MODULE 1

INTRODUCTION

Ever since computers were invented, we have wondered whether they might be made to learn. If we could understand how to program them to learn-to improve automatically with experience-the impact would be dramatic.

- Imagine computers learning from medical records which treatments are most effective for new diseases
- Houses learning from experience to optimize energy costs based on the particular usage patterns of their occupants.
- Personal software assistants learning the evolving interests of their users in order to highlight especially relevant stories from the online morning newspaper

A successful understanding of how to make computers learn would open up many new uses of computers and new levels of competence and customization

Some successful applications of machine learning

- Learning to recognize spoken words
- Learning to drive an autonomous vehicle
- Learning to classify new astronomical structures
- Learning to play world-class backgammon

Why is Machine Learning Important?

- Some tasks cannot be defined well, except by examples (e.g., recognizing people).
- Relationships and correlations can be hidden within large amounts of data. Machine Learning/Data Mining may be able to find these relationships.
- Human designers often produce machines that do not work as well as desired in the environments in which they are used.
- The amount of knowledge available about certain tasks might be too large for explicit encoding by humans (e.g., medical diagnostic).
- Environments change over time.
- New knowledge about tasks is constantly being discovered by humans. It may be difficult to continuously re-design systems “by hand”.

WELL-POSED LEARNING PROBLEMS

Definition: A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks in T, as measured by P, improves with experience E.

To have a well-defined learning problem, three features needs to be identified:

1. The class of tasks
2. The measure of performance to be improved
3. The source of experience

Examples

1. ***Checkers game:*** A computer program that learns to play ***checkers*** might improve its performance as measured by its ability to win at the class of tasks involving playing checkers games, through experience obtained by playing games against itself.

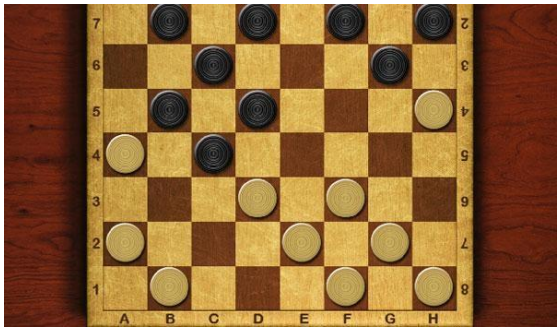


Fig: Checker game board

***A checkers learning problem*:**

- Task T: playing checkers
- Performance measure P: percent of games won against opponents
- Training experience E: playing practice games against itself

2. ***A handwriting recognition learning problem:***
    - Task T: recognizing and classifying handwritten words within images
    - Performance measure P: percent of words correctly classified
    - Training experience E: a database of handwritten words with given classifications
3. ***A robot driving learning problem*:**
    - Task T: driving on public four-lane highways using vision sensors
    - Performance measure P: average distance travelled before an error (as judged by human overseer)
    - Training experience E: a sequence of images and steering commands recorded while observing a human driver

DESIGNING A LEARNING SYSTEM

The basic design issues and approaches to machine learning are illustrated by designing a program to learn to play checkers, with the goal of entering it in the world checkers tournament

1. Choosing the Training Experience
2. Choosing the Target Function
3. Choosing a Representation for the Target Function
4. Choosing a Function Approximation Algorithm
    1. Estimating training values
    2. Adjusting the weights
5. The Final Design

1. Choosing the Training Experience

- The first design choice is to choose the type of training experience from which the system will learn.
- The type of training experience available can have a significant impact on success or failure of the learner.

There are three attributes which impact on success or failure of the learner

1. Whether the training experience provides ***direct or indirect feedback*** regarding the choices made by the performance system.

    For example, in checkers game:
    In learning to play checkers, the system might learn from ***direct training examples*** consisting of ***individual checkers board states*** and ***the correct move for each***.

    Indirect training examples consisting of the ***move sequences*** and ***final outcomes*** of various games played. The information about the correctness of specific moves early in the game must be inferred indirectly from the fact that the game was eventually won or lost.

    Here the learner faces an additional problem of ***credit assignment***, or determining the degree to which each move in the sequence deserves credit or blame for the final outcome. Credit assignment can be a particularly difficult problem because the game can be lost even when early moves are optimal, if these are followed later by poor moves.
    Hence, learning from direct training feedback is typically easier than learning from indirect feedback.

