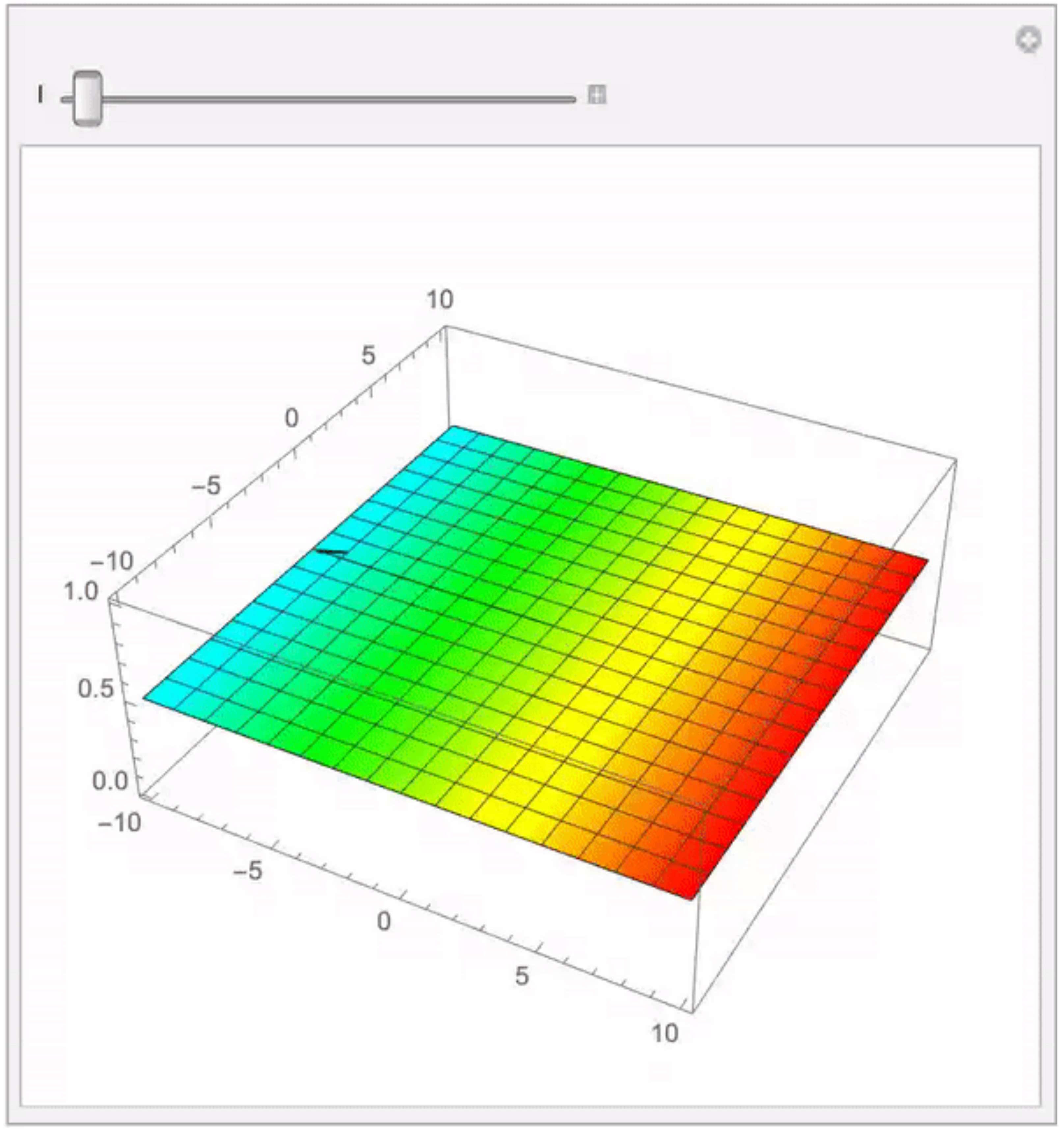
$\sigma(w^\top x)$ for $\|w\| = 1$

The transition between the two levels happens at the hyperplane $w^\perp = \{v : v^\top w = 0\}$

