COMP47750
Machine Learning with Python

Nearest Neighbour Classifiers

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original slides by Derek Greene

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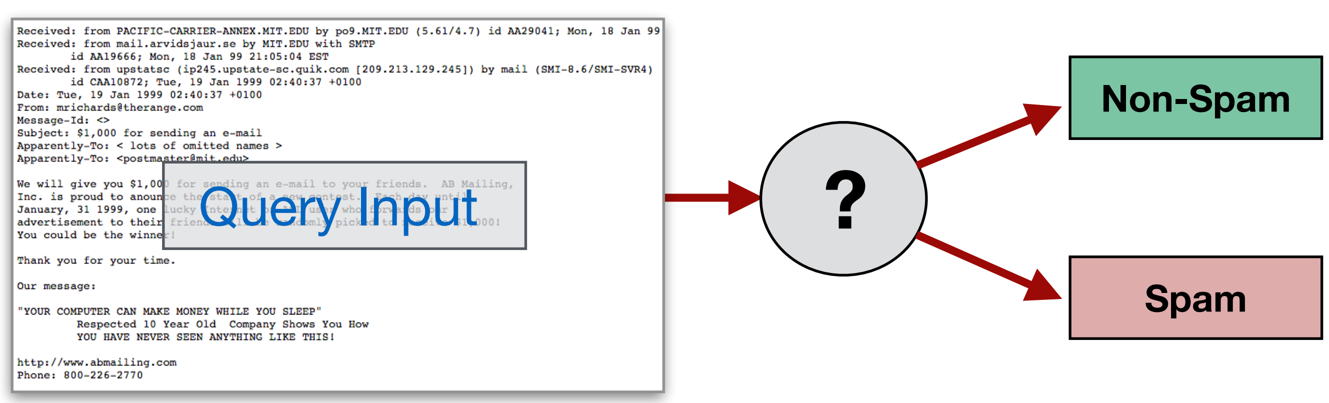
Overview

- Eager v Lazy Classification Strategies
- Distance-based Models
- Feature Spaces
- Measuring Distance
- Data Normalisation
- Nearest Neighbours
- *k*-Nearest Neighbour Classifier (*k*NN)
- Weighted *k*NN
- *k*NN in scikit-learn in Python

Reminder: Classification

- Supervised Learning: Algorithm that learns a function from manually-labelled training examples.
- Classification: Training examples, usually represented by a set of descriptive features, help decide the *class* to which a new unseen query input belongs.
- Binary Classification: Assign one of two possible target class labels to the new query input.



- Multiclass Classification: Assign one of *M>2* possible target class labels to the new query input.

Eager v Lazy Classifiers

- Eager Learning Classification Strategy
  - Classifier builds a full model during an initial training phase, to use later when new query examples arrive.
  - More offline setup work, less work at run-time.
  - Generalise before seeing the query example.
- Lazy Learning Classification Strategy
  - Classifier keeps all the training examples for later use.
  - Little work is done offline, wait for new query examples.
  - Focus on the local space around the examples.

- Distance-based Models: Many learning algorithms are based on generalising from training data to unseen data by exploiting the distances (or similarities) between the two.

Example: Athlete Selection

- Training set of performance ratings for 20 college athletes, where each athlete is described by 2 continuous features: *speed*, *agility*.
- Each athlete has a target class label indicating whether they were selected for the university athletics team: 'Yes' or 'No'.

Athlete	***Speed***	***Agility***	***Selected***
x1	2.50	6.00	No
x2	3.75	8.00	No
x3	2.25	5.50	No
x4	3.25	8.25	No
x5	2.75	7.50	No
x6	4.50	5.00	No
x7	3.50	5.25	No
x8	3.00	3.25	No
x9	4.00	4.00	No
x10	4.25	3.75	No

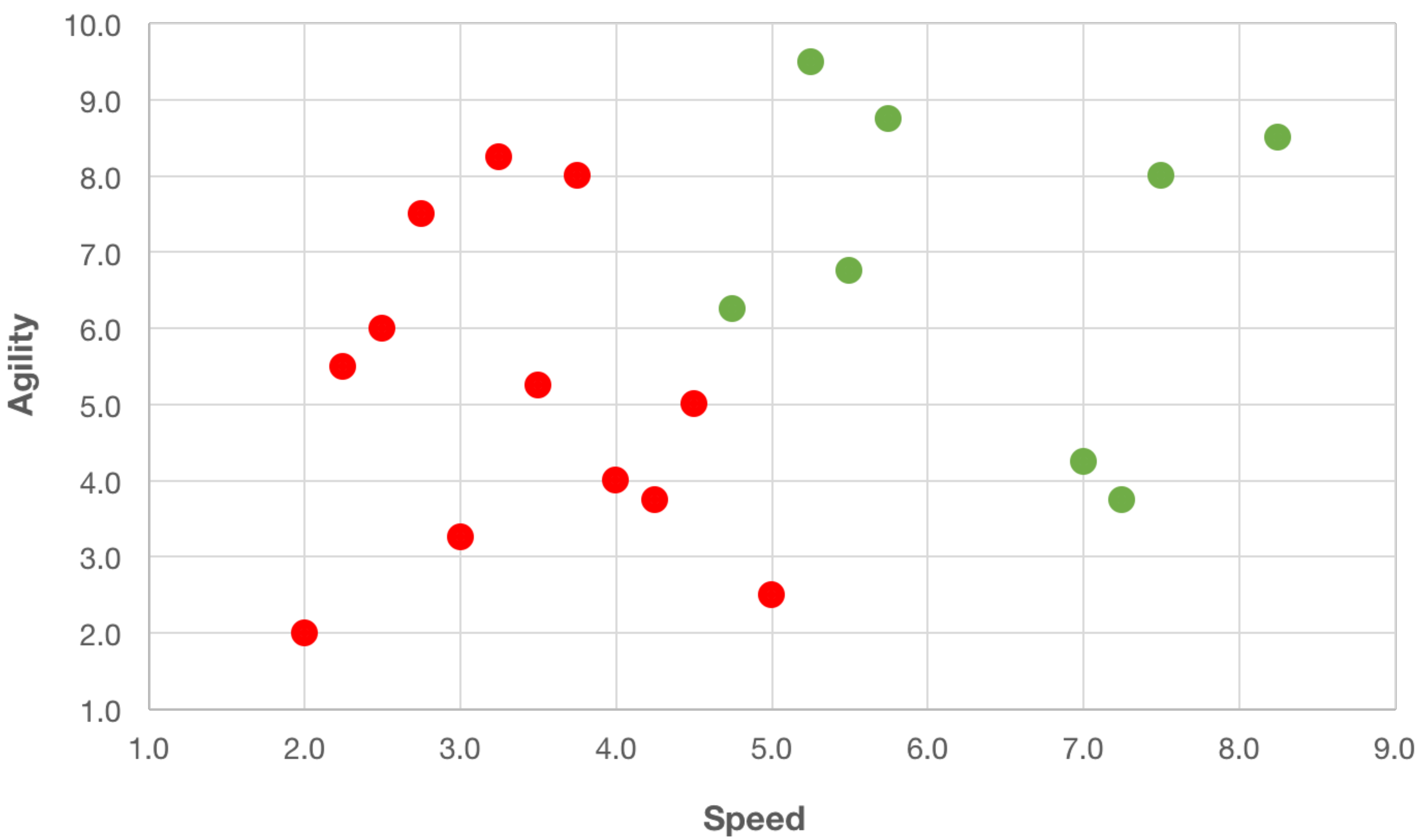
Athlete	***Speed***	***Agility***	***Selected***
x11	2.00	2.00	No
x12	5.00	2.50	No
x13	8.25	8.50	Yes
x14	5.75	8.75	Yes
x15	4.75	6.25	Yes
x16	5.50	6.75	Yes
x17	5.25	9.50	Yes
x18	7.00	4.25	Yes
x19	7.50	8.00	Yes
x20	7.25	3.75	Yes

