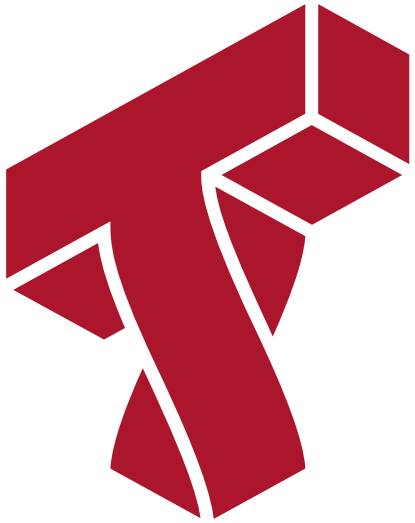


Lecture 4: Classification and Logistic Regression

Part 1: Classification

So far, every supervised learning algorithm that we've seen has been regression

We will next look at classification. First, let's define what classification is.

Review: Regression vs. Classification

Consider a training dataset $\mathcal{D} = \{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(n)}, y^{(n)})\}$.

We distinguish between supervised learning problems depending on the targets $y^{(i)}$:

1. **Regression**: The target space is continuous: $\mathcal{Y} \subseteq \mathbb{R}$.
2. **Classification**: The target space is discrete: $\mathcal{Y} = \{y_1, y_2, \ldots y_K\}$.

   Each of the K discrete values corresponds to a *class* that we want to predict

An Example: Classifying Iris Flowers

Our running example for classification problems will be the **iris flower dataset**.

This is a classical dataset originally published by R. A. Fisher in 1936.

Image source: Machine Learning in R for Beginners

Let's import the dataset from `sklearn`.

```
import warnings; warnings.filterwarnings('ignore')
from sklearn import datasets
iris = datasets.load_iris(as_frame=True)
print(iris.DESCR)
```

```
.. _iris_dataset:

Iris plants dataset
--------------------

**Data Set Characteristics:**

    :Number of Instances: 150 (50 in each of three classes)
    :Number of Attributes: 4 numeric, predictive attributes and the class
    :Attribute Information:
        - sepal length in cm
        - sepal width in cm
        - petal length in cm
        - petal width in cm
        - class:
                - Iris-Setosa
                - Iris-Versicolour
                - Iris-Virginica

    :Summary Statistics:

    ============== ==== ==== ======= ===== ====================
                    Min  Max   Mean    SD   Class Correlation
    ============== ==== ==== ======= ===== ====================
    sepal length:   4.3  7.9   5.84   0.83    0.7826
    sepal width:    2.0  4.4   3.05   0.43   -0.4194
    petal length:   1.0  6.9   3.76   1.76    0.9490  (high!)
```

Below, we print out five random rows of this dataset.

```
import pandas as pd
iris_X, iris_y = iris.data, iris.target
pd.concat([iris_X, iris_y], axis=1).sample(5) # sample 5 random rows from the data
```

	sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)	target
1	4.9	3.0	1.4	0.2	0
104	6.5	3.0	5.8	2.2	2
46	5.1	3.8	1.6	0.2	0
13	4.3	3.0	1.1	0.1	0
112	6.8	3.0	5.5	2.1	2

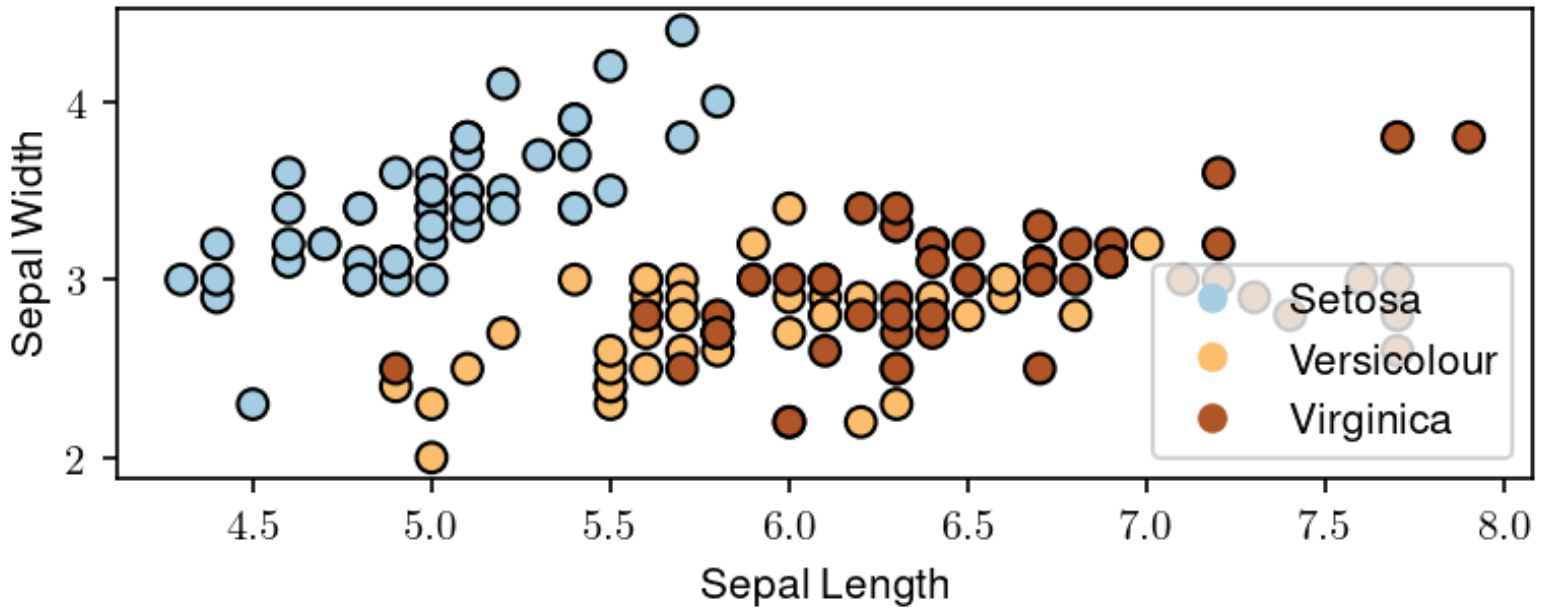
Understanding Classification

How is classification different from regression?

- **Regression**: fit a curve that passes close to the targets $y^{(i)}$.
- **Classification**: find boundaries separating the classes in the feature space
- Classification model outputs often have a simple **probabilistic interpretation**: they are probabilities that a data point belongs to a given class

Let's look at an example on the Iris dataset. We visualize this dataset using the first 2 attributes using `matplotlib`.

```
import matplotlib.pyplot as plt # Code from: https://scikit-learn.org/stable/auto_examples/datasets/plot_iris_dataset.html
plt.rcParams.update({ "figure.figsize": [6, 2], "figure.dpi": 150, "text.usetex": True, "font.family": "Helvetica"})
p1 = plt.scatter(iris_X.iloc[:, 0], iris_X.iloc[:, 1], c=iris_y, edgecolor='k', s=50, cmap=plt.cm.Paired)
plt.xlabel('Sepal Length'); plt.ylabel('Sepal Width')
plt.legend(handles=p1.legend_elements()[0], labels=['Setosa', 'Versicolour', 'Virginica'], loc='lower right');
```



Let's train a classification algorithm called **logistic regression**.

```
from sklearn.linear_model import LogisticRegression

logreg = LogisticRegression(C=1e5)
X, Y = iris_X.to_numpy()[:,:2], iris_y.copy()
logreg.fit(X, Y);
```

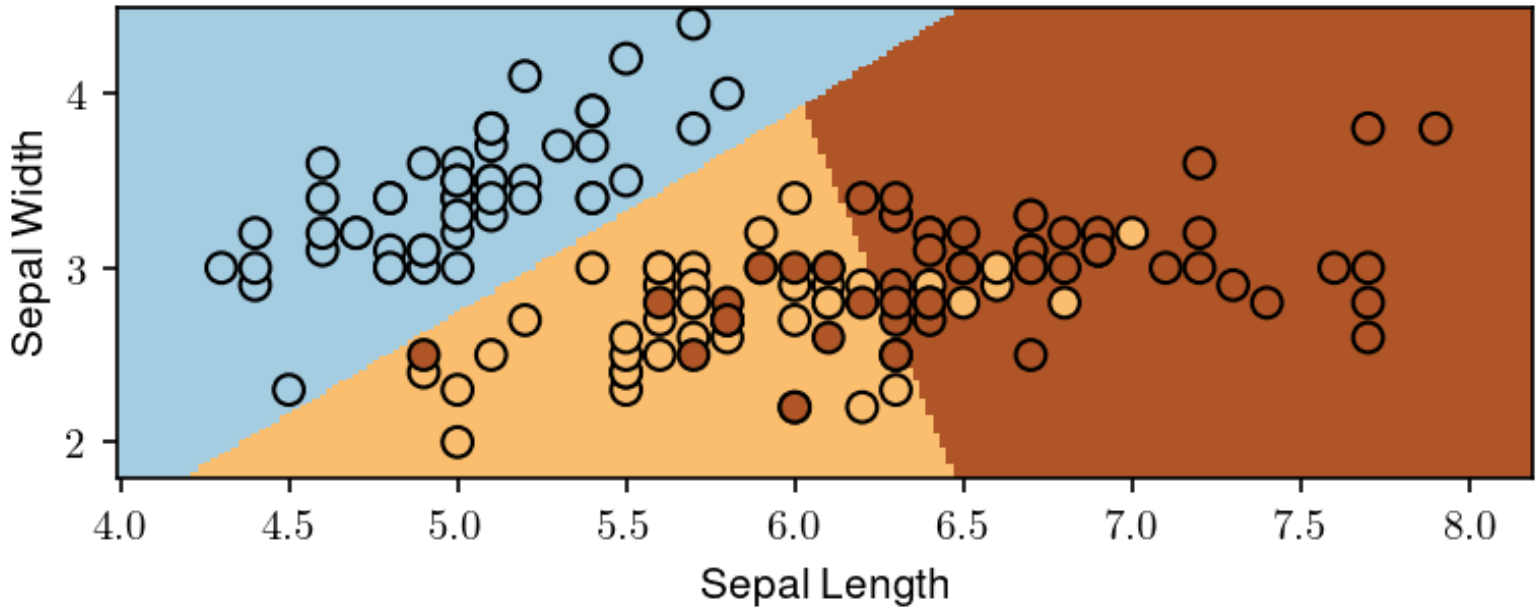
Note: logistic regression actually a **classification** algorithm.

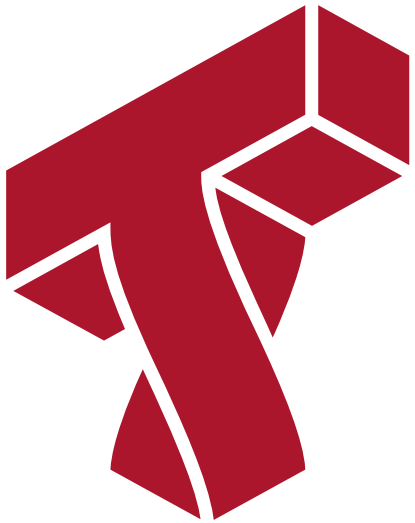
The regions below are predicted to be associated with the blue, brown, and yellow classes. The lines between them are the decision boundaries.

```
import numpy as np
xx, yy = np.meshgrid(np.arange(4, 8.2, .02), np.arange(1.8, 4.5, .02))
Z = logreg.predict(np.c_[xx.ravel(), yy.ravel()])

# Put the result into a color plot
plt.pcolormesh(xx, yy, Z.reshape(xx.shape), cmap=plt.cm.Paired)

# Plot also the training points
plt.scatter(X[:, 0], X[:, 1], c=Y, edgecolors='k', cmap=plt.cm.Paired, s=50)
plt.xlabel('Sepal Length'); plt.ylabel('Sepal Width');
```





Part 2: Logistic Regression

We are now going to define our first classification algorithm: logistic regression.

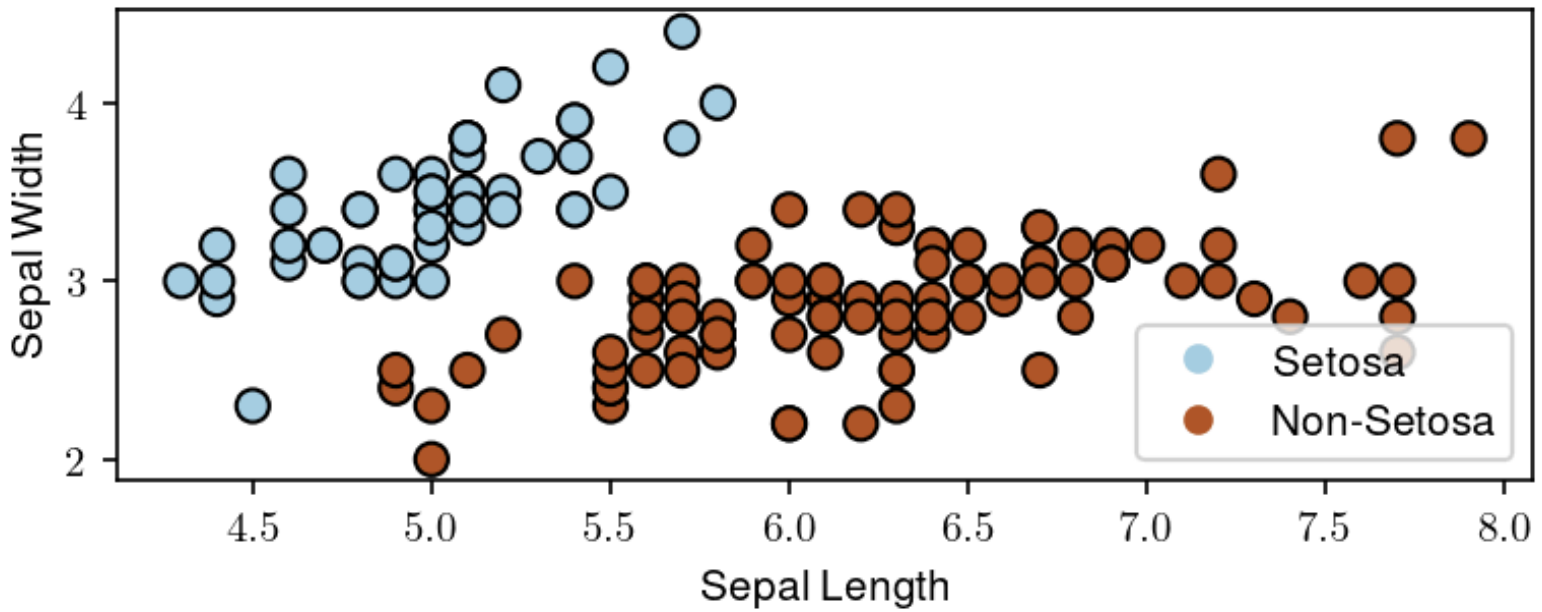
Binary Classification

- We will to start by looking at **binary** (two-class) classification.
- To keep things simple, we will use the Iris dataset.