2. The degree to which the ***learner controls the sequence of training examples***

   For example, in checkers game:
   The learner might depends on the ***teacher*** to select informative board states and to provide the correct move for each.

   Alternatively, the learner might itself propose board states that it finds particularly confusing and ask the teacher for the correct move.

   The learner may have complete control over both the board states and (indirect) training classifications, as it does when it learns by playing against itself with ***no teacher present***.

3. How well it represents the ***distribution of examples*** over which the final system performance P must be measured

   For example, in checkers game:
   In checkers learning scenario, the performance metric P is the percent of games the system wins in the world tournament.

   If its training experience E consists only of games played against itself, there is a danger that this training experience might not be fully representative of the distribution of situations over which it will later be tested.
   It is necessary to learn from a distribution of examples that is different from those on which the final system will be evaluated.

2. Choosing the Target Function

The next design choice is to determine exactly what type of knowledge will be learned and how this will be used by the performance program.

Let's consider a checkers-playing program that can generate the legal moves from any board state.
The program needs only to learn how to choose the best move from among these legal moves. We must learn to choose among the legal moves, the most obvious choice for the type of information to be learned is a program, or function, that chooses the best move for any given board state.

1. Let ***ChooseMove*** be the target function and the notation is

   $$ChooseMove : B \rightarrow M$$

   which indicate that this function accepts as input any board from the set of legal board states B and produces as output some move from the set of legal moves M.

ChooseMove is a choice for the target function in checkers example, but this function will turn out to be very difficult to learn given the kind of indirect training experience available to our system

2. An alternative target function is an ***evaluation function*** that assigns a ***numerical score*** to any given board state
   Let the target function V and the notation

$$V : B \rightarrow R$$

   which denote that V maps any legal board state from the set B to some real value. Intend for this target function V to assign higher scores to better board states. If the system can successfully learn such a target function V, then it can easily use it to select the best move from any current board position.

Let us define the target value V(b) for an arbitrary board state b in B, as follows:

- If b is a final board state that is won, then V(b) = 100
- If b is a final board state that is lost, then V(b) = -100
- If b is a final board state that is drawn, then V(b) = 0
- If b is a not a final state in the game, then V(b) = V(b'),

Where b' is the best final board state that can be achieved starting from b and playing optimally until the end of the game

3. Choosing a Representation for the Target Function

Let's choose a simple representation - for any given board state, the function ***c*** will be calculated as a linear combination of the following board features:

- x_1: the number of black pieces on the board
- x_2: the number of red pieces on the board
- x_3: the number of black kings on the board
- x_4: the number of red kings on the board
- x_5: the number of black pieces threatened by red (i.e., which can be captured on red's next turn)
- x_6: the number of red pieces threatened by black

Thus, learning program will represent as a linear function of the form

$$\hat{V}(b) = w_0 + w_1 x_1 + w_2 x_2 + w_3 x_3 + w_4 x_4 + w_5 x_5 + w_6 x_6$$

Where,

- w_0 through w_6 are numerical coefficients, or weights, to be chosen by the learning algorithm.
- Learned values for the weights w1 through w6 will determine the relative importance of the various board features in determining the value of the board
- The weight w_0 will provide an additive constant to the board value

4. Choosing a Function Approximation Algorithm

In order to learn the target function **f** we require a set of training examples, each describing a specific board state b and the training value $V_{train}(b)$ for b.

Each training example is an ordered pair of the form $(b, V_{train}(b))$.

For instance, the following training example describes a board state b in which black has won the game (note $x_2 = 0$ indicates that red has no remaining pieces) and for which the target function value $V_{train}(b)$ is therefore +100.

$$((x_1=3, x_2=0, x_3=1, x_4=0, x_5=0, x_6=0), +100)$$

Function Approximation Procedure

1. Derive training examples from the indirect training experience available to the learner
2. Adjusts the weights w_i to best fit these training examples

1. Estimating training values

   A simple approach for estimating training values for intermediate board states is to assign the training value of $V_{train}(b)$ for any intermediate board state b to be $\hat{V}$(Successor(b))

   Where ,
   - $\hat{V}$ is the learner's current approximation to V
   - Successor(b) denotes the next board state following b for which it is again the program's turn to move

   Rule for estimating training values

$$\mathbf{V_{train}(b) \leftarrow \hat{V}(Successor(b))}$$

2. Adjusting the weights

Specify the learning algorithm for choosing the weights w_i to best fit the set of training examples $\{(b, V_{train}(b))\}$

A first step is to define what we mean by the bestfit to the training data.