Scaling w makes the transition faster or slower

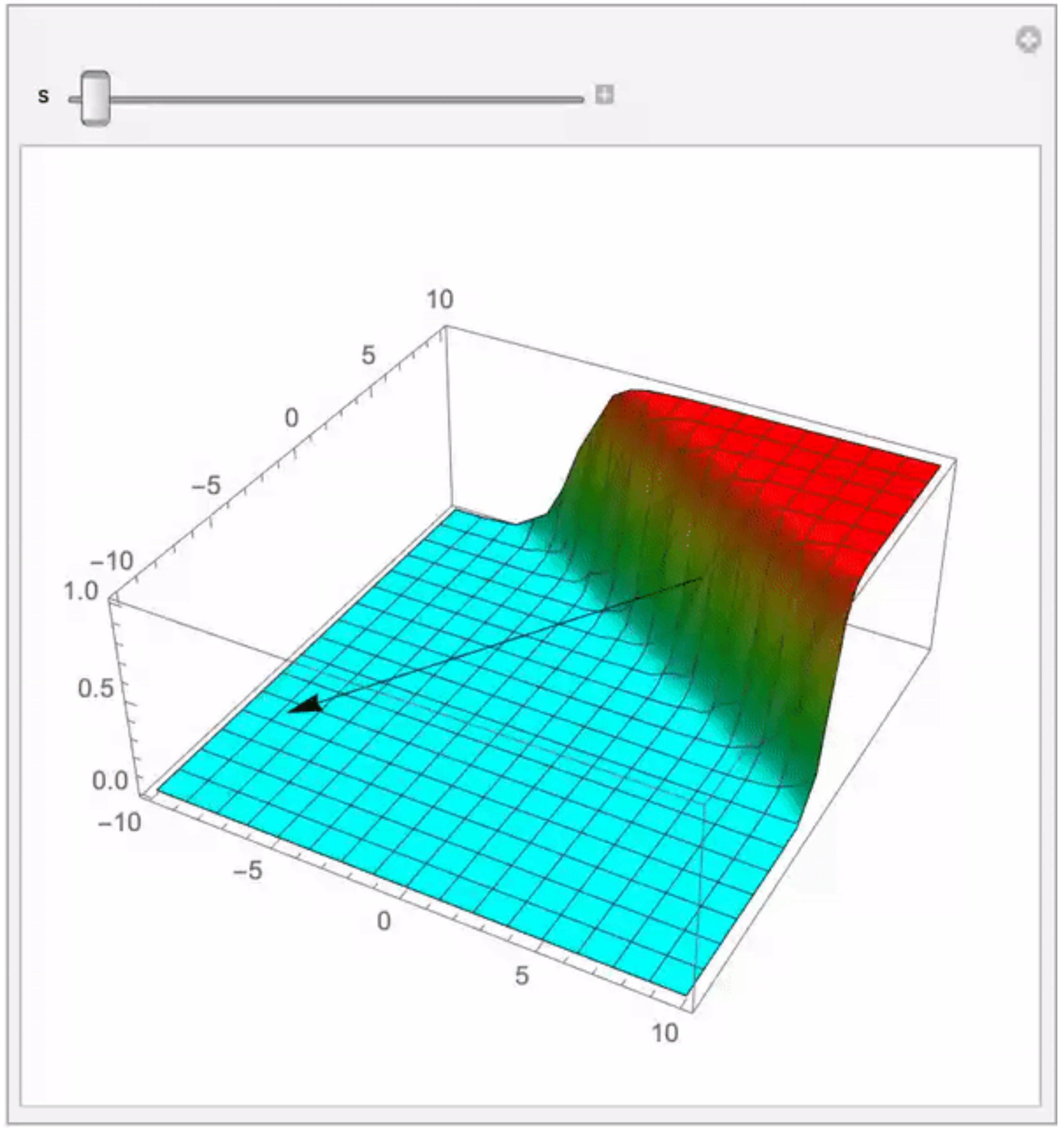


$\sigma(t \cdot w_1^\top x)$ for $t \in [e^{-10}, e^{10}]$

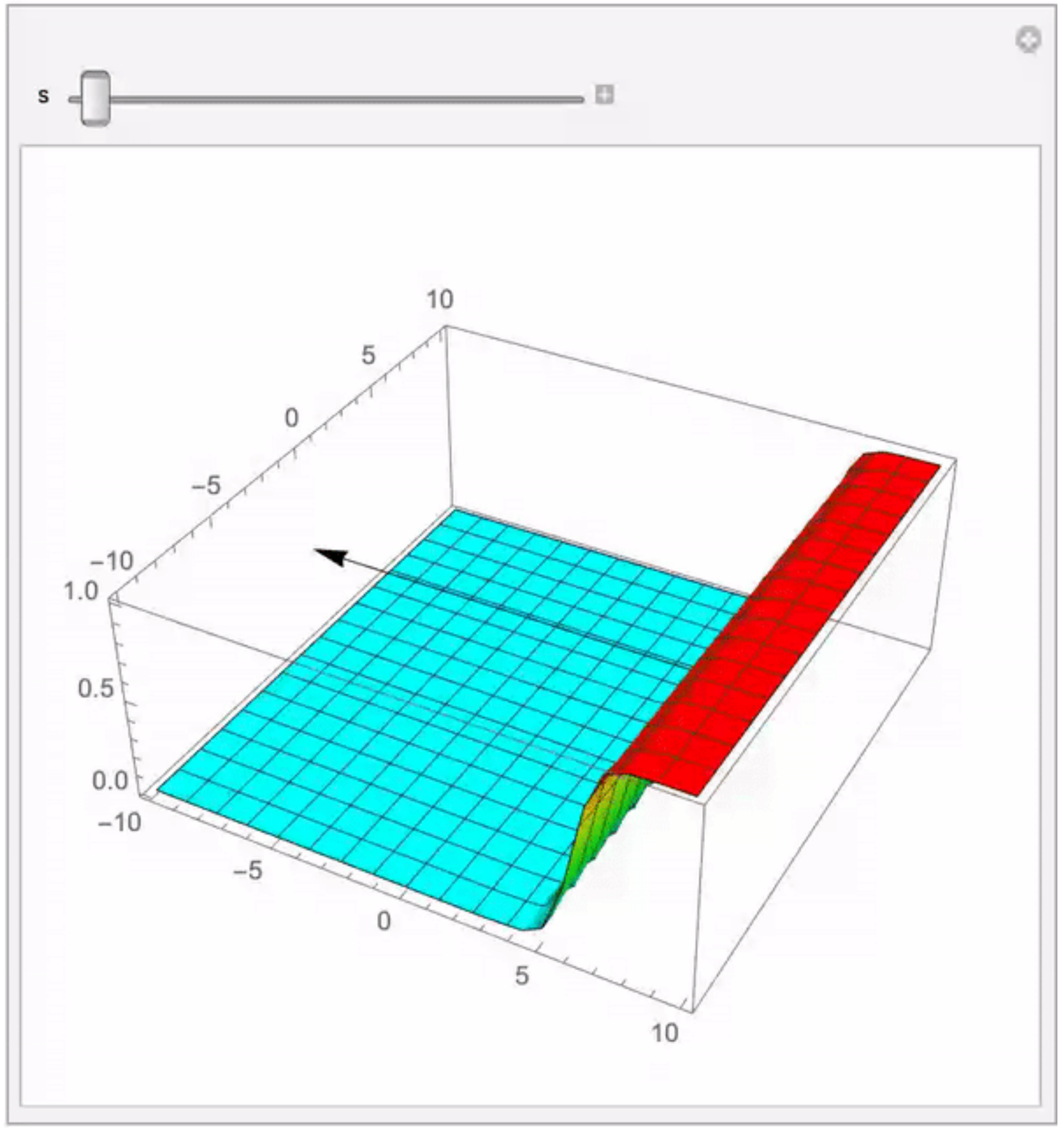


$\sigma(t \cdot w_2^\top x)$ for $t \in [e^{-10}, e^{10}]$

Changing w_0 shifts the decision region along the w vector



$\sigma(w_1^\top x + w_0)$ for $w_0 \in [-6,6]$



$\sigma(w_2^\top x + w_0)$ for $w_0 \in [-6,6]$

The transition happens at the hyperplane $\{v : v^\top w + w_0 = 0\}$

What about the bias term?

We should consider a **shift** w_0 as there is no reason for the transition hyperplane to pass through the origin:

$$p(1 \mid x) = \sigma(w^\top x + w_0)$$

However, for simplicity, we will prefer to **add the constant** 1 to the feature vector

$$x = \begin{pmatrix} x \\ 1 \end{pmatrix}$$

It is crucial for allowing to shift the decision region

Note that **both options are equivalent**

Maximum likelihood estimation (MLE) is a method of estimating the parameters of a statistical model

