Nearest Neighbour Classifiers

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CSC411: Machine Learning and Data Mining, Winter 2017
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The Task

• 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: \((x_1^{(1)}, x_2^{(1)}, \ldots, x_m^{(1)})\) Label: \(y^{(1)}\)
    Train Example 2: \((x_1^{(2)}, x_2^{(2)}, \ldots, x_m^{(2)})\) Label: \(y^{(2)}\)
    ...
    Train Example N: \((x_1^{(N)}, x_2^{(N)}, \ldots, x_m^{(N)})\) Label: \(y^{(N)}\)

  • Test set:
    Test Example 1: \((x_1^{(N+1)}, x_2^{(N+1)}, \ldots, x_m^{(N+1)})\) Label: \(y^{(N+1)}\)
    Test Example 2: \((x_1^{(N+2)}, x_2^{(N+2)}, \ldots, x_m^{(N+2)})\) Label: \(y^{(N+2)}\)
    ...
    Test Example K: \((x_1^{(N+K)}, x_2^{(N+K)}, \ldots, x_m^{(N+K)})\) Label: \(y^{(N+K)}\)
Face Recognition Example

• 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
Nearest Neighbour Classification

• Task: classify the test example
  \[ x = (x_1, x_2, \ldots, x_m) \]
• Idea: find the \( k \) nearest neighbours of \( x \) in the training set, and output the majority label
• The distance between \( x^{(1)} \) and \( x^{(2)} \) could be
  \[ |x^{(1)} - x^{(2)}| = \sqrt{\sum_i \left( x_i^{(1)} - x_i^{(1)} \right)^2} \] ("Euclidean/L2 distance")
  \[ \max_i |x_i^{(1)} - x_i^{(2)}| \] ("L-infinity distances")
  \[ -\frac{x^{(1)} \cdot x^{(2)}}{|x^{(1)}||x^{(2)}|} = -\cos\theta_{x^{(1)},x^{(2)}} \]
  • Minus the cosine of the angle between the vectors \( x^{(1)} \) and \( x^{(2)} \)
• By default, we use the Euclidean distance
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?

Large k: relatively simple boundary, no small “islands” in the data. Small changes in x do no 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?