One common approach is to define the best hypothesis, or set of weights, as that which minimizes the squared error E between the training values and the values predicted by the hypothesis.

$$E \equiv \sum_{\langle b, V_{train}(b)\rangle \in \text{ training examples}} (V_{train}(b) - \hat{V}(b))^2$$

Several algorithms are known for finding weights of a linear function that minimize E. One such algorithm is called the ***least mean squares, or LMS training rule***. For each observed training example it adjusts the weights a small amount in the direction that reduces the error on this training example

LMS weight update rule :- For each training example $(b, V_{train}(b))$

Use the current weights to calculate $\hat{V}(b)$

For each weight w_i, update it as

$$w_i \leftarrow w_i + \eta\,(V_{train}(b) - \hat{V}(b))\,x_i$$

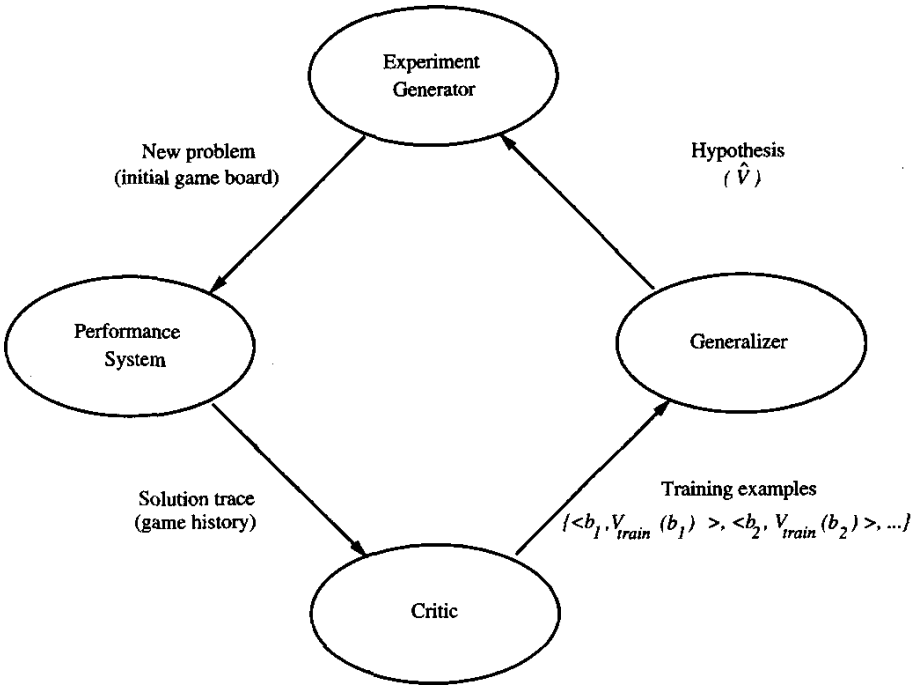
Here η is a small constant (e.g., 0.1) that moderates the size of the weight update.

Working of weight update rule

- When the error $(V_{train}(b) - \hat{V}(b))$ is zero, no weights are changed.
- When $(V_{train}(b) - \hat{V}(b))$ is positive (i.e., when $\hat{V}(b)$ is too low), then each weight is increased in proportion to the value of its corresponding feature. This will raise the value of $\hat{V}(b)$, reducing the error.
- If the value of some feature x_i is zero, then its weight is not altered regardless of the error, so that the only weights updated are those whose features actually occur on the training example board.