Q. Will a new athlete **q** be selected: 'Yes' or 'No'?

Athlete	***Speed***	***Agility***	***Selected***
q	3.00	8.00	???

Feature Spaces

- A feature space is a *D*-dimensional coordinate space used to represent the input examples for a given problem, with one coordinate for each descriptive feature.
- **Example:** Use a feature space to visually position the 20 athletes in a 2-dimensional coordinate space (i.e. *agility* versus *speed*):

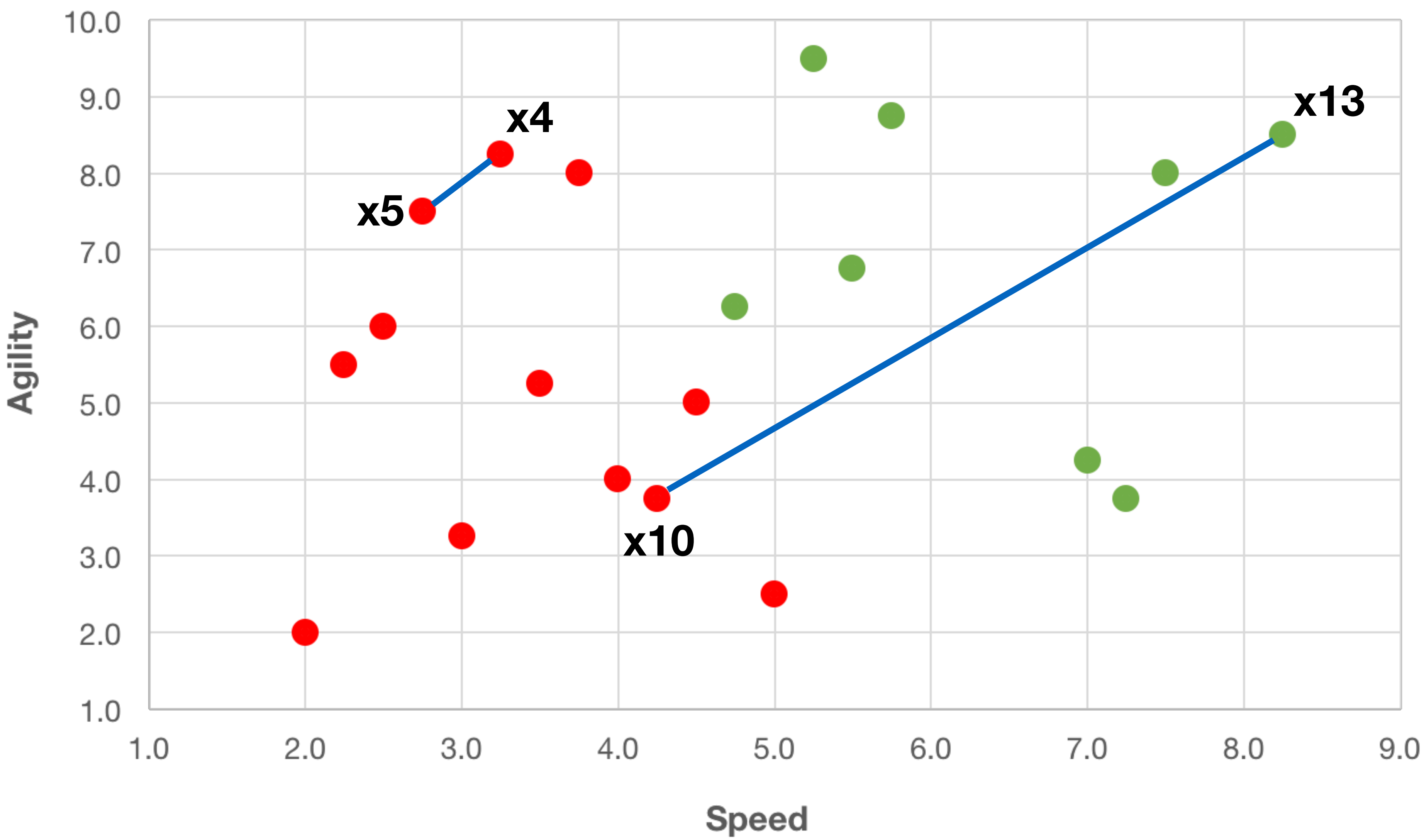


Training set of 20 examples (athletes)

Each example described by 2 feature values: *agility* & *speed*

Measuring Distance

- Measuring the distance (or similarity) between two examples is fundamental to many ML algorithms.
- Many measures can be used to calculate distance. There is no "best" distance measure. The choice is highly problem-dependent.



Examples *x4* and *x5* have a low distance (high similarity)

Examples *x10* and *x13* have a high distance (low similarity)

Measuring Distance

- Distance function: A suitable function to measure how distant (or similar) two input examples are from one another are in some *D*-dimensional feature space.

- Local distance function: Measure the distance between two examples based on a single feature.

Athlete	*Speed*	*Agility*
x1	2.50	6.00
x2	3.75	8.00

  - e.g. what is distance between **x1** and **x2** in terms of *Speed*?
  - e.g. what is distance between **x1** and **x2** in terms of *Agility*?

- Global distance function: Measure the distance between two examples based on the combination of the local distances across all features.
  - e.g. what is distance between **x1** and **x2** based on both *Speed* and *Agility*?

Measuring Distance

- Overlap function: Simplest local distance measure. Returns 0 if the two values for a feature are equal and 1 otherwise. Generally suitable for categorical data.

