Computer Science 760 Notes
Machine Learning

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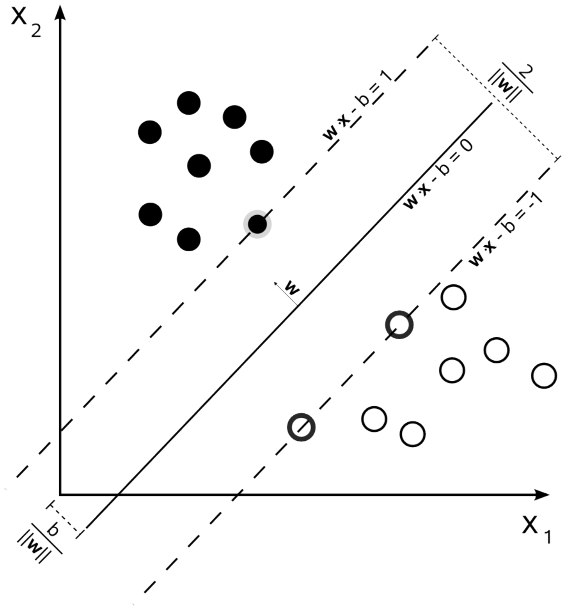
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1 Decision Tree Learning

1.1 Information Gain

Information gain is used to determine the (feature to) split
Information theory: entropy and information gain:

(i) Entropy $= H(X) = -\sum_{x \in X} P(X=x) \log_2 P(X=x)$

(ii) Conditional entropy $= H(Y|X) = -\sum_{x \in X} P(Y|X=x)$, where
$H(Y|X=x) = \sum_{y\ inY} P(Y=y|X=x) \log_2 P(Y=y|X=x)$

(iii) Mutual information (information gain) $= I(X,Y) = H(Y) - H(Y|X)$

Alternative metric: Gini coefficient, i.e. product of probabilities for each of (2) outcomes for the feature

Limitation of information gain: biased toward tests with many outcomes (i.e. features with many possible values)
C4.5 uses gain ratio: $SplitInfo(D,S) = -\sum_{k \in S} |D_k|/|D| \log_2(D_k/D)$, and $GainRatio = I(D,S)/SplitInfo(D,S)$

1.2 Decision Tree Algorithms

Overfitting: $h \in H$ overfits the training data D if there is an alternative model $h' \in H$ such that $error(h) > error(h')$ yet $error_D(h) < error_D(h)$
Avoiding overfitting in decision tree learning:

(i) Early stopping: stop if further splitting not justified by statistical test

(ii) Post-pruning: grow large tree, then prune nodes using tuning set
Iteratively eliminate nodes until further reductions reduce accuracy

Lookahead: instead of evaluating using information gain, look ahead to see what splits at the next level would be, and measure information gain at a deeper level

Continuous features: use threshold-based boolean attribute, treshold determined by sorting examples according to the featurem and generating candidate thresholds between adjacent examples with different class values
Threshold chosen from candidates based on information gain

Training examples with missing attribute values: possible strategies

(i) At node n, upon encountering a missing feature value, assign it the value most common among examples at node n, or most common among examples at the node n that also have the same class value

(ii) Assign fractional value to attribute for the example and pass fractional example to children for purposes of evaluating information gain

2 Instance-Based Learning

2.1 K-nearest Neighbor

k-nearest neighbor classification: given an instance x_q to classify, find k training-set instances that are most simimlar or x_q
Return the class value: $\hat{y} = argmax_{v \in values(Y)} \sum_{i=1}^{k} \delta(v, y_i)$
Various determinations of distance:

(i) Hamming distance: number of features with differing values

(ii) Euclidean distance: $\delta(x_i, x_j) = \sqrt{\sum_f (x_{if} - x_{jf})^2}$

(iii) Manhattan distance: $\delta(x_i, x_j) = \sum_f (x_{if} - x_{jf})^2$

k-nearest neighbor regression: given an instance x_q, find the k nearest training-set instances and return $\sum_{i=1}^{k} \delta(v, y_i)$
Distance-weighted nearest neighbor: instances contribute to prediction according to their distance from x_q

k-nearest neighbor does almost nothing at training time, and offsets costs to classification/prediction time
Strategies to speed up k-nearest neighbor

(i) Don't retain every training instance: edited nearest neighbor
Select subset of instances that still provide accurate classifications:

  (a) Incremental deletion: delete from memory all training instances redundant to classification
  (b) Incremental growth: if training instances insufficient to classify training instance, add to memory

(ii) Use data structure to look up nearest neighbors (k-d tree)

k-d trees (A^* instance search): each node stores one instance, and splits on the median value of the feature having the highest variance
Nodes are pushed to the A^* priority queue with the value indicating the minimum possible distance to the query based on the threshold for the split

Strenghts of instance based learning: simple, efficeint training, easily adapts to on-line nearning, rubust to noisy data, etc.
Limitations: sensitive to range of feature values, senstivie to irrelevant and correlated features, inefficient classification, no insight into problem domain (i.e. lacks modeling of problem)

2.2 Linear Locally Weighted Regression

Locally weighted linear regression: $f(x) = w_0 + w_1 a_1(x) + \ ... \ + w_n a_n(x)$
Local approximations to have query point fit local training examples:

1. Minimize squared error over just k nearest neighbors:
   $E_1(x_q) = (1/2) \sum_{x \in k \text{ nearest neighbors of } x_q} (f(x) - \hat{f}(x))^2$
2. Minimize squared error over entire set of D of training examples, using decreasing function K:
   $E_2(x_q) = (1/2) \sum_{x \in D} (f(x) - \hat{f}(x))^2 K(d(x_q, x))$
3. Combination of the previous: let N be k nearest neighbors of x_q

$$\frac{1}{2} \sum_{x \in N} (f(x) - \hat{f}(x))^2 K(d(x_q, x))$$

3 Probability and Bayesian Learning

Note: for more rigourous details, see Heckerman's Bayesian Network Learning Tutorial

3.1 Probabilistic Machine Learning Concepts

Recall Bayes theorem: $P(A|B) = P(B|A)P(A)/P(B)$

Brute-force MAP learning algorithm:

(i) Given information D, for each hypothesis $h \in H$, calculate the posterior probability $P(h|D) = P(D|h)P(h)/P(D)$

(ii) Output hypothesis h_{MAP} with highest posterior probability $h_{MAP} = argmax_{h \in H} P(h|D)$

Other probabalisitic concepts in machine learning:

(i) Maximum likelihood and least-squared error hypotheses

(ii) Maximum likelihood hypotheses for predicting probabilities

(iii) Minimum description length principle

(iv) Bayes optimal classification: $argmax_{v_j \in V} \sum_{h_i \in H} P(v_j|h_i)P(h_i|D)$

(v) Gibb's Algorithm: choose hypothesis $h \in H$ at random, according to posterior probaiblity distribution over H, and use h to predict the classification of the next instance x

3.2 Bayesian networks

A Bayesian network consists of a directed acyclic graph and a set of conditional probability distributions
In the each Directed Acyclic Graph (DAG):

(i) Each node denotes a random variable

(ii) An edge from X to Y represents that X directly influences Y

(iii) Each node X contains a conditional probability distribution representing $P(X|Parents(X))$

(iv) Each variable X is independent of its non-descendants given its parents

(v) Each variable X is independent of all others given its Markov blanket

Advantages of Bayesian network representation:

(i) Captures indepdendence and conditional indpendence where they exist

(ii) Encodes the relevant portion fo the full joint distribution

(iii) Graphical representation gives insight into complexity of inference

Inference task: given values for some variables in the network (evidence) and set of query variables, compute posterior distribution over query variables
Hidden variables: neither evidence nor the query variables
Baysean networks allow for any set to be evidence and any set to be query
Inference by enumeration: consider the chain rule $P(x_1, ..., x_n) = P(x_1)P(x_2|x_1)P(x_3|x_2, x_1)...P(x_n|x_{n-1}, ..., x_1)$
Posterior probability on query variables can be found via independence, chain rule, and marginalization

Parameter learning task: given set of training instances and graph structure, infer parameter of conditional probability distributions
Strcture learning task: given set of training instances, infer graph structure (and possibly parameters of CPDs)
For parameter learning, use maximum a posteriori (MAP) estimation: e.g. m-estimates $P(X = x) = (n_x + p_x m)/(\sum_{v \in Values(X)} n_v) + m$, where p_x is prior probability of value x, m is number of virtual instances, and n_v is number of occurences of value v

3.3 Expectation Maximization

Missing data (hidden variables, values missing at random): values can be imputed using Expectation Maximization (EM)
Iterate until convergence:

(i) Expectation step: using current model, compute expectation over missing values (missing temporarily take expected values)

(ii) Maximization step: update model parameters with those that maximize probability of data (MLE or MAP)

Note that k-means unsupervised clustering is a form of expectation maximization
Expectation maximation can be hard (takes most likely value) or soft (expectation is probabiltiy distribution)

Expectation maximation for parameter learning:

(i) Expecation step: compute probability of each completion of incomplete data points, i.e. answering query over missing variables given others

(ii) Maximization step: use completed data set to update Dirchlet distributions, except counts can be fractional, update conditional probability tables

Subtelty for parameter learning: overcounting based on number of iterations required to converge to settings for missing values. After each expectation step, reset Dirichlet distributions before repeating maximization step

Problems with expectation maximization: only finds local optimum, deterministic with respect to priors

3.4 Learning Network Structure

Chow-Liu algorithm: learns tree structure that maximizes likelihood of training data

(i) Compute weight $I(X_i, X_j)$ of each possible edge (X_i, X_j)

(ii) Find maximum-weight spanning tree: use mutual information to calculate
$I(X,Y) = \sum_{x \in valuesX} \sum_{y \in valuesY} P(x,y) \log_2 P(x,y)/(P(X)P(Y))$

Prim's algorithm (given (V, E)):

(a) $V_{new} = \{v\}$ where $v \in V$ (arbitrary)
(b) $E_{new} = \{\}$
(c) Repeat until $V_{new} = V$: choose edge (u, v) in E with max weight where u is in V_{new} and v is not. Add v to V_{new} and (u, v) to E_{new}
(d) Return $(V_{new}, E_{new}$, a maximum spanning tree

Kruskal's algorithm (given (V, E)):

    (i) $E_{new} = \{\}$
    (ii) For each (u, v) in E ordered by weight (high to low):
    Pop (u, v) from E and add to E_{new} if it does not create a cycle
    (iii) Return V and E_{new}, a maximum spanning tree

(iii) Assign edge directions in maximimum-weight spanning tree
Pick a node for the root, assign edge direction

Heuristic search for structure learning: each state in search space represents Bayes net structure
Search approach requires specification of

(i) Scoring function: $score(G, D) = \sum_i score(X_i, Parents(X_i) : D)$
Thus, a network can be scored by summing terms over nodes, and changes can be efficently scored via a local search

(ii) State transition operators: adding an edge, deleting in edge, reversing an edge

(iii) Search algorithm: hill climbing or sparse candidate search

Bayesian network hill climibing search: greedy algorithm
Bayesian network sparse candidate search (given data set D, initial network B_0, parameter k):

(i) Let $i = 0$

(ii) Repeat until convergence:

    (a) Increment i
    (b) Restrict step: select for each variable X_j a set $C^i_j(|C^i_k|)$ of candidate parents
    (c) Maximize step: find network B_i maximizing score among networks where $\forall X_j, Parents(X_j) \subset C^i_j$

(iii) Return B_i

Restriction step in sparse candidate search:
Fpr the first iteration: candidate parents computed using mutual information
$I(X, Y) = \sum_{x,y} P(x, y) \log (P(x, y)/(P(x)P(y)))$
Kullback-Liebler divergence: distance measure between two distributions P and Q

$$D_{KL} = (P(X)||Q(X)) = \sum_x P(x) \log \frac{P(x)}{Q(x)}$$

KL-divergence assesses discrepancy between network's estimate $P_{net}(X, Y)$ and empirical estimate
$M(X, Y) = D_{KL}(P(X, Y)||P_{net}(X, Y))$

Algorithm for restriction step in sparse candidate (given data D, current network B_i, parameter k):

(i) For each variable X_j

    (a) Calculate $M(X_j, X_i)$ for all $X_j \neq X_i$ such that $X_l \notin Parents(X_j)$
    (b) Choose highest ranking $X_l...X_{k-s}$ where $s = |Parents(X_j)|$
    (c) Include current parents in candidate set to ensure monotonic score improvements
    $C^i_j = Parents(X_j) \cup X_l...X_{k-s}$

(ii) Return C^i_j for all X_j

Scoring function for structure learning: maxmize data probability, but penalize complexity
General approach: $argmax_{G,\theta_G} \log P(D|G, \theta_G) - f(n)|\theta_G|$
Akaike information criterion (AIC) $f(n) = 1$, Bayesian Information Criterion (BIC) $f(n) = \log(n)/2$

3.5 Naive Bayes and Tree Augmented Network

Naive Bayes assumption: all features X_i are conditionally independent given class Y
$P(X_1, ..., X_n, Y) = P(Y)\Pi_{i=1}^{n} P(X_i|Y)$
Unaugmented tree starts with edge from node Y to each feature $X_1, ..., X_n$
Learning: estimate $P(Y = y)$ for each value of Y, estimate $P(X_i = x|Y = y)$ for each X_i
Classification done using Bayes rule:

$$P(Y = y|X) = \frac{P(y)P(X|y)}{\sum\limits_{y' \in values(Y)} P(y')P(X|y')} = \frac{P(y)\prod\limits_{i=1}^{n} P(x_i|y)}{\sum\limits_{y'=values(Y)} (P(y')\prod\limits_{i=1}^{n} P(x_i|y'))}$$

Tree Augmented Network (TAN) algorithm: learns tree structure to augment edges of naive Bayes network

(i) Compute weight $I(X_i, X_j|Y)$ for each possible edge (X_i, X_j) between features

(ii) Find maximum weight spanning tree (MST) for graph over $X_l ... X_n$

(iii) Assign edge direction in MST

(iv) Construct a TAN model by adding node for Y and an edge for Y to each X_i

4 Machine Learning Methdology

4.1 Partitioning of Data

Evaluation of learning models: given instance set X and probability distribution D defining the probaiblity of encountering an $x \in X$, learner must learn target concept (function) $f \in H$
Evaluation methdology seeks to answer two questions: what is the best accuracy for a hypothesis h, learned from n instances, applied to future instances drawn according to D, and what is the probably error in this accuracy estimate

Distinction between sample error and true error:

(i) Sample error: error of h with respect ot target function f and data sample S
$error_S(h) = (1/n) \sum_{x \in S} \delta(f(x), h(x))$, where $\delta(a, b) = 1$ if $a \neq b$, 0 otherwise

(ii) True error: $error_D(h) = Pr_{x \in D}[f(x) \neq h(x)]$

Limitations of singular training/test partitions:

(i) Not enough data for sufficiently large training and test sets

(ii) Single training set does not show how sensitive accuracy is to particular training sample

Random resampling: repeatedly partitioning data into training and test sets
Stratified sampling: statify instances by class and select (i.e. maintain class proportions)
Cross validation: partition data into n subsamples. Iteratively test on one subset, train on rest
Leave-one-out cross validation: n is the number of instances

4.2 Performance Evaluation

Receiver Operating Characteristic (ROC) curve: true positive-rate vs false positive-rate as threshold as confidence of an instance being positive is varied
Algorithm for creating an ROC curve:

(i) Sort test-set prediction according to confidence that each instance is positive

(ii) Step through sorted list from high to low confidence

    (a) Locate threshold between instances with opposite classes
    (b) Compute TPR, FPR for instances above threshold
    (c) Output (FPR, TPR) coordinate

Points plotted on ROC curve can be interpolated to form convex hull
Having a high TPR or low FPR does not indicate accuracy in unbalanced data sets

Alternative accuracy metric: recall and precision

(i) Recall (TP rate) = TP/(actual positives) = TP/(TP + FN)

(ii) Precision = TP/(predicted positives) = TP/(TP + FP)

Precision/recall curve: plots prevision vs. recall as threshold as confidence of an instance being positive is varied

Single ROC/PR curve with cross-validation: multiple approaches

(i) Assume confidence values comparable across folds
Pool predicitons from all test sets and plot curve from pooled predictions

(ii) Plot individual curves for all test sets, viewing each as function
Plot average curve for set of functions

ROC and PR curves allow predictive performance to be assessed at various levels of confidence, assume binary classification, and can be summarized by the integral
ROC curves: insensitive to class distribution changes, can identify optimal classification thresholds for tasks with differential misclassification costs
PR curves: show fraction of predictions that are false positives, suited for tasks with many negative instances

4.3 Confidence Intervals and Learning Tasks

Avoiding pitfalls: questions when applying learning tasks

(i) Held-aside test data should be representative of collecting new data

(ii) Folds of cross validation should only use training data for the fold
At no point in preprocessing should test case labels be accessed

(iii) Repeated modificiations of learning algorithm or preprocessing could lead to overfitting

Confidence intervals on error: suppose we have learned model h, test set S containing n instances drawn independently of each other and independent of h, with $n \geq 30$, and h makes r errors over the n instances
Estimate of error is $error_S(h) = r/n$
With approximately N probability, the true error is in the interval

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

where z_N is a constant that depends on N, e.g. $z_{0.95} = 1.96$
Confidence interval follows from normal approximation of binomial distribution
An $N\%$ confidence interval on parameter p is an interal that is expected with $N\%$ probability to contain p
In using confidence intervals, consider (central limit theorem) that a large number independent, identically distribution random variables approximately follows a normal distribution

Difference in error of two hypotheses: $\hat{d} = error_S(h_1) - error_S(h_2)$
$N\%$ confidence interval for d is:

$$\hat{d} \pm z_N \sqrt{\frac{error_{S_1}(h_1)(1 - error_{S_1}(h_1))}{n_1} + \frac{error_{S_2}(h_2)(1 - error_{S_2}(h_2))}{n_2}}$$

4.4 Comparing Learning Models and Hypotheses

Consider δs as observed values of a set of independent, identically distributed variables
Null hypothesis: the 2 learning systems have the same accuracy
Alternative hypothesis: one system is more accurate than the other
Hypothesis test:

(i) Use paired t-test to determine probability p that mean of δs would arise from null hypothesis

(ii) If p is sufficiently small (usually $p < 0.05$), reject null hypothesis

Comparing systems using a paired t-test:

(i) Calculate sample mean: $\bar{\delta} = (1/n) \sum_{i=1}^{n} \delta_i$

(ii) Calculate t statistic:

$$t = \frac{\bar{\delta}}{\sqrt{\frac{1}{n(n-1)} \sum_{i=1}^{n} (\delta_i - \bar{\delta})^2}}$$

(iii) Determine corresponding p-value: use t in table for t-distribution with $n - l$ degrees of freedom

t-tests compare two learning systems, tests like McNemar's χ^2 test compares two learned models

Scatter plots for pairwise method comparison: can compare thwo methods A and B by plotting $(Aperf., Bperf.)$ across numerous data sets
Lesion studies: determine relevant contributions to learning system performance by removing (lesioning) components

5 Computational Learning Theory

5.1 PAC Learning

Computational learning theory concerns itself with:

(i) Sample complexity: how many training examples needed to converge on hypothesis

(ii) Computational complexity: how much computational effort needed for learner to converge

(iii) Mistake bound: how many misclassifications before learner converges on hypothesis

Learning setting composed of:

(i) Set of instances X

(ii) Set of hypotheses H

(iii) Set of possible target concepts C

(iv) Unknown probability distribution D over instances

Learner is given set D of training instances $(x, c(x))$ for some target concept $c \in C$
Learning task is to output hypothesis h modeling c

True error of hypothesis: how often h is wrong on future instances drawn from D:
$error_D(h) = P_{x \in D}(c(x) \neq h(x))$
Traning error: how often h is wrong on instances in training set d
$error_D(h) = P(x \in D)(c(x) \neq h(x)) = (1/|D|) \sum_{x \in D} \delta(c(x) \neq h(x))$

Probably Approximately Correct (PAC) Learning: consider class C of possible target concepts defined over set of instances X each of length n, and a learner L using hypothesis space H

Formal definition of PAC Learnable:
C is PAC learnable by L if for all $c \in C$, distributions D over C, ε and δ such that $0 < \varepsilon, \delta < 0.5$:
Learner L will, with probability greater than $(1 - \delta)$, output hypothesis $h \in H$ such that $error_D(h) \leq \varepsilon$, in time polynomial to $1/\varepsilon, 1/\delta, n, size(c)$

Suppose hypotheses consistent with m training instances
PAC learnability determined by whether:

(i) m grows polynomially in the relevant parameters

(ii) Processing time per training example is polynomial

Consistency with respect to training example set $D = \{(x_1, c(x_1), ..., (x_m, c(x_m)))\}$, and hypothesis h

$$consistent(h, D) = \forall((x, c(x)) \in D)h(x) = c(x)$$

Version space: $VS_{H,D} = \{h \in H | consistent(h, D)\}$
Version space $VS_{H,D}$ is ε-exhausted with repsect to concept c and data set D if:
$(\forall h \in VS_{H,D})error_D(h) < \varepsilon$

The probability that VS_{HD} is not ε-exhausted is no greater than $|H|e^{-\varepsilon m}$
Proof: probability that some hypothesis with error greater than ε is consistent with m training instance is $(1-\varepsilon)^m$, there are at most $|H|$ such hypotheses, and since $(1-\varepsilon) \geq e^{-\varepsilon}$ when $0 \leq \varepsilon \leq 1$, the bound is $|H|e^{-\varepsilon m}$

The probability must be reduced below δ: $|H|e^{-\varepsilon m} \geq \delta$
Solving for m yields the number of examples needed for PAC learnability:

$$m \geq \frac{1}{\varepsilon}\left(\ln|H| + \ln\frac{1}{\delta}\right)$$

5.2 Hypothesis Spaces

Agnostic learning setting: don't assume $c \in H$
Learner returns hypothesis h that makes fewest errors in training
For training set error to be less than $error_D(h) + \varepsilon$, m examples sufficient, where

$$m \geq \frac{1}{2\varepsilon^2}\left(\ln|H| + \ln\frac{1}{\delta}\right)$$

If H is infinite, for measure of hypothesis space complexity, use in place of $|H|$ the largest subset of X for which H can guarantee zero training error regardless of target function

A set of instances D is shattered by a hypothesis space H if and only if for every dichotomy of D, there is a hypothesis in H consistent with the dichotomy
The VC dimension of H defined over instance space X is the size of the largest finite subset of X that is shattered by H

A concept class is PAC learnable if it has finite VC dimension
The VC dimension for finite H: $VC - dim(H) \leq \log_2|H|$
Proof: suppose $VC - dim(H) = d$, and for d instances

(i) There are at most 2^d different possible labelings

(ii) H must represent at most 2^d hypotheses, so $2^d \leq |H|$

(iii) Thus $d \leq \log_2|H|$, so $VC - dim(H) \leq \log_2|H|$

Using $VC - dim(H)$ as a measure of complexity of H, the bound can be defined as

$$m \geq \frac{1}{\varepsilon}\left(4\log_2\frac{2}{\delta} + 8VC - dim(H)\log_2\frac{13}{\varepsilon}\right)$$

Lower bound on sample complexity: given target concept C

$$m < max\left[\frac{1}{\varepsilon}\log|\frac{1}{\delta}|, \frac{VC - dim(C) - 1}{32\varepsilon}\right]$$

5.3 Mistake Bound

Learning setting (i.e. on-line learning setting): for $t = 1, 2, ...$

(i) Learner receives instance x_t

(ii) Learner predicts $h(x_t)$

(iii) Learner receives label $c(x_t)$ and updates model h

Mistake bound model addresses how many mistakes will be made before the target concept is learned

Mistake bound model analysis of halving algorithm
Halving algorithm is as follows:

```
(i) $VS_1 = H$
(ii) For $t = 1$ to $T$:
    (a) Given training instance $(x_t, c(x_t))$, $h'(x_t) = MajorityVote(VS_t, x_t)$
    (b) Eliminate all wrong $h$ from version space (at least half)
        $VS_{t+1} = \{h \in VS_t | h(x_t) = c(x_t)\}$
(iii) Return $VS_{t+1}$
```

Maximum number of mistakes is $M_{Halving}(C) = \lfloor \log_2 |H| \rfloor$

Optimal mistake bounds: suppose C is an arbitrary nonempty concept class
An optimal mistake bound is defined as $Opt(C) = min_{A \in \text{Learning Algorithms}} M_A(C)$
$M_{Opt}(C)$ is defined as the number of mistakes made given:

1. The hardest target concept to learn
2. The hardest training sequence and distribution
3. Using the best algorithm to determine the concept

Optimal mistake bound is $VC - dim(C) \leq M_{Opt}(C) \leq M_{Halving}(C) \leq log_2(|C|)$
In short $M_{Opt}(C) \geq VC - dim(C)$, the mistake bound is no lower than the concept's VC-dimension

Mistake bound model analysis of weighted majority algorithm
Weighted majority algorithm is as follows: given predictors $A = \{a_1, ..., a_n\}$, learning rate $0 \leq \beta < 1$

```
(i) For all $i$, initialize $w_i = 1$
(ii) For each training instance $(x, c(x))$:
    (a) Initialize $q_0$ and $q_0$ to 0
    (b) For each predictor $a_i$: $q_{a_i(x)} = q_{a_i(x)} + w_i$
    (c) If $q_1 > q_0$ then $h(x) = 1$, else if $q_0 > q_1$ then $h(x) = 0$, else $h(x) = random(0, 1)$
    (d) For each predictor $a_i$: if $a_i(x) \neq c(x)$ then $w_i = \beta w_i$
```

If k is minimum number of mistakes made by the best predictor in A on training set D, then maximum number of mistakes for $\beta = 1/2$ is $2.4(k + log_2 n)$

6 Ensemble Methods

6.1 Ensembles and Bagging

Ensemble: set of learned models, individual decisions combined to predict for new instances
Ensemble accuracy is built on two conditions:

(i) Errors made by individual predictors are (at least somewhat) uncorrelated

(ii) Predictor error rates are better than guessing

Ensembles overcome a few problems with single hypotheses:

(i) Statistical problem: hypothesis space is too large for amount of available training data

(ii) Computational problem: learning algorithm cannot guarantee finding the best hypothesis in space

(iii) Representational problem: hypothesis space does not contain good approximation to true concept

Classifier error can't be completely uncorrelated, but diversity in classifiers can be improved by:

(i) Choosing a variety of learning algorithms

(ii) Choosing a variety of settings for learning algorithms

(iii) Choosing different subsamples of the training set (bagging)

(iv) Using different probability distributions over training instances (boosting)

(v) Choosing different features and subsamples (random forests)

Bagging (Bootstrap aggregation):

(i) Learning: given learner L, training set $D = \{(x_1, y_1), ..., (x_m, y_m)\}$
For $i = 1$ to T: h_i is model learned using L on m randomly drawn instances with replacement from D

(ii) Classification: given test instance x, predict y to be plurality vote of $h_1(x), ..., h_T(x)$

(iii) Regression: given test instance x, predict y to be mean of $h_1(x), ..., h_T(x)$

Bootstrap replicates: sampled training set, each containing m instances
Bagging works best with unstable learning methods (i.e. small changes in D result in large changes in learned models)

6.2 Adaptive Boosting

Weak PAC learning algorithm: cannot PAC learn for arbitrary ε or δ, though hypotheses slightly better than random geussing
Boosting: uses weak PAC learner L as subroutine to create strong PAC learner for the same concept class

Adaptive Boosting (AdaBoost): given learner L, number of stages T, training set $D = \{(x_1, y_1), ..., (x_m, y_m)\}$

(i) Initialize instance weights: $w_1(i) = 1/m$ for all i

(ii) For $t = 1$ to T

   (a) Normalize weights: For all i: $p_t(i) = w_t(i)/(\sum_j w_t(j))$

(b) h_t is model learned using L on D and p_t

(c) Calculate weighted error: $\varepsilon_t = \sum_i p_t(i)(1 - \delta(h_t(x_i), y_i))$

(d) If $\varepsilon_t > 0.5$: $T = t - 1$, break

(e) $\beta_t = \varepsilon_t/(1 - \varepsilon_t)$

(f) For all i where $h_t(x_i) = y_i$
Downweight correct examples: $w_{t+1}(i) = w_t(i)\beta_t$

Return: $h(x) = argmax_y \sum_{t=1}^{T} \log(1/\beta_t)\delta(h_t(x), y)$

AdaBoost calls base learner L with probability distribution p_t specified by weights on instances
Implementation methods:

(i) Adapt L to learn from weighted instances

(ii) Sample large ($>> m$) unweighted set of instances according to p_t

6.3 Random Forests and Multi-Class problems

Random Forests: set of randomized decision trees, i.e. training sets drawn as in bagging
To select split at node: randomly select (without replacement) f feature splits from F (where $f << |F|$), choosing the best feature split from among those in R, no pruning

Consider a learning task with $k > 2$ classes:
Some learning methods can use one model to predict k classes
Alternative approach: learn 1 class vs the rest

Error correcting output codes (ECOC): each class represented by multi-bit code word.
Classifer is function for each bit
ECOC ensemble: each class represented by codeword $y_1y_2...y_n$, where y_i is predicted by ith classifier
To classify instance x using ECOC ensemble, T classifiers

(i) Form vector $h(x) = (h_1(x), ..., h_T(x))$, where $h_i(x)$ is prediction of model for ith bit

(ii) Find codeword c with smallest hamming distance from $h(x)$

(iii) Predict the class associated with c

ECOC should satisfy two properties:

1. Row separation: each codeword well separated in Hamming distance from every other codeword

2. Column separation: bit positions should be uncorrelated with other bit positions

7 Neural Networks and Deep Learning

7.1 Perceptrons

Perceptron: input units $x_1, ..., x_n$ and output unit o, and input weights $w_1, ...w_n$
$o = 1$ if $w_0 + \sum_{i=1}^{n} w_i x_i > 0$, 0 otherwise
Perceptron training rule:

(i) Randomly initialize weights

(ii) Iterate through training instances until convergence

  (a) Calculate output for given instance:
  $o = 1$ if $w_0 + \sum_{i=1}^{n} w_i x_i > 0$, 0 otherwise

  (b) Update each weight: $w_i = w_i + \Delta w_i$, where $\Delta w_i = \eta(y - o)x_i$

Perceptrons can only represent linearly separable concepts:
Decision boundary given by 1 if $w_0 + w_1 x_1 + ... + w_n x_n > 0$

7.2 Neural Network Gradient Descent

Multilayer networks use backpropogation algorithm
Key insight: require neural network to be differentiable, and use gradient descent in weight space
Let training set $D = \{(\hat{x}_1, y_1), ..., (\hat{x}_2, y_1)\}$, then the error measure is $E(w) = (1/2) \sum_{d \in D} (y_d - o_d)^2$
Gradient descent in weight space: on each iteration

(i) Calculate gradient of E: $\nabla E(w) = [\partial E/\partial w_0, \partial E/\partial w_1, ..., \partial E/\partial w_n]$

(ii) Step in opposite direction, $\Delta w = -\eta \nabla E(w)$, so $\Delta w_i = -\eta(\partial E/\partial w_i)$

Sigmoid function: to be able to differentiate E with respect to w_i, network represents continuous function
Use sigmoid function instead of threshold function for hidden and output units: $f(x) = 1/(1 + e^{-x})$
Input to sigmoid function: $w_0 + \sum_{i=1}^{n} w_i x_i$

Batch training is standard gradient descent. Calculates error for entire set before changing weights
Batch neural network training: given network structure and training set $D = \{(\hat{x}_1, y_1), ..., (\hat{x}_n, y_n)\}$

(i) Initialize all weights in w to small random numbers

(ii) Until stopping criteria is met:

  (a) Initialize the error $E(w) = 0$

  (b) For each $(\hat{x}_i, y_i)$ in the training set:
  Input $\hat{x}_i$ to network and compute output o_i
  Then increment the error $E(w) = E(w) + (1/2)(y_i - o_i)^2$

  (c) Calculate the gradient: $\nabla E(w) = [\partial E/\partial w_0, \partial E/\partial w_1, ..., \partial E/\partial w_n]$

  (d) Update the weights: $\Delta w = -\eta \nabla E(w)$

Online training is stochastic gradient descent, calculates error gradient and steps for each instance
Online neural network training: given network structure and training set $D = \{(\hat{x}_1, y_1), ..., (\hat{x}_2, y_1)\}$

(i) Initialize the error $E(w) = 0$

(ii) Until stopping criteria is met: for each $(\hat{x}_i, y_i)$ in the training set

(a) Input $\hat{x}_i$ to network and compute output o_i

(b) Calculate the error $E(w) = (1/2)(y_i - o_i)^2$

(c) Calculate the gradient: $\nabla E(w) = [\partial E/\partial w_0, \partial E/\partial w_1, ..., \partial E/\partial w_n]$

(d) Update the weights: $\Delta w = -\eta \nabla E(w)$

Gradient descent finds local minimum (global minimum for single-layer network)

To compute the derivative $\partial E/\partial w_i$, use the chain rule

$$\frac{\partial E}{\partial w_i} = \frac{\partial E}{\partial o}\frac{\partial o}{\partial net}\frac{\partial net}{\partial w_i}, \text{ where } net = w_0 + \sum_{i=1}^{n} w_i x_i$$

Condier the simple case of stochastic gradient descent: derive the following

$$\frac{E_d}{w_i} = \frac{\partial}{\partial w_i}\frac{1}{2}(y_d - o_d)^2 = (y_d - o_d)(-x_{di})$$

Consider the case of gradient descent with a sigmoid output and no hidden units: $o_d = 1/(1 + e^{-net_d})$
A useful property in this case: $\partial o_d/\partial net_d = o_d(1 - o_d)$

$$\begin{aligned}
\frac{\partial E_d}{\partial w_i} &= \frac{\partial}{\partial w_i}\frac{1}{2}(y_d - o_d)^2 \\
&= (y_d - o_d)\frac{\partial}{\partial w_i}(y_d - o_d) \\
&= (y_d - o_d)\left(-\frac{\partial o_d}{\partial w_i}\right) \\
&= -(y_d - o_d)\frac{\partial o_d}{\partial net_d}\frac{\partial net_d}{\partial w_i} \\
&= -(y_d - o_d)o_d(1 - o_d)\frac{\partial net_d}{\partial w_i} \\
&= -(y_d - o_d)o_d(1 - o_d)x_{di}
\end{aligned}$$

7.3 Backpropagation and Network Representation

Notation on backpropgation:

(i) w_{ij} is the weight to unit j from i

(ii) o_i is the output of unit i, this is x_i if i is an input unit

(iii) net_j is the sum $w_0 + \sum_{i=1}^{n} w_i x_i$ into unit j

Each weight is changed by $\Delta w_{ji} = -\eta(\partial E/\partial w_{ji}) = -\eta(\partial E/\partial net_j)(\partial net_j/\partial w_{ji})$
Let $\delta_j = -\partial E/\partial net_j$, and note that $o_i = \partial net_j/\partial w_{ji}$, then $\delta_{wi} = \eta\delta_j o_i$
Since $\delta_j = -\partial E/\partial net_j$, the following substitutions apply

(i) $\delta_j = o_j(1 - o_j)(y_j - o_j)$ if j is an output unit

(ii) $\delta_j = o_j(1 - o_j)\sum_k \delta_k w_{kj}$ if j is a hidden unit

Backpropogation algorithm:

(i) Calculate error of output units j: $\delta_j = o_j(1 - o_j)(y_j - o_j)$

(ii) Determine updates for weights from hidden units i to output units j: $\Delta w_{ji} = \eta \delta_j o_i$

(iii) Calculate error of hidden units j: $o_j(1 - o_j) \sum_k \delta_k w_{kj}$

(iv) Determine updates for weights to hidden units using hidden unit errors: $\Delta_{ji} = \eta \delta_j o_i$

To increase learning rate, momentum term is used: $\Delta w_{ji}(n) = \eta \delta_j x_{ji} + \alpha \Delta w_{ji}(n-1)$
Effect is to apply small component of direction of previous update to current update

Neural netowork and backpropgation jargon:

(i) Activation: the output value of a hidden or output unit

(ii) Epoch: one pass through the training instances during gradient descent

(iii) Tranfer function: function used to compute output of a hidden/output unity from net input

Initializing weights: should be small values to ensure large sigmoid derivative (i.e. faster learning) and random to break symmetry, typically $[-0.01, 0.01]$
Early stopping: return weights that minimize error on separate validation set
Input feature encoding for neural networks:

(i) Nominal features represented using 1-of-k enconding: feature vector $(x_1, x_2, ..., x_k)$
$x_i = 1$ if ith name, otherwise $x_i = 0$

(ii) Ordinal features can use thermometer encoding: feature vector $(x_1, x_2, ..., x_k)$
$x_i = 1$ if $i < n$ for nth feature strength, 0 otherwise

(iii) Real valued features can be represented using individual, normalized inputs

Output encoding for neural networks:

(i) Regression tasks use outputs with linear transfer functions

(ii) Binary classification tasks use single sigmoid output unit

(iii) k-ary classification tasks use k sigmoid or softmax output units
Softmax: $o_i = e^{net_i} / \sum_{j \in outputs} e_{net_j}$

Recurrent neural networks: Elman networks (hiddens to inputs), Jordan networks (outputs to inputs)

7.4 Deep Learning

Learning representaiton: additional hidden units compose new features from original input features
Competing intuitions on deep learning:

(i) Limits to 2-layer network (input, hidden, ouput)
Representation theorem: 2-layer network with sigmoid activation can represent any continuous function
Adding more hidden layers does not improve accuracy, and often degrades it under backpropogation

(ii) Deeper networks are better: can represent n-variable parity function with polynomial number of nodes, but needs exponentially many with a single hidden layer
Additional layers allows for more interesting derived features to be composed

Training deep neural networks: autoencoder networks trained to reconstruct the inputs
Encouraging an autoencoder to generalize:

(i) Bottleneck: use fewer hidden units than inputs

(ii) Sparsity: use penalty function encouraging most hidden unit activations to be near 0

(iii) Denoising: train to predict true input from corrected input

(iv) Contractive: force encoder to have small derivatives

Stacking autoencoders for deep networks:

1. Train autoencoder to represent x, i.e. hidden layer h_1 reconstructs x
2. Discard output layer, train autoencoder to represent h_1, repeat for k layers
3. Discard ouptut layer, train weights on last layer for supervised task, i.e. h_k predicts y
4. Fine tuning: run backpropogation on entire network to fine-tune weights for supervised task

8 Support Vector Machines

8.1 Linear Classifiers

Key vector concepts:

(i) Dot product: $w\dot{x} = w^T x = \sum_i w_i x_i$

(ii) 2-norm Euclidean length: $||\hat{x}||_2 = \sqrt{\sum_i |x_i|^2}$

Suppose classes are -1, $+1$, then the linear classifier is $h(x) = 1$ if $(\sum_{i=1}^n w_i x_i) + b > 0$, -1 otherwise
An instance (x, y) will be correctly classified if $y(w^T x + b) > 0$

SVM learning chooses hyperplane separator that maximizes the margin
Let x_+ and x_- be the closest positive/negative instances to hyperplane
Let $hatw$ be a length 1 vector in the same direction as w. Then the margin is gven by

$$margin_D(h) = \frac{1}{2}\hat{w}^T(x_+ - x_-) = \frac{1}{||w||_2}$$

Hard-margin SVM: given training set $D = \{(x^{(1)}, y^{(1)}), ..., (x^{(m)}, y^{(m)})\}$
Maximizing margin is equivalent to constrained optimzation problem:
Free parameters are w and b: minimize $1/2||w||_2^2$
Constraints: $y^{(i)}(w^T x^{(i)} + b) \geq 1$ for $i = 1, 2, ..., m$

Soft-margin SVM: nonlinearly-separable (noisy) data, slack variables (denoted ξ) to tolerate errors
Free parameters are $w, b, \xi^{(1)}, ..., \xi^{(m)}$, mimnimize $1/2||w||_2^2 + C\sum)i = 1^m \xi^{(i)}$
Constraints: $y^{(i)}(w^T x^{(i)} + b) \geq 1 - \xi^{(i)}$, where $\xi^{(i)} \geq 0$, for $i = 1, 2, ..., m$
The constant C determines relative importance of maximizing margin vs minimizing slack

8.2 Nonlinear Classifiers

For any data set, mapping ϕ to higher-dimensional space makes data linearly separable
Feature vectors are mapped as such: $\phi(x) = (\phi_1(x), \phi_2(x), ..., \phi_k(x))$
Nonlinear case: $h(x) = 1$ if $w \cdot \phi(x) + b > 0$, -1 otherwise, where w is higher-dimensional vector

Kernel trick: dot product between two higher-dimensional mappings can sometimes be implemnted by a kernel function. Dot product computed without explicitly mapping instances to higher-dimensional space
Example (quadratic kernel): $k(x, z) = (x \cdot z + 1)^2 = \phi(x) \cdot \phi(z)$

Given training set $D = \{(x^{(1)}, y^{(1)}), ..., (x^{(m)}, y^{(m)})\}$. Suppose weight vector can be represented as linear combination of training instances: $w = \sum_{i=1}^m \alpha_i x^{(i)}$
Then the linear SVM can be represented as $\sum_{i=1}^m \alpha_i x^{(i)} \cdot x + b$
A nonlinear SVM can be represented as:

$$\sum_{i=1}^m \alpha_i \phi(x^{(i)}) \cdot \phi(x) + b = \sum_{i=1}^m \alpha_i k(x^{(i)}, x) + b$$

Primal and dual formulations of hard-margin SVM (with kernel):

(i) Primal: $argmax_{(w,b)}(1/2)||w||_2^2$ with constraints $y^{(i)}(w^T x^{(i)} + b) \geq 1$ for $i = 1, 2, ..., m$

(ii) Primal (kernel): $argmax_{(w,b)}(1/2)||w||_2^2$ with constraints $y^{(i)}(w^T \phi(x^{(i)}) + b) \geq 1$

(iii) Dual: has constraints $\alpha_i \geq 0$ for $i = 1, 2, ..., m$, and $\sum_{i=1}^{m} \alpha_i y^{(i)} = 0$

$$\underset{\alpha_1,\dots,\alpha_m}{argmax} \left(\sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{j=1}^{m} \sum_{k=1}^{m} \alpha_j \alpha_k y^{(j)} y^{(k)} (x^{(j)} \cdot x^{(k)}) \right)$$

(iv) Dual with kernel: same constraints, but maximizing

$$\underset{\alpha_1,\dots,\alpha_m}{argmax} \left(\sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{j=1}^{m} \sum_{k=1}^{m} \alpha_j \alpha_k y^{(j)} y^{(k)} k(x^{(j)}, x^{(k)}) \right)$$

Support vectors: final solution is sparse linear combination of the training instances
Instances with $\alpha_i > 0$ are support vectors, lie on margin boundary

Support vector regression:

(i) Minimization task:

$$\underset{w,b,\xi^{(m)},\hat{\xi}^{(m)},\dots,\hat{\xi}^{(m)}}{argmax} \frac{1}{2}||w||_2^2 + C \sum_{i=1}^{m} \left(\xi^{(i)} + \hat{\xi}^{(i)} \right)$$

(ii) Subject to constraints:

$$\begin{gathered} (w^T x^{(i)} + b) - y^{(i)} \leq \varepsilon + \xi^{(i)} \\ y^{(i)} - (w^T x^{(i)} + b) \leq \varepsilon + \hat{\xi}^{(i)} \\ \xi^{(i)}, \hat{\xi}^{(i)} \geq 0 \end{gathered}$$

8.3 Kernel functions

Kernel matrix (Gram matrix): represents pairwise similarities for instances in the training set

$$\begin{bmatrix} k(x^{(1)}, x^{(1)}) & k(x^{(1)}, x^{(2)}) & \dots & k(x^{(1)}, x^{(m)}) \\ k(x^{(2)}, x^{(1)}) & k(x^{(2)}, x^{(2)}) & \dots & k(x^{(2)}, x^{(m)}) \\ \vdots & \vdots & \ddots & \vdots \\ k(x^{(1)}, x^{(1)}) & k(x^{(1)}, x^{(2)}) & \dots & k(x^{(1)}, x^{(m)}) \end{bmatrix}$$

Some common kernels:

1. Polynomial of degree d: $k(x, z) = (x \cdot z)^d$
2. Polynomial of degree up to d: $k(x, z) = (x \cdot z + 1)^d$
3. Radial basis function (Gaussian): $k(x, z) = e^{-\gamma||x-z||^2}$
   The feature mapping is infinite-dimensional: suppose $\gamma = 1/2$
   $k(x, z) = e^{-(1/2)||x||^2} e^{-(1/2)||z||^2} \sum_{n=0}^{\infty} (x \cdot z)^n / n!$

A kernel is valid if there is some ϕ such that $k(x, z) = \phi(x) \cdot \phi(z)$
Holds for a symmetric function $k(x, z)$ if and only if kernel matrix K is positive semidefinite for any training set, meaning $\forall v (v^T K v \geq 0)$
Given a valid kernel, following operators can be used to make new kernels

(i) Addition: $k_a(x, v) + k_b(x, v) = k(x, v)$
Mapping composition: $\phi(x) = (\phi_a(x), \phi_b(x))$

(ii) Nonnegative scalar multiplication: $k(x,v) = \gamma k_a(x,v)$, where $\gamma > 0$
Mapping composition: $\phi(x) = \sqrt{\gamma}\phi_a(x)$

(iii) Multiplication: $k(x,v) = k_a(x,v)k_b(x,v)$
Mapping composition: $\phi_l(x) = \phi_{ai}(x)\phi_{bj}(x)$

(iv) Composition with positive semidefinite matrix A: $k(x,v) = x^T Av$
Mapping composition: $\phi(x) = L^T x$ where $A = LL^T$

(v) Function multiplication: $f(x)f(v)k_a(x,v)$
Mapping composition: $\phi(x) = f(x)\phi_a(x)$

8.4 SVMs by Sequential Minimal Optimization

Perceptron learning, like SVMs, finds linear separator by adjusting weights on misclassified examples
Sequential Minimal Optimization (SMO): maintains sum of example weights times example label
When SMO adjusts weight of one example, must adjust weight of another

Weight vector for perceptron is weighted sum of examples:
$(w_1, w_2, ..., w_N) = \sum_{i=1}^{M} \alpha_i(x_1^i, x_2^i, ..., x_N^i)$
Perceptron learning chooses example, and if mislabeled, adds to its weight
SMO is similar, but with constraint: $\sum_{i=1}^{m} \alpha_i y^{(i)} = 0$
Thus, when adding β to weight α_i, either

(i) Subtract β from a_j for example with same sign/class label, or

(ii) Add β to a_j for example with oppositve sign/class label

At each step, two examples chosen for weight revision. Size of revision depends on error difference
For a soft-margin SVM, size of change subject to constraint $0 \leq \alpha \leq C$

Recall the perceptron learning rule: $w = w + \eta Ex$, where error $E = (y - o)$
Final weight vector is weighted combination of examples, where weight on example is sum of terms $-\eta E$
Thus, corresponding prediction in SVM is: $u = \sum_{j=1}^{N} y_j \alpha_j K(x_j, x) - b$

Changes from perceptron rule to SMO rule:

(i) Given constraint: $\sum_{i=1}^{N} y_i \alpha_i = 0$
Weight adjustment: $\alpha_1 = \alpha_1 + y_1\eta(E_2 - E_1)$, and adjust α_2 so that $y_1\alpha_1 + y_2\alpha_2$ unchanged

(ii) Instead of constant, use a learning rate of $(K(x_1,x_1) + K(x_2,x_2) - 2K(x_1,x_2))^{-1}$
When x_1 and x_2 are similar (i.e. $K(x_1,x_2)$ is larger), step size is larger

(iii) Given constraint: $\forall i(0 \leq \alpha \leq C)$
Any changes to any α must be clipped to follow constraint

Single SMO step:

(i) Given examples e_1 and e_2, set $\alpha_2' = \alpha_2 + (y_2(E_1 - E_2))/\eta$

(ii) Clip value in natural way:
If $y_1 = y_2$, then $L = max(0, \alpha_2 + \alpha_1 - C)$ and $H = min(C, \alpha_2 + \alpha_1)$
Otherwise, $L = max(0, \alpha_2 - \alpha_1)$, and $min(C, C + \alpha_2 - \alpha_1)$

(iii) If $\alpha_2' \geq H$, then set $\alpha_2'' = H$, if $\alpha_2' \leq L$, set $\alpha_2'' = L$, otherwise unchanged

(iv) Set $\alpha_1' = \alpha_1 + y_1 y_2(\alpha_2 - \alpha_2'')$

Karush-Kuhn-Tucker (KKT) conditions: neccesary and sufficient for this SVM

(i) $\alpha = 0$ iff example correctly labeled with room to spare, i.e. $y_i u_i \geq 1$

(ii) $\alpha = C$ iff example incorrectly labeled or on the margin, i.e. $y_i u_i \leq 1$

(iii) $0 < \alpha < C$ iff example is barely correctly labeled (i.e. a support vector)

SMO algorithm: input C, kernel, kernel parameters, ε value

(i) Initalize b and all αs to 0

(ii) Repeat the following until KTT satisfied (to within ε)

(iii) Find example e_1 that violates KTT

(iv) Choose second example e_2

  (a) Maximize $|E_1 - E_2|$ to maximize step size
  (b) If unchanged, randomly choose unbound example
  (c) If unchanged, randomly choose example
  (d) If unchanged, re-choose e_1

(v) Update α_1 and α_2 in one step

(vi) Compute new threshold b

  (a) Compute b_1 and b_2 as follows

$$b_1 = E_1 + y_1(\alpha_1' - \alpha_1)K(x_1, x_1) + y_2(\alpha_2'' = \alpha_2)K(x_1, x_2) + b$$
$$b_2 = E_2 + y_1(\alpha_1' - \alpha_1)K(x_1, x_2) + y_2(\alpha_2'' = \alpha_2)K(x_2, x_2) + b$$

  (b) Let $b = (b_1 + b_2)/2$

9 Reinforcement Learning

9.1 Learning Value Function

Reinforcement learning consists of a set of states S, set of actions A. At each time t, agent observes state $s_t \in S$ and chooses action $a_t \in A$. Agent receives reward r_t, changes to state s_{t+1}

Markov decision process: Markov assumption is that only previous state, action matters

(i) Markovian state transition: $P(s_{t+1} \mid s_t, a_t, s_{t-1}, a_{t-1}, ...) = P(s_{t+1}|s_t, a_t)$

(ii) Markovian reward: $P(r_t \mid s_t, a_t, s_{t-1}, a_{t-1}, ...) = P(r_t|s_t, a_t)$

(iii) Goal: learn policy that maximizes $E(r_t + \gamma r_{t+1} + \gamma^2 r_{t+2} + \gamma^3 r_{t+3} + ...)$
Where $0 \leq \gamma < 1$, for every possible starting state s_0

Learning task: a control policy $\pi : S \to A$ that maximizes $\sum_{t=0}^{\infty} \gamma^t E(r_t)$ from every $s \in S$
Value function for a policy: given π, define $V^\pi(s) = \sum_{t=0}^{\infty} \gamma^t E(r_t)$
Optimal policy is given by: $\pi^* = argmax_\pi V^\pi(s)$ for all s, has value function $V^*(s)$
Knowing $V^*(s)$, $r(s_t, a)$ and $P(s_t \mid s_{t-1}, a_{t-1})$ allows computing $\pi^*(s)$

$$\pi^*(s_t) = \underset{a\in A}{argmax} \left(r(s_t, a) + \gamma \sum_{s\in S} P(s_{t+1} = s \mid s_t, a) V^*(s) \right)$$

Value iteration for learning V^*

(i) Arbitrarily initialize $V(s)$

(ii) Iterate until policy is good enough (e.g. policy converges):
For each $s \in S$, set the variable $V(s)$ as such

$$V(s) = \max_{a\in A}(Q(s, a)) \text{ where}$$
$$Q(s, a) = r(s, a) + \gamma \sum_{s'\in S} P(s' \mid s, a) V(s')$$

9.2 Q Function Learning

Suppose the case that $P(s_t \mid s_{t-1} a_{t-1})$ is unknown
Define a function Q, related to V^*

$$V^*(s) = E(r(s, \pi^*(s))) + \gamma E_{s' \mid s, \pi^*(s)}(V^*(s'))$$
$$Q(s, a) = E(r(s, a)) + \gamma E_{s' \mid s, \pi^*(s)}(V^*(s'))$$

If agent knows $Q(s, a)$ it choose optimal action without knowing/learning $P(s' \mid s, a)$
$\pi(s) = argmax_{a\in A} Q(s, a)$, and $V^*(s) = max_{a\in A} Q(s, a)$

Q learning for determinisitic worlds:

(i) For each s, a, initialize table entry $Q(s, a) = 0$

(ii) Observe the current state s

(iii) Iterate forever:

  (a) Select an action a and execute

(b) Receive immediate reward r, observe new state s'

(c) Update table entry $Q(s,a) = r + \gamma \max_{a'} Q(s',a')$

(d) Update $s = s'$

Q learning for nondeterministic models:

(i) For each s, a, initialize table entry $Q(s,a) = 0$

(ii) Observe the current state s

(iii) Iterate forever:

  (i) Select an action a and execute it

  (ii) Receive immediate reward r, observe new state s'

  (iii) Update table entry $Q_n(s,a) = (1-\alpha_n)Q_{n-1}(s,a) + \alpha_n(r + \gamma \max_{a'} Q_{n-1}(s',a')$
  Where $\alpha_n = 1/(1 + visits_n(s,a))$

  (iv) Update $s = s'$

Model-free Q learning: only need to know which actions legal, choose next state with highest Q
Model-based V learning: need next-states function, choose next state with highest V value

Exploration vs exploitation: sometimes choose random actions (exploration)
Select actions probabilistically according to: $P(a_i \mid s) = c^{Q(s,a_i)} / \sum_j c^Q(s,a_j)$, where $c > 0$ determine how strongly selection favors higher Q values

Compact representations of Q functions: e.g. neural net
Q learning with function approximation:

(i) Measure sensors, sense state s_0

(ii) Predict $Q(s_0, a)$ for each action a

(iii) Select action a (with exploration factor)

(iv) Apply action a and sense new state s_1 and reward r

(v) Calculate action a' that maximizes $Q_n(s_1, a')$

(vi) Train with new instance, $x = s_0$

$$y = (1-\alpha)Q(s_0,a) + \alpha \left(r + \gamma \max_{a'} Q(s_1, a') \right)$$

10 Rule Learning and Inductive Logic Programming

10.1 Relational Learning via FOIL

Hypothesis space: propositional rules (conjunection of tests and implied class from satisfied conjunction)
Note: any decision tree can be converted into equivalent set of rules
Relational learning: learning a rule in first order logic based on related factors

FOIL algorithm for relational learning: given tuples (instances) of target relation and extentionally represented background relations, learn set of rules (mostly) covering positive tuples of target relation, but not negative tuples
Consider a graph traveral problem input: learning $can-reach(x_1, x_2)$ relation

(i) Instances of target relation: tuple set $\{(+,(x_1,x_2)) \mid can-reach(x_1,x_2)\}$

(ii) Instances of target relation: tuple set $\{(-,(x_1,x_2)) \mid \neg can-reach(x_1,x_2)\}$

(iii) Extentionally defined background relations: $linked-to$ is set of tuples represented adjacent nodes in the graph

FOIL algorithm learns relation: $can-reach(x_1,x_2) = linked-to(x_1,x_2)$, and
$can_reach(x_1,x_2) = linked_to(x_1,x_3) \wedge can-reach(x_3,x_2)$

FOIL algorithm subroutine: $LearnRuleSet$(Tuples T of target relation, background relations B)

(i) Initialize $S = \{\}$, then:

(ii) Repeat until no (few) positive tuples left in T:
$R = LearnRule(T,B)$, $S = S \cup R$, $T = T-$positive tuples covered by R

(iii) Return S

FOIL algorithm subroutine: $LearnRule$(Tuples T of target relation, background relations B)

(i) Initialize $R = \{\}$, then:

(ii) Repeat until no (few) negative tuples left in T:
$L =$ best literal, based on T and B to right-hand side or R
$R = R \cup L$ and $T =$new set of tuples that satisfy L

(iii) Return R

Literals in FOIL: given current rule $R(X_1, X_2, \dots, X_k) = L_1 \wedge \dots \wedge L_n$
FOIL considers adding several types of literals:

(i) $X_j = X_k$ or $X_j \neq X_k$, where X_j and X_k either appear in LHS of the rule, or were introduced by a previous literal

(ii) $Q(V_1, V_2, ..., V_a)$ or $\neg Q(V_1, V_2, ..., V_a)$, where at least of of V_is has to be in LHS of the rule or introduced by a previous literal, where Q is abackground relation

(iii) $X_j = c$ or $X_j \neq c$ where c is a constant

(iv) $X_j > a$, $X_j \leq a$, $X_j > X_k$, or $X_j \leq X_k$ where X_j and X_k are numeric variables and a is a numeric constant

Evaluating literals in FOIL:

$$FOIL\_Gain(L,R) = t(Info(R_0) - Info(R_1))$$
$$FOIL\_Gain(L,R) = t\left(\log_2 \frac{p_1}{p_1+n_1} - \log_2 \frac{p_0}{p_0+n_0}\right)$$

Given the following substitutions:

(i) $p_0 = \#$ of positive tuples covered by R

(ii) $n_0 = \#$ of negative tuples covered by R

(iii) $p_1 = \#$ of positive tuples covered by $R \wedge L$

(iv) $n_1 = \#$ of negative tuples covered by $R \wedge L$

(v) $t = \#$ of positive tuples of R also covered by $R \wedge L$

10.2 Background on Rule Learning and ILP

Skolem normal form: formal logic statemetns without existential quantifiers

(i) Process is applied to one sentence at a time and applied only to entire sentence (outermost quantifier first). Each sentence initially has empty vector of free variables

(ii) Replace $\forall X A(X)$ with $A(X)$ and add X to vector of free variables

(iii) Replace $\exists X A(X)$ with $A(x(V))$: x is new function symbol, V is the current vector of free variables