We will attempt to distinguish class 0 *(Iris Setosa)* from the other two classes, using only the first two features in the dataset

```
iris_y2 = iris_y.copy()
iris_y2[iris_y2==2] = 1  # rename class two to class one

# plot also the training points
p1 = plt.scatter(iris_X.iloc[:, 0], iris_X.iloc[:, 1], c=iris_y2, edgecolor='k', s=60, cmap=plt.cm.Paired)
plt.xlabel('Sepal Length'); plt.ylabel('Sepal Width')
plt.legend(handles=p1.legend_elements()[0], labels=['Setosa', 'Non-Setosa'], loc='lower right');
```



Review: Ordinary Least Squares

Recall that in ordinary least squares, we fit a linear model of the form

$$f(x) = \sum_{j=0}^{d} \theta_j \cdot x_j = \theta^\top x.$$

It minimizes the mean squared error (MSE)

$$J(\theta) = \frac{1}{2n} \sum_{i=1}^{n} (y^{(i)} - \theta^\top x^{(i)})^2$$

on a dataset $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(n)}, y^{(n)})\}$.

We could use least squares to solve our classification problem, setting $\mathcal{Y} = \{0, 1\}$.

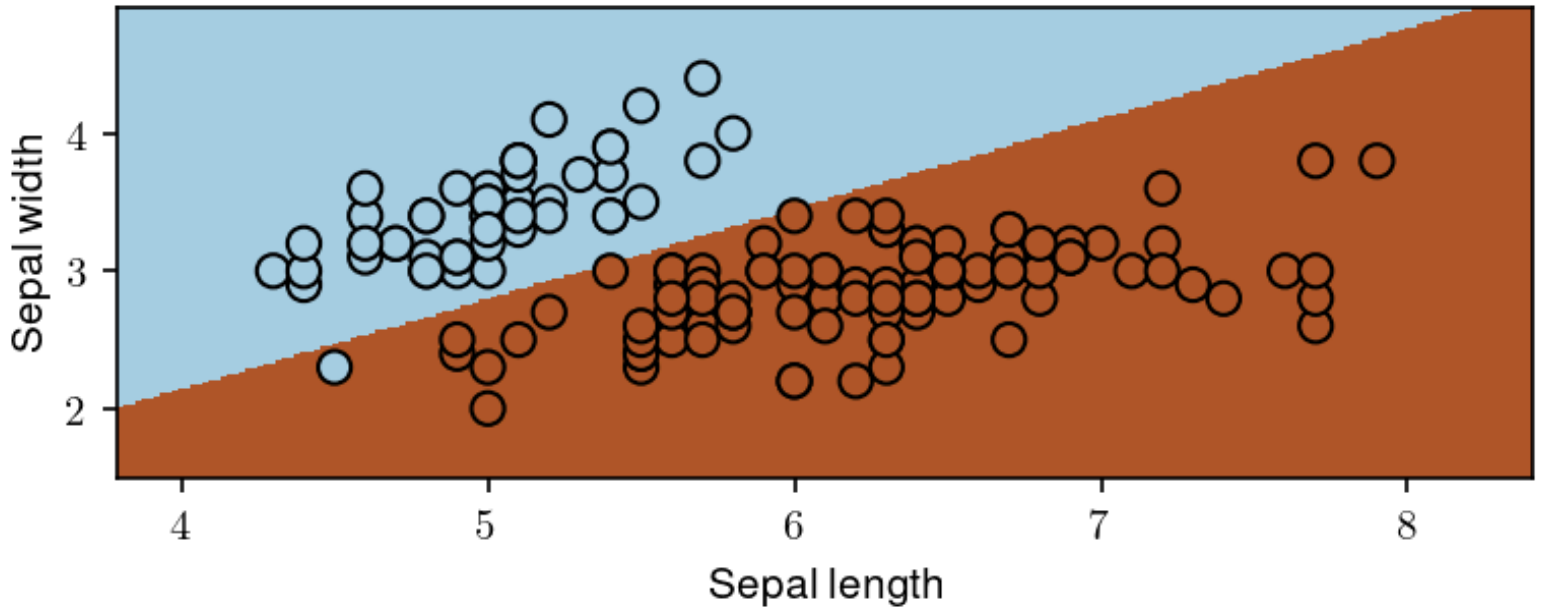
```
from sklearn.linear_model import LinearRegression

linreg = LinearRegression()
X, Y = iris_X.to_numpy()[:,:2], iris_y2
linreg.fit(X, Y);
```

Ordinary least squares returns a decision boundary that is not unreasonable.

```
# Plot the decision boundary by assigning a color to each point in the mesh
x_min, x_max = X[:, 0].min() - .5, X[:, 0].max() + .5
y_min, y_max = X[:, 1].min() - .5, X[:, 1].max() + .5
h = .02  # step size in the mesh
xx, yy = np.meshgrid(np.arange(x_min, x_max, h), np.arange(y_min, y_max, h))
Z = linreg.predict(np.c_[xx.ravel(), yy.ravel()])
Z[Z>0.5] = 1.; Z[Z<0.5] = 0.

plt.pcolormesh(xx, yy, Z.reshape(xx.shape), cmap=plt.cm.Paired)
plt.scatter(X[:, 0], X[:, 1], c=Y, edgecolors='k', cmap=plt.cm.Paired, s=60)
plt.xlabel('Sepal length'); plt.ylabel('Sepal width');
```



However, applying OLS is problematic for a few reasons.

- **Unbounded outputs**: There is nothing to prevent outputs larger than one or smaller than zero, which is conceptually wrong
- **Performance issues:** At least one point is misclassified, and others are too close to the decision boundary.

Logistic Regression: The Model

Logistic regression is a classification algorithm where f_θ has the form

$$f_\theta(x) = \sigma(\theta^\top x) = \frac{1}{1 + \exp(-\theta^\top x)}.$$

This is a composition of a linear model $\theta^\top x$ with

$$\sigma(z) = \frac{1}{1 + \exp(-z)},$$

which is the *sigmoid* or *logistic* function.

