DSC 255 - MACHINE LEARNING FUNDAMENTALS

CROSS-VALIDATION

SANJOY DASGUPTA, PROFESSOR



COMPUTER SCIENCE & ENGINEERING
HALICIOĞLU DATA SCIENCE INSTITUTE



K-nearest neighbor classification

Classify a point using the labels of its k-nearest neighbors among the training points.

MNIST:	K	1	3	5	7	9	11
	Test error (%)	3.09	2.94	3.13	3.10	3.43	3.34

In real life, there's no test set. How to decide which k is best?

K-nearest neighbor classification

Classify a point using the labels of its k-nearest neighbors among the training points.

In real life, there's no test set. How to decide which k is best?

1 Hold-out set:

- Let S be the training set.
- Choose a subset V ⊂ S as a validation set.
- What fraction of V is misclassified by the k-nearest neighbors in S \ V ?

K-nearest neighbor classification

Classify a point using the labels of its k-nearest neighbors among the training points.

In real life, there's no test set. How to decide which k is best?

Hold-out set:

- Let S be the training set.
- Choose a subset $V \subset S$ as a validation set.
- What fraction of V is misclassified by the k-nearest neighbors in S \ V ?

2 Leave-one-out cross-validation:

- For each point $x \in S$, find the k-nearest neighbors in $S \setminus \{x\}$.
- What fraction are misclassified?

Cross-validation

How to estimate the error of k-NN for a particular k?

10-fold cross-validation

- Divide the training set into 10 equal pieces.
- Training set (call it S): 60,000 points
- Call the pieces S_1 , S_2 , ..., S_{10} : 6,000 points each.
- For each piece S_i :
 - \triangleright Classify each point in S_i using k-NN with training set $S S_i$
 - \triangleright Let \in_i = fraction of S_i that is incorrectly classified
- Take the average of these 10 numbers:

estimated error with
$$k$$
-NN = $\frac{\epsilon_1 + \dots + \epsilon_{10}}{10}$