dm22s1

Topic 09 : Classification1

Part 01 : Overview

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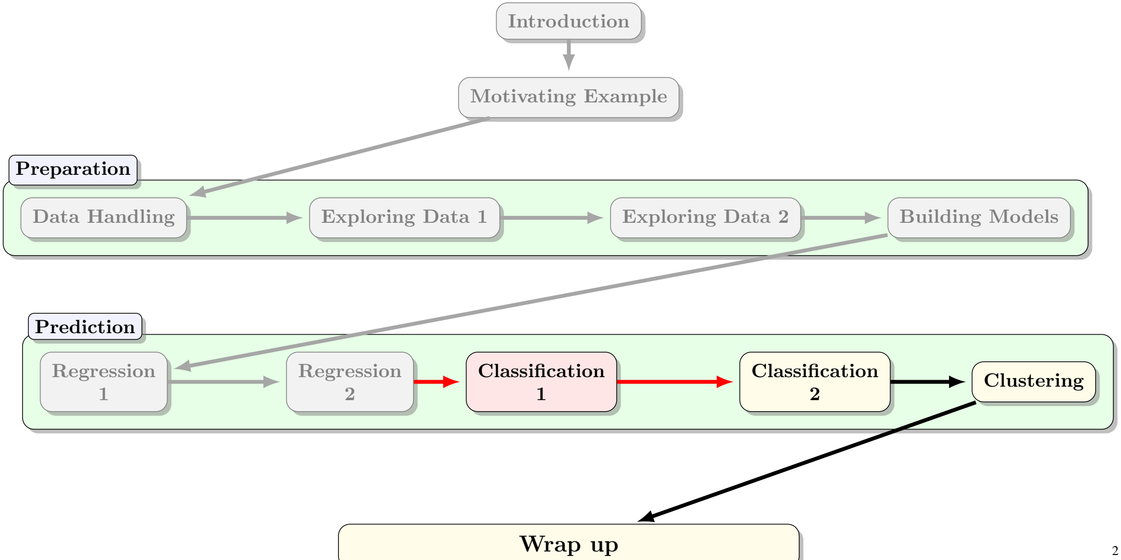
Outline

- How classification differs from regression
- Classification metrics
- Logistic regression in practice - Iris dataset
- Logistic regression - how it works

Data Mining (Week 9)



Acknowledgment

Thanks to Dr Kieran Murphy for many of today’s slides.

Outline

Introduction to Classification

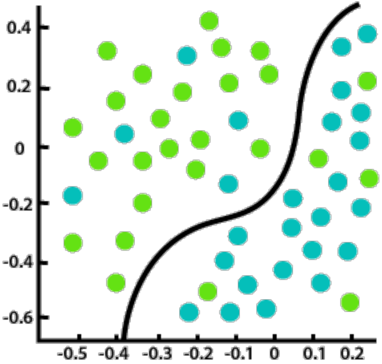
Definition 1 (Classification)

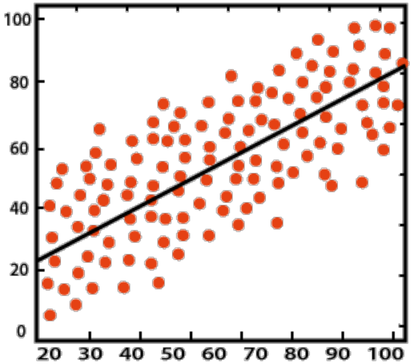
Classification aims to learn a function that takes attribute values and predicts a categorical/qualitative value, such as membership of a class, existence of an effect, etc. The attributes can be categorical or numeric. As with linear regression, classification is an example of supervised learning. It differs from regression because regression predicts a numeric response.

- Some *classifiers* generate class membership probabilities (numeric) en route to predicting class membership (of the most likely class), so the distinction is not always clear-cut.
- There is essentially one regression algorithm (with many variants/enhancements/implementations) but there are *many* classification algorithms.
- You have seen 1 already (KNN) and we introduce another algorithm today.