5. The Final Design

The final design of checkers learning system can be described by four distinct program modules that represent the central components in many learning systems



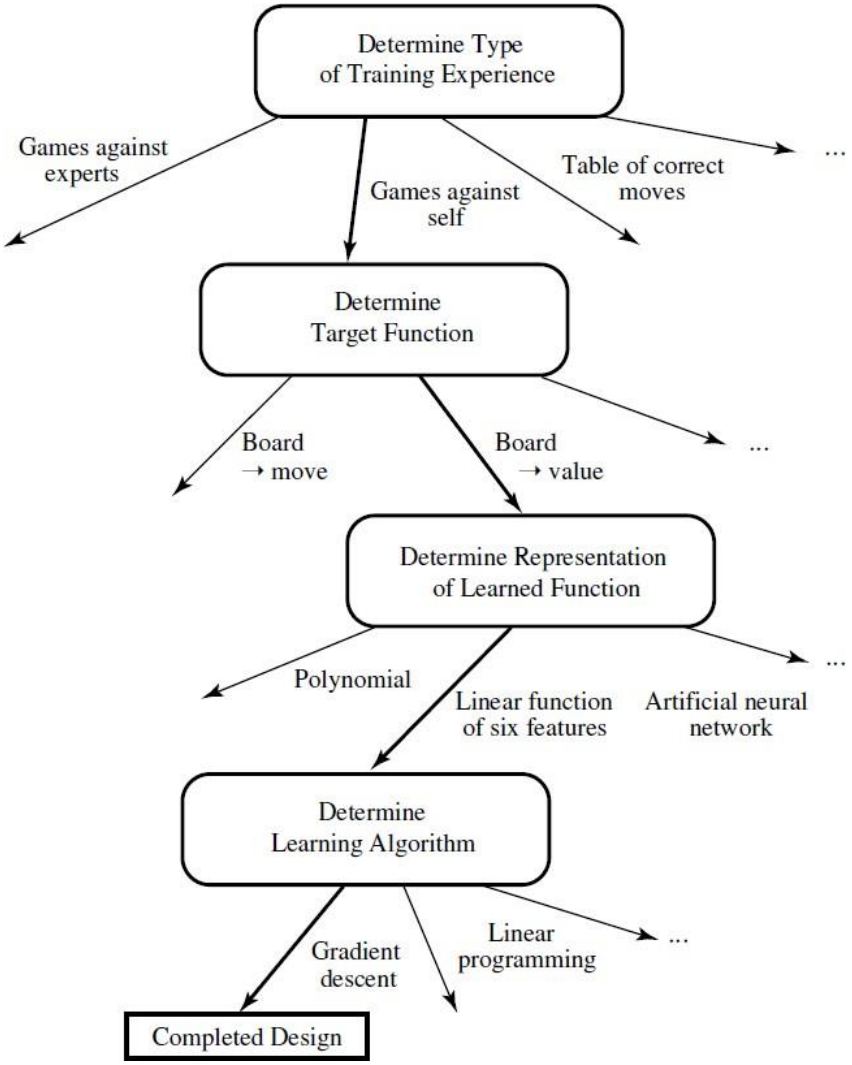
1. **The Performance System** is the module that must solve the given performance task by using the learned target function(s). It takes an instance of a new problem (new game) as input and produces a trace of its solution (game history) as output.

2. **The Critic** takes as input the history or trace of the game and produces as output a set of training examples of the target function

3. **The Generalizer** takes as input the training examples and produces an output hypothesis that is its estimate of the target function. It generalizes from the specific training examples, hypothesizing a general function that covers these examples and other cases beyond the training examples.

4. **The Experiment Generator** takes as input the current hypothesis and outputs a new problem (i.e., initial board state) for the Performance System to explore. Its role is to pick new practice problems that will maximize the learning rate of the overall system.

The sequence of design choices made for the checkers program is summarized in below figure



PERSPECTIVES AND ISSUES IN MACHINE LEARNING

Issues in Machine Learning

The field of machine learning, and much of this book, is concerned with answering questions such as the following

- What algorithms exist for learning general target functions from specific training examples? In what settings will particular algorithms converge to the desired function, given sufficient training data? Which algorithms perform best for which types of problems and representations?
- How much training data is sufficient? What general bounds can be found to relate the confidence in learned hypotheses to the amount of training experience and the character of the learner's hypothesis space?

- When and how can prior knowledge held by the learner guide the process of generalizing from examples? Can prior knowledge be helpful even when it is only approximately correct?
- What is the best strategy for choosing a useful next training experience, and how does the choice of this strategy alter the complexity of the learning problem?
- What is the best way to reduce the learning task to one or more function approximation problems? Put another way, what specific functions should the system attempt to learn? Can this process itself be automated?
- How can the learner automatically alter its representation to improve its ability to represent and learn the target function?