Given i.i.d. samples $(z_1, \cdots, z_N) \sim p(z_1, \cdots, z_N | w)$, the MLE finds the **parameters** w_* **under which the observations** $z_1, \cdots, z_N$ **are the most likely**:

$$w_* = \arg\max \underset{\textbf{Likelihood function}}{\mathscr{L}(w)} := p(z_1, \cdots, z_N | w) \underset{\textbf{i.i.d. obs}}{=} \prod_{n=1}^{N} p(z_n | w)$$

Often more convenient to work with the **negative log-likelihood**:

$$w_* = \arg\min[-\log(\mathscr{L}(w))] = \arg\min \sum_{n=1}^{N} -\log(p(z_n | w))$$

This estimator is **consistent***: if the data are generated according to the model, the MLE converges to the true parameter when $n \to \infty$

In practice, data are not generated according to it, but it still provides a theoretical justification

*under mild technical conditions

MLE for logistic regression

<u>Assumption:</u> The inputs $\mathbf{X}$ do not depend on the parameter w we choose:

$$\mathscr{L}(w) = p(\mathbf{y}, \mathbf{X} \,|\, w) = p(\mathbf{X} \,|\, w) p(\mathbf{y} \,|\, \mathbf{X}, w) \underset{\mathbf{X} \perp\!\!\!\perp w}{=} p(\mathbf{X})\ p(\mathbf{y} \,|\, \mathbf{X}, w)$$

cst independant of w

$$\begin{aligned} p(\mathbf{y} \mid \mathbf{X}, w) &= \Pi_{n=1}^{N}\ p(y_n \,|\, x_n, w) \\ &= \Pi_{n:y_n=1}\ p(y_n = 1 \,|\, x_n, w)\ \Pi_{n:y_n=0}\ p(y_n = 0 \,|\, x_n, w) \\ &= \Pi_{n=1}^{N}\ \sigma(x_n^\top w)^{y_n}[1 - \sigma(x_n^\top w)]^{1-y_n} \end{aligned}$$

The likelihood is proportional to:

$$\boxed{\mathscr{L}(w) \propto \prod_{n=1}^{N} \sigma(x_n^\top w)^{y_n}[1 - \sigma(x_n^\top w)]^{1-y_n}}$$

Minimum of the negative log likelihood

It is more convenient to work with the negative log-likelihood:

$$
\begin{aligned}
-\log\big(p(\mathbf{y}\,|\,\mathbf{X}, w)\big) &= -\log\big(\textstyle\prod_{n=1}^{N} \sigma(x_n^\top w)^{y_n}[1-\sigma(x_n^\top w)]^{1-y_n}\big) \\
&= -\textstyle\sum_{n=1}^{N} y_n \log \sigma(x_n^\top w) + (1-y_n)\log\big(1-\sigma(x_n^\top w)\big) \\
&= \textstyle\sum_{n=1}^{N} y_n \log\left(\frac{1-\sigma(x_n^\top w)}{\sigma(x_n^\top w)}\right) - \log\big(1-\sigma(x_n^\top w)\big) \\
&= \textstyle\sum_{n=1}^{N} - y_n x_n^\top w + \log\big(1+e^{x_n^\top w}\big)
\end{aligned}
$$

