MSc Data Mining

Topic 05 : Classification

Part 02 : Logistic Regression

Dr Bernard Butler and Dr Kieran Murphy

Department of Computing and Mathematics, SETU Waterford.
(bernard.butler@setu.ie; kmurphy@wit.ie)

Spring Semester, 2023

Outline

- Relationship with linear regression
- (Sigmoid) Logistic function

Outline

Linear Regression I

Dataset

Take the IRIS dataset (4 features, target discrete with 3 levels $[0, 1, 2]$) and simplify it by* taking only the first feature, and merging class 1 ('versicolor') and class 2 ('virginica').

1
```
X, y, target_names = iris.data[:,:1], iris.target, iris.target_names
y[y>1] = 1
target_names = np.array([target_names[0], 'other'])
```

So we have target

2
```
y
```

```
array([0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
       0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1,
       1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1])
```

and target names of

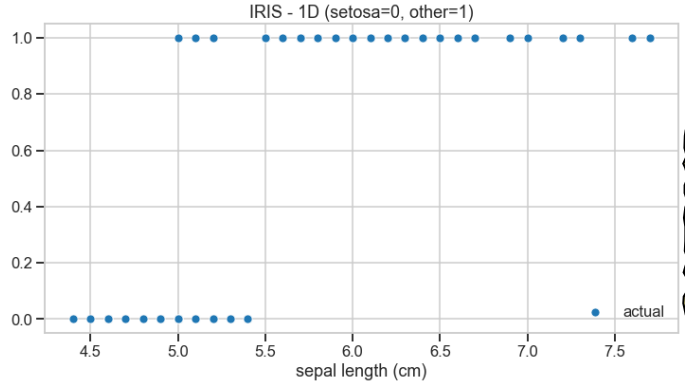
3
```
target_names
```

```
array(['setosa', 'other'], dtype='<U6')
```

*Python for Data Science — Cheat Sheet Numpy Basics

Linear Regression II

```
plt.figure(figsize=(12,6))
sns.scatterplot(x=X_test.T[0],y=y_test, label="actual")
plt.xlabel(iris.feature_names[0])
plt.title("IRIS – 1D (setosa=0, other=1)")
plt.legend(loc="lower right")
plt.show()
```



From the graph, it looks like we could predict class using sepal length, in particular if sepal length is <5.5 then predict `setosa` else predict `other`.
How many observations will be miss-classified then?

Linear Regression III

Following standard procedure we split data . . .

```
5 from sklearn.model_selection import train_test_split
  X_train, X_test, y_train, y_test = train_test_split(X, y, train_size=0.6, random_state=666)
```

. . . import and create instance of model (`LinearRegression`) . . .

```
6 from sklearn.linear_model import LinearRegression
  model = LinearRegression()
```

. . . fit model (using training data — feature(s) and target) . . .

```
7 model.fit(X_train, y_train)
```

. . . predict (using feature(s) in test data) . . .

```
8 y_pred = model.predict(X_test)
```

Linear Regression III

Following standard procedure we split data . . .

```
9 from sklearn.model_selection import train_test_split
  X_train, X_test, y_train, y_test = train_test_split(X, y, train_size=0.6, random_state=666)
```

. . . import and create instance of model (`LinearRegression`) . . .

```
10 from sklearn.linear_model import LinearRegression
   model = LinearRegression()
```

. . . fit model (using training data — feature(s) and target) . . .

```
11 model.fit(X_train, y_train)
```

. . . predict (using feature(s) in test data) . . .

```
12 y_pred = model.predict(X_test)
```

Linear Regression III

Following standard procedure we split data . . .

```
13 from sklearn.model_selection import train_test_split
   X_train, X_test, y_train, y_test = train_test_split(X, y, train_size=0.6, random_state=666)
```

. . . import and create instance of model (`LinearRegression`) . . .

```
14 from sklearn.linear_model import LinearRegression
   model = LinearRegression()
```

. . . fit model (using training data — feature(s) and target) . . .

```
15 model.fit(X_train, y_train)
```

. . . predict (using feature(s) in test data) . . .

```
16 y_pred = model.predict(X_test)
```