CONCEPT LEARNING

- Learning involves acquiring general concepts from specific training examples. Example: People continually learn general concepts or categories such as "bird," "car," "situations in which I should study more in order to pass the exam," etc.
- Each such concept can be viewed as describing some subset of objects or events defined over a larger set
- Alternatively, each concept can be thought of as a Boolean-valued function defined over this larger set. (Example: A function defined over all animals, whose value is true for birds and false for other animals).

Definition: Concept learning **-** Inferring a Boolean-valued function from training examples of its input and output

A CONCEPT LEARNING TASK

Consider the example task of learning the target concept "Days on which ***Aldo*** enjoys his favorite water sport"

Example	Sky	AirTemp	Humidity	Wind	Water	Forecast	EnjoySport
1	Sunny	Warm	Normal	Strong	Warm	Same	Yes
2	Sunny	Warm	High	Strong	Warm	Same	Yes
3	Rainy	Cold	High	Strong	Warm	Change	No
4	Sunny	Warm	High	Strong	Cool	Change	Yes

Table: Positive and negative training examples for the target concept ***EnjoySport.***

The task is to learn to predict the value of ***EnjoySport*** for an arbitrary day, based on the values of its other attributes?

What hypothesis representation is provided to the learner?

- Let's consider a simple representation in which each hypothesis consists of a conjunction of constraints on the instance attributes.
- Let each hypothesis be a vector of six constraints, specifying the values of the six attributes *Sky, AirTemp, Humidity, Wind, Water*, and *Forecast*.

For each attribute, the hypothesis will either

- Indicate by a "?' that any value is acceptable for this attribute,
- Specify a single required value (e.g., Warm) for the attribute, or
- Indicate by a "Φ" that no value is acceptable

If some instance ***x*** satisfies all the constraints of hypothesis ***h***, then ***h*** classifies ***x*** as a positive example (***h(x) = 1***).

The hypothesis that ***PERSON*** enjoys his favorite sport only on cold days with high humidity is represented by the expression

(?, Cold, High, ?, ?, ?)

The most general hypothesis-that every day is a positive example-is represented by

(?, ?, ?, ?, ?, ?)

The most specific possible hypothesis-that no day is a positive example-is represented by

(Φ, Φ, Φ, Φ, Φ, Φ)

Notation

- The set of items over which the concept is defined is called the ***set of instances***, which is denoted by X.

Example: X is the set of all possible days, each represented by the attributes: Sky, AirTemp, Humidity, Wind, Water, and Forecast

- The concept or function to be learned is called the ***target concept***, which is denoted by c.

c can be any Boolean valued function defined over the instances X

$$c: X \rightarrow \{O, 1\}$$

Example: The target concept corresponds to the value of the attribute ***EnjoySport*** (i.e., c(x) = 1 if ***EnjoySport*** = Yes, and c(x) = 0 if ***EnjoySport*** = No).

- Instances for which c(x) = 1 are called ***positive examples***, or members of the target concept.
- Instances for which c(x) = 0 are called ***negative examples***, or non-members of the target concept.
- The ordered pair (x, c(x)) to describe the training example consisting of the instance x and its target ***concept value c(x).***
- ***D*** to denote the set of available training examples

- The symbol ***H*** to denote the set of all possible hypotheses that the learner may consider regarding the identity of the target concept. Each hypothesis ***h*** in ***H*** represents a Boolean-valued function defined over ***X***

$$h: X \rightarrow \{O, 1\}$$

The goal of the learner is to find a hypothesis h such that h(x) = c(x) for all x in X.

- Given:
  - Instances X: Possible days, each described by the attributes
    - *Sky* (with possible values Sunny, Cloudy, and Rainy),
    - *AirTemp* (with values Warm and Cold),
    - *Humidity* (with values Normal and High),
    - *Wind* (with values Strong and Weak),
    - *Water* (with values Warm and Cool),
    - *Forecast* (with values Same and Change).

  - Hypotheses *H*: Each hypothesis is described by a conjunction of constraints on the attributes *Sky, AirTemp, Humidity, Wind, Water*, and *Forecast*. The constraints may be "?" (any value is acceptable), "Φ" (no value is acceptable), or a specific value.

