Logistic Regression: From Theory to Decision Boundaries

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Introduction

This document explores logistic regression, a fundamental classification algorithm in machine learning:

- **From Linear to Logistic Regression**: We explain why linear regression fails for classification and motivate the need for a different approach.
- **The Sigmoid Function**: We introduce the sigmoid (logistic) function and explain how it transforms outputs into probabilities.
- **The Decision Boundary**: We derive the decision boundary that separates classes in feature space.
- **Binary Cross-Entropy Loss**: We explain why we use log-loss instead of mean squared error.
- **Gradient Descent for Logistic Regression**: We derive the update rules for optimizing the model.
- **Worked Example**: We train a logistic regression classifier on a simple 2D dataset.

From Linear to Logistic Regression

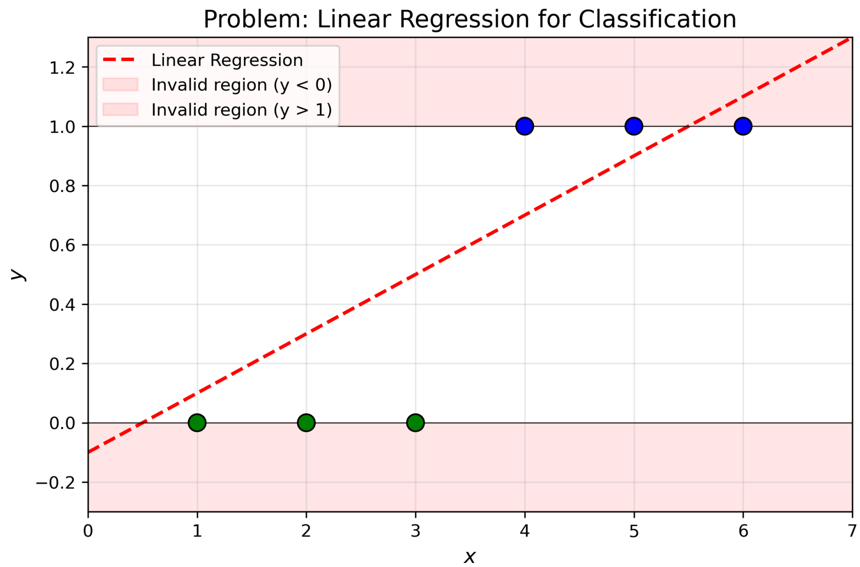
In **linear regression**, we predict a continuous output:

$$\hat{y} = w \cdot x + b.$$

However, in **classification**, we want to predict a discrete label (e.g., 0 or 1). If we use linear regression directly, the output could be any value from $-\infty$ to $+\infty$. This is problematic because:

- Probabilities must lie in $[0, 1]$.

- A prediction of $\hat{y} = 2.5$ or $\hat{y} = -0.3$ has no clear interpretation.
- Mean squared error with a linear model creates a non-convex optimization landscape.



The figure above illustrates the problem: a linear fit can produce values outside the valid range $[0, 1]$.

The Solution: Logistic Regression

Instead of directly predicting y, we pass the linear combination $z = w \cdot x + b$ through a **sigmoid function** that squashes the output to $(0, 1)$.

The Sigmoid Function

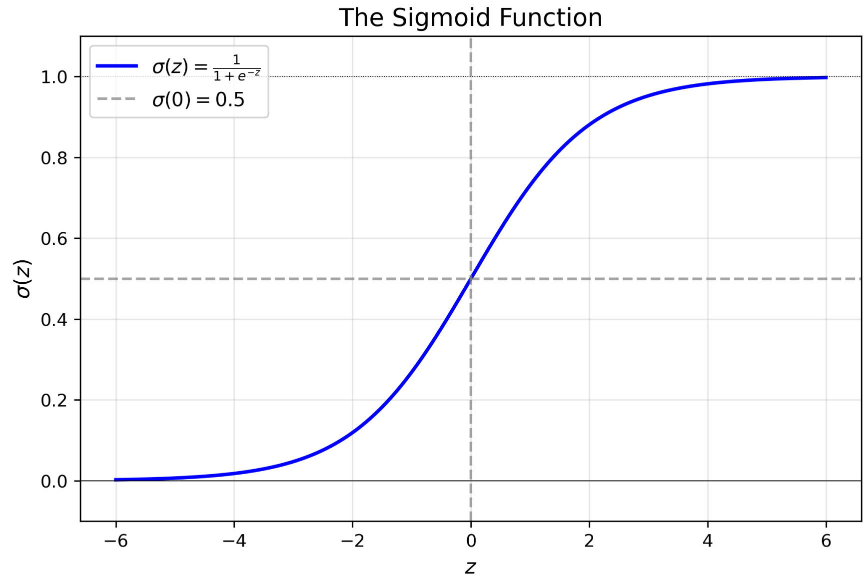
The **sigmoid function** (also called the logistic function) is defined as:

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

Key Properties

1. **Range**: The output is always in $(0, 1)$, making it interpretable as a probability.
2. **Center**: When $z = 0$, we have $\sigma(0) = \frac{1}{1+1} = 0.5$.
3. **Asymptotic behavior**:
   - As $z \to +\infty$, $\sigma(z) \to 1$.
   - As $z \to -\infty$, $\sigma(z) \to 0$.

4. **Smooth and differentiable**: This is essential for gradient-based optimization.



The Logistic Regression Model

Combining the linear function with the sigmoid, the logistic regression model is:

$$\hat{y} = \sigma(w \cdot x + b) = \frac{1}{1 + e^{-(w \cdot x + b)}}.$$

The output $\hat{y}$ is interpreted as $P(y = 1 \mid x)$, the probability that the input x belongs to class 1.

The Decision Boundary

To make a final classification, we apply a **threshold** (typically 0.5):

- If $\hat{y} \geq 0.5$, predict class 1.
- If $\hat{y} < 0.5$, predict class 0.

Deriving the Boundary

The threshold $\hat{y} = 0.5$ occurs when $\sigma(z) = 0.5$, which happens when $z = 0$.

For a two-dimensional input $x = (x_1, x_2)$ with weights $w = (w_1, w_2)$ and bias b:

$$z = w_1 x_1 + w_2 x_2 + b = 0.$$

Solving for x_2:

$$x_2 = -\frac{w_1}{w_2} x_1 - \frac{b}{w_2}.$$

This is a **linear equation** of the form $x_2 = m x_1 + c$, where:

- Slope: $m = -\frac{w_1}{w_2}$
- Intercept: $c = -\frac{b}{w_2}$

The decision boundary is therefore a straight line in 2D (or a hyperplane in higher dimensions).

Binary Cross-Entropy Loss

Why Not Mean Squared Error?

For linear regression, we minimize the mean squared error (MSE). However, MSE is problematic for logistic regression:

1. **Non-convexity**: When combined with the sigmoid, MSE creates a cost surface with many local minima.
2. **Weak gradients**: When the prediction is far from the target, the sigmoid saturates and gradients become very small.

The Log-Loss Function

Instead, we use **Binary Cross-Entropy** (also called log-loss):

$$J(w, b) = -\frac{1}{m} \sum_{i=1}^{m} \left[y_i \log(\hat{y}_i) + (1 - y_i) \log(1 - \hat{y}_i) \right].$$

Intuition

- When $y_i = 1$: The cost is $-\log(\hat{y}_i)$. If $\hat{y}_i \approx 1$, cost ≈ 0. If $\hat{y}_i \approx 0$, cost $\to \infty$.
- When $y_i = 0$: The cost is $-\log(1 - \hat{y}_i)$. If $\hat{y}_i \approx 0$, cost ≈ 0. If $\hat{y}_i \approx 1$, cost $\to \infty$.

This function heavily penalizes "confident and wrong" predictions, which is exactly what we want.

Convexity

A key advantage of binary cross-entropy is that it is **convex** when used with the sigmoid function, guaranteeing a unique global minimum.

Gradient Descent for Logistic Regression

To minimize the cost function, we use gradient descent.

Computing the Gradients

The gradients of $J(w, b)$ with respect to the parameters are:

$$\frac{\partial J}{\partial w} = \frac{1}{m} \sum_{i=1}^{m} (\hat{y}_i - y_i) x_i,$$

$$\frac{\partial J}{\partial b} = \frac{1}{m} \sum_{i=1}^{m} (\hat{y}_i - y_i).$$

Note: These have the same form as linear regression gradients, but $\hat{y}_i = \sigma(w \cdot x_i + b)$ instead of a linear prediction.

Update Rules

At each iteration, we update the parameters:

$$w := w - \alpha \cdot \frac{\partial J}{\partial w} = w - \frac{\alpha}{m} \sum_{i=1}^{m} (\hat{y}_i - y_i) x_i,$$

$$b := b - \alpha \cdot \frac{\partial J}{\partial b} = b - \frac{\alpha}{m} \sum_{i=1}^{m} (\hat{y}_i - y_i),$$

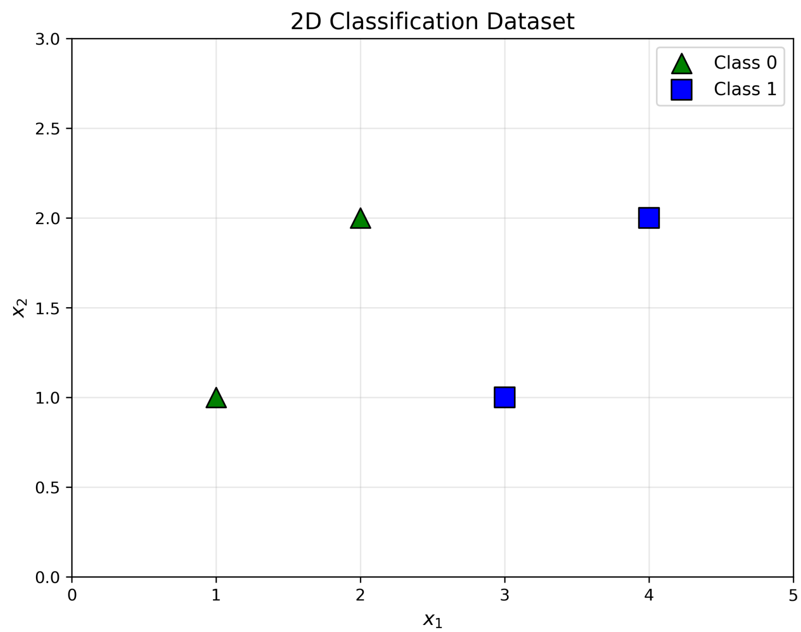
where α is the learning rate.

Worked Example: 2D Classification

We now apply logistic regression to a simple 2D dataset with 4 data points.

1. The Dataset

Point	x_1	x_2	y (class)
1	1	1	0
2	2	2	0
3	3	1	1
4	4	2	1



2. Model Setup

Our model is:

$$\hat{y} = \sigma(w_1 x_1 + w_2 x_2 + b).$$

We initialize:

- Weights: $w_1 = 0$, $w_2 = 0$
- Bias: $b = 0$
- Learning rate: $\alpha = 0.5$

3. Initial State (Iteration 0)

With $w = (0, 0)$ and $b = 0$, for any input x:

$$z = 0 \cdot x_1 + 0 \cdot x_2 + 0 = 0 \quad \Rightarrow \quad \hat{y} = \sigma(0) = 0.5.$$

All predictions are 0.5, meaning the model has no discriminative power yet.
The initial cost is:

$$J = -\frac{1}{4} \sum_{i=1}^{4} [y_i \log(0.5) + (1 - y_i) \log(0.5)] = -\log(0.5) = \ln(2) \approx 0.693.$$

4. First Gradient Descent Step

Compute the gradients. Since $\hat{y}_i = 0.5$ for all points and the true labels are $y = (0, 0, 1, 1)$:

$$\hat{y}_i - y_i = (0.5 - 0, 0.5 - 0, 0.5 - 1, 0.5 - 1) = (0.5, 0.5, -0.5, -0.5).$$

Gradient for w_1:

$$\frac{\partial J}{\partial w_1} = \frac{1}{4}\sum_{i=1}^{4}(\hat{y}_i - y_i)x_{i,1} = \frac{1}{4}[0.5(1) + 0.5(2) + (-0.5)(3) + (-0.5)(4)]$$

$$= \frac{1}{4}[0.5 + 1 - 1.5 - 2] = \frac{-2}{4} = -0.5.$$

Gradient for w_2:

$$\frac{\partial J}{\partial w_2} = \frac{1}{4}\sum_{i=1}^{4}(\hat{y}_i - y_i)x_{i,2} = \frac{1}{4}[0.5(1) + 0.5(2) + (-0.5)(1) + (-0.5)(2)]$$

$$= \frac{1}{4}[0.5 + 1 - 0.5 - 1] = 0.$$

Gradient for b:

$$\frac{\partial J}{\partial b} = \frac{1}{4}[0.5 + 0.5 - 0.5 - 0.5] = 0.$$

Update parameters:

$$w_1 := 0 - 0.5 \cdot (-0.5) = 0.25,$$

$$w_2 := 0 - 0.5 \cdot 0 = 0,$$

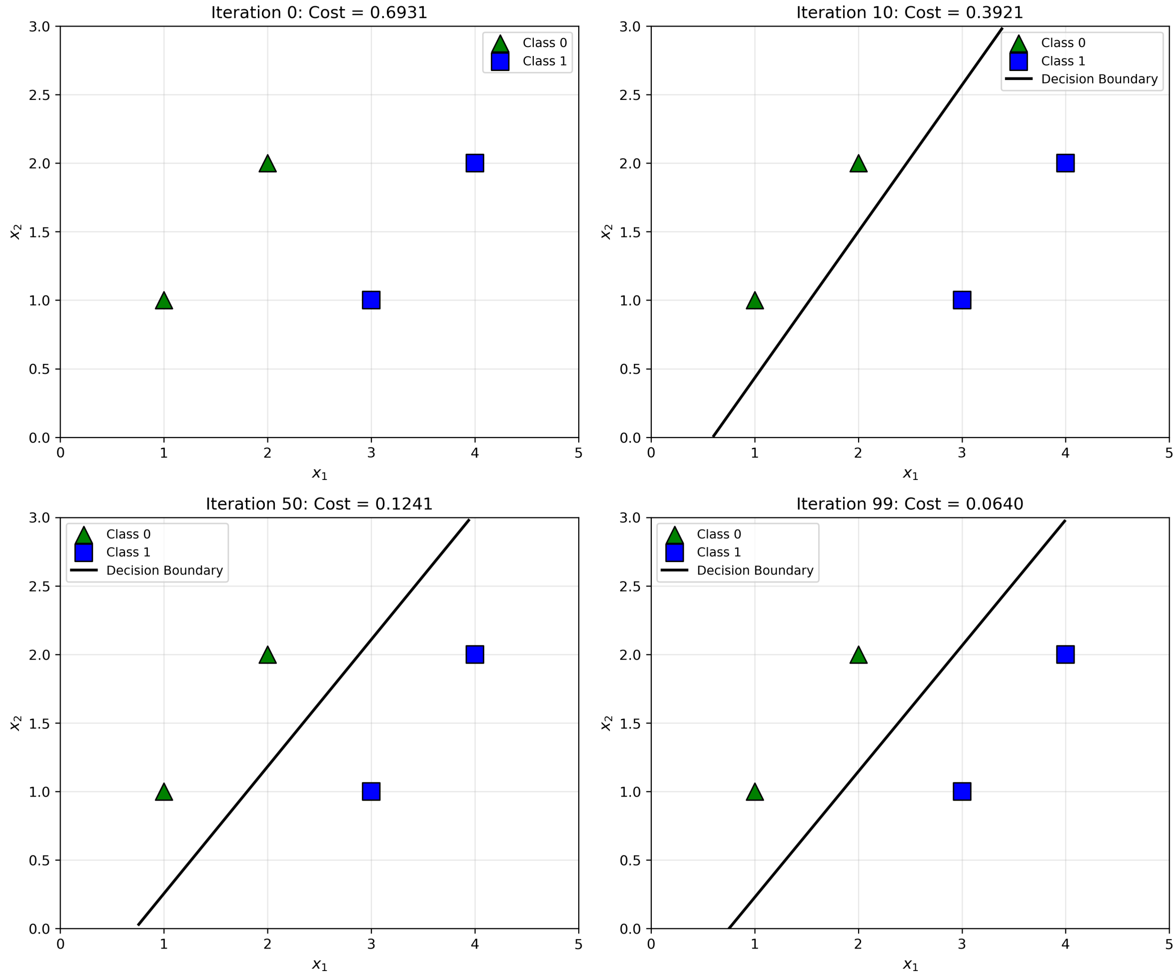
$$b := 0 - 0.5 \cdot 0 = 0.$$

After iteration 1: $w = (0.25, 0)$, $b = 0$, Cost ≈ 0.625.

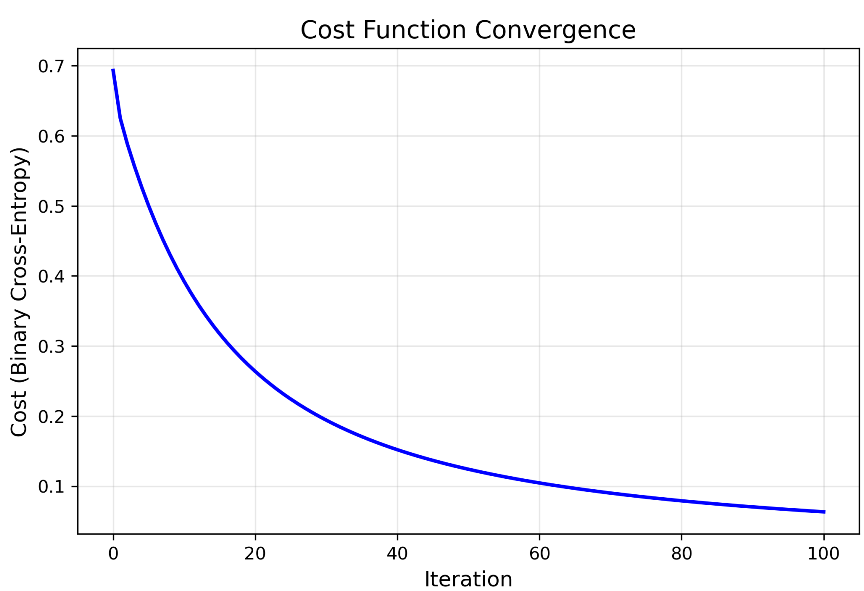
5. Gradient Descent Progress

Continuing the iterations:

Iteration	w_1	w_2	b	Cost
0	0.0000	0.0000	0.0000	0.6931
1	0.2500	0.0000	0.0000	0.6250
2	0.2789	-0.1185	-0.0744	0.5882
3	0.3571	-0.2037	-0.1280	0.5565
10	0.7863	-0.7354	-0.4687	0.3921
50	2.0726	-2.2368	-1.5028	0.1241
100	2.7805	-3.0275	-2.0951	0.0633



6. Cost Convergence



The cost decreases monotonically, demonstrating the convexity of the binary cross-entropy loss.

7. Final Decision Boundary

After 100 iterations, the learned parameters are:

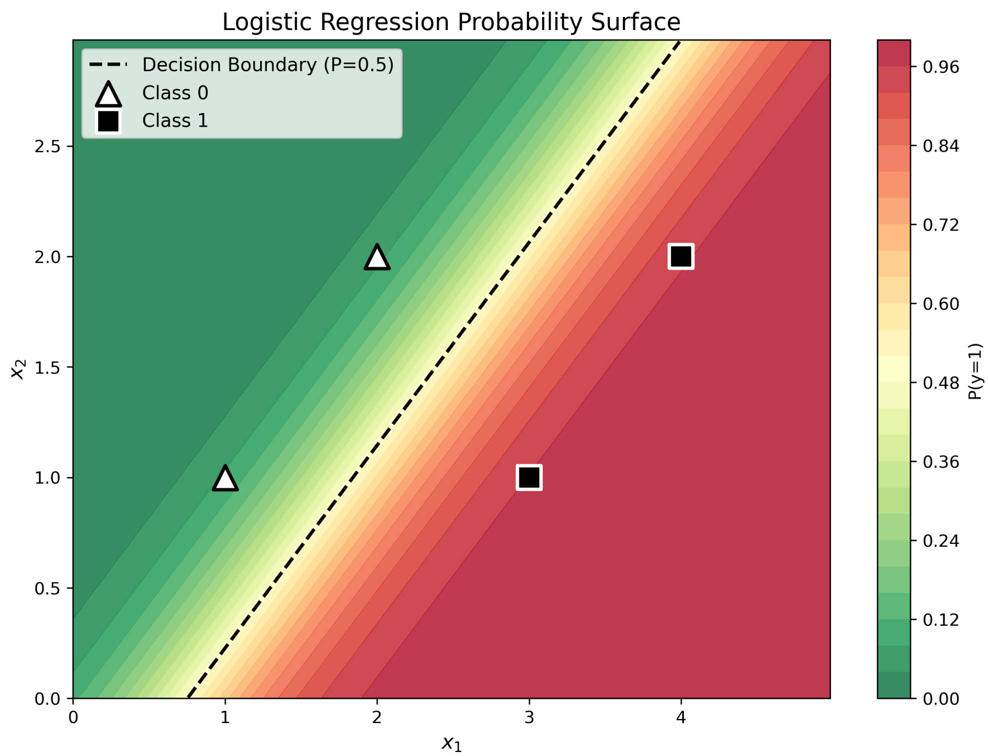
$$w_1 \approx 2.78, \quad w_2 \approx -3.03, \quad b \approx -2.10.$$

The decision boundary is where $w_1x_1 + w_2x_2 + b = 0$:

$$2.78x_1 - 3.03x_2 - 2.10 = 0.$$

Solving for x_2:

$$x_2 = \frac{2.78}{3.03}x_1 - \frac{2.10}{3.03} \approx 0.92x_1 - 0.69.$$



The probability surface shows smooth transitions from low probability (green, class 0) to high probability (red, class 1), with the decision boundary at $P = 0.5$.

Conclusion

We have covered the key concepts of logistic regression:

1. **The Problem**: Linear regression outputs unbounded values; classification needs probabilities.

2. **The Sigmoid Function**: Transforms $z \in (-\infty, \infty)$ to $(0, 1)$.
3. **The Decision Boundary**: A linear surface where $w \cdot x + b = 0$.
4. **Binary Cross-Entropy**: A convex loss function that penalizes incorrect confident predictions.
5. **Gradient Descent**: Iteratively minimizes the loss by updating w and b.

Connection to Neural Networks

Logistic regression can be viewed as a **single-layer neural network** with one neuron and a sigmoid activation. By stacking multiple layers of such units with non-linear activations, we obtain deep neural networks capable of learning complex, non-linear decision boundaries.

Matrix Form of Logistic Regression

For efficiency and scalability, logistic regression is often formulated using matrix operations, allowing vectorized computations over multiple samples and features simultaneously.

Vectorized Predictions

Consider a dataset with n samples and d features. We augment the feature matrix X (shape (n, d)) with a column of ones for the bias term, resulting in $\tilde{X}$ of shape $(n, d+1)$. The weight vector $\mathbf{w}$ (including the bias weight) is of shape $(d + 1, 1)$.

The linear combination is:

$$\mathbf{z} = \tilde{X}\mathbf{w},$$

and the predictions are:

$$\hat{\mathbf{y}} = \sigma(\mathbf{z}) = \frac{1}{1 + e^{-\mathbf{z}}},$$

where σ is applied element-wise.

Vectorized Loss and Gradients

The binary cross-entropy loss is:

$$J(\mathbf{w}) = -\frac{1}{n}\sum_{i=1}^{n}\left[y_i \log \hat{y}_i + (1 - y_i)\log(1 - \hat{y}_i)\right],$$

which vectorizes to:

$$J(\mathbf{w}) = -\frac{1}{n}\left(\mathbf{y}^T \log \hat{\mathbf{y}} + (\mathbf{1} - \mathbf{y})^T \log(\mathbf{1} - \hat{\mathbf{y}})\right).$$

The gradient with respect to $\mathbf{w}$ is:

$$\frac{\partial J}{\partial \mathbf{w}} = \frac{1}{n}\tilde{X}^T(\hat{\mathbf{y}} - \mathbf{y}).$$

Gradient descent updates: $\mathbf{w} \leftarrow \mathbf{w} - \alpha\frac{\partial J}{\partial \mathbf{w}}$.

Extension to Neural Networks

Logistic regression is fundamentally a single-layer feedforward neural network. To build deeper networks, we stack multiple layers of affine transformations followed by non-linear activations.

For a 2-layer network (1 hidden layer with h units):

- Hidden layer: $\mathbf{Z}^{(1)} = \tilde{X}\mathbf{W}^{(1)} + \mathbf{b}^{(1)}$, $\mathbf{A}^{(1)} = \sigma(\mathbf{Z}^{(1)})$
- Output layer: $\mathbf{Z}^{(2)} = \mathbf{A}^{(1)}\mathbf{W}^{(2)} + \mathbf{b}^{(2)}$, $\hat{\mathbf{y}} = \sigma(\mathbf{Z}^{(2)})$

where $\mathbf{W}^{(1)}$ is $(d+1, h)$, $\mathbf{W}^{(2)}$ is $(h, 1)$, and biases are broadcasted.

Training uses backpropagation to compute gradients layer-by-layer, generalizing the logistic regression gradients. This enables learning complex, non-linear decision boundaries, with logistic regression as the simplest case (no hidden layers).