Classification vs Regression

Supervised data models have a target.
If target is quantitate (continuous) then have a regression model, if categorical then classification model.





Classification models aim to:
- predict class/label for each new observation,
- define a decision boundary between classes,
- and possibly the probability of being in each class.

Regression models aim to
- predict a continuous value for each new observation.

Classification vs Regression

- Unlike regression, statistical distributions play a limited role in evaluating a classifier:
    - Scope for hypothesis testing is limited (there is no equivalent of the `statsmodels` diagnostic output (covered in topic 8).
    - Rely on empirical metrics — accuracy, precision, recall, f1-score, auc, ...
- Classification metrics tend to be easier to use/understand than those in regression — classification metrics are based on counts of correct (or incorrect) cases divided by a subset of cases.
- Central concept in classification model is the confusion matrix:

		Predicted		
		Negative	Positive	
Actual	Negative	✔ True Negative (TN)	Type I error False Positive (FP)	N
	Positive	Type II error False Negative (FN)	✔ True Positive (TP)	P
		$\hat{N}$	$\hat{P}$	T

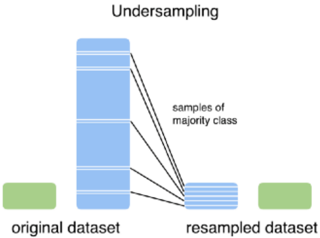
Unbalanced Classification Datasets

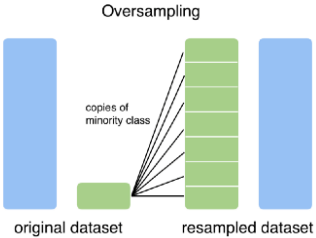
Practical classification datasets are often unbalanced — where the frequency of the classes in the target are very uneven:

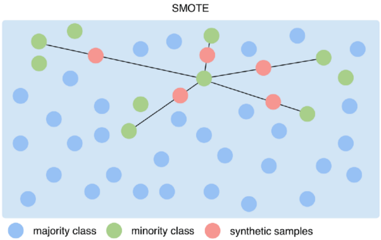
- Telecommunication customer churn datasets. Churn rate of 2%–10%.
- Credit Card Fraud Detection 0.172% (492 frauds / 284,807 transactions).
- National Institutes of Health Chest X-Ray Dataset 14 cases, (size 13 to 3,044) in 5,606 cases

Solutions

Use suitable metrics and/or







Summary of Classification Models

Model	Data Pre-processing*		Impact from		Summary
	Normalisation	Scaling	Collinearity	Outliers	
KNN	✔	✔	✔	✘	• Local approximation, lazy learner • Heavy computational requirements
Logistic Regression	✔	✘	✔	✔	• Descriptive with good accuracy • Reasonable computational requirements
Naïve Bayes	NA	NA	✔	✘	• Works with categorical features only • Suitable for small train datasets
Decision Tree	✘	✘	✔	✔	• Easy to setup and interpret (XAI). • Robust to missing data but not to noise. • Slow training for larger sets.
Random Forest (Not this module)	✘	✘	✘	✘	• High prediction accuracy • Limited explainability • Works with both continuous and categorical features
Support Vector Classifier (Not this module)	✘	✘	✘/✔	✔	• High prediction accuracy • Explainability depends on kernel • Computational effort depends on kernel
Neural Networks (Not this module)	✘	✔	✔	✔	• High prediction accuracy • Self-extract features • Heavy computational requirements

*Use `StandardScaler`, or `RobustScaler` if have outliers.

Lazy vs Eager Learners

Lazy learner

Stores training data (or only minor processing) and uses this to compute prediction when given test data.

- Does not generalise until after training
- Does not produce a standalone model
- Training data must be kept for prediction
- Local approximations
- Often based on *search*
- If new data is just added to the training data, it can respond more easily to changing conditions

Eager learner

Builds a model from the train set, before receiving new data for prediction

- Training has an extra goal: to generalise from the data
- Training has an extra output: standalone model
- Training data can be discarded after use
- Local and/or global approximations
- Based on *computation*
- Models *drift* with time, so not suited to highly dynamic contexts, as it needs retraining

Usually an (eager) model requires much less memory than a (lazy) training set.

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Outline

A Non-perfect Test — Type I and Type II Errors

Consider an imperfect test with two outcomes, there are four possible outcomes:

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		Predicted: Negative	Predicted: Positive	
Actual	Negative	✔ True Negative (TN)		N
	Positive		✔ True Positive (TP)	P
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Confusion Matrix

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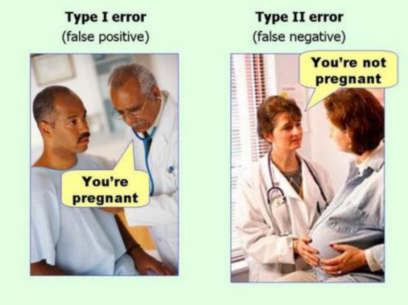
- If the test is applied to $T = P + N = \hat{P} + \hat{N}$ observations / subjects / instances then we have four independent quantities TP, TN, FP, and FN.
- How do we combines these quantities into a single metric ?
- The fraction of correct results seems like a good idea

$$\text{accuracy} = \frac{TP + TN}{P + N}$$

But what happens, if we are testing for an rare event? Maximising accuracy will result in the test always returning negative.



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- Depending on the conditions we often modify the test to reduce probability of the type of error we don't want at the expense of increasing the probability of the other — think court case vs medical condition.

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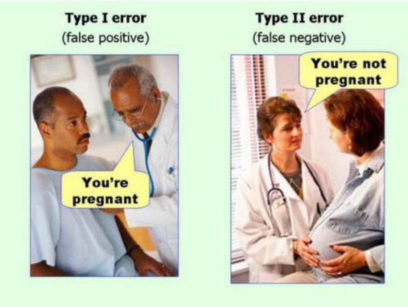

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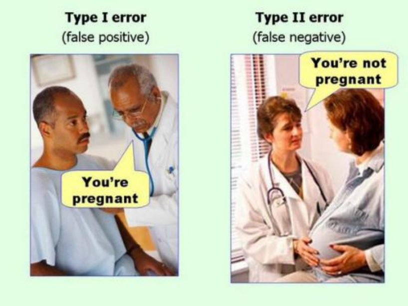

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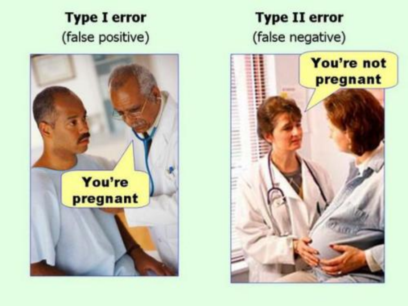

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Confusion matrix (Contingency table) Metrics I

$$\textbf{Accuracy} = \frac{\text{TP} + \text{TN}}{\text{P} + \text{N}}$$

(How often is the classifier correct?)

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- False negative rate (FNR) $= \dfrac{FN}{\text{P}} = 1 - TPR$
- **Sensitivity** = **Recall** = True positive rate (TPR) $= \dfrac{TP}{\text{P}} = 1 - FNR$
  (Of positive cases that exist how many did we mark positive?)
- **Specificity** $= \dfrac{\text{TN}}{\text{N}} = 1 - \text{FPR}$
  (When it's actually no, how often does we predict no?)
  (Of cases that are negative, how many did we mark negative?)
- False positive rate (FPR) = false acceptance $= \dfrac{FP}{\text{N}} = 1 - \text{Specificity}$
- **Precision** = positive predictive value (PPV) $= \dfrac{TP}{\hat{\text{P}}} = \dfrac{TP}{\text{TP} + \text{FP}}$
  (Of cases that we marked positive, how many were correct?)

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Accuracy — how well model is trained and performs in general

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Recall — important when the costs of false negatives are high

Precision — important when the costs of false positives are high

Confusion matrix (Contingency table) Metrics II

F_1 Score

The F-measure or balanced F-score (F_1 score) is the harmonic mean of precision and recall:

$$F_1 = 2\left[\frac{1}{\frac{1}{\text{precision}} + \frac{1}{\text{recall}}}\right] = 2\left[\frac{\text{precision} \times \text{recall}}{\text{precision} + \text{recall}}\right]$$

A word of Caution . . .

Consider the three binary classifiers A, B and C

	A		B		C	
	T	F	T	F	T	F
T	0.9	0.1	0.8	0	0.78	0
F	0	0	0.1	0.1	0.12	0.1

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Metric	**A**	**B**	**C**	(best)
Accuracy	0.9	0.9	0.88	**AB**
Precision	0.9	1.0	1.0	**BC**
Recall	1.0	0.888	0.8667	**A**
F-score	0.947	0.941	0.9286	**A**

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Yet look at the performance metrics – B is never the clear winner.

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F-score	0.947	0.941	0.9286	**A**

Clearly classifier *A* is useless since it always predicts label T regardless of the input. Also, B is slightly better than C (lower off- diagonal total).
Yet look at the performance metrics – B is never the clear winner.

We use some metrics because they are easy to understand, and not because they always give the "correct" result.

Mutual Information is a Better Metric

The mutual information between predicted and actual label (case) is defined

$$I(\hat{y}, y) = \sum_{\hat{y}=\{0,1\}} \sum_{y=\{0,1\}} p(\hat{y}, y) \log \frac{p(\hat{y}, y)}{p(\hat{y})p(y)}$$

where $p(\hat{y}, y)$ is the joint probability distribution function.
This gives the intuitively correct rankings $B > C > A$

Metric	**A**	**B**	**C**
Accuracy	0.9	0.9	0.88
Precision	0.9	1.0	1.0
Recall	1.0	0.888	0.8667
F-score	0.947	0.941	0.9286
Mutual information	**0**	**0.1865**	**0.1735**

Micro Average vs Macro Average Performance

In a multi-class classifier we have more than two classes. To combine the metrics for individual classes to get an overall system metrics, we can apply either

Micro-Average Method
: Sum up the individual true positives, false positives, and false negatives of the system for different classes and then apply totals to get the statistics.

Macro-average Method
: Average the precision and recall of the system on different classes.

See `classification_report` from `sklearn.metrics` (Example: IRIS dataset)

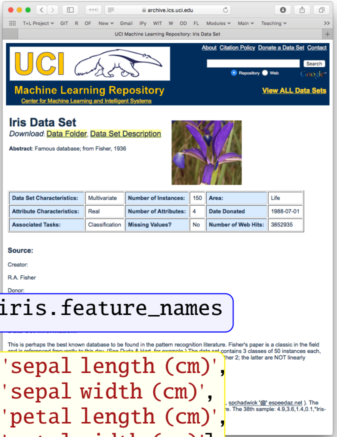
```
              precision   recall f1-score  support

      setosa       1.00     0.95     0.97       19
  versicolor       0.81     0.74     0.77       23
   virginica       0.71     0.83     0.77       18

    accuracy                         0.83       60
   macro avg       0.84     0.84     0.84       60
weighted avg       0.84     0.83     0.84       60
```

Outline

Example: IRIS Dataset — Load




```
iris.feature_names
```

```
['sepal length (cm)',
 'sepal width (cm)',
 'petal length (cm)',
 'petal width (cm)']
```

```python
from sklearn import datasets
iris = datasets.load_iris()

df = pd.DataFrame(iris.data)
df.columns = iris.feature_names
df['target'] = iris.target_names[iris.target]
df.sample(4)
```

	sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)	target
107	7.3	2.9	6.3	1.8	virginica
35	5.0	3.2	1.2	0.2	setosa
22	4.6	3.6	1.0	0.2	setosa
129	7.2	3.0	5.8	1.6	virginica

The data set contains, four numeric features, 3 classes of 50 instances each, where each class refers to a type of iris plant. One class is linearly separable from the other 2; the latter are NOT linearly separable from each other.

Example: IRIS Dataset — Preprocess Data

We will cover some classifiers in a moment, but for now just treat the classifiers (`LogisticRegression`) as a black box and focus on the general process:

Extract the data (features and target)

Split dataset into `train` and `test`

† Python for Data Science — Cheat Sheet Numpy Basics

Example: IRIS Dataset — Preprocess Data

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Extract the data (features and target)

The IRIS dataset has 4 features, but to simplify visualisation we are only going to use the first two[†] ('sepal length' and 'sepal width'):

```
dataset_name = "IRIS"
X, y, target_names = iris.data[:,:2], iris.target, iris.target_names
```

Split dataset into `train` and `test`

[†] Python for Data Science — Cheat Sheet Numpy Basics

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```
dataset_name = "IRIS"
X, y, target_names = iris.data[:,:2], iris.target, iris.target_names
```

Split dataset into `train` and `test`

We will keep 40% of the data for testing. Setting the parameter `random_state` to a value means that we will get a random — but still reproducible — split.

```
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)
```
.

[†] Python for Data Science — Cheat Sheet Numpy Basics

Example: IRIS Dataset — Fit Model and Predict

Select classifier

Train model

Predict

Example: IRIS Dataset — Fit Model and Predict

Select classifier

Scikit-learn supports a large set of classifiers, and aims to have a consistent interface to all. First import classifier and create instance ...

```
from sklearn.linear_model import LogisticRegression
model = LogisticRegression(max_iter=500)
```

Train model

Predict

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model = LogisticRegression(max_iter=500)
```

Train model

Then we train (fit) the classifier/model using only the features (`X_train`) and targets (`y_train`) from the train dataset . . .

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

```
LogisticRegression(max_iter=500)
```

Predict

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Train model

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

```
LogisticRegression(max_iter=500)
```

Predict

Now that model is trained, we can use it to generate predictions, using the features (`X_test`) from the test dataset ...

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

Example: IRIS Dataset — Evaluate I

Scoring and confusion matrix

Example: IRIS Dataset — Evaluate I

Scoring and confusion matrix

We could just compute the score using whatever metric we have picked ...

```
from sklearn.metrics import accuracy_score
accuracy_score(y_test, y_pred)
```

```
0.8333333333333334
```

But this needs context, and even if good can hide critical flaws. Lets look at the confusion matrix ...

```
from sklearn.metrics import confusion_matrix
cm = confusion_matrix(y_test,y_pred)
cm
```

```
array([[18, 1,  0],
       [ 0, 17,  6],
       [ 0,  3, 15]])
```

or, to get a nicer output, convert to a DataFrame ...

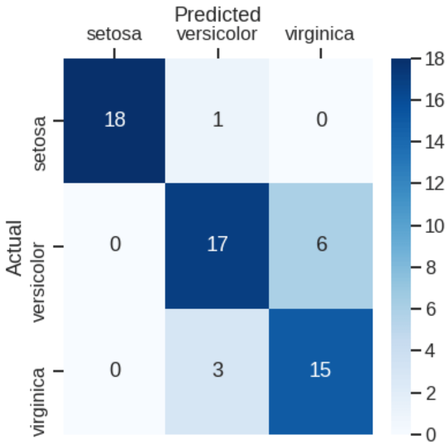
```
df_cm = pd.crosstab(target_names[y_test],target_names[y_pred])
df_cm.index.name = 'Actual'
df_cm.columns.name = 'Predicted'
df_cm
```

Predicted	**setosa**	**versicolor**	**virginica**
Actual			
setosa	18	1	0
versicolor	0	17	6
virginica	0	3	15

Example: IRIS Dataset — Evaluate II

The confusion matrix is fundamental in evaluating a classifier, so find a presentation/visualisation that you like and use it. Here I have a heat map representation that I tend to use.

Predicted	**setosa**	**versicolor**	**virginica**
Actual			
setosa	18	1	0
versicolor	0	17	6
virginica	0	3	15




```
plt.figure(figsize=(6,6))
g = sns.heatmap(df_cm, annot=True, cmap="Blues")
g.xaxis.set_ticks_position("top")
g.xaxis.set_label_position('top')
```

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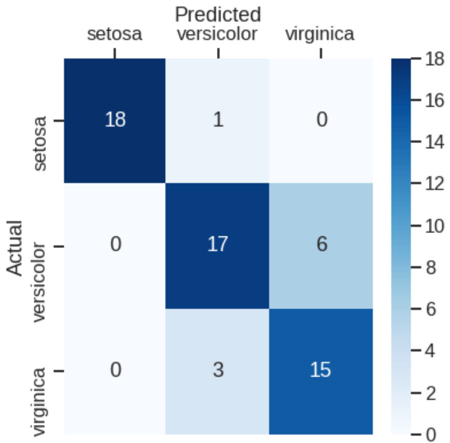

The first class `setosa` was only misclassified once, while the classifier had more difficulty between the second two classes.

```
plt.figure(figsize=(6,6))
g = sns.heatmap(df_cm, annot=True, cmap="Blues")
g.xaxis.set_ticks_position("top")
g.xaxis.set_label_position('top')
```

Example: IRIS Dataset — Evaluate III

The classification report, constructed from the confusion matrix, summaries the most common metrics per class and for overall averages ...

```python
from sklearn.metrics import classification_report
print(classification_report(y_test, y_pred, target_names=target_names))
```

Predicted	setosa	versicolor	virginica
Actual			
setosa	18	1	0
versicolor	0	17	6
virginica	0	3	15

```
              precision    recall  f1-score   support

      setosa       1.00      0.95      0.97        19
  versicolor       0.81      0.74      0.77        23
   virginica       0.71      0.83      0.77        18

    accuracy                           0.83        60
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weighted avg       0.84      0.83      0.84        60
```

Example: IRIS Dataset — Evaluate III

The classification report, constructed from the confusion matrix, summaries the most common metrics per class and for overall averages ...

```python
from sklearn.metrics import classification_report
print(classification_report(y_test, y_pred, target_names=target_names))
```

precision (setosa) = $18/(18+0) = 1$

recall (setosa) = $18/(18+1) = 0.95$

Predicted	setosa	versicolor	virginica
Actual			
setosa	18	1	0
versicolor	0	17	6
virginica	0	3	15

	precision	recall	f1−score	support
setosa	1.00	0.95	0.97	19
versicolor	0.81	0.74	0.77	23
virginica	0.71	0.83	0.77	18
accuracy			0.83	60
macro avg	0.84	0.84	0.84	60
weighted avg	0.84	0.83	0.84	60

accuracy = $(18+17+15)/60 = 0.83$

f1-score (virginica) = $2/(1/0.71+1/0.83) = 0.77$

Outline

Motivation

Linear regression is a very powerful and flexible prediction model (Topics 7 and 8)

Can it be used to predict categorical variables, perhaps coded as numbers?

- Pros
  - Linear regression provides a principled way of combining the contributions of the predictors, whether they are numeric or not.
  - There is a lot of well-established theory and practice, e.g., in respect of collinearity.
  - The model is extremely flexible, e.g., predictors can be nonlinear functions of the features.
  - Implementations can use computing resources efficiently.
- Cons
  - Prediction is numeric value, needs to be converted to a categorical value.
  - Conversion function introduces unwelcome features, e.g., ordering and scaling, that do not apply to nominal variables.
  - Interpretation of linear regression in terms of classification performance is tricky because the conversion function needs to balance continuity against evaluating to either 0 or 1.

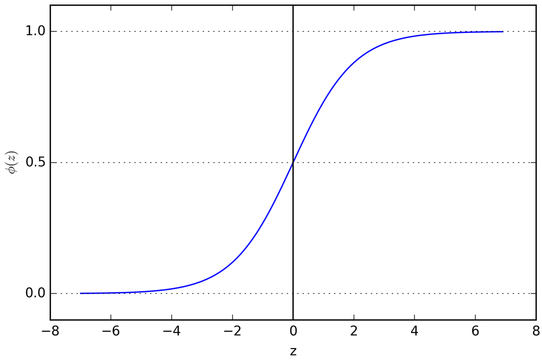
So—is there any hope for using linear regression in classification?

Probability view of Classification

When we predict a nominal value, it is equivalent to saying that the probability that a given observation takes that value is high and that it takes any other value is low.

- Probabilities are numeric, but their range is restricted to $[0, 1]$.
- We need a function of the predictors with the following properties
  - it has the range $[0, 1]$
  - it is defined over a domain which is $(-\infty, \infty)$
  - it can evaluate to 0 or 1, depending on its input.
- A line (like $y = \beta_0 + \beta_1 x$), such as we used in previous topics, does not have these properties
- Ideally, the function should be smooth and well-behaved everywhere, *and* evaluate to 0 or 1 as appropriate.
- Note that the classes are labeled as 0 or 1 (binary classification).

Introducing the logistic function



Definition 2 (logistic function)

The curve above is given by the logistic function, which can be written as $p(z) = \frac{e^z}{1+e^z}$. Letting $z = \beta_0 + \beta_1 X$, we have $p(X) = \frac{e^{\beta_0+\beta_1 X}}{1+e^{\beta_0+\beta_1 X}}$ for some β_0 and β_1.

Predicting the (log) odds ratio

$$
\begin{aligned}
p(X) &= \frac{e^{\beta_0+\beta_1 X}}{1+e^{\beta_0+\beta_1 X}} && (1)\\
\implies e^{\beta_0+\beta_1 X} &= p(X) + e^{\beta_0+\beta_1 X} p(X)\\
\implies (1-p(X))e^{\beta_0+\beta_1 X} &= p(X)\\
\implies \frac{p(X)}{1-p(X)} &= e^{\beta_0+\beta_1 X}\\
\implies \log\left(\frac{p(X)}{1-p(X)}\right) &= \beta_0 + \beta_1 X && (2)
\end{aligned}
$$

The expression on the left of (2) is called the *log-Odds Ratio* (or $\text{logit}(X)$). When $p(X) \to 1$, $\text{logit}(X) \to \infty$ and when $p(X) \to 0$, $\text{logit}(X) \to -\infty$, as required.
The expression on the right of (2) is a linear form in β, as used in linear regression.
For training: Compute logit(X) from the training labels and use linear regression to get $\{\beta_i\}$.
For prediction: Substitute X, $\{\beta_i\}$ in the logistic function (1) to obtain class $\text{round}(p(X))$.

Logistic regression summary

Training

Given (labeled) training data, convert the label to the equivalent logit value and use *maximum likelihood estimation* to look for the parameters β that make the observed data as likely as possible. Extension to multiple predictors is trivial.

Prediction

Given the fitted β, just evaluate the logistic function for a specific X. The resulting $p(X)$ will hopefully be near 0 or 1 and can be interpreted according to how "success" ($p = 1$) is defined.

Extension to categorical predictors

As with linear regression: create dummy (binary) indicator (0,1)-valued variables, one for each level of the categorical predictor.

Extension to non-binary predicted values

We can convert to extra indicator variables, but at some cost in complexity. Therefore, logistic regression is best suited to binary prediction.

Logistic regression in python

Python's `scikit-learn` and `statsmodel` libraries provide a general interface to model fitting that abstracts away logistic functions and other details.

Method (Recognising the Handwritten Digits)

```python
from sklearn.linear_model import LogisticRegression

# Get and configure a LogisticRegression object, with an L2 regularisation penalty
clf = LogisticRegression(penalty='l2')

# Fit the training data
clf.fit(Xtrain, ytrain)

# Using the beta parameters that have just been learned and are in clf, predict (recognise) the test data
ypred = clf.predict(Xtest)
```

Outline

Review of Regression 1

- Classification is one of the most common machine learning tasks
- For regression, the focus is on residuals, for classification it is on the confusion matrix
- Performance metrics are based on ratios and independent of the algorithm used
- Trade-offs are needed: Type 1 vs Type 2 errors and associated classification metrics
- Builds upon all the existing EDA, model building and multivariate analysis we saw before

Next topic - we introduce 2 new classification algorithms