The Logistic Function

To address the fact that the output of linear regression is not in $[0, 1]$, we will *squeeze* it into that range using

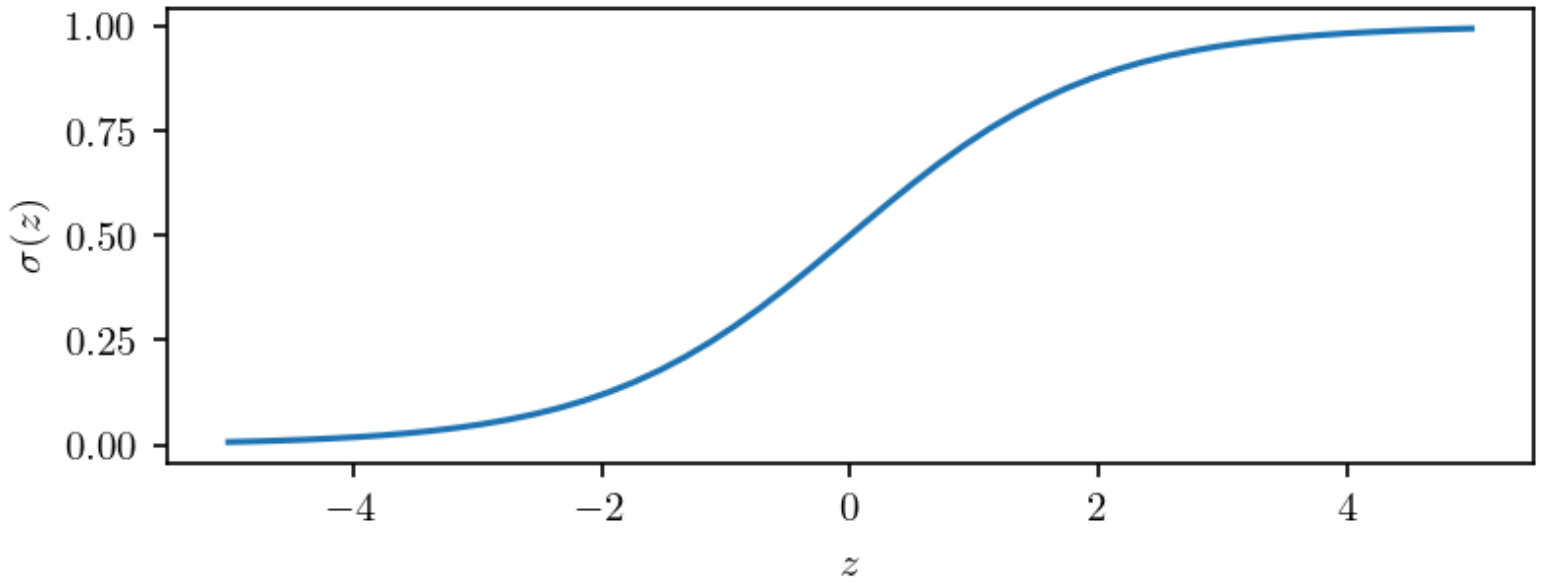
$$\sigma(z) = \frac{1}{1 + \exp(-z)}.$$

This is known as the *sigmoid* or *logistic* function.

The logistic function $\sigma : \mathbb{R} \to [0, 1]$ "squeezes" points from the real line into $[0, 1]$.

```
def sigmoid(z):
    return 1/(1+np.exp(-z))

z = np.linspace(-5, 5)
plt.plot(z, sigmoid(z))
plt.xlabel('$z$'); plt.ylabel(r'$\sigma(z)$');
```



The Logistic Function: Properties

The sigmoid function is defined as

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

A few observations:

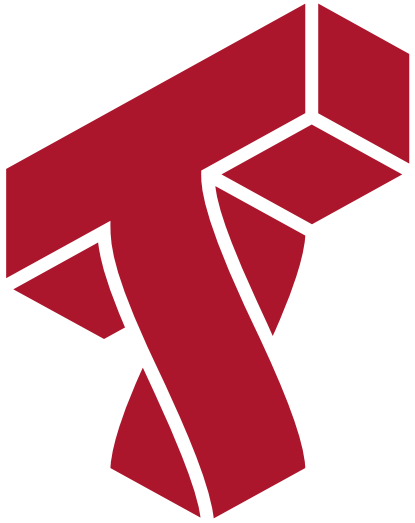
- The function tends to 1 as $z \to \infty$ and tends to 0 as $z \to -\infty$.
- Thus, models of the form $\sigma(\theta^\top x)$ output values between 0 and 1, which is suitable for binary classification.
- It is easy to show that the derivative of $\sigma(z)$ has a simple form: $\frac{d\sigma}{dz} = \sigma(z)(1 - \sigma(z))$.

Probabilistic Interpretations

The logistic model can be interpreted to output a probability, and defines a conditional probability distribution as follows:

$$P_\theta(y = 1|x) = \sigma(\theta^\top x)$$
$$P_\theta(y = 0|x) = 1 - \sigma(\theta^\top x).$$

Recall that a probability over $y \in \{0, 1\}$ is called Bernoulli.



Part 3: Maximum Likelihood

In order to train a logistic regression model, we need to define an objective.

We derive this objective using the principle of maximum likelihood.

Recall: Supervised Learning Models

A model is a function f_θ that maps inputs $x \in \mathcal{X}$ to targets $y \in \mathcal{Y}$.

Model Type	How To Use	Example
$f_\theta : \underbrace{\mathcal{X}}_{\text{input}} \to \underbrace{\mathcal{Y}}_{\text{output}}$	$y_{\text{pred}} = f_\theta(x)$	$y_{\text{pred}} = \theta^\top x$

Probabilistic Supervised Learning Models

A probabilistic model parameterizes a *probability* over y_{pred} given x.

$$P_\theta(y = y_{\text{pred}}|x)$$

Given $x \in \mathcal{X}$, the model outputs a *conditional probability* $P(y|x)$ over targets $y \in \mathcal{Y}$.

For example, our logistic regression model f_θ defines ("parameterizes") a probability distribution $P_\theta(y|x)$ as follows:

$$P_\theta(y=1|x) = \sigma(\theta^\top x)$$
$$P_\theta(y=0|x) = 1 - \sigma(\theta^\top x).$$

For each x, $P_\theta(y|x)$ is a valid probability over $y \in \{0, 1\}$.

This is a more general recipe for a probabilistic model:

- Given an x, we have **a formula for** $P_\theta(y|x)$ as a function of x and θ.
- The formula assigns higher probabilities ("**scores**") to more likely y.
- These **scores sum to 1** over all y, hence they're valid probabilities.

We usually use the following notation to denote probabilistic models:

$$P_\theta(y|x) : \mathcal{X} \to \underbrace{(\mathcal{Y} \to [0,1])}_{\text{probability } P(y|x) \text{ over } \mathcal{Y}} .$$

Why Probabilistic Models?

There are two reasons why we will be interested in probabilistic models.

- **Confidence Estimation**: Oftentimes, we want to know if the model is certain in its prediction.
- **Learning Objective**: Probabilistic models can be used to define a principled learning objective.

Conditional Maximum Likelihood

We can train any model that defines a probability distribution $P_\theta(y|x)$ by optimizing the *conditional maximum likelihood* objective

$$\max_\theta \ell(\theta) = \max_\theta \frac{1}{n} \sum_{i=1}^{n} \log P_\theta(y^{(i)}|x^{(i)}).$$

defined over a dataset $\mathcal{D} = \{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(n)}, y^{(n)})\}$.

We want to choose the weights such that the true label $y^{(i)}$ has the highest possible probability under $P_\theta(y|x^{(i)})$ for each $x^{(i)}$.

Example: Flipping a Random Coin

Consider a simple example in which we repeatedly toss a biased coin and record the outcomes.

- There are two possible outcomes: heads (H) and tails (T). A training dataset consists of tosses of the biased coin, e.g., $\mathcal{D} = \{H, H, T, H, T\}$
- **Assumption:** true probability distribution is $P_{\text{data}}(y)$, $y \in \{H, T\}$
- Our task is to determine the probability θ of seeing heads.

Example: Flipping a Random Coin

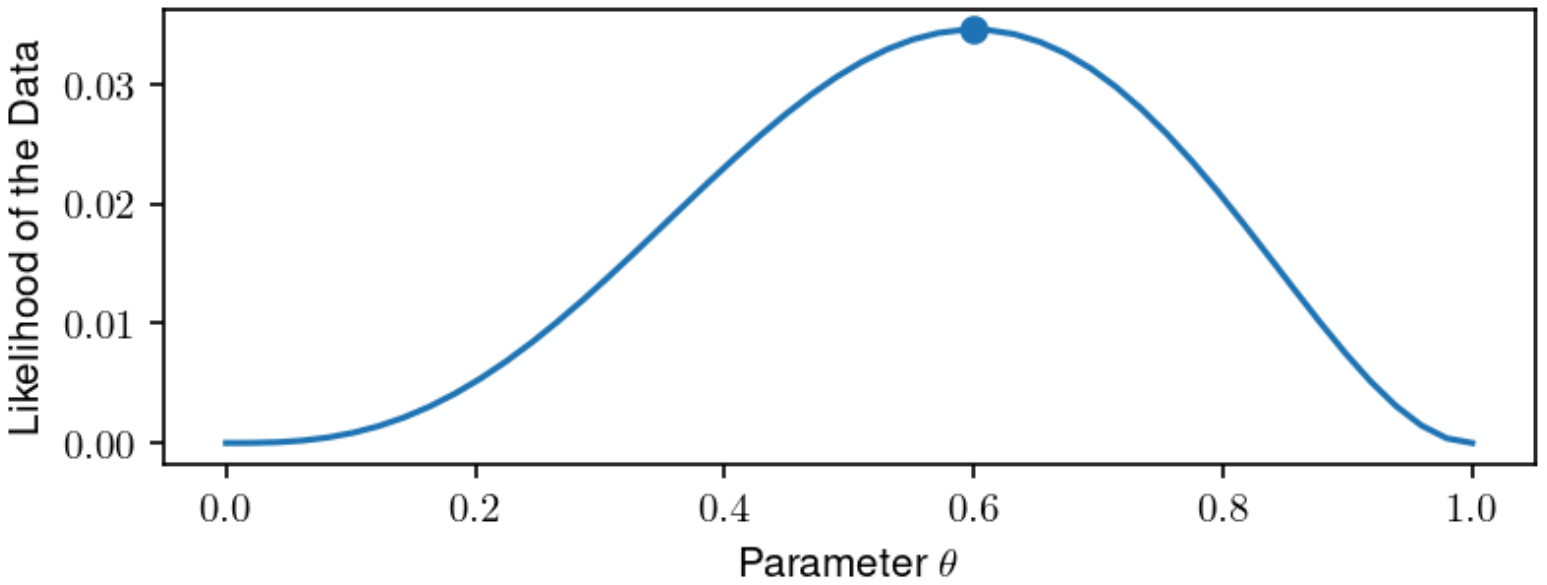
How should we choose θ if 3 out of 5 tosses are heads? Let's apply maximum likelihood:

- Our dataset is $\mathcal{D} = \{y^{(1)}, y^{(2)}, y^{(3)}, y^{(4)}, y^{(5)}\} = \{H, H, T, H, T\}$
- Our model is $P_\theta(y) = \theta$ if $y = H$ and $P_\theta(y) = 1 - \theta$ if $y = T$, and there is a single parameter $\theta \in [0, 1]$
- The likelihood of the data is $L(\theta) = \prod_{i=1}^{n} P_\theta(y^{(i)}) = \theta \cdot \theta \cdot (1 - \theta) \cdot \theta \cdot (1 - \theta)$.

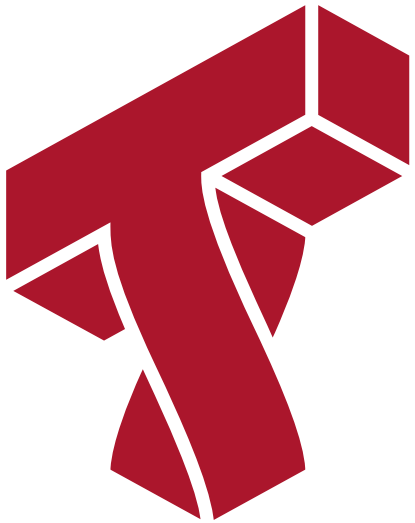
We optimize for θ which makes $\mathcal{D}$ most likely. What is the solution?

```
# our dataset is {H, H, T, H, T}; if theta = P(x=H), we get:
coin_likelihood = lambda theta: theta*theta*(1-theta)*theta*(1-theta)

theta_vals = np.linspace(0,1)
plt.ylabel('Likelihood of the Data'); plt.xlabel(r'Parameter $\theta$')
plt.scatter([0.6], [coin_likelihood(0.6)])
plt.plot(theta_vals, coin_likelihood(theta_vals));
```



The likelihood $L(\theta)$ is maximized by $\theta = 0.6$, which is also what we expect intuitively since 3/5 tosses are heads.



Part 4: Learning in Logistic Regression

We will use maximum likelihood to learn the parameters of a logistic regression model.

Logistic Regression

Recall that a logistic model defines ("parameterizes") a probability distribution $P_\theta(y|x) : \mathcal{X} \times \mathcal{Y} \to [0, 1]$ as follows:

$$P_\theta(y = 1|x) = \sigma(\theta^\top x)$$
$$P_\theta(y = 0|x) = 1 - \sigma(\theta^\top x).$$

When $y \in \{0, 1\}$, can write this more compactly as

$$P_\theta(y|x) = \sigma(\theta^\top x)^y \cdot (1 - \sigma(\theta^\top x))^{1-y}$$

Let's implement a logistic regression model in `numpy`.

```
def f(X, theta):
    """The sigmoid model we are trying to fit.

    Parameters:
    theta (np.array): d-dimensional vector of parameters
    X (np.array): (n,d)-dimensional data matrix

    Returns:
    y_pred (np.array): n-dimensional vector of predicted targets
    """
    return sigmoid(X.dot(theta))
```

Applying Maximum Likelihood

Following the principle of maximum likelihood, we want to optimize the following objective defined over a binary classification dataset
$\mathcal{D} = \{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \ldots, (x^{(n)}, y^{(n)})\}$.

$$\begin{aligned}
\ell(\theta) &= \frac{1}{n} \sum_{i=1}^{n} \log P_\theta(y^{(i)} \mid x^{(i)}) \\
&= \frac{1}{n} \sum_{i=1}^{n} \log \sigma(\theta^\top x^{(i)})^{y^{(i)}} \cdot (1 - \sigma(\theta^\top x^{(i)}))^{1-y^{(i)}} \\
&= \frac{1}{n} \sum_{i=1}^{n} y^{(i)} \cdot \log \sigma(\theta^\top x^{(i)}) + (1 - y^{(i)}) \cdot \log(1 - \sigma(\theta^\top x^{(i)})).
\end{aligned}$$

This objective is also often called the log-loss, or cross-entropy.

Observe that this objective asks the model to:

- Output a large score $\sigma(\theta^\top x^{(i)})$ (a score close to one) if $y^{(i)} = 1$
- Output a score that's small (close to zero) if $y^{(i)} = 0$.

$$\ell(\theta) = \frac{1}{n} \sum_{i=1}^{n} y^{(i)} \cdot \log \sigma(\theta^\top x^{(i)}) + (1 - y^{(i)}) \cdot \log(1 - \sigma(\theta^\top x^{(i)})).$$

Let's implement the log-likelihood objective.

```
def log_likelihood(theta, X, y):
    """The cost function, J(theta0, theta1) describing the goodness of fit.

    We added the 1e-6 term in order to avoid overflow (inf and -inf).

    Parameters:
    theta (np.array): d-dimensional vector of parameters
    X (np.array): (n,d)-dimensional design matrix
    y (np.array): n-dimensional vector of targets
    """
    return (y*np.log(f(X, theta) + 1e-6) + (1-y)*np.log(1-f(X, theta) + 1e-6)).mean()
```

Review: Gradient Descent

If we want to minimize an objective $J(\theta)$, we may start with an initial guess θ_0 for the parameters and repeat the following update:

$$\theta_i := \theta_{i-1} - \alpha \cdot \nabla_\theta J(\theta_{i-1}).$$

Gradient of the Log-Likelihood

We want to use gradient descent to maximize the log-likelihood.
Hence our objective is $J(\theta) = -\ell(\theta)$

The gradient of the negative log-likelihood is

$$\nabla_\theta J(\theta) = \nabla_\theta \left[-\ell(\theta)\right] = \frac{1}{n} \sum_{i=1}^{n} \left(\sigma(\theta^\top x^{(i)}) - y^{(i)}\right) \cdot x^{(i)}$$

Interestingly, this expression looks similar to the gradient of the mean squared error, which we derived in the previous lecture.

Let's implement the gradient.

```
def loglik_gradient(theta, X, y):
    """The cost function, J(theta0, theta1) describing the goodness of fit.

    Parameters:
    theta (np.array): d-dimensional vector of parameters
    X (np.array): (n,d)-dimensional design matrix
    y (np.array): n-dimensional vector of targets

    Returns:
    grad (np.array): d-dimensional gradient of the MSE
    """
    return np.mean((f(X, theta)-y) * X.T, axis=1)
```

Let's now implement gradient descent.

```
threshold = 5e-5
step_size = 1e-1

theta, theta_prev = np.zeros((3,)), np.ones((3,))
opt_pts = [theta]
opt_grads = []
iter = 0
iris_X['one'] = 1
X_train = iris_X.iloc[:,[0,1,-1]].to_numpy()
y_train = iris_y2.to_numpy()

while np.linalg.norm(theta - theta_prev) > threshold:
    if iter % 50000 == 0:
        print('Iteration %d. Log-likelihood: %.6f' % (iter, log_likelihood(theta, X_train, y_train)))
    theta_prev = theta
    gradient = loglik_gradient(theta, X_train, y_train)
    theta = theta_prev - step_size * gradient
    opt_pts += [theta]
    opt_grads += [gradient]
    iter += 1
```

```
Iteration 0. Log-likelihood: -0.693145
Iteration 50000. Log-likelihood: -0.021506
Iteration 100000. Log-likelihood: -0.015329
Iteration 150000. Log-likelihood: -0.012062
Iteration 200000. Log-likelihood: -0.010076
```

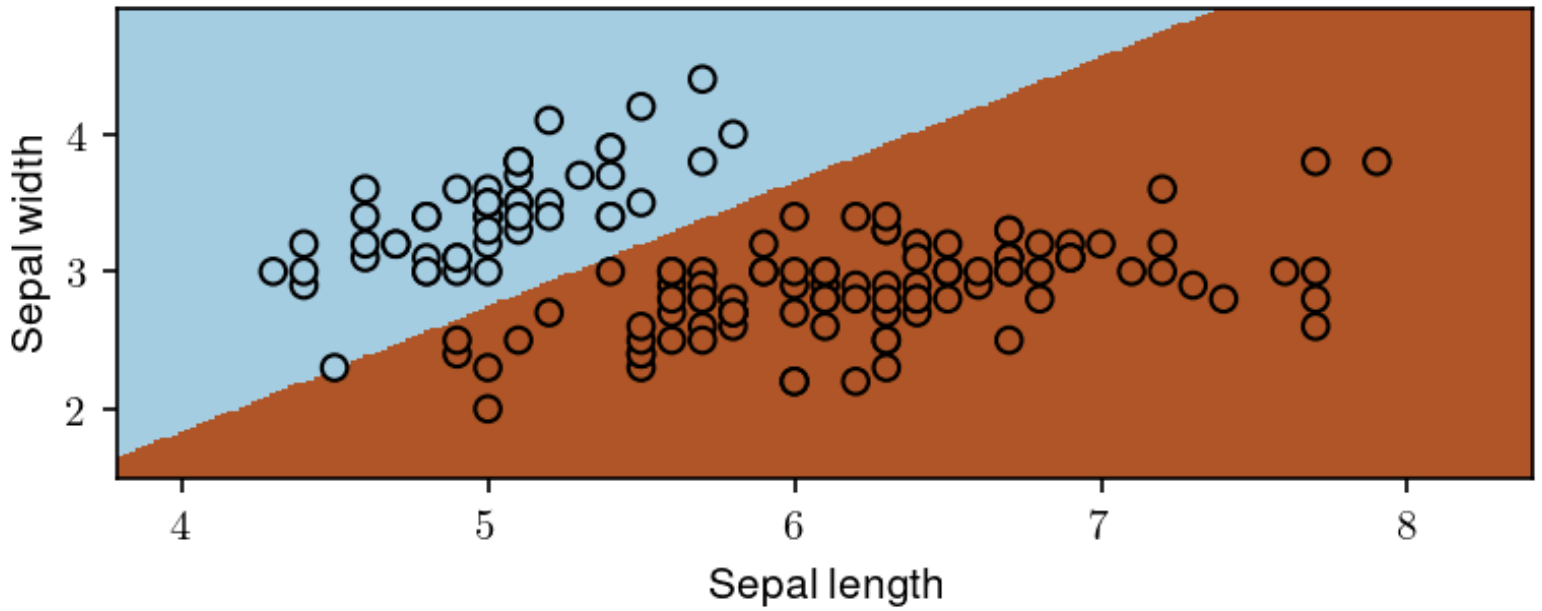
Let's now visualize the result.

```
xx, yy = np.meshgrid(np.arange(x_min, x_max, .02), np.arange(y_min, y_max, .02))

# predict using the learned model
Z = f(np.c_[xx.ravel(), yy.ravel(), np.ones(xx.ravel().shape)], theta)
Z[Z<0.5] = 0; Z[Z>=0.5] = 1

plt.pcolormesh(xx, yy, Z.reshape(xx.shape), cmap=plt.cm.Paired)

plt.scatter(X[:, 0], X[:, 1], c=Y, edgecolors='k', cmap=plt.cm.Paired)
plt.xlabel('Sepal length'); plt.ylabel('Sepal width');
```



Observations About Logistic Regression

Logistic regression finds a linear decision boundary.

This is the set of points for which $P(y = 1|x) = P(y = 0|x)$.

Equivalently:

$$0 = \log \frac{P(y = 1|x)}{P(y = 0|x)} = \log \frac{\frac{1}{1+\exp(-\theta^\top x)}}{1 - \frac{1}{1+\exp(-\theta^\top x)}} = \theta^\top x$$

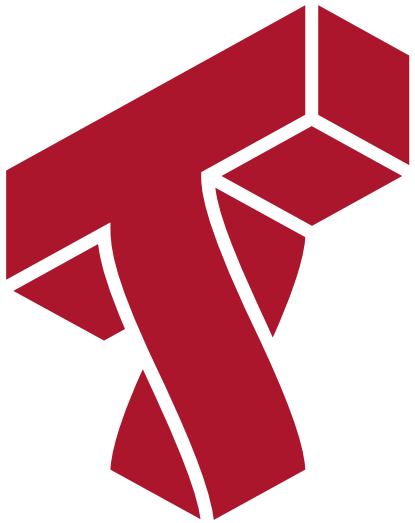
The set of x for which $0 = \theta^\top x$ is a linear surface.

Unlike least squares, we don't have a closed form solution (a formula) for the optimal θ.

We can nonetheless find it numerically via gradient descent.

Algorithm: Logistic Regression

- **Type**: Supervised learning (binary classification)
- **Model family**: Linear decision boundaries.
- **Objective function**: Cross-entropy, a special case of log-likelihood.
- **Optimizer**: Gradient descent.
- **Probabilistic interpretation**: Parametrized Bernoulli distribution.



Part 5: Multi-Class Classification

Let's look at an extension of logistic regression to an arbitrary number of classes.

Multi-Class Classification

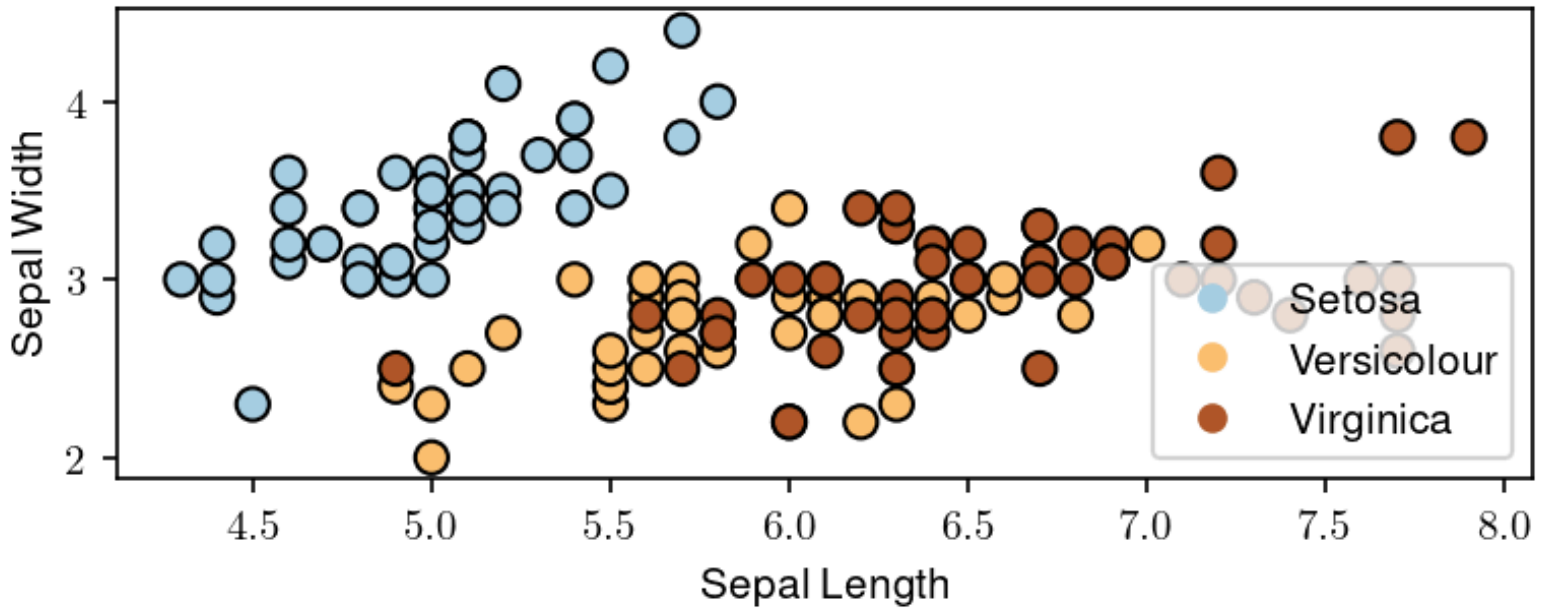
Logistic regression only applies to binary classification problems.
What if we have an arbitrary number of classes K?

- The simplest approach is the **"one vs. all" approach**:

  Train one classifier for each class to distinguish that class from all the others.
- This works, but is not very elegant.
- Alternatively, we may fit a probabilistic model that outputs multi-class probabilities.

Let's load a fully multiclass version of the Iris dataset.

```
# https://scikit-learn.org/stable/auto_examples/neighbors/plot_classification.html
p1 = plt.scatter(iris_X.iloc[:, 0], iris_X.iloc[:, 1], c=iris_y,
            edgecolor='k', s=60, cmap=plt.cm.Paired)
plt.xlabel('Sepal Length'); plt.ylabel('Sepal Width')
plt.legend(handles=p1.legend_elements()[0], labels=['Setosa', 'Versicolour', 'Virginica'], loc='lower right');
```



The Softmax Function

The logistic function $\sigma : \mathbb{R} \to [0, 1]$ "squeezes" the score $z \in \mathbb{R}$ of a class into a probability in $[0, 1]$.

The *softmax* function $\vec{\sigma} : \mathbb{R}^K \to [0, 1]^K$ is a multi-class version of σ

- It takes in a K-dimensional *vector* of class scores $\vec{z} \in \mathbb{R}$
- It "squeezes" $\vec{z}$ into a length K *vector* of probabilities in $[0, 1]^K$

The k-th component of the output of the softmax function $\vec{\sigma}$ is defined as

$$\sigma(\vec{z})_k = \frac{\exp(z_k)}{\sum_{l=1}^{K} \exp(z_l)}.$$

Softmax takes a vector of scores $\vec{z}$, exponentiates each score z_k, and normalizes the exponentiated scores such that they sum to one.

Softmax Regression: Model Class

Softmax regression is a multi-class classification algorithm which uses a model $f_\theta : \mathcal{X} \to [0,1]^K$ that generalizes logistic regression.

Softmax regression works as follows:

1. Given an input x, we compute K scores, one per class. The score

$$z_k = \theta_k^\top x$$

   of class k is a linear function of x and parameters θ_k for class k

1. We "squeeze" the vector of scores $\vec{z}$ into $[0,1]^K$ using the softmax function $\vec{\sigma}$ and we output $\vec{\sigma}(\vec{z})$, a vector of K probabilities.

The parameters of this model are $\theta = (\theta_1, \theta_2, \ldots, \theta_K)$, and the parameter space is $\Theta = \mathbb{R}^{K \times d}$.

The output of the model is a *vector* of class membership probabilities, whose k-th component $f_\theta(x)_k$ is

$$f_\theta(x)_k = \sigma(\theta_k^\top x)_k = \frac{\exp(\theta_k^\top x)}{\sum_{l=1}^{K} \exp(\theta_l^\top x)},$$

where each $\theta_l \in \mathbb{R}^d$ is the vector of parameters for class ℓ and $\theta = (\theta_1, \theta_2, \ldots, \theta_K)$.

Softmax Regression: Probabilistic Interpretation

The softmax model outputs a vector of probabilities, and defines a conditional probability distribution as follows:

$$P_\theta(y = k|x) = \vec{\sigma}(\vec{z})_k = \frac{\exp(\theta_k^\top x)}{\sum_{l=1}^{K} \exp(\theta_l^\top x)}.$$

Recall that a probability over $y \in \{1, 2, \ldots, K\}$ is called Categorical.

Softmax Regression: Learning Objective

We again maximize likelihood over a dataset $\mathcal{D}$.

$$L(\theta) = \prod_{i=1}^{n} P_\theta(y^{(i)} \mid x^{(i)}) = \prod_{i=1}^{n} \vec{\sigma}(\vec{z}^{(i)})_{y^{(i)}}$$
$$= \prod_{i=1}^{n} \left(\frac{\exp(\theta_{y^{(i)}}^\top x^{(i)})}{\sum_{l=1}^{K} \exp(\theta_l^\top x^{(i)})} \right).$$

We optimize this using gradient descent.

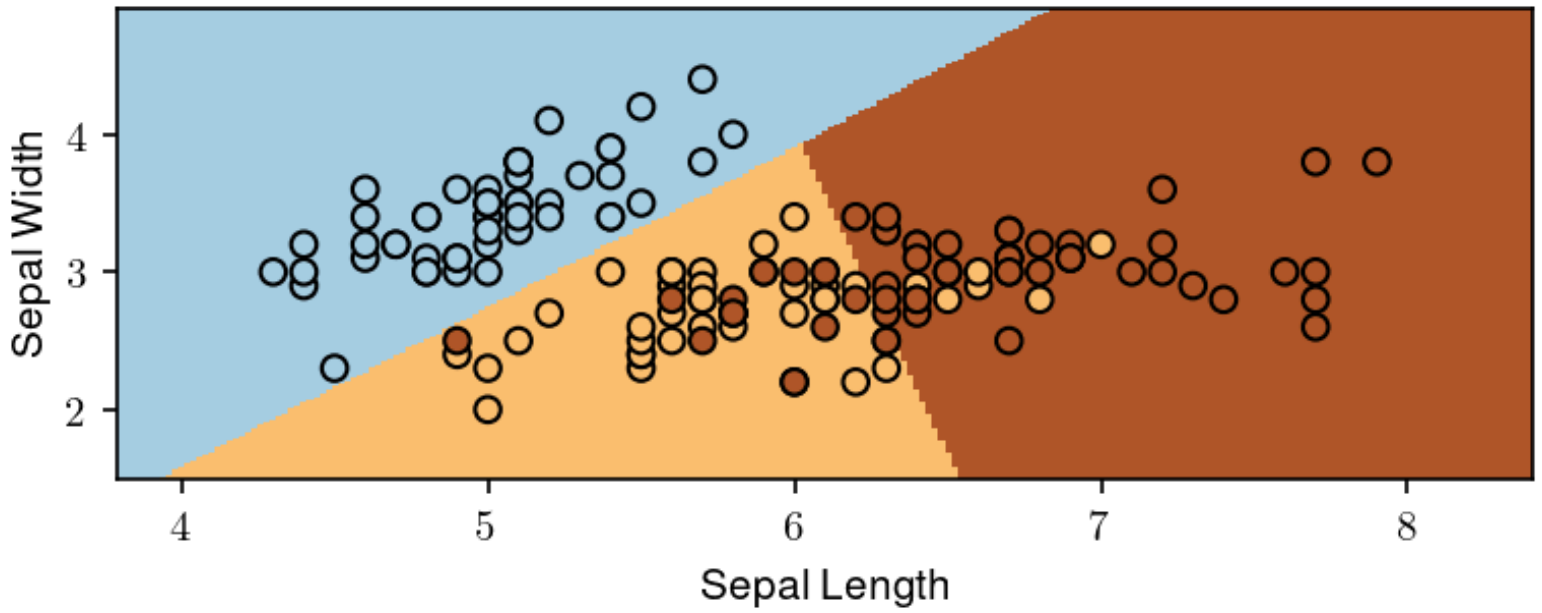
Let's now apply softmax regression to the Iris dataset by using the implementation from `sklearn`.

```
# https://scikit-learn.org/stable/auto_examples/linear_model/plot_iris_logistic.html
from sklearn.linear_model import LogisticRegression
logreg = LogisticRegression(C=1e5, multi_class='multinomial')

logreg.fit(X, iris_y) # Create an instance of Softmax and fit the data.
Z = logreg.predict(np.c_[xx.ravel(), yy.ravel()])

plt.pcolormesh(xx, yy, Z.reshape(xx.shape), cmap=plt.cm.Paired)

plt.scatter(X[:, 0], X[:, 1], c=iris_y, edgecolors='k', cmap=plt.cm.Paired)
plt.xlabel('Sepal Length'); plt.ylabel('Sepal Width');
```



Algorithm: Softmax Regression

- **Type**: Supervised learning (multi-class classification)
- **Model family**: Linear decision boundaries.
- **Objective function**: Softmax loss, a special case of log-likelihood.
- **Optimizer**: Gradient descent.
- **Probabilistic interpretation**: Parametrized categorical distribution.

Conclusion and Key Ideas

In summary, the key takeaways are:

- Do **classification** by taking a regression model and mapping the output into $[0, 1]$
  e.g., via sigmoid or softmax
- ML models usually have **probabilistic interpretations** as $P_\theta(y|x)$
- Any probabilistic model can be trained using **maximum likelihood**:

$$\max_\theta \sum_{i=1}^{n} P_\theta(y^{(i)}|x^{(i)})$$

Next class: regularization, further analysis