  - Target concept *c*: ***EnjoySport*** : X → {0, 1}
  - Training examples *D*: Positive and negative examples of the target function

- Determine:
  - A hypothesis h in H such that *h(x) = c(x)* for all *x* in X.

Table: The ***EnjoySport*** concept learning task.

The inductive learning hypothesis

Any hypothesis found to approximate the target function well over a sufficiently large set of training examples will also approximate the target function well over other unobserved examples.

CONCEPT LEARNING AS SEARCH

- Concept learning can be viewed as the task of searching through a large space of hypotheses implicitly defined by the hypothesis representation.
- The goal of this search is to find the hypothesis that best fits the training examples.

Example:
Consider the instances X and hypotheses H in the *EnjoySport* learning task. The attribute Sky has three possible values, and *AirTemp, Humidity, Wind, Water, Forecast* each have two possible values, the instance space X contains exactly

3.2.2.2.2.2 = 96 distinct instances
5.4.4.4.4.4 = 5120 syntactically distinct hypotheses within H.

Every hypothesis containing one or more "Φ" symbols represents the empty set of instances; that is, it classifies every instance as negative.

1 + (4.3.3.3.3.3) = 973. Semantically distinct hypotheses

General-to-Specific Ordering of Hypotheses

Consider the two hypotheses

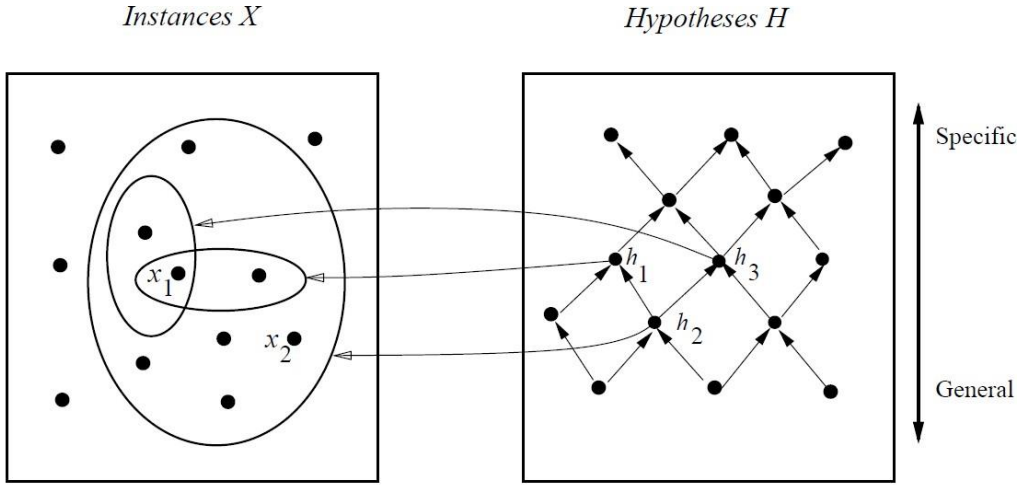
h_1 = (Sunny, ?, ?, Strong, ?, ?)
h_2 = (Sunny, ?, ?, ?, ?, ?)

- Consider the sets of instances that are classified positive by h_l and by h_2.
- h_2 imposes fewer constraints on the instance, it classifies more instances as positive. So, any instance classified positive by h_l will also be classified positive by h_2. Therefore, h_2 is more general than h_l.

Given hypotheses h_j and h_k, h_j is more-general-than or- equal do h_k if and only if any instance that satisfies h_k also satisfies h_i

Definition: Let h_j and h_k be Boolean-valued functions defined over X. Then h_j is ***more general-than-or-equal-to*** h_k (written $h_j \geq h_k$) if and only if

$$(\forall\, x \in X)\, [(h_k(x) = 1) \rightarrow (h_j(x) = 1)]$$



x_1 = <Sunny, Warm, High, Strong, Cool, Same>
x_2 = <Sunny, Warm, High, Light, Warm, Same>

h_1 = <Sunny, ?, ?, Strong, ?, ?>
h_2 = <Sunny, ?, ?, ?, ?, ?>
h_3 = <Sunny, ?, ?, ?, Cool, ?>

- In the figure, the box on the left represents the set X of all instances, the box on the right the set H of all hypotheses.
- Each hypothesis corresponds to some subset of X-the subset of instances that it classifies positive.
- The arrows connecting hypotheses represