

# Linear Models for Classification

Master's Degree in Bioinformatics and Computational Biology - Machine Learning

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▶ **Questionnaire**

Please, fill in the questionnaire regarding your prior knowledge about this topic.



## Introduction



# Supervised Learning: Classification (I)



## Definition (Classification Problem)

A **classification problem** is a supervised learning problem where the outputs are discrete.



## Examples (Classification Problems)

- ▶ Predicting if a patient has a certain disease or not depending on medical data.
- ▶ Distinguishing the species of captured fish using the data provided by several sensors.
- ▶ Discerning the type of object that appears in a picture.



# Supervised Learning: Classification (II)



## Elements of a Supervised Learning Problem

**Data** Set of input–output pairs,  $\mathcal{D} = \{(\mathbf{x}_i, y_i)\}_{i=1}^N$ .

**Features** Vector of attributes (independent/input variables, covariates...),  $\mathbf{x}_i \in \mathcal{X}$ .

**Label** Target (dependent variable, outcome...),  $y_i \in \mathcal{Y}$ .

**Model** Mapping from the input to the output space,  $f_{\theta} : \mathcal{X} \rightarrow \mathcal{Y}$ , with  $\theta$  the model parameters.

**Learning Algorithm** Procedure to obtain a model based on the data,  $\mathcal{A} : \mathcal{D} \rightarrow f_{\theta}(\cdot)$ .

- ▶ In a classification setting  $\mathcal{Y} = \{\mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_M\}$ .
- ▶ In many situations, specially after preprocessing the data,  $\mathcal{X} = \mathbb{R}^d$ .
- ▶ The resultant model assigns to each input a certain class,  $f_{\theta} : \mathcal{X} \rightarrow \{\mathcal{C}_1, \mathcal{C}_2, \dots, \mathcal{C}_M\}$ .



# Binary Classification and Linear Models

- ▶ The most important classification scenario is when  $M = 2$  (**binary classification**).
  - If  $M > 2$ , there are encoding techniques to transform the problem into several binary subproblems.
- ▶ The classes are usually denoted as  $\mathcal{C}_0$  and  $\mathcal{C}_1$ , and they are represented with a 0/1 (or  $-1/1$ ) encoding.
  - The labels are transformed to:

$$t_i = \begin{cases} 0 & \text{if } y_i = \mathcal{C}_0, \\ 1 & \text{if } y_i = \mathcal{C}_1. \end{cases}$$

- ▶ “Simplest” approaches to classification:
  - Ignore the input: **constant model** (usually, **majority class**).
  - Define the output as a linear combination of the inputs plus a **transformation: linear model**.
    - Simple. Robust (small variance). Interpretable. Easy to train. Easy to predict.
    - Limited flexibility. Under-fitting (large bias).



## Binary Linear Classification





# Binary Linear Classifier

- ▶ For simplicity,  $\mathcal{X} = \mathbb{R}^d$ .
- ▶ The data becomes  $\mathcal{D} = \{(\mathbf{x}_i, t_i)\}_{i=1}^N$ , with  $\mathbf{x}_i = (x_{i,1}, x_{i,2}, \dots, x_{i,d}) \in \mathbb{R}^d$  and  $t_i \in \{0, 1\}$ .

- ▶ The corresponding linear model is a hyperplane, with parameters  $\theta = \{b, \mathbf{w}\}$ .
  - $b \in \mathbb{R}$  is the intercept or bias term.
  - $\mathbf{w} = (w_1, w_2, \dots, w_d) \in \mathbb{R}^d$  is the normal vector of the hyperplane.
  - The model is defined as:

$$f_{\theta}(\mathbf{x}) = \begin{cases} 0 & \text{if } b + \mathbf{w}^T \mathbf{x} < 0, \\ 1 & \text{if } b + \mathbf{w}^T \mathbf{x} \geq 0. \end{cases}$$

- The hyperplane divides the space into two halves, one for class  $\mathcal{C}_0$  and the other for class  $\mathcal{C}_1$ .
- ▶ The **learning algorithm** will determine  $b$  and  $\mathbf{w}$  using  $\mathcal{D}$ .



# Binary Linear Classifier - Exercise



## Exercise

[▶ Questionnaire](#)

Given a 2-dimensional binary linear classification model with parameters  $\theta = \{b, \mathbf{w}\}$ , with  $b = 1$  and  $\mathbf{w} = (1, 2)^\top$ .

- 1 Compute the output of the model for  $\mathbf{x}_1 = (1, 1)^\top$ .
- 2 Compute the output of the model for  $\mathbf{x}_2 = (1, -2)^\top$ .
- 3 Compute the output of the model for  $\mathbf{x}_3 = (0, 0)^\top$ .



Notebook

Binary Linear Classification: First Example



## Quality of the Model

- ▶ A procedure is needed to determine the bias  $b$  and the vector  $\mathbf{w}$ , optimizing the **quality** of the model.
- ▶ The quality of the model has to be defined. Usually from two points of view:


**Fitness** A fitness term  $\mathcal{F}_{\mathcal{D}}(\boldsymbol{\theta})$  measures how well the model fits the training data.

**Complexity** A regularization term  $\mathcal{R}(\boldsymbol{\theta})$  penalizes the complexity of the model.



### Fitness Term for a Classification Linear Model

**Correct Prediction** For the  $i$ -th pattern,



$$c_i = \begin{cases} 0 & \text{if } t_i \neq f_{\boldsymbol{\theta}}(\mathbf{x}_i) \\ 1 & \text{if } t_i = f_{\boldsymbol{\theta}}(\mathbf{x}_i) \end{cases} = \begin{cases} 0 & \text{if } (t_i = 0, b + \mathbf{w}^T \mathbf{x}_i \geq 0) \text{ or } (t_i = 1, b + \mathbf{w}^T \mathbf{x}_i < 0), \\ 1 & \text{if } (t_i = 0, b + \mathbf{w}^T \mathbf{x}_i < 0) \text{ or } (t_i = 1, b + \mathbf{w}^T \mathbf{x}_i \geq 0). \end{cases}$$

**Accuracy**  $\text{Acc}(b, \mathbf{w}) = \mathbb{E}[C] \approx \frac{1}{N} \sum_{i=1}^N c_i.$



## Quality of the Model - Exercise



## Exercise

[▶ Questionnaire](#)

Given a 2-dimensional binary linear classification model with parameters  $\theta = \{b, \mathbf{w}\}$ , with  $b = 1$  and  $\mathbf{w} = (1, 2)^\top$ , and for the following data:

$x_{i,1}$	$x_{i,2}$	$t_i$
1	1	1
1	-2	0
0	0	0

- 1 Compute the accuracy.



Notebook

Binary Linear Classification: Quality of the Model



# Training a Linear Classifier: Using the Regression Framework

- ▶ The most common choice for evaluating the model is the accuracy.

- It is a sensible and intuitive measure.
- It is **non-convex**.
- It is **non-differentiable**.
- It is **discontinuous**.

- 
- ▶ Optimizing the accuracy is a problem that cannot (in general) be tackled directly.

- 
- ▶ An alternative idea could be to train a Linear Regression model.

- Labels  $-1/1$ .
- The predicted label is determined by taking the sign of the output.



Notebook

Binary Linear Classification: Training a Regression Linear Model





# Training a Linear Classifier: Logistic Regression (I)



- ▶ A different quality measure is needed.
    - It should be simpler to optimize than the accuracy.
    - It should not penalize points far from the decision boundary (but on the correct side).
- 
- ▶ A probabilistic approach can be helpful.
  - ▶ In particular, the main framework is **Logistic Regression**.
    - The linear model is used to estimate the posterior probability of one class.
    - A sigmoid transformation is used.

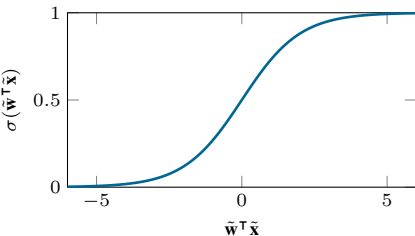


## Training a Linear Classifier: Logistic Regression (II)

- Denoting by  $\tilde{\mathbf{x}} = [1, \mathbf{x}]$  and by  $\tilde{\mathbf{w}} = [b, \mathbf{w}]$ , the posterior probabilities are defined as:

$$p(\mathcal{C}_1 | \tilde{\mathbf{x}}; \tilde{\mathbf{w}}) = \sigma(\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}) = \frac{1}{1 + e^{-\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}}},$$

$$p(\mathcal{C}_0 | \tilde{\mathbf{x}}; \tilde{\mathbf{w}}) = 1 - p(\mathcal{C}_1 | \tilde{\mathbf{x}}; \tilde{\mathbf{w}}) = 1 - \frac{1}{1 + e^{-\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}}} = \frac{e^{-\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}}}{1 + e^{-\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}}} = \frac{1}{1 + e^{\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}}} = \sigma(-\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}).$$



- $\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}} < 0 \Rightarrow p(\mathcal{C}_1 | \tilde{\mathbf{x}}; \tilde{\mathbf{w}}) < 0.5$ : Class  $\mathcal{C}_0$  is predicted.
- $\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}} \geq 0 \Rightarrow p(\mathcal{C}_1 | \tilde{\mathbf{x}}; \tilde{\mathbf{w}}) \geq 0.5$ : Class  $\mathcal{C}_1$  is predicted.

# Training a Linear Classifier: Logistic Regression - Exercise



## Exercise

[▶ Questionnaire](#)

Given a 2-dimensional binary linear classification model with parameters  $\theta = \{b, \mathbf{w}\}$ , with  $b = 1$  and  $\mathbf{w} = (1, 2)^\top$ .

- 1 Compute the probability of  $\mathbf{x}_1$  belonging to class  $\mathcal{C}_1$  for  $\mathbf{x}_1 = (1, 1)^\top$ .
- 2 Compute the probability of  $\mathbf{x}_2$  belonging to class  $\mathcal{C}_1$  for  $\mathbf{x}_2 = (1, -2)^\top$ .
- 3 Compute the probability of  $\mathbf{x}_3$  belonging to class  $\mathcal{C}_0$  for  $\mathbf{x}_3 = (0, 0)^\top$ .



## Training a Linear Classifier: Maximum Likelihood (I)

- The probabilistic interpretation can help to define a quality measure.

## Exercise

[► Questionnaire](#)

- In the following dataset, both  and  have been randomly generated with probabilities  $\pi_1$  and  $1 - \pi_1$ , respectively:




Between the following options, what is the most likely value of  $\pi_1$ ? Why?


- 0 %.
- 5 %.
- 50 %.
- 95 %.
- 100 %.




# Training a Linear Classifier: Maximum Likelihood (II)

- The **likelihood** of the data is a common choice to quantify the quality of a probabilistic model:



$$\mathcal{L}(\mathcal{D}; \tilde{\mathbf{w}}) = \prod_{i=1}^N p(t_i | \tilde{\mathbf{x}}_i; \tilde{\mathbf{w}}) = \prod_{i=1}^N \underbrace{p(\mathcal{C}_0 | \tilde{\mathbf{x}}_i; \tilde{\mathbf{w}})^{1-t_i} p(\mathcal{C}_1 | \tilde{\mathbf{x}}_i; \tilde{\mathbf{w}})^{t_i}}_{\begin{cases} p(\mathcal{C}_0 | \tilde{\mathbf{x}}_i; \tilde{\mathbf{w}}) & \text{if } t_i = 0, \\ p(\mathcal{C}_1 | \tilde{\mathbf{x}}_i; \tilde{\mathbf{w}}) & \text{if } t_i = 1. \end{cases}}.$$


- The **Cross Entropy (CE)** error is defined as the minus log-likelihood:

$$\begin{aligned} \text{CE}(\tilde{\mathbf{w}}) &= -\log \mathcal{L}(\mathcal{D}; \tilde{\mathbf{w}}) \\ &= \sum_{i=1}^N (-(1-t_i) \log(p(\mathcal{C}_0 | \tilde{\mathbf{x}}_i; \tilde{\mathbf{w}})) - t_i \log(p(\mathcal{C}_1 | \tilde{\mathbf{x}}_i; \tilde{\mathbf{w}}))) \\ &= \sum_{i=1}^N (-(1-t_i) \log(1 - \sigma(\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_i)) - t_i \log(\sigma(\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_i))). \end{aligned}$$




## Training a Linear Classifier: Maximum Likelihood - Exercise



## Exercise

[▶ Questionnaire](#)

Given a 2-dimensional binary linear classification model with parameters  $\theta = \{b, \mathbf{w}\}$ , with  $b = 1$  and  $\mathbf{w} = (1, 2)^\top$ , and for the following data:

$x_{i,1}$	$x_{i,2}$	$t_i$
1	1	1
1	-2	0
0	0	0

- 1 Compute the likelihood of this model.



## Training a Linear Classifier: Maximum Likelihood (III)

- ▶ The minimizer of  $\text{CE}(\tilde{\mathbf{w}})$  is the maximizer of  $\mathcal{L}(\mathcal{D}; \tilde{\mathbf{w}})$ .
- ▶ The learning algorithm for training a Linear Logistic Regression model consists in solving the problem:

$$\min_{\tilde{\mathbf{w}} \in \mathbb{R}^{d+1}} \{\text{CE}(\tilde{\mathbf{w}})\} = \min_{\tilde{\mathbf{w}} \in \mathbb{R}^{d+1}} \left\{ \sum_{i=1}^N \left( -(1 - t_i) \log(1 - \sigma(\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_i)) - t_i \log(\sigma(\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_i)) \right) \right\}.$$

- ▶ How is this problem solved?
  - It is **convex**: there are no local minima.
  - It is **differentiable**: the optima are characterized by the zeros of the gradient.



## Training a Linear Classifier: Optimization (I)

$$\min_{\tilde{\mathbf{w}} \in \mathbb{R}^{d+1}} \{\text{CE}(\tilde{\mathbf{w}})\} = \min_{\tilde{\mathbf{w}} \in \mathbb{R}^{d+1}} \left\{ \sum_{i=1}^N (-(1-t_i) \log(1 - \sigma(\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_i)) - t_i \log(\sigma(\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_i))) \right\}.$$

$$\begin{aligned} \nabla_{\tilde{\mathbf{w}}} \text{CE}(\tilde{\mathbf{w}}) &= \sum_{i=1}^N (-(1-t_i) \nabla_{\tilde{\mathbf{w}}} \log(1 - \sigma(\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_i)) - t_i \nabla_{\tilde{\mathbf{w}}} \log(\sigma(\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_i))) \\ &= \sum_{i=1}^N ((1-t_i) \sigma(\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_i) \tilde{\mathbf{x}}_i - t_i (1 - \sigma(\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_i)) \tilde{\mathbf{x}}_i) \\ &= \sum_{i=1}^N \sigma(\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_i) \tilde{\mathbf{x}}_i - t_i \sigma(\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_i) \tilde{\mathbf{x}}_i - t_i \tilde{\mathbf{x}}_i + t_i \sigma(\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_i) \tilde{\mathbf{x}}_i \\ &= \sum_{i=1}^N (\sigma(\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_i) - t_i) \tilde{\mathbf{x}}_i. \end{aligned}$$



More detail in the appendix  
Gradient of the Sig-  
moid Transformation.



## Gradient-Based Optimization: Iterative Methods

► Can the problem  $\nabla_{\theta} \mathcal{F}(\theta^*) = \mathbf{0}$  be directly solved?

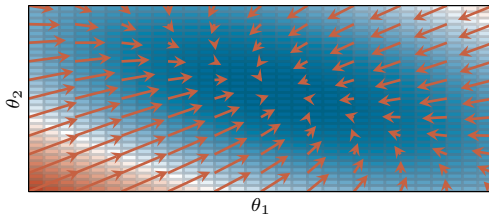


- Only for simple cases.
- In several dimensions, it implies solving a system of  $d$  equations (one for each partial derivative).
- This condition does not imply minimum (valley), it may be a maximum or a saddle point.

► But the gradient points in the direction of greatest increase:

- $-\nabla_{\theta} \mathcal{F}$  points in the direction of **steepest descent**.
- This can be used to define where to go next.

$$\mathcal{F}(\theta + \epsilon) \approx \mathcal{F}(\theta) + \nabla_{\theta} \mathcal{F}(\theta)^{\top} \epsilon \implies \mathcal{F}(\theta - \eta \nabla_{\theta} \mathcal{F}(\theta)) \approx \mathcal{F}(\theta) - \eta \|\nabla_{\theta} \mathcal{F}(\theta)\|_2^2 \leq \mathcal{F}(\theta).$$



# Gradient Descent

- It is a simple (yet useful) optimization algorithm that is often used in Machine Learning (ML) to find the local minimum.

## Gradient Descent: Algorithm

**Require:** Objective function  $\mathcal{F}$ , starting point  $\theta^{(0)}$

**Ensure:**  $\theta^{(t-1)} \in \mathbb{R}^d$  an approximate local minimum of  $\mathcal{F}(\theta)$

**for**  $t = 1, 2, \dots$  **do**

$\mathbf{g} \leftarrow \nabla_{\theta} \mathcal{F}(\theta^{(t-1)})$

**if**  $\mathbf{g} \approx \mathbf{0}$  **then**

**return**  $\theta^{(t-1)}$

**end if**

$\theta^{(t)} \leftarrow \theta^{(t-1)} - \eta^{(t)} \mathbf{g}$

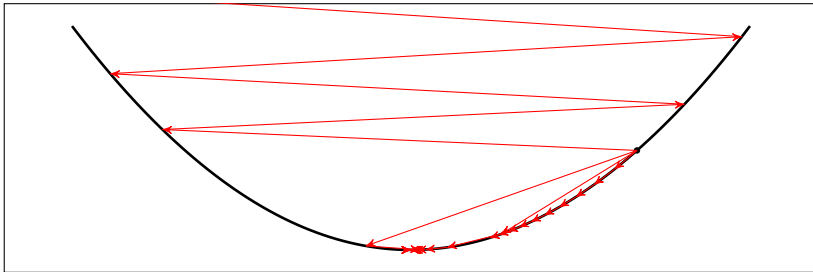
**end for**

- ▷ Start at a random point.
- ▷ Arrive to a valley.
- ▷ Several steps.
- ▷ Stop, look for the direction most downhill.
- ▷ If there is not direction downhill, stop.
- ▷ Take a step in that direction.



## Gradient Descent: Step-Size

- ▶ The step-size  $\eta^{(t)}$  has to be set at each iteration  $t$ .
- ▶ This is a crucial issue:
  - ① If the step-size is too **small**, the algorithm will require too many epochs (iterations) to converge and can become trapped in local minima more easily.
  - ② If the step-size is **large**, the convergence will also be slow.
  - ③ If the step-size is **too large**, gradient descent will overshoot the minima and diverge.
- ▶ In some cases, **optimal** step-sizes can be computed.
- ▶ There are heuristics that guarantee convergence, but only to **local minima**, and usually slowly and zigzagging.



## Training a Linear Classifier: Optimization (II)

- ▶ In summary, the Linear Logistic Regression Model is the solution of the following problem:

$$\min_{\tilde{\mathbf{w}} \in \mathbb{R}^{d+1}} \left\{ \sum_{i=1}^N (-(1-t_i) \log(1 - \sigma(\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_i)) - t_i \log(\sigma(\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_i))) \right\}.$$

- ▶ There is not closed-form solution to the resultant equation for the stationary points:

$$\nabla_{\tilde{\mathbf{w}}} \text{CE}(\tilde{\mathbf{w}}) = \sum_{i=1}^N (\sigma(\tilde{\mathbf{w}}^\top \tilde{\mathbf{x}}_i) - t_i) \tilde{\mathbf{x}}_i = \mathbf{0}.$$

- ▶ An iterative algorithm, such as **gradient descent**, should be used.

### Linear Logistic Regression Model

- ▶ The model can be trained iteratively by updating the weights as:

$$\tilde{\mathbf{w}}^{(s+1)} = \tilde{\mathbf{w}}^{(s)} - \eta^{(s)} \sum_{i=1}^N \left( \sigma\left(\left(\tilde{\mathbf{w}}^{(s)}\right)^\top \tilde{\mathbf{x}}_i\right) - t_i \right) \tilde{\mathbf{x}}_i.$$



Notebook

Binary Linear Classification: Optimization



## Summary



# Linear Models for Classification: Summary



- ▶ A **classification** problem is a supervised problem with discrete targets.

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- ▶ A simple yet useful classification model is the **linear model**.
  - The decision boundary is a hyperplane dividing the space.

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- ▶ In order to train the linear model, an **optimization problem** is usually solved.
- ▶ The **accuracy**, the more natural choice, is hard to optimize in practice.

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- ▶ The **likelihood** is used instead, leading to the **Logistic Regression** model.
  - The resultant problem can be solved iteratively using gradient descent.



# Linear Models for Classification

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Introduction

Supervised Learning: Classification

Binary Classification and Linear Models

Binary Linear Classification

Binary Linear Model

Quality of the Model

Learning Algorithm

Summary





## Additional Material

### Additional Material

#### Gradient of the Sigmoid Transformation



# Expressions for the Gradient of the Sigmoid Transformation

- The linear model with sigmoid transformation satisfies the following equations:

$$\begin{aligned}\nabla_{\tilde{\mathbf{w}}} \sigma(\tilde{\mathbf{w}}^T \tilde{\mathbf{x}}) &= \nabla_{\tilde{\mathbf{w}}} \frac{1}{1 + e^{-\tilde{\mathbf{w}}^T \tilde{\mathbf{x}}}} = \frac{1}{(1 + e^{-\tilde{\mathbf{w}}^T \tilde{\mathbf{x}}})^2} e^{-\tilde{\mathbf{w}}^T \tilde{\mathbf{x}}} \tilde{\mathbf{x}} = \frac{1}{1 + e^{-\tilde{\mathbf{w}}^T \tilde{\mathbf{x}}}} \frac{e^{-\tilde{\mathbf{w}}^T \tilde{\mathbf{x}}}}{1 + e^{-\tilde{\mathbf{w}}^T \tilde{\mathbf{x}}}} \tilde{\mathbf{x}} \\ &= \sigma(\tilde{\mathbf{w}}^T \tilde{\mathbf{x}})(1 - \sigma(\tilde{\mathbf{w}}^T \tilde{\mathbf{x}}))\tilde{\mathbf{x}};\end{aligned}$$

$$\nabla_{\tilde{\mathbf{w}}} \log(\sigma(\tilde{\mathbf{w}}^T \tilde{\mathbf{x}})) = \frac{1}{\sigma(\tilde{\mathbf{w}}^T \tilde{\mathbf{x}})} \nabla_{\tilde{\mathbf{w}}} \sigma(\tilde{\mathbf{w}}^T \tilde{\mathbf{x}}) = (1 - \sigma(\tilde{\mathbf{w}}^T \tilde{\mathbf{x}}))\tilde{\mathbf{x}};$$

$$\nabla_{\tilde{\mathbf{w}}} \log(1 - \sigma(\tilde{\mathbf{w}}^T \tilde{\mathbf{x}})) = \nabla_{\tilde{\mathbf{w}}} \log(\sigma(-\tilde{\mathbf{w}}^T \tilde{\mathbf{x}})) = -(1 - \sigma(-\tilde{\mathbf{w}}^T \tilde{\mathbf{x}}))\tilde{\mathbf{x}} = -\sigma(\tilde{\mathbf{w}}^T \tilde{\mathbf{x}})\tilde{\mathbf{x}}.$$

- These properties are one of the reasons why this function is so commonly used.

