CS760: Machine Learning Exam Review

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1 Topics

1. Decision Tree Learning
2. Instance-based Learning, K-Nearest Neighbor
3. ML Methodology
4. Linear and Logistic Regression
5. Bayesian Network Learning
6. Neural Networks
7. Deep Neural Networks
8. Learning Theory
9. Support Vector Machines

2 Decision Tree Learning

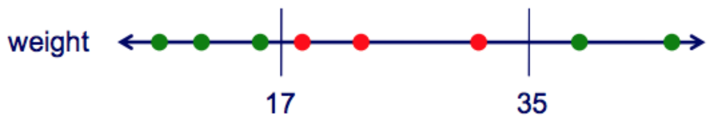
2.1 Goals

- DT representation
- Standard approach
- Occam's razor
- Entropy / IG
- Types of DT Splits
- Test sets / unbiases accuracy estimates
- Overfitting
- Pruning
- Tuning (validation) sets

- Regression trees
- m-of-splits
- Lookahead

2.2 Notes

- Splits on nominal features have one branch per value
- Splits on continuous features use a threshold
- Candidate Splits on continuous features
  - sorts the values
  - split thresholds in intervals between different classes



- The simplest tree with accurate classification will be the best on unseen data
- **Occams razor**: Simpler models are better
- IG Limitation: biased towards tests with many outcomes
- Avoiding overfitting:
  1. Early stopping: stop if further splitting not justified by statistical test (ID3)
  2. Post pruning: grow a large tree, prune back some nodes, more robust
- Pruning: grow a complete tree, remove the nodes that most improves tuning-set accuracy until further pruning is harmful
- Regression Trees: CART does least squares regression
- Lookahead
  1. myopia: an important feature seems to not be informative until use in conjunction with other features
  2. Replaces the InfoGain step with an EvaluateSplit step
  3. Choose the best info gain that would result from a 2-level subtree

2.3 Relevant Equations

$$H(Y) = -\sum_{y \in \text{values}(Y)} P(y) \log_2 P(y)$$

Entropy:

$$H(Y \mid X) = \sum_{x \in \text{values}(X)} P(X = x)\, H(Y \mid X = x)$$

where

$$H(Y \mid X = x) = -\sum_{y \in \text{values}(Y)} P(Y = y \mid X = x)\, \log_2 P(Y = y \mid X = x)$$

$$\text{InfoGain}(D,S) = H_D(Y) - H_D(Y \mid S)$$

D indicates that we're calculating probabilities using the specific sample *D*

Information Gain:

$$= \sum_{L \in \text{leaves}} \sum_{i \in L} (y_i - \hat{y}_i)^2$$

Least Squares Regression in CART

3 Instance-Based Learning

3.1 Goals

1. k-NN classification
2. k-NN regression
3. edited nearest neighbor
4. k-d trees for nearest neighbor identification
5. locally weighted regression
6. inductive bias

3.2 Notes

1. Determining similarity/distance

(a) Hamming distance: count number of features for which 2 instances differ (discrete only)

(b) Euclidean distance: $d(x^{(i)}, x^{(j)}) = \sqrt{\sum_f (x_f^{(i)} - x_f^{(j)})^2}$

(c) Manhattan distance: $d(x^{(i)}, x^{(j)}) = \sum_f |x_f^{(i)} - x_f^{(j)}|$

(d) If a mix of continuous/discrete features, refer to equations

2. Normalization

   - Determine mean and stddev for feature x_i

$$\mu_i = \frac{1}{|D|}\sum_{d=1}^{|D|} x_i^{(d)} \qquad \sigma_i = \sqrt{\frac{1}{|D|}\sum_{d=1}^{|D|}\left(x_i^{(d)} - \mu_i\right)^2}$$

   - Standard each feature

$$\hat{x}_i^{(d)} = \frac{x_i^{(d)} - \mu_i}{\sigma_i}$$

$$\hat{y} \leftarrow \frac{1}{k}\sum_{i=1}^{k} y^{(i)}$$

3. k-NN Regression

4. Speeding up k-NN

   - Don't retain every training instance
   - Use smart data structure to look up nearest neighbors (ie k-d tree)

5. Edited instance-based learning
   Incremental deletion, start will all train inst in memory. If other instances provide correct classification for $(x^{(i)}, y^{(i)})$, delete it
   Incremental growth, start with empty memory. If other instances don't correctly classify $(x^{(i)}, y^{(i)})$, add it to memory

6. k-d trees

   (a) Similar to DT

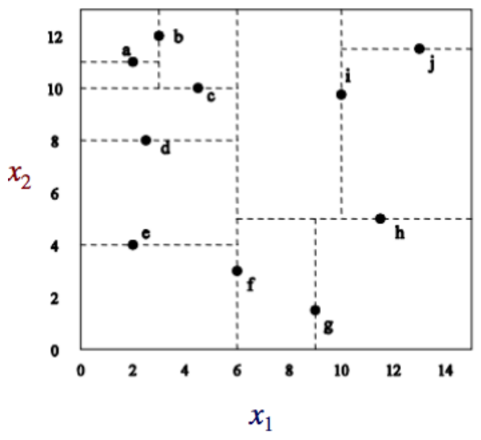
   (b) Each node stores one instance

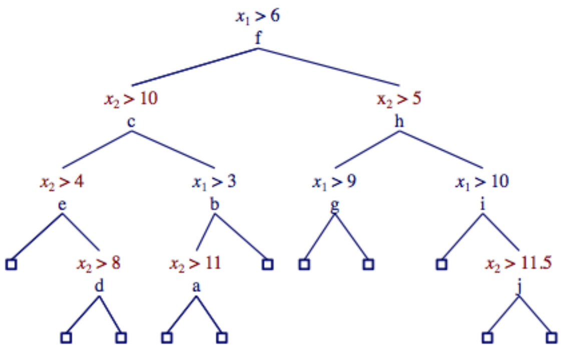
   (c) Each node splits on median value of feature with highest variance

   (d) Implemented using priority queue storing nodes considered and their lower bound on distance to query instance

   (e) k-d trees are sensitive to irrelevant features, **locally weighted regression**

Example:





7. Locally weighted regression

   prediction/learning task

   - find the weights w_i for each $x^{(q)}$ by minimizing

   $$E(\mathbf{x}^{(q)}) = \sum_{i=1}^{k}\left(f(\mathbf{x}^{(i)}) - y^{(i)}\right)^2$$

   - this is done at prediction time, specifcally for $x^{(q)}$
   - can do this using gradient descent (to be covered soon)

8. Stengths of instance-based learning

   (a) simple to implement

   (b) adapts well to online training

   (c) robust to noisy training data with k ¿ 1

   (d) good in practice

9. Limits of instance-based learning

   (a) sensitive to range of feature values

   (b) potentially sensitive to irrelevant and correlated features

   (c) can be inefficient

   (d) no explicit model

3.3 Equations

$$d(\mathbf{x}^{(i)},\mathbf{x}^{(j)}) = \sum_f \begin{cases} \left|x_f^{(i)} - x_f^{(j)}\right| & \text{if } f \text{ is continuous} \\ 1-\delta\left(x_f^{(i)},x_f^{(i)}\right) & \text{if } f \text{ is discrete} \end{cases}$$

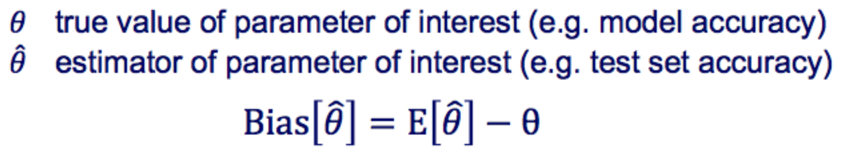
4 ML Methodology

4.1 Goals

- bias of an estimator
- test sets
- learning curves
- stratified sampling
- cross validation
- confustion matrices
- TP, FP, TN, FN
- ROC curves
- precision-recall curves
- true positive rate (TPR)
- positive predictive value (PPV)
- false positive rate (FPR)

4.2 Notes

- Bias of an estimator



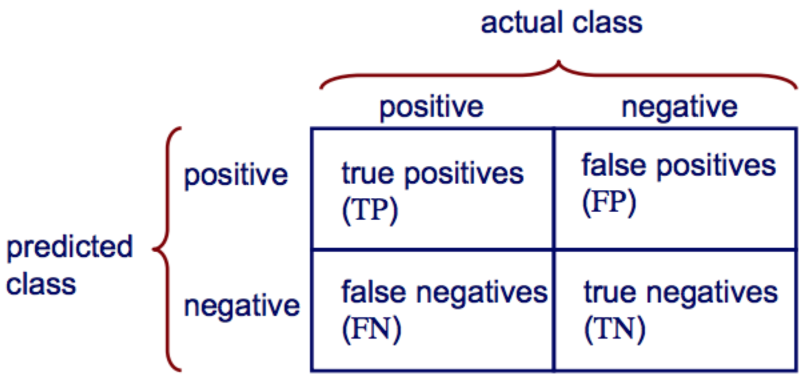
θ true value of parameter of interest (e.g. model accuracy)

$\hat{\theta}$ estimator of parameter of interest (e.g. test set accuracy)

$$\text{Bias}[\hat{\theta}] = \text{E}[\hat{\theta}] - \theta$$

- **Learning curves**: Assesses the accuracy of a learning method as a function of training-set size. Randomly select s instances from train set and train, eval on test set. Repeat n times (optional)
- **Stratified Sampling**: Ensure that class proportions are maintained in training and validation sets
- **Cross Validation**: Partition data into n subsamples, iteratively leave on sub-sample out for the test set, train on rest
  - 10-fold is common when learning is not time-consuming
  - leave-one-out: n = num instances
  - stratified cross val
  - **NOTE**: CV evaluates a learning method, not individually learned model

- Confusion Matricies help us understand what types of mistakes a learned model makes



		actual class	
		positive	negative
predicted class	positive	true positives (TP)	false positives (FP)
	negative	false negatives (FN)	true negatives (TN)

$$\text{accuracy} = \frac{TP + TN}{TP + FP + FN + TN}$$

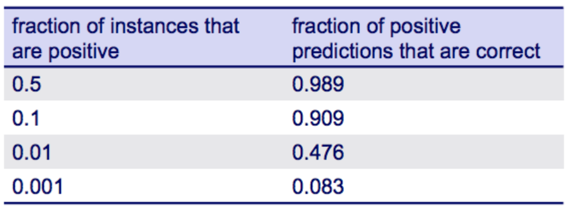
$$\text{error} = 1 - \text{accuracy} = \frac{FP + FN}{TP + FP + FN + TN}$$

- When is accuracy a bad measure?
  - there is a large class skew
  - differential misclassifaction costs (ie medical domain)
  - most interested in subset of high-confidence predictions
- Alternative accuracy metrics

$$\text{true positive rate (recall)} = \frac{TP}{\text{actual pos}} = \frac{TP}{TP + FN}$$

$$\text{false positive rate} = \frac{FP}{\text{actual neg}} = \frac{FP}{TN + FP}$$

  - **ROC curves**: TP vs FP, Order instances according to predicted positive confidence. Thresholds are where there is a pos instance on high side, neg on low side



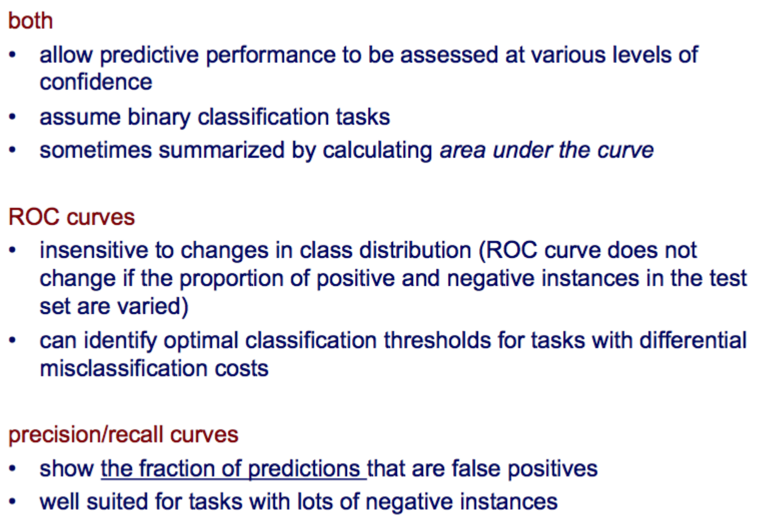
fraction of instances that are positive	fraction of positive predictions that are correct
0.5	0.989
0.1	0.909
0.01	0.476
0.001	0.083

- **Precision/recall curves**

$$\text{recall (TP rate)} = \frac{\text{TP}}{\text{actual pos}} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

$$\text{precision (positive predictive value)} = \frac{\text{TP}}{\text{predicted pos}} = \frac{\text{TP}}{\text{TP} + \text{FP}}$$

- ROC vs PR curve comparison:



both

- allow predictive performance to be assessed at various levels of confidence
- assume binary classification tasks
- sometimes summarized by calculating *area under the curve*

ROC curves

- insensitive to changes in class distribution (ROC curve does not change if the proportion of positive and negative instances in the test set are varied)
- can identify optimal classification thresholds for tasks with differential misclassification costs

precision/recall curves

- show the fraction of predictions that are false positives
- well suited for tasks with lots of negative instances

tl;dr: ROC good for varied distributions, PR good for many negative instances

4.3 Equations

5 ML Methology (pt2)

5.1 Goals

- confidence intervals for error
- pairwise t-tests for comparing learning systems
- scatter plots for comparing learning systems
- lesion studies
- model selection
- validation (tuning) sets
- internal cross validation

5.2 Notes

- Confidence intervals on error
  Given n test instances, and r = num errors:

  $$error_S(h) = \frac{r}{n}$$

  With approximately C% probability, the true error lies in the interval

  $$error_S(h) \pm z_C \sqrt{\frac{error_S(h)(1 - error_S(h))}{n}}$$

  where z_C is a constant that depends on C (e.g. for 95% confidence, z_C =1.96)

5.3 Equations