Athlete	*Gender*	*Nationality*
x1	Female	Irish
x2	Male	Irish
x3	Male	Italian

For feature *Gender*

$$d_g(x1,x2) = 1$$
$$d_g(x1,x3) = 1$$
$$d_g(x2,x3) = 0$$

For feature *Nationality*

$$d_n(x1,x2) = 0$$
$$d_n(x1,x3) = 1$$
$$d_n(x2,x3) = 1$$

- Hamming distance: Global distance function which is the sum of the overlap differences across all features - i.e. number of features on which two examples disagree.

$$d(x1,x2) = 1 + 0 = 1$$
$$d(x1,x3) = 1 + 1 = 2$$
$$d(x2,x3) = 0 + 1 = 1$$

Overlap distance for *Gender* +
Overlap distance for *Nationality*

Measuring Distance

- Absolute difference: For numeric data, we can calculate absolute value of the difference between values for a feature.

Athlete	Speed	Agility
x1	2.50	6.00
x2	3.75	8.00
x3	2.25	5.50

For feature *Speed*

$d_S(x1,x2) = |2.50-3.75| = 1.25$
$d_S(x1,x3) = |2.50-2.25| = 0.25$
$d_S(x2,x3) = |3.75-2.25| = 1.5$

For feature *Agility*

$d_S(x1,x2) = |6.0-8.0| = 2.0$
$d_S(x1,x3) = |6.0-5.5| = 0.5$
$d_S(x2,x3) = |8.0-5.5| = 2.5$

- Again we can compute a global distance between two examples by summing the local distances over all features.

$d(x1,x2) = 1.25 + 2.0 = 3.25$
$d(x1,x3) = 0.25 + 0.5 = 0.75$
$d(x2,x3) = 1.5 + 2.5 = 4.0$

Absolute difference for *Speed* +
Absolute difference for *Agility*

- For *ordinal features*, calculate the absolute value of the difference between the two positions in the ordered list of possible values.

e.g. Ordinal Feature *Dosage*:
{Low,Medium,High} = {1, 2, 3}

```
diff(Low,High) = |1-3| = 2
diff(Medium,Low) = |2-1| = 1
diff(High,High) = |3-3| = 0
```

Measuring Distance

- Euclidean distance: Most common measure used to quantify distance between two examples with numeric features.
- Given by the "straight line" distance between two points in a Euclidean coordinate space - e.g. a feature space.
- Calculated as the square root of sum of squared differences for each feature *f* representing a pair of examples.
- The output is a real value ≥ 0, where a larger value indicates two examples are more distant (i.e. less similar to one another).

Input:
2 examples
p and **q**

$$\mathrm{ED}(\mathbf{p}, \mathbf{q}) = \sqrt{\sum_{f \in F} (q_f - p_f)^2}$$

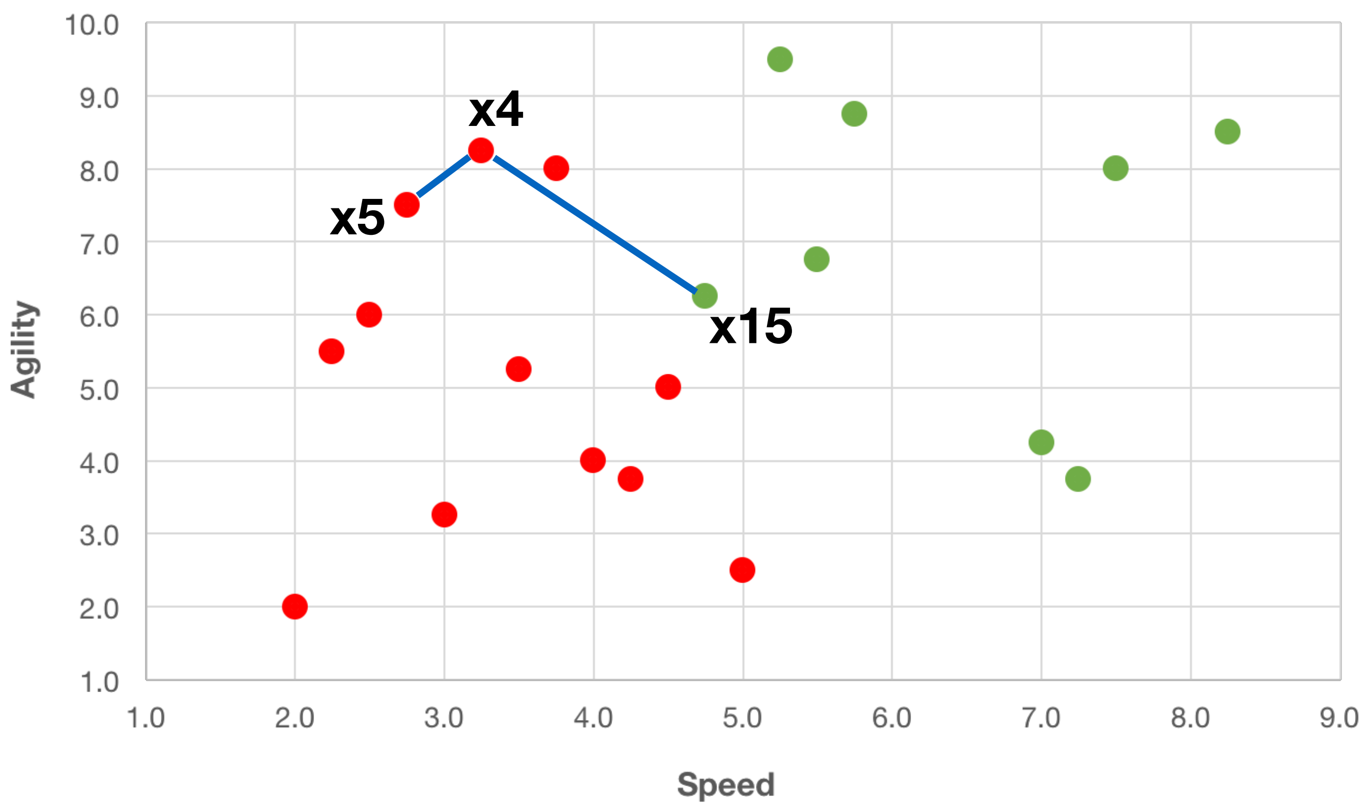
Calculate square of the difference between the examples on feature *f*

For each feature *f* in the full set of features *F*

Measuring Distance

- **Example:** Apply Euclidean distance, where *F* consists of 2 numeric features: *speed*, *agility*

$$\mathrm{ED}(\mathbf{p},\mathbf{q}) = \sqrt{\sum_{f \in F} (q_f - p_f)^2}$$



Athlete	*Speed*	*Agility*
x4	3.25	8.25
x15	4.75	6.25

$$ED(x4, x15) = \sqrt{(3.25 - 4.75)^2 + (8.25 - 6.25)^2}$$
$$= \sqrt{6.25} = 2.5$$

Athlete	*Speed*	*Agility*
x4	3.25	8.25
x5	2.75	7.50

$$ED(x4, x5) = \sqrt{(3.25 - 2.75)^2 + (8.25 - 7.50)^2}$$
$$= \sqrt{0.81} = 0.9$$

Heterogeneous Distance Functions

- In many datasets, the features associated with examples will have different types (e.g. continuous, categorical, ordinal etc).
- We can create a global measure from different local distance functions, using an appropriate function for each feature.

