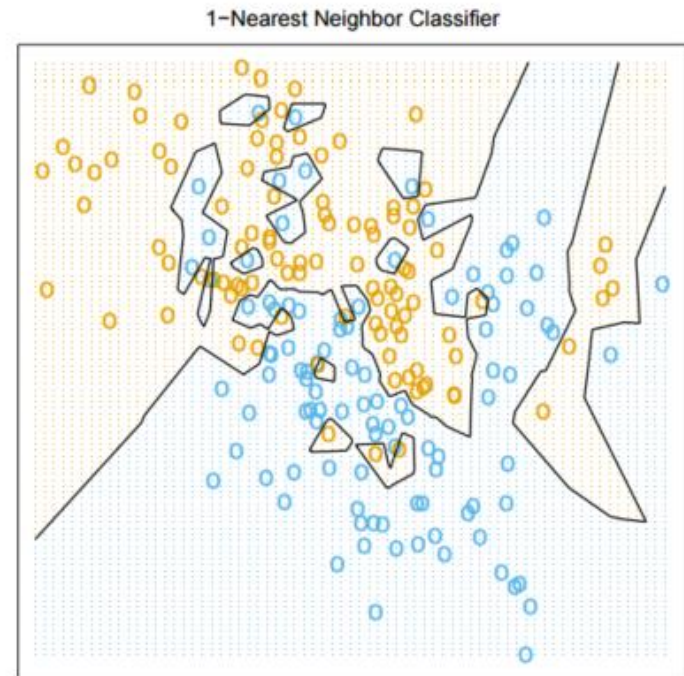


Nearest Neighbour Classifiers



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ESLII, Friedman, Hastie and Tibshirani

SML310: Projects in Data Science, Fall 2019

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The Task: Supervised Learning

• Given a set of labelled examples (the *training set*), determine/predict the labels of a set of unlabelled examples (the *test set*)

• Training set:

Train Example 1: $(x_1^{(1)}, x_2^{(1)}, \dots, x_m^{(1)})$ Label: $y^{(1)}$

Train Example 2: $(x_1^{(2)}, x_2^{(2)}, \dots, x_m^{(2)})$ Label: $y^{(2)}$

...

Train Example N: $(x_1^{(N)}, x_2^{(N)}, \dots, x_m^{(N)})$ Label: $y^{(N)}$

• Test set:

Test Example 1: $(x_1^{(N+1)}, x_2^{(N+1)}, \dots, x_m^{(N+1)})$ Label: $y^{(N+1)}$

Test Example 2: $(x_1^{(N+2)}, x_2^{(N+2)}, \dots, x_m^{(N+2)})$ Label: $y^{(N+2)}$

...

Test Example K: $(x_1^{(N+K)}, x_2^{(N+K)}, \dots, x_m^{(N+K)})$ Label: $y^{(N+K)}$

Task: Face Recognition

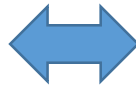
- Training set: photos of musicians with names (“labels”)
- Test set: photos of musicians whose name we want to figure out
 - Note: generally, we *will* know the labels for the test set, but we pretend we don’t. We can then predict the labels using our algorithm and compare the answers the algorithm gives to the correct answers to figure out the performance of our algorithm.
- An estimate for the performance of the algorithm on *new data*: the proportion of the examples in the test set that were correctly classified

What Justin Bieber Looks like to a Computer

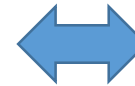
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114 112 171 234 212 108 26 36 27 32 35 27 41 28 28 30 23 51 80 101 111 114 116 115 122 122 124 126 128 127 130 136 198 219 172 50 31 99 92 127 123 131 152 150 176 131
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Images ↔ Vectors

Dark Gray	Dark Gray	White	White
Dark Gray	Dark Gray	White	White
Dark Gray	Dark Gray	White	White
Light Gray	Light Gray	Light Gray	Light Gray



60	60	255	255
60	60	255	255
60	60	255	255
128	128	128	128



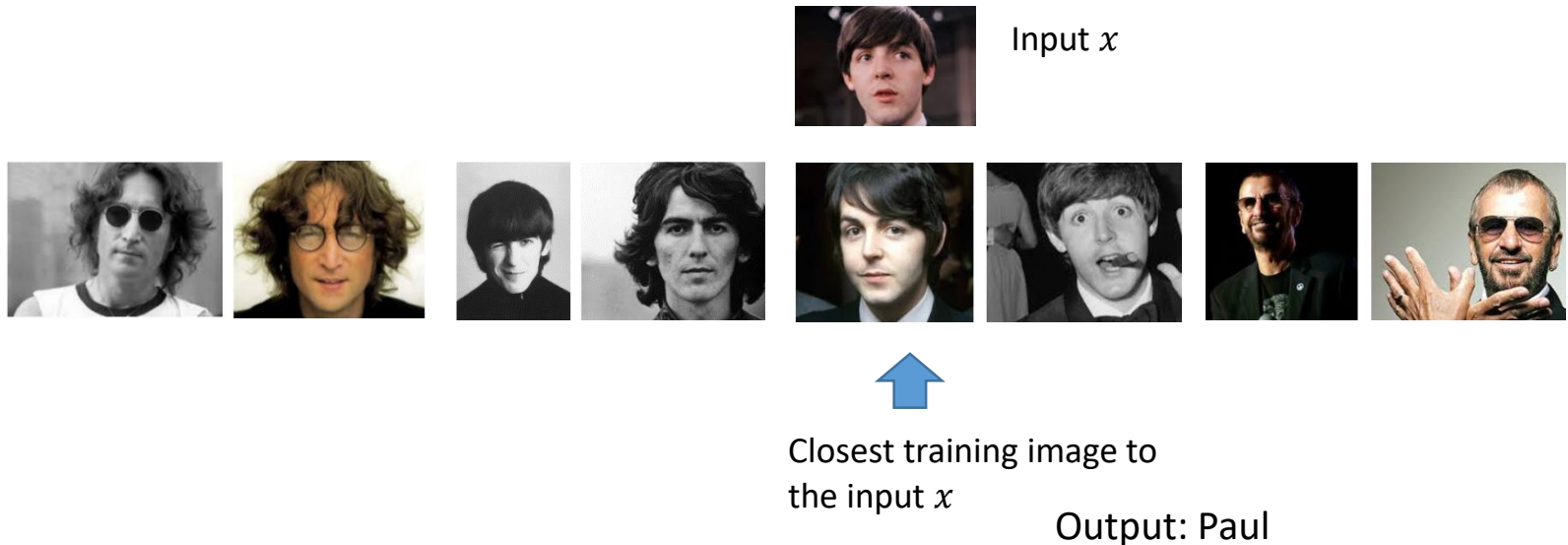
60
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60
255
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128
128
128
128

The Face Recognition Task

- Training set:
 - $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \dots, (x^{(N)}, y^{(N)})\}$
 - $x^{(i)}$ is a k -dimensional vector consisting of the intensities of all the pixels in the i -th photo (20×20 photo $\rightarrow x^{(i)}$ is 400-dimensional)
 - $y^{(i)}$ is the *label* (i.e., name)
- Test phase:
 - We have an input vector x , and want to assign a label y to it
 - Whose photo is it?

Face Recognition using 1-Nearest Neighbors (1NN)

- Training set: $\{(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \dots, (x^{(N)}, y^{(N)})\}$
- Input: x
- 1-Nearest Neighbor algorithm:
 - Find the training photo/vector $x^{(i)}$ that's as "close" as possible to x , and output the label $y^{(i)}$



Are the two images a and b close?

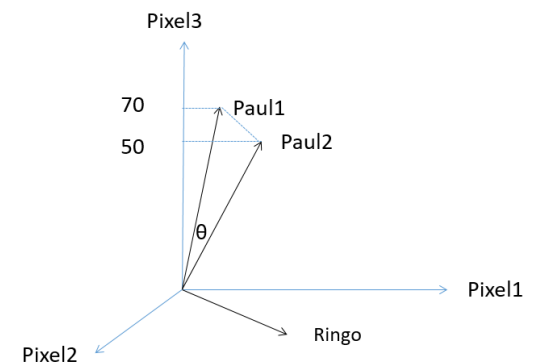
- Key idea: think of the images as *vectors*
 - Reminder: to turn an image into a vector, simply “flatten” all the pixels into a 1D vector
- Is the distance between the endpoints of vectors a and b small?

$$|a - b| = \sqrt{\sum_i (a_i - b_i)^2} \text{ small}$$

- Is the cosine of the angle between the vectors a and b large?

$$\cos \theta_{ab} = \frac{a \cdot b}{|a||b|} = \frac{\sum_i a_i b_i}{\sqrt{\sum_i a_i^2} \sqrt{\sum_i b_i^2}} \text{ large}$$

By the law of cosines



k-Nearest Neighbour Classification

- For an example x
 - Find the k closest examples (neighbours) to x in the training set
 - Output the plurality label for the k closest examples

- Can use various distance functions:

- Euclidian (L2): $\text{dist}(a, b) = \sqrt{\sum_i (a_i - b_i)^2}$ (default)

- L-infinity: $\text{dist}(a, b) = \max_i |a_i - b_i|$

- L-zero: $\text{dist}(a, b) = \#\{a_i \neq b_i\}$

- Negative cosine: $\text{dist}(a, b) = -\frac{a \cdot b}{|a||b|}$

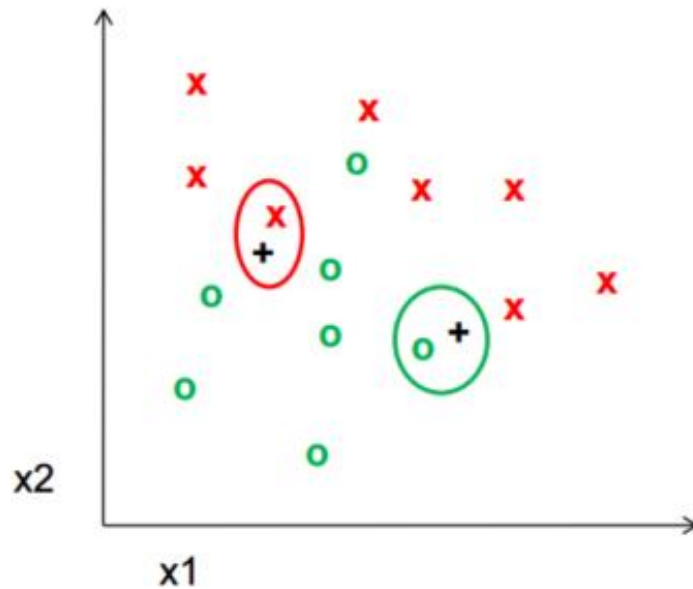
1-nearest neighbour

Task: classify the test set of “+”

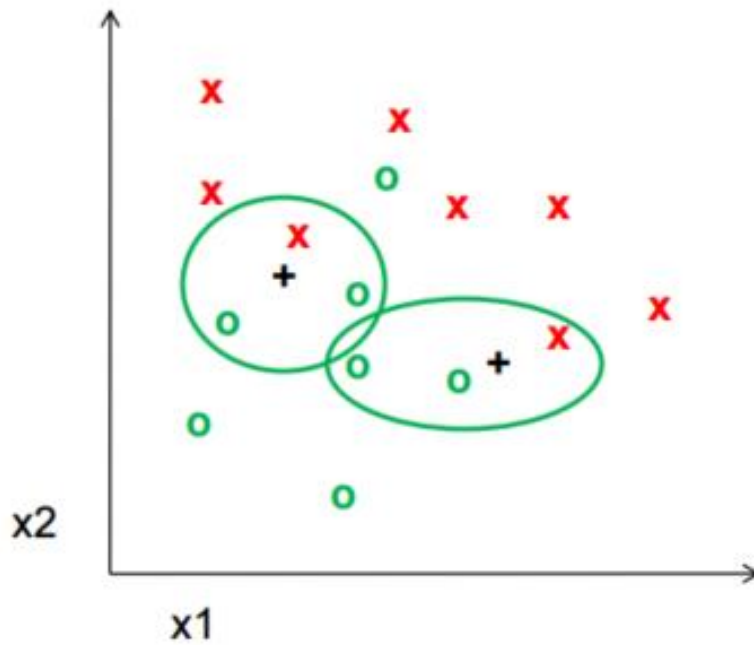
The labels for the training set are GREEN and RED

The examples are 2-dimensional

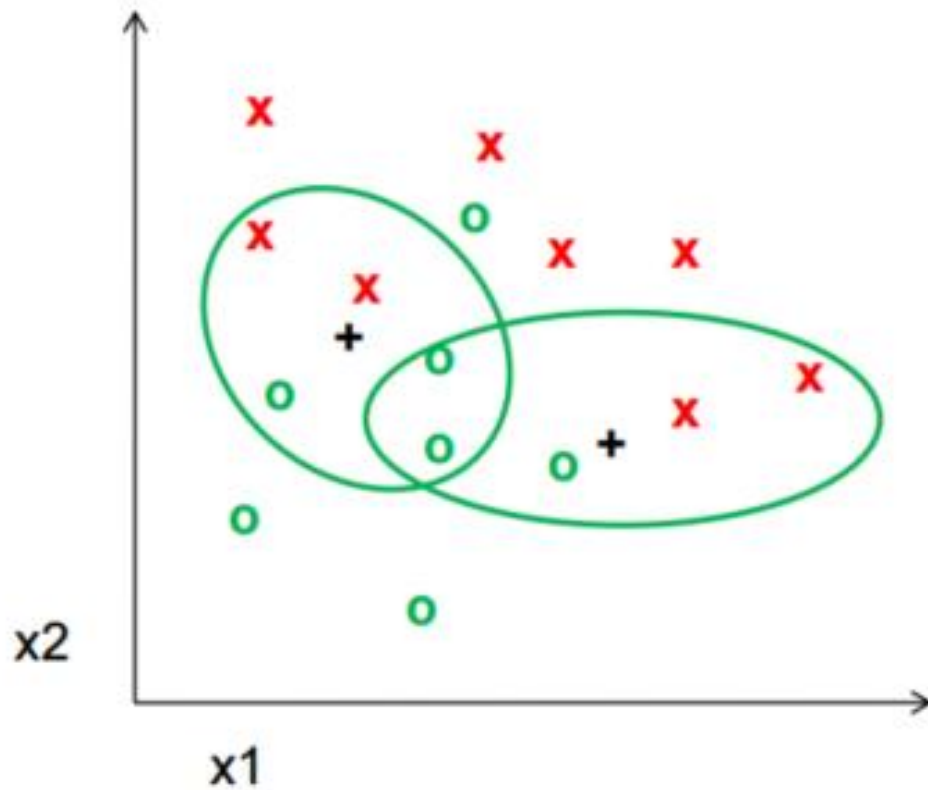
Use L2/Euclidean distance



3-nearest neighbour



5-nearest neighbour

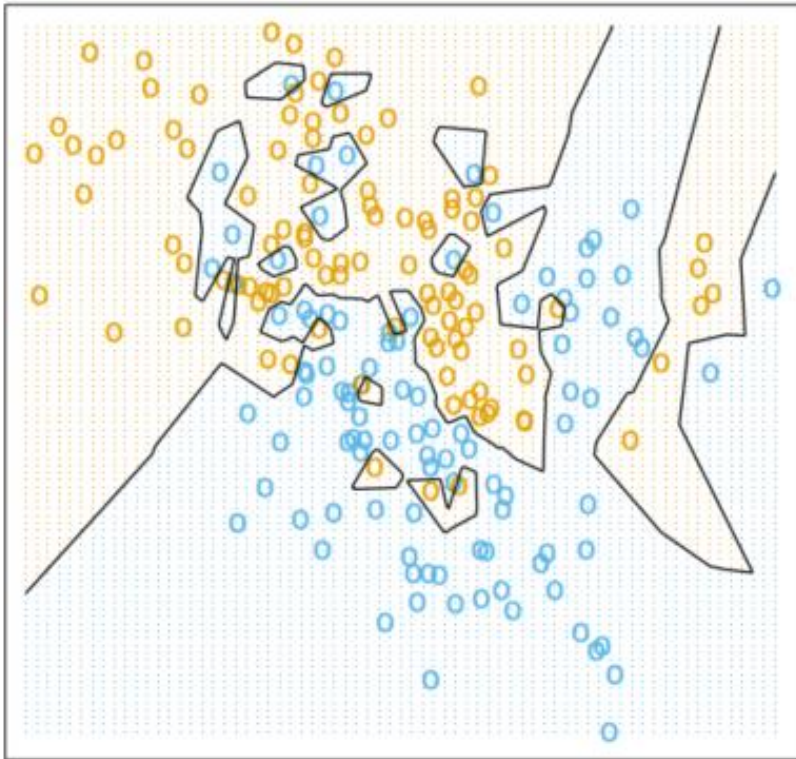


How do we determine K?

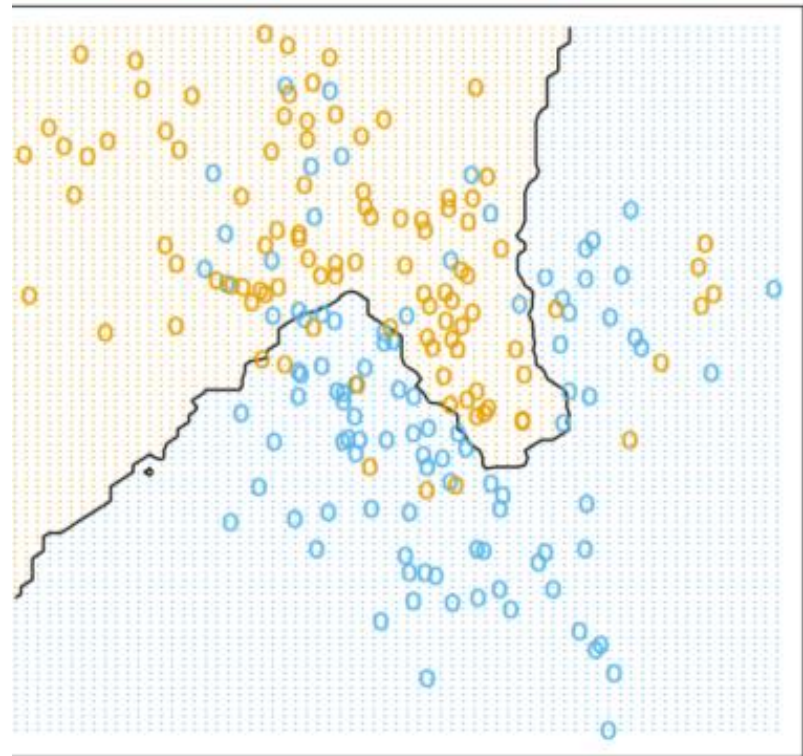
- Try different values, and see which works best on the test set?
 - Could do that, but then we are selecting the best K for our particular test set. This means that the performance on our test set is now an overestimate of how well we'd do on *new data*
- Solution: set aside a *validation set* (which is separate from both the training and the test set), and select the K for the best performance on the validation set, but report the results on the test set
 - Generally, the performance on the validation set will be better than on the test set
 - What about the performance on the *training set*?

What does the best K say about the data?

1-Nearest Neighbor Classifier



15-Nearest Neighbor Classifier



Large k : relatively simple boundary, no small "islands" in the data. Small changes in x do not generally change the label

Small k : a complex boundary between the labels. Small changes in x often change the labels

Why not let K be very small?

- Great for the performance on the training set!
 - Perfect performance guaranteed for $k = 1$
- If the test data does not look exactly like the training data, the performance on the test data will be worse for k that is too small
 - The training data could be noisy (e.g., in the orange region, data points are sometimes blue with probability 5%, randomly)
 - This is an example of *overfitting* – building a classifier that works well on the training set, but does not generalize well to the test set

Why not let K be very large?

Distance Functions

- For images, why might the cosine distance make sense?
- For images, why might the Euclidean distance make sense?