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

We obtain the following cost function we will minimize to learn the parameter w_*

$$\boxed{w_* = \arg\min L(w) := \frac{1}{N}\sum_{n=1}^{N} - y_n x_n^\top w + \log\big(1+e^{x_n^\top w}\big)}$$

*If we are considering $y \in \{-1,1\}$, we will have a different function

** minimizing L is exactly equivalent to maximize the likelihood $\mathscr{L}$ since $p(X) \perp\!\!\!\perp w$

A side note on logistic loss

In logistic regression, the **negative log likelihood** is equivalent to ERM for the **logistic loss** (a surrogate for 0-1 loss, as discussed yesterday)

- Logistic loss for $y \in \{0,1\}$:

$$\ell(y, g(x)) = -yg(x) + \log(1 + \exp(g(x)))$$

- Logistic loss for $y \in \{-1,1\}$:

$$\ell(y, g(x)) = \log(1 + \exp(-yg(x)))$$

Note: the logistic loss can be applied in modern machine learning as well: $g(x)$ can represent the output of a neural network

Gradient of the negative log likelihood

To minimize L, let's first look at its stationary points by computing its gradient:

$$\nabla L(w) = \nabla \left[\frac{1}{N} \sum_{n=1}^{N} \log\left(1 + e^{x_n^\top w}\right) - y_n x_n^\top w \right] = \frac{1}{N} \sum_{n=1}^{N} \frac{e^{x_n^\top w} x_n}{1 + e^{x_n^\top w}} - y_n x_n = \frac{1}{N} \sum_{n=1}^{N} \left(\sigma(x_n^\top w) - y_n\right) x_n$$

Which can be written under the matrix form $\mathbf{X} = \begin{bmatrix} x_1^\top \\ \vdots \\ x_n^\top \end{bmatrix} \in \mathbb{R}^{n \times d}$ and $\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \in \mathbb{R}^n$

$$\nabla L(w) = \frac{1}{N} \mathbf{X}^\top \left(\sigma(\mathbf{X} w) - \mathbf{y}\right)$$

- Same gradient as in LS but with σ
- No closed form solution to $\nabla L(w) = 0$
- Good news: the cost function L is convex

Convexity of the loss function L

Claim: The function

$$L(w) = \frac{1}{N}\sum_{n=1}^{N} - y_n x_n^\top w + \log\left(1 + e^{x_n^\top w}\right)$$

is convex in the weight vector w

Proof: L is obtained through simple convexity preserving operations:

1. Positive combinations of convex functions is convex
2. Composition of a convex and a linear functions is convex
3. A linear function is both convex and concave
4. $\eta \mapsto \log(1 + e^{\eta})$ is convex

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Proof of 4: $h(\eta) := \log(1 + e^{\eta})$ is cvx

$$h'(\eta) = \frac{e^{\eta}}{1 + e^{\eta}} = \sigma(\eta)$$

$$h''(\eta) = \sigma'(\eta) = \frac{e^{\eta}}{(1 + e^{\eta})^2} \geq 0$$

Proof of the convexity of L

$$\begin{cases} \text{2. Composition of a convex and a linear functions is convex} \\ \text{4. } \eta \mapsto \log(1 + e^{\eta}) \text{ is convex} \end{cases}$$

$$\log\left(1 + e^{x_n^\top w}\right) \text{ is convex}$$

3. A linear function is both convex and concave

$$-y_n x_n^\top w \text{ is convex}$$

1. Positive combinations of convex functions is convex

$$L(w) = \frac{1}{N} \sum_{n=1}^{N} - y_n x_n^\top w + \log\left(1 + e^{x_n^\top w}\right) \text{ is convex}$$

Second proof: Hessian of L is psd

The Hessian $\nabla^2 L$ is the **matrix** whose entries are the **second derivatives** $\frac{\partial^2}{\partial w_i \partial w_j} L(w)$

$$
\begin{aligned}
\nabla^2 L(w) &= \nabla [\, \nabla L(w)]^\top \\
&= \nabla \left[\tfrac{1}{N} \textstyle\sum_{n=1}^N x_n \big(\sigma(x_n^\top w) - y_n\big)\right]^\top \\
&= \tfrac{1}{N} \textstyle\sum_{n=1}^N \nabla \sigma(x_n^\top w) x_n^\top = \tfrac{1}{N} \textstyle\sum_{n=1}^N \sigma(x_n^\top w)\big(1 - \sigma(x_n^\top w)\big) x_n x_n^\top
\end{aligned}
$$

It can be written under the matrix form:

$$\nabla^2 L(w) = \frac{1}{N} \mathbf{X}^\top S \mathbf{X}, \quad \text{where } S = \text{diag}\Big[\sigma(x_n^\top w)\big(1 - \sigma(x_n^\top w)\big)\Big] \succcurlyeq 0$$

➡ L is convex since $\nabla^2 L(w) \succcurlyeq 0$

How to minimize the convex function L?

Gradient descent:

$$\begin{cases} w_0 \in \mathbb{R}^d \\ w_{t+1} = w_t - \frac{\gamma_t}{N} \sum_{n=1}^{N} \big(\sigma(x_n^\top w_t) - y_n\big) x_n \end{cases}$$

can be slow

Stochastic gradient descent

$$\begin{cases} w_0 \in \mathbb{R}^d \\ w_{t+1} = w_t - \gamma_t \big(\sigma(x_{n_t}^\top w_t) - y_{n_t}\big) x_{n_t} \end{cases}$$ where $\mathbb{P}[n_t = n] = 1/N$

is faster but converges slower

Newton's method uses second order information

Newton's method **minimizes** the **quadratic approximation**:

$$L(w) \sim L(w_t) + \nabla L(w_t)^\top (w - w_t) + \frac{1}{2}(w - w_t)^\top \nabla^2 L(w_t)(w - w_t) := \phi_t(w)$$

$$\tilde{w} = \arg\min \phi_t(w) \implies \nabla L(w_t) + \nabla^2 L(w_t)(\tilde{w} - w_t) = 0$$

Newton's method: $$w_{t+1} = w_t - \gamma_t \nabla^2 L(w_t)^{-1} \nabla L(w_t)$$

The step-size is needed to ensure convergence (damped Newton's method)

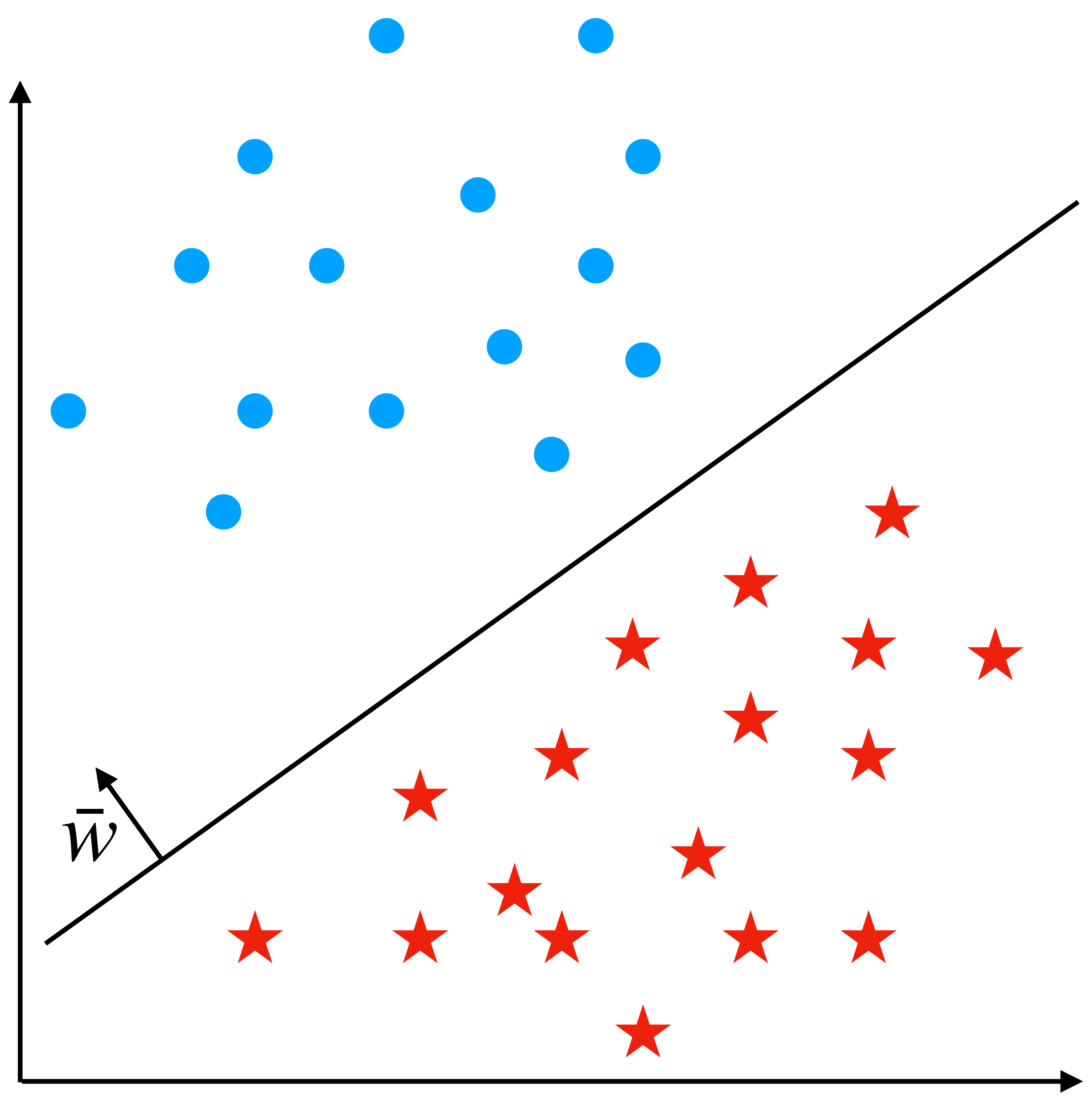
The convergence is typically **faster than with gradient descent** but the **computational complexity is higher** (computing Hessian and solving a linear system)

Problem when the data are linearly separable

$$\inf_{w} L(w) = 0 = \lim_{\alpha \to \infty} L(\alpha \cdot \bar{w})$$

The inf value is not attained for a finite w

If we use an optimization algorithm, the weights will go to ∞



$$L(w) = \frac{1}{N} \sum_{n=1}^{N} -y_n x_n^\top w + \log\left(1 + e^{x_n^\top w}\right)$$

Solution: add a ℓ_2-regularization

➡ **ridge logistic regression**:

$$\frac{1}{N} \sum_{n=1}^{N} -y_n x_n^\top w + \log\left(1 + e^{x_n^\top w}\right) + \frac{\lambda}{2}\|w\|_2^2$$

- Optimization perspective: stabilize the optimization process
- Statistical perspective: avoid overfitting

Recap

- Logistic regression:
  - Maps inputs to output class probabilities
  - Exhibits robustness towards unbalanced data and extreme values
- How to solve logistic regression?
  - By minimizing the negative log-likelihood (a.k.a. logistic loss)
  - Using gradient methods or second-order methods
- Not ideal when data is linearly separable?
  - Weights go to infinity
  - A solution is to add a penalty term, e.g. ℓ_2-regularization