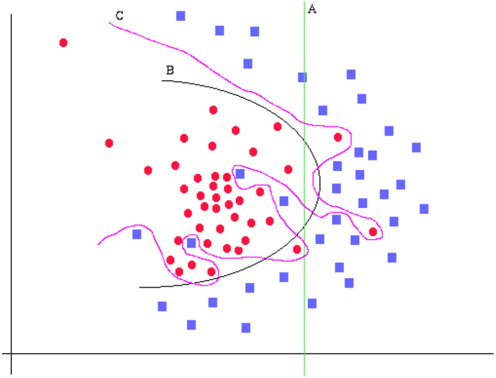
Model Selection

COMP4211

THE DEPARTMENT OF COMPUTER SCIENCE & ENGINEERING
計算機科學及工程學系

Example



which one is the best?

Training Error

given:

- target function f
- hypothesis/model h (e.g., a particular neural network)
- distribution $\mathcal{D}$ of the instances
- training set S (of size n) drawn from $\mathcal{D}$

training error

- proportion of examples in S that h misclassifies

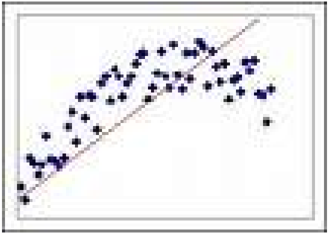
$$error_S(h) \equiv \frac{1}{n} \sum_{x \in S}^{n} \delta(f(x) \neq h(x))$$

  - $\delta(f(x) \neq h(x))$ is 1 if $f(x) \neq h(x)$, and 0 otherwise
- what we can measure

How to Select the “Best” Hypothesis?

use how many hidden units / hidden layers?

use the network that minimizes the training error?



what we want to obtain is a model with low testing error

Testing Error

testing error

- probability that h will misclassify an instance drawn at random according to $\mathcal{D}$

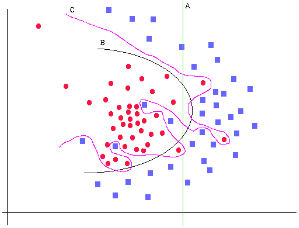
$$error_{\mathcal{D}}(h) \equiv Pr_{x \in \mathcal{D}}[f(x) \neq h(x)]$$

typically, use a test set to estimate the testing error

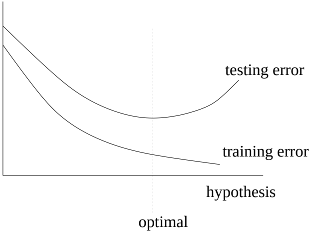
$$error_{test}(h) \equiv \frac{1}{|testSet|} \sum_{x \in testSet}^{n} \delta(f(x) \neq h(x))$$

- the test patterns should be drawn independently from the training patterns
- the testing data should not be used in any way to learn the hypothesis

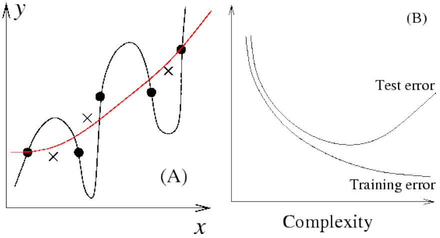
How to Select the "Best" Hypothesis?...



- intuitively, the model should be not too simple (too few hidden units) nor too complex (too many hidden units)



Overfitting

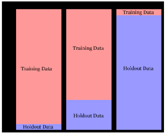


hypothesis $h \in H$ overfits the training data if there is an alternative hypothesis $h' \in H$ such that

- h has smaller error than h' over the training examples, but
- h has a larger error than h' over the entire distribution of instances

How to Select the "Best" Hypothesis?...

- the test data should not be used!
- partition the available (training) data into two sets
  - training set: used to form the learned hypothesis
  - validation set: used to estimate the accuracy of this hypothesis over subsequent data



- once the evaluation is complete, all the data can be used to train the final hypothesis (optional)
- generally,
  - the larger the training set, the better the hypothesis
  - the larger the validation set, the more accurate is error estimation

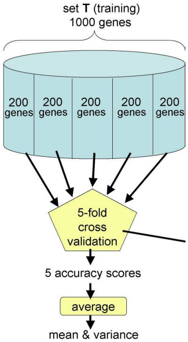
Example

withhold one-third of the available examples for the validation set, using the other two-thirds for training

How to make Error Estimation more reliable?

repeat the process with different subsamples

k-fold Cross-validation



1. the m available examples are partitioned into k disjoint subsets, each of size m/k
2. the learning procedure is then run k times, each time
   - using one of these subsets as the validation set, and
   - combining the other subsets for the training set
3. average the performance on the validation sets over the k runs

k-fold Cross-validation...

each example is used

- in the validation set once, and
- in the training set for the other $k - 1$ folds

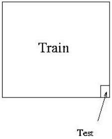
a high proportion of the available data $(1 - \frac{1}{k})$ is used for training, while making use of all the data in computing the error

how many times do we need to perform training?

- e.g., $k \sim 10$

leave-one-out cross-validation ($k = m$)

- train on $m - 1$ examples and validate on 1 example
- useful for small data sets



k-fold Stratified Cross-validation

another problem:

- examples in the training set of each fold may not be representative
- e.g., all the examples of a certain class are missing
- $\rightarrow$ the classifier cannot learn to predict this class

how to ensure that each class is represented with approximately equal proportions in both the training and validation sets?

- partition the m examples into k folds such that each class is uniformly distributed among the k folds
- the class distribution in each fold is similar to that in the original data set
- e.g., 10-fold (stratified) cross-validation