Athlete	***Speed***	***Agility***	***Gender***	***Nationality***
x1	2.50	6.00	Female	Irish
x2	3.75	8.00	Male	Irish
x3	2.25	5.50	Male	Italian

Use absolute difference for continuous features *Speed* & *Agility*

Use overlap for categorical features *Gender* & *Nationality*

```
d(x1,x2) = 1.25 + 2.0 + 1 + 0 = 4.25
d(x1,x3) = 0.25 + 0.5 + 1 + 1 = 2.75
d(x2,x3) = 1.5 + 2.5 + 0 + 1 = 5.0
```

Global distance calculated as sum over individual local distances

- Often domain expertise is required to choose an appropriate distance function for a particular dataset.

Data Normalisation

- Numeric features often have different ranges, which can skew certain distance functions.
- So that all features have similar range, we apply *feature normalisation*.
- Min-max normalisation:
  Use min and max values for a given feature to rescale to the range [0,1]

Example	*Age*
x1	24
x2	19
x3	50
x4	40
x5	23
x6	68
x7	45
x8	33
x9	80
x10	58

$$z_i = \frac{x_i - \min(x)}{\max(x) - \min(x)}$$

- Example: Feature *Age*

$$\min(x) = 19$$

$$\max(x) = 80$$

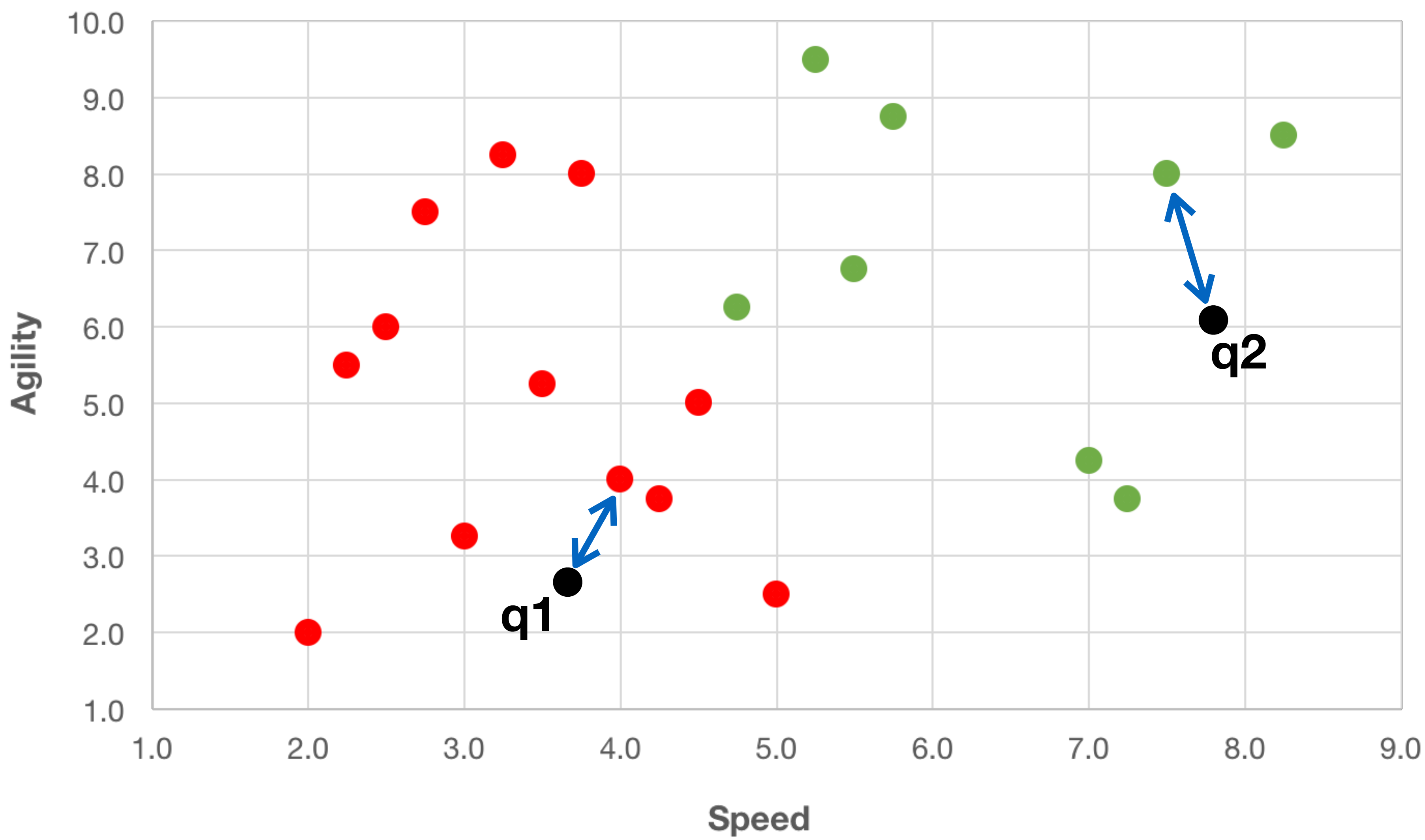
$$\max(x) - \min(x) = 61$$

Age (Non-normalised)	24	19	50	40	23	68	45	33	80	58
Age (Normalised)	0.08	0.00	0.51	0.34	0.07	0.80	0.43	0.23	1.00	0.64

Nearest Neighbour Classifier

Lazy learning approach: Do not build a model for the data. Identify most similar previous example(s) from the training set for which a label has already been assigned, using some distance function.

Nearest neighbour rule (1NN): For a new query input **q**, find a single labelled example **x** closest to **q**, and assign **q** the same label as **x**.



Assign **q1** to 'No' class

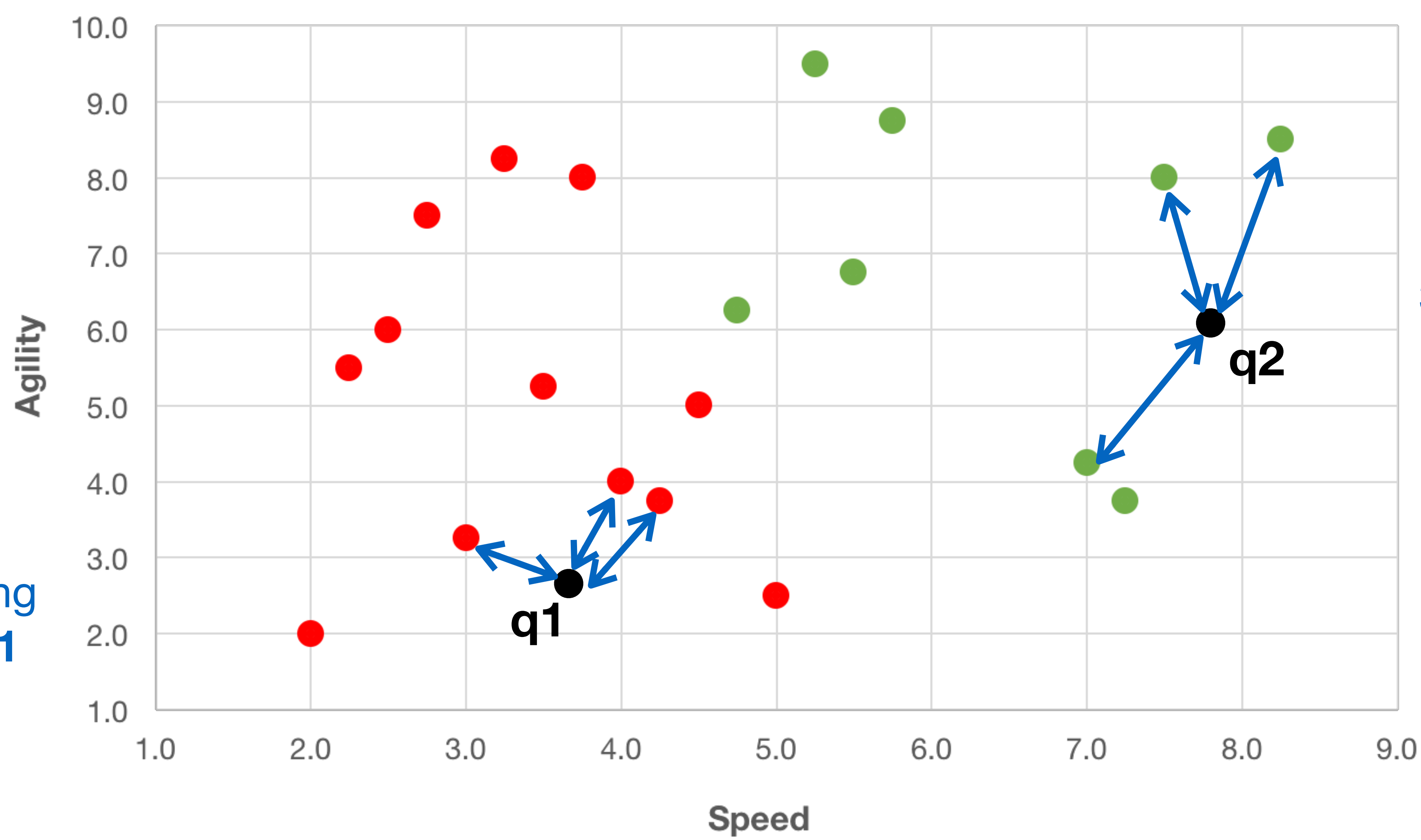
Assign **q2** to 'Yes' class

k-Nearest Neighbour Classifier

k-Nearest neighbours (kNN): The NN approach naturally generalises to the case where we use *k* nearest neighbours from the training set to assign a label to a new query input.

Example: For new query inputs, calculate distance to all training examples. Find *k=3* nearest examples (i.e. with smallest distances).

3 nearest training examples to **q1**

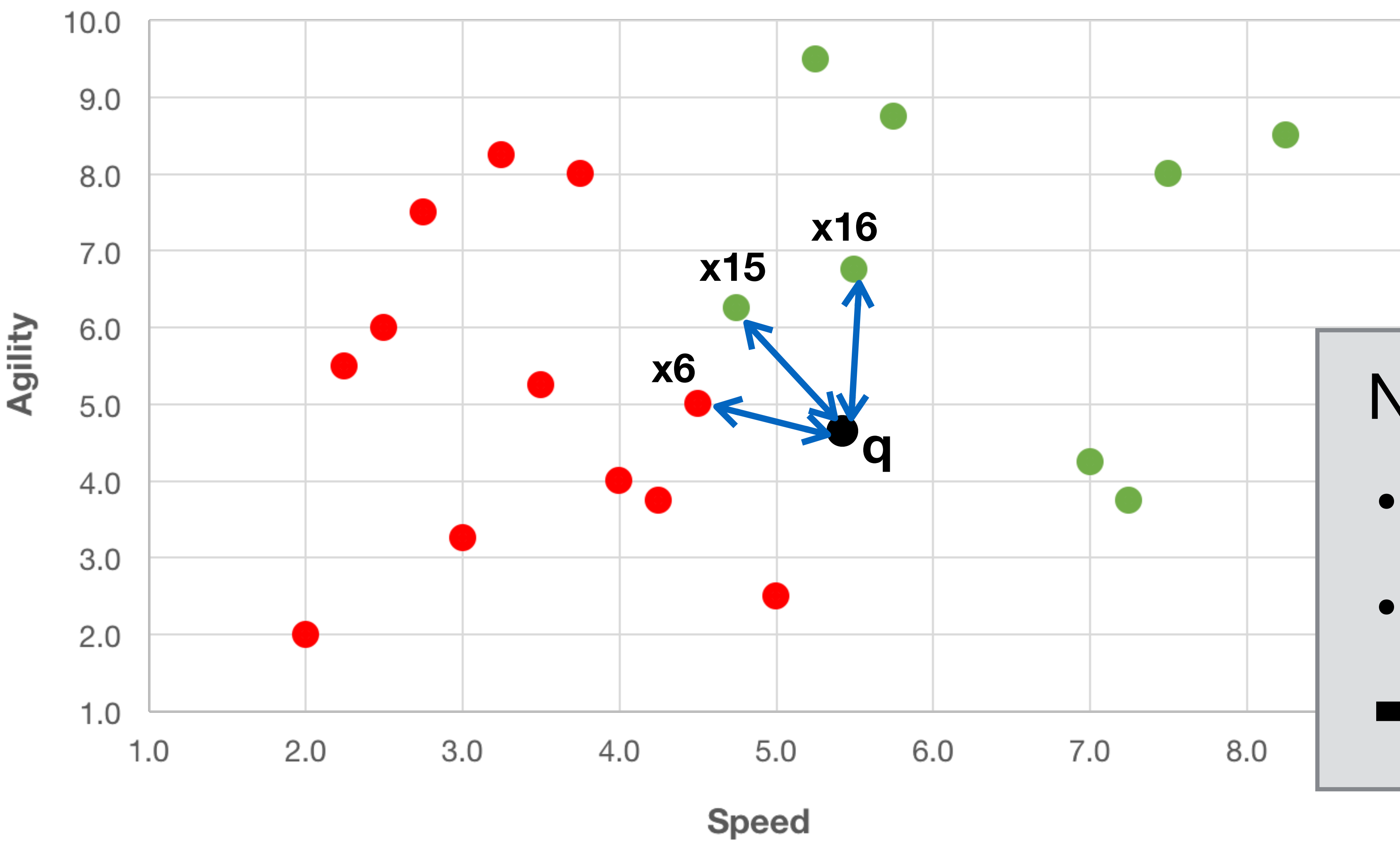


3 nearest training examples to **q2**

k-Nearest Neighbour Classifier

Majority voting: The decision on a label for a new query example is decided based on the "votes" of its *k* nearest neighbours. The label for the query is the majority label of its neighbours.

Example: Measure distance from **q** to all training examples. Find the *k=3* nearest examples, and use their labels as votes.



Neighbour counts

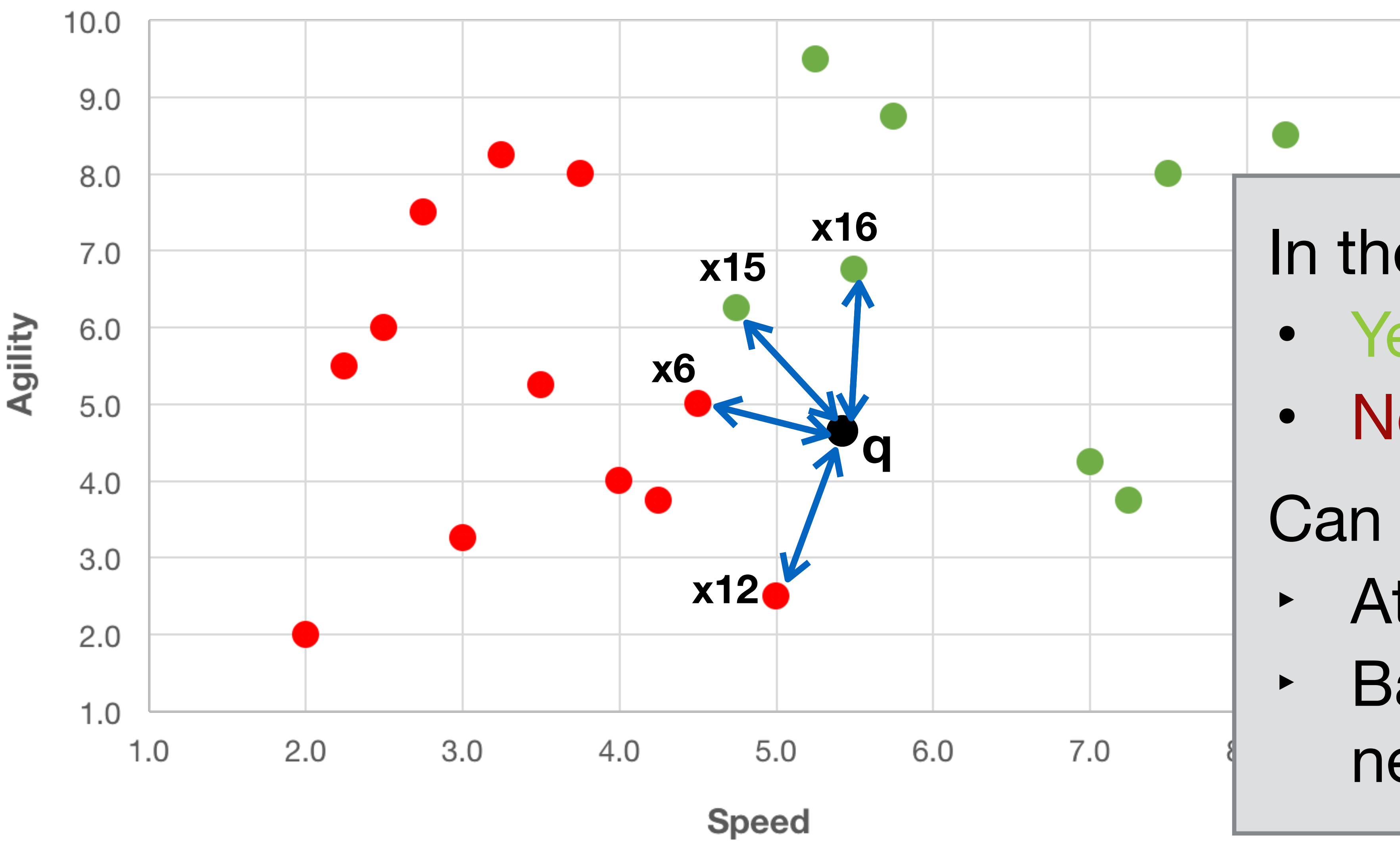
- Yes = 2 votes
- No = 1 vote

➡ Majority says Yes!

k-Nearest Neighbour Classifier

Majority voting: The decision on a label for a new query example is decided based on the “votes” of its *k* nearest neighbours. The label for the query is the majority label of its neighbours.

Example: Measure distance from **q** to all training examples.
Find the *k=4* nearest examples, and use their labels as votes.



In the case that…

- Yes = 2 votes
- No = 2 votes

Can break ties…

- At random
- Based on sum of neighbour distances

Example: kNN Classification (*k*=3)

- Training set of 20 athletes - 8 labelled as 'Yes', 12 as 'No'.
- Each athlete described by 2 continuous features: *Speed*, *Agility* Euclidean distance would be an appropriate distance function.

Athlete	Speed	Agility	Selected
x1	2.50	6.00	No
x2	3.75	8.00	No
x3	2.25	5.50	No
x4	3.25	8.25	No
x5	2.75	7.50	No
x6	4.50	5.00	No
x7	3.50	5.25	No
x8	3.00	3.25	No
x9	4.00	4.00	No
x10	4.25	3.75	No

Athlete	Speed	Agility	Selected
x11	2.00	2.00	No
x12	5.00	2.50	No
x13	8.25	8.50	Yes
x14	5.75	8.75	Yes
x15	4.75	6.25	Yes
x16	5.50	6.75	Yes
x17	5.25	9.50	Yes
x18	7.00	4.25	Yes
x19	7.50	8.00	Yes
x20	7.25	3.75	Yes

Will a new input example **q** be classified as 'Yes' or 'No'?

Athlete	Speed	Agility	Selected
q	5.00	7.50	???

Example: kNN Classification (*k*=3)

- Measure distance between **q** and all 20 training examples.

Athlete	Speed	Agility	Selected	Distance
x1	2.50	6.00	No	2.915
x2	3.75	8.00	No	1.346
x3	2.25	5.50	No	3.400
x4	3.25	8.25	No	1.904
x5	2.75	7.50	No	2.250
x6	4.50	5.00	No	2.550
x7	3.50	5.25	No	2.704
x8	3.00	3.25	No	4.697
x9	4.00	4.00	No	3.640
x10	4.25	3.75	No	3.824

Athlete	Speed	Agility	Selected	Distance
x11	2.00	2.00	No	6.265
x12	5.00	2.50	No	5.000
x13	8.25	8.50	Yes	3.400
x14	5.75	8.75	Yes	1.458
x15	4.75	6.25	Yes	1.275
x16	5.50	6.75	Yes	0.901
x17	5.25	9.50	Yes	2.016
x18	7.00	4.25	Yes	3.816
x19	7.50	8.00	Yes	2.550
x20	7.25	3.75	Yes	4.373

q	5.00	7.50	???

- Rank the training examples and identify set of 3 examples with the smallest distances.

Athlete	Speed	Agility	Selected	Distance
x16	5.50	6.75	Yes	0.901
x15	4.75	6.25	Yes	1.275
x2	3.75	8.00	No	1.346

- Yes = 2 votes
- No = 1 vote

➡ Majority says Yes, so assign label Yes to **q**

Weighted kNN

- Weighted voting: In this approach, some training examples have a higher weight than others.
- Instead of using a binary vote of 1 for each nearest neighbour, typically closer neighbours get higher votes when deciding on the predicted label for a query example.
- Inverse distance-weighted voting: Simplest strategy is to take a neighbour's vote to be the inverse of their distance from the query (i.e. 1/Distance). We then sum over the weights for each class.

$$d(q, x16) = 0.901$$

$$\Rightarrow \text{weight}(x16) = \frac{1}{d(q, x16)} = \frac{1}{0.901} = 1.109$$

$$d(q, x2) = 1.346$$

$$\Rightarrow \text{weight}(x2) = \frac{1}{d(q, x2)} = \frac{1}{1.346} = 0.743$$

Example: Weighted kNN (*k*=3)

- Measure distance between **q** and all 20 training examples.

Athlete	Speed	Agility	Selected	Distance
x1	2.50	6.00	No	2.915
x2	3.75	8.00	No	1.346
x3	2.25	5.50	No	3.400
x4	3.25	8.25	No	1.904
x5	2.75	7.50	No	2.250
x6	4.50	5.00	No	2.550
x7	3.50	5.25	No	2.704
x8	3.00	3.25	No	4.697
x9	4.00	4.00	No	3.640
x10	4.25	3.75	No	3.824

Athlete	Speed	Agility	Selected	Distance
x11	2.00	2.00	No	6.265
x12	5.00	2.50	No	5.000
x13	8.25	8.50	Yes	3.400
x14	5.75	8.75	Yes	1.458
x15	4.75	6.25	Yes	1.275
x16	5.50	6.75	Yes	0.901
x17	5.25	9.50	Yes	2.016
x18	7.00	4.25	Yes	3.816
x19	7.50	8.00	Yes	2.550
x20	7.25	3.75	Yes	4.373

- Rank the training examples and identify set of 3 examples with the smallest distances. Assign weights based on 1/Distance, and sum weights for each class.

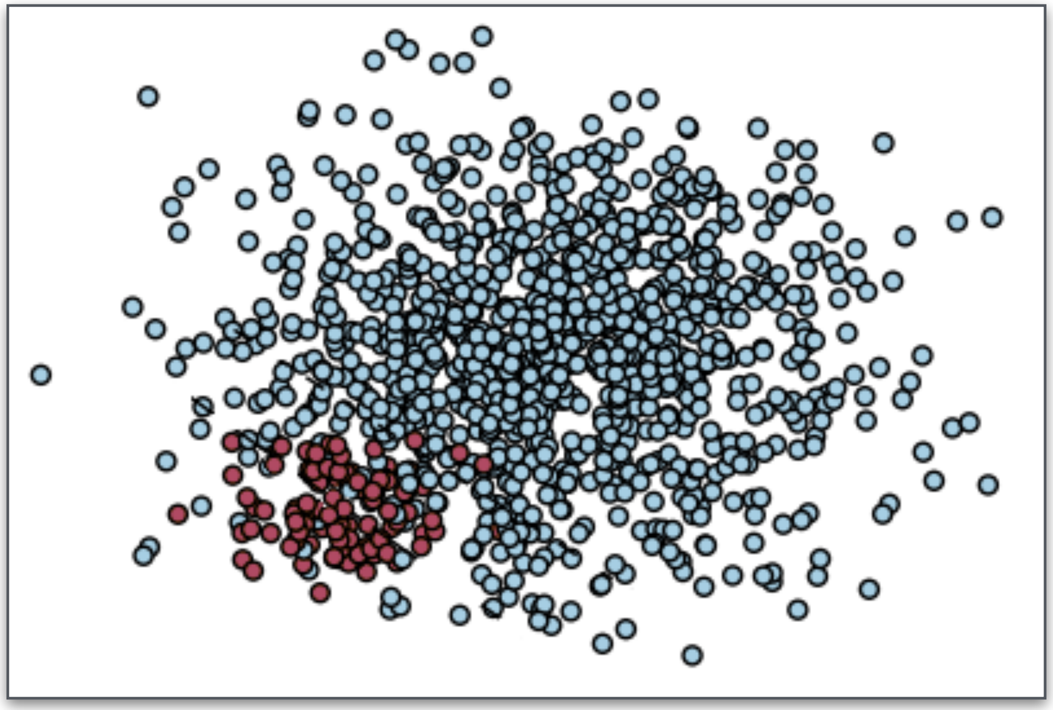
Athlete	Speed	Agility	Selected	Distance	Weight
x16	5.50	6.75	Yes	0.901	1.109
x15	4.75	6.25	Yes	1.275	0.784
x2	3.75	8.00	No	1.346	0.743

- Weights for Yes = 1.109 + 0.784 = 1.893
- Weights for No = 0.743

➡ Majority says Yes

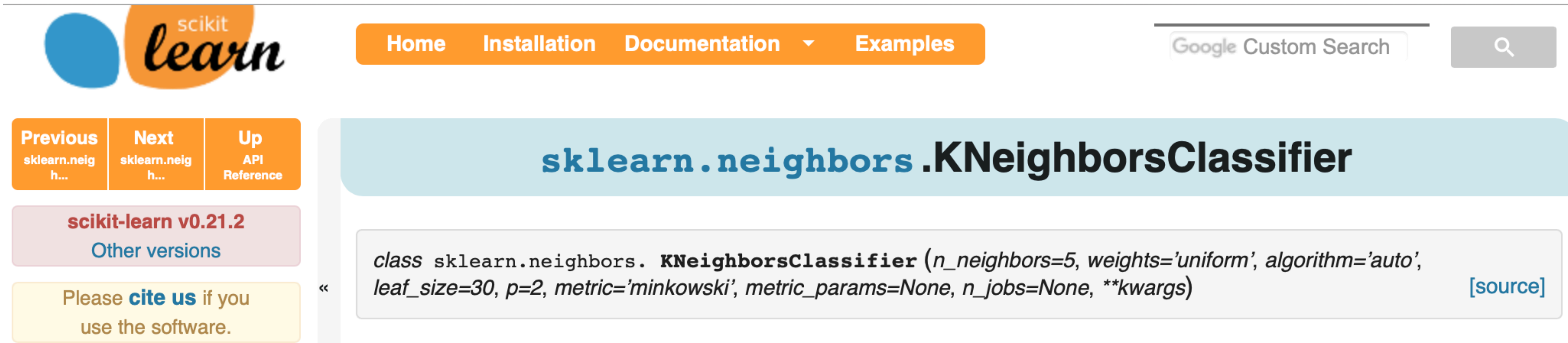
Parameter Tuning

- A simple 1-NN classifier is easy to implement. But it will be susceptible to "noise" in the data. A misclassification will occur every time a single noisy example is retrieved.
- We might decide to vary the neighbourhood size parameter *k* to improve the predictive performance of kNN.
- Choosing between different settings of an algorithm is often referred to as *hyperparameter tuning* or *model selection*.
- Using a larger (e.g. $k > 2$) can sometimes make the classifier more robust and overcome this problem.
- But when *k* is large ($k \rightarrow N$) and classes are *unbalanced*, we always predict the majority class.



k-NN with Scikit Learn

Code Notebook:
02-kNN



- Examples in Notebook 02-kNN
  - Loading a dataset
  - Finding nearest neighbours
  - Training a k-NN classifier
  - Scaling features
  - Weighting Instances

Load a dataset into Python

- Load a csv file into a Pandas dataframe in Python

```
athlete = pd.read_csv('AthleteSelection.csv',index_col = 'Athlete')
athlete.head()

y = athlete.pop('Selected').values
X = athlete.values
```

- X contains the features
- y contains the targets

	Speed	Agility	Selected
Athlete			
x1	2.50	6.00	0
x2	3.75	8.00	0
x3	2.25	5.50	0
x4	3.25	8.25	0
x5	2.75	7.50	0

Train a k-NN classifier

Set up classifier

```
forecast_kNN = KNeighborsClassifier(n_neighbors=3)
```

Train it

```
forecast_kNN.fit(X,y)
```

Setup queries examples

```
xinput = np.array([[8.,70.,11.],
                   [8,69,15]])
```

Make predictions

```
forecast_kNN.predict(xinput)
```

	Temperature	Humidity	Wind_Speed	Go-Out
0	6	85	30	0
1	14	90	35	0
2	15	86	8	1
3	21	56	15	1
4	17	67	9	1

Test on the Training Data

- Use training data as test (not a good idea)
- *k* = *3* so one misclassification

```
y_dash = forecast_kNN.predict(X)
print('     y:',y)
print('y_dash:',y_dash)

     y: [0 0 1 1 1 0 1 0 1 1 1 1 1 0 1 0 0 0]
y_dash: [0 0 1 1 1 0 1 0 1 1 1 1 1 0 1 0 1 0]
```

```
confusion = confusion_matrix(y, y_dash)
print("Confusion matrix:\n{}".format(confusion))

Confusion matrix:
[[ 7  1]
 [ 0 10]]
```

What would we expect to happen when k=1? (Try it.)

Normalizing (Scaling) Data

- Normaize data so all features have the same influence
  - Two popular models
    - N(0,1)
    - MinMax typically range (0,1)

Set up Scaler	`scaler = preprocessing.StandardScaler().fit(X)`
Scale the data	`X_scaled = scaler.transform(X)` `q_scaled = scaler.transform([q])`
Retrain the classifier	`forecast_kNN_S.fit(X_scaled,y)`
Make predictions	`forecast_kNN_S.kneighbors(q_scaled)`

Instance weighting

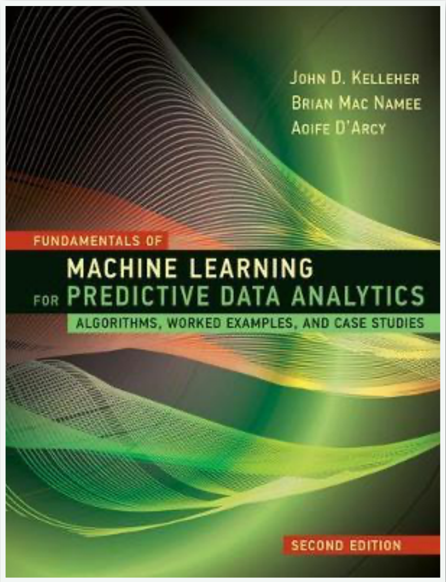
- Give nearer neighbours a bigger weight (vote)
  - based on distance

```
forecast_kNN_SW = KNeighborsClassifier(n_neighbors=3,weights='distance')
forecast_kNN_SW.fit(X_scaled,y)
y_dash = forecast_kNN_SW.predict(X_scaled)
confusion = confusion_matrix(y, y_dash)
print("Confusion matrix:\n{}".format(confusion))
print('\n     y:',y)
print('y_dash:',y_dash)

Confusion matrix:
[[ 8  0]
 [ 0 10]]

     y: [0 0 1 1 1 0 1 0 1 1 1 1 1 0 1 0 0 0]
y_dash: [0 0 1 1 1 0 1 0 1 1 1 1 1 0 1 0 0 0]
```

Additional Reading Materials

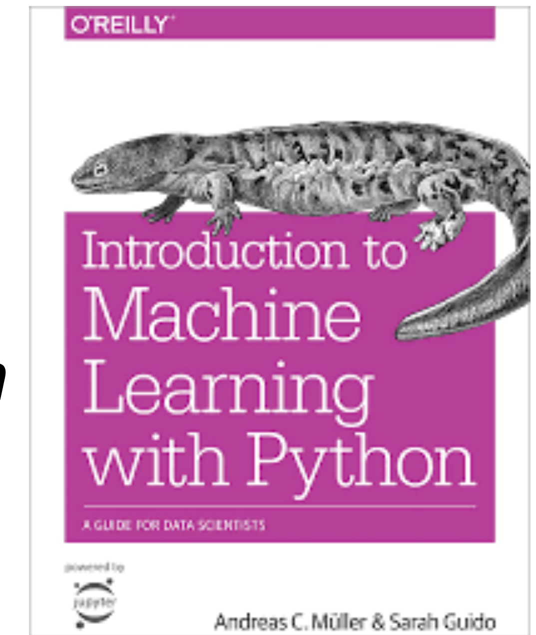


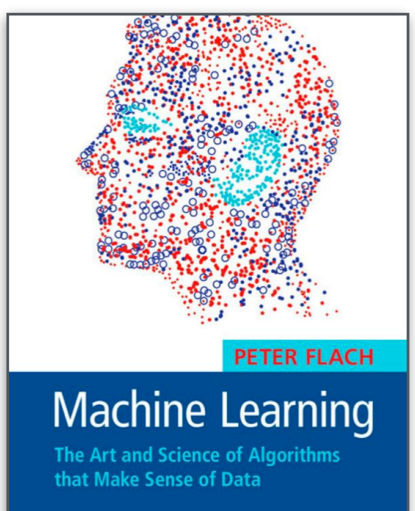
Fundamentals of Machine Learning for Predictive Data Analytics

John D. Kelleher, Brian Mac Namee, Aoife D'Arcy

Introduction to ML with Python

Andreas Muller & Sarah Guido





Machine Learning: The Art and Science of Algorithms that Make Sense of Data

Peter Flach

Machine Learning
McGraw-Hill

Tom M. Mitchell