Linear Regression III

Following standard procedure we split data . . .

```
17 from sklearn.model_selection import train_test_split
   X_train, X_test, y_train, y_test = train_test_split(X, y, train_size=0.6, random_state=666)
```

. . . import and create instance of model (LinearRegression) . . .

```
18 from sklearn.linear_model import LinearRegression
   model = LinearRegression()
```

. . . fit model (using training data — feature(s) and target) . . .

```
19 model.fit(X_train, y_train)
```

. . . predict (using feature(s) in test data) . . .

```
20 y_pred = model.predict(X_test)
```

Linear Regression III

Following standard procedure we split data . . .

21
```
from sklearn.model_selection import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y, train_size=0.6, random_state=666)
```

. . . import and create instance of model (LinearRegression) . . .

22
```
from sklearn.linear_model import LinearRegression
model = LinearRegression()
```

. . . fit model (using training data — feature(s) and target) . . .

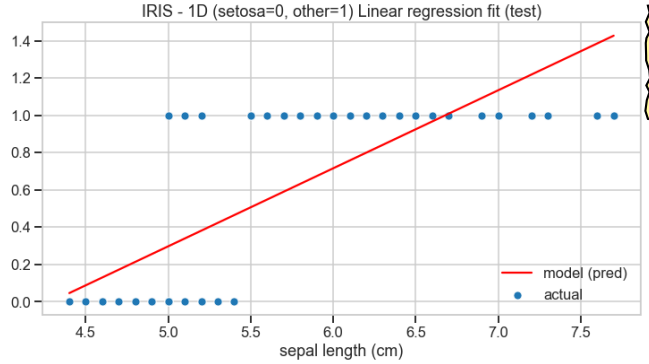
23
```
model.fit(X_train, y_train)
```

. . . predict (using feature(s) in test data) . . .

24
```
y_pred = model.predict(X_test)
```

Linear Regression III

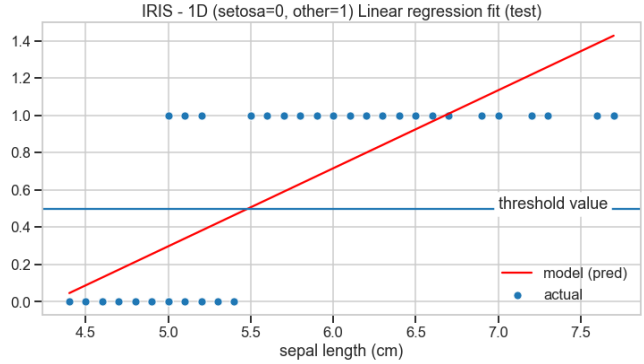
```
25 plt.figure(figsize=(12,6))
sns.scatterplot(x=X_test.T[0],y=y_test, label="actual")
sns.lineplot(x=X_test.T[0], y=y_pred, color='red', label="model (pred)")
plt.xlabel(iris.feature_names[0])
plt.title("IRIS - 1D (setosa=0, other=1) Linear regression fit (test)")
plt.legend(loc="lower right")
plt.show()
```



This is called a linear probability model. It has the advantages that much of the regression statistical theory can be applied to it.
But output is in range $(-\infty, \infty)$, we want 0 or 1

Linear Regression III

```
plt.figure(figsize=(12,6))
sns.scatterplot(x=X_test.T[0],y=y_test, label="actual")
sns.lineplot(x=X_test.T[0], y=y_pred, color='red', label="model (pred)")
plt.xlabel(iris.feature_names[0])
plt.title("IRIS - 1D (setosa=0, other=1) Linear regression fit (test)")
plt.legend(loc="lower right")
plt.show()
```

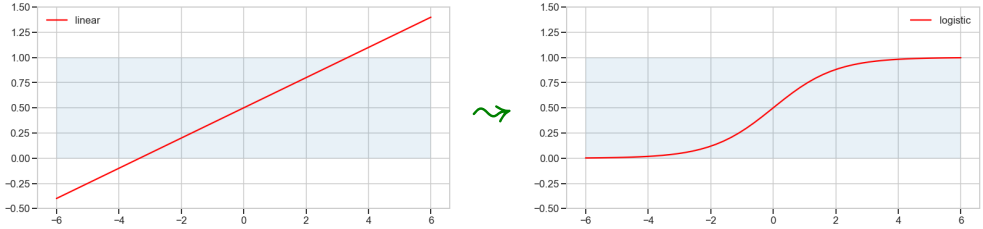


This is called a linear probability model. It has the advantages that much of the regression statistical theory can be applied to it.
But output is in range $(-\infty, \infty)$, we want 0 or 1

Pick a threshold value, default is 0.5.
If $y <$ `threshold`
    predict 0
else
    predict 1

. . . it would be nice . . .

Can we ~~replace~~ map the infinite interval $(-\infty, \infty)$ to a finite interval, say to $(0, 1)$?



A Sigmoid function[†] is any function that has a stretched S-shaped curve. One example of a sigmoid function is the

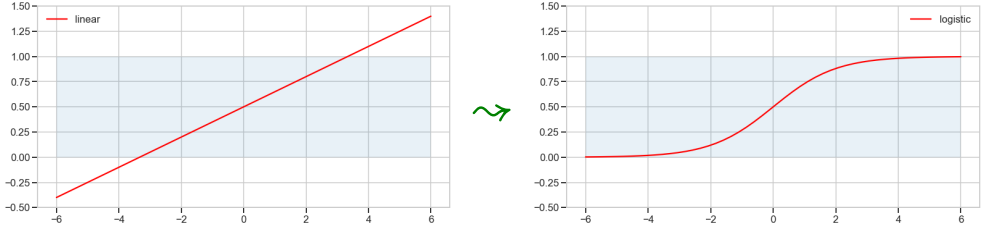
Logistic function, σ

$$\sigma(x) = \frac{1}{1 + \exp(-x)} = \frac{1}{1 + e^{-x}} = \frac{e^x}{1 + e^x}$$

[†] Sigmoid function (Wikipedia), and Logistic function (Wikipedia),

. . . it would be nice . . .

Can we ~~replace~~ map the infinite interval $(-\infty, \infty)$ to a finite interval, say to $(0, 1)$?



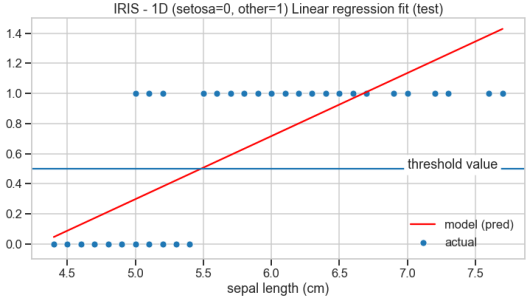
A Sigmoid function[†] is any function that has a stretched S-shaped curve. One example of a sigmoid function is the

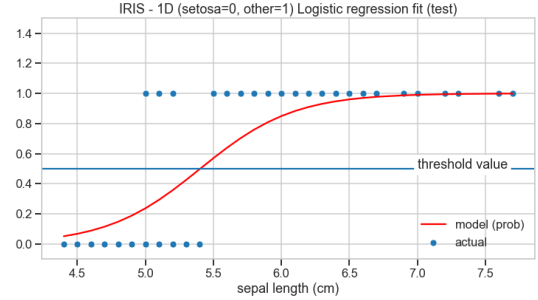
Logistic function, σ

$$\sigma(x) = \frac{1}{1 + \exp(-x)} = \frac{1}{1 + e^{-x}} = \frac{e^x}{1 + e^x}$$

[†] Sigmoid function (Wikipedia), and Logistic function (Wikipedia),

Linear Regression vs Logistic Regression





Linear Regression Model

$y = mx + c$

$x \rightsquigarrow y$

Logistic Regression Model

$y = \sigma(z)$ where $z = mx + c$

$x \rightsquigarrow z \rightsquigarrow y$

Aside: The function linking, z, the output of linear step, to y, the model output is called a link function.

Aside: Of all the Sigmoid functions, why pick Logistic? I

First a little bit of mathematical manipulation ...

$$y = \sigma(z) = \frac{1}{1 + e^{-z}} \qquad \text{definition of } \sigma(z)$$

$$y + ye^{-z} = 1 \qquad \text{multiply both sides by } (1 + e^{-z})$$

$$e^{-z} = \frac{1 - y}{y} \qquad \text{solve for } e^{-z}$$

$$e^{z} = \frac{y}{1 - y} \qquad \text{invert both sides}$$

$$z = \ln\left(\frac{y}{1 - y}\right) \qquad \text{apply logs}$$

So we have

$$y = \frac{1}{1 + e^{-z}} \iff z = \ln\left(\frac{y}{1 - y}\right)$$

Aside: Of all the Sigmoid functions, why pick Logistic? II

- If y represents a probability, then
$$\frac{y}{1-y}$$
represent the odds — an alternative measure of the likelihood of a particular outcome[‡].
- Then
$$z = \ln\left(\frac{y}{1-y}\right)$$
is the log-odds, or the logit.
- This implies that increasing one of the independent variables multiplicatively scales the odds of the given outcome at a constant rate, with each independent variable having its own parameter. So the feature coefficients in a logistic regression have a similar interpretation (but not the same!) as in linear regression.

[‡]Odds are defined as the ratio of the number of events that produce that outcome relative to the number that do not.

Logistic Regression — Probability of being in Predicted Class

Unlike some classifiers, the `LogisticRegression` classifier can also report on the probability of an observation being in the predicted class[§].

27
```
y_prob = model.predict_proba(X_test)
y_prob
```

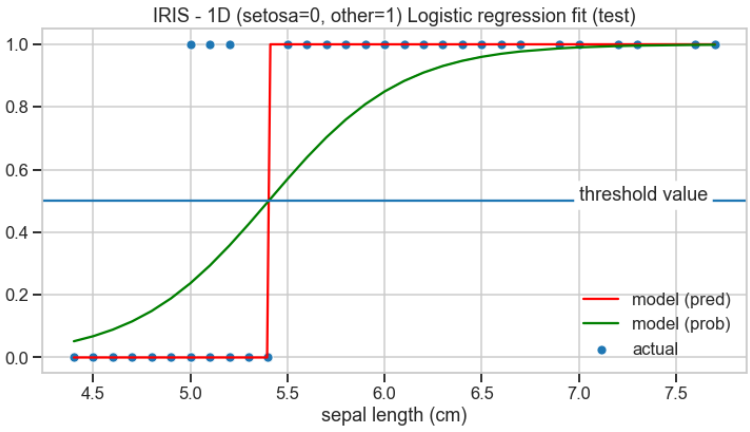
```
array([[0.36106274, 0.63893726],
       [0.24038055, 0.75961945],
       [0.76292166, 0.23707834],
       [0.24038055, 0.75961945],
       [0.91120554, 0.08879446],
       [0.43024916, 0.56975084],
       [0.29719846, 0.70280154],
       [0.03992405, 0.96007595],
       [0.06912596, 0.93087404],
       [0.43024916, 0.56975084],
       [0.02275676, 0.97724324],
       [0.93203415, 0.06796585],
```

28
```
y_log_prob = model.predict_log_proba(X_test)
y_log_prob
```

```
array([[-1.01870355e+00, -4.47949007e-01],
       [-1.42553199e+00, -2.74937692e-01],
       [-2.70599925e-01, -1.43936465e+00],
       [-1.42553199e+00, -2.74937692e-01],
       [-9.29867864e-02, -2.42143102e+00],
       [-8.43390801e-01, -5.62556133e-01],
       [-1.21335515e+00, -3.52680729e-01],
       [-3.22077634e+00, -4.07428849e-02],
       [-2.67182500e+00, -7.16313014e-02],
       [-8.43390801e-01, -5.62556133e-01],
       [-3.78289290e+00, -2.30196948e-02],
       [-7.03858210e-02, -2.68874994e+00],
```

[§]This is a big deal as it allows us to punish learners when they miss-classify based on how confident the classifier was — cross entropy loss functions (week 6 & 7).

Logistic Regression



Predicted	other	setosa
Actual		
other	38	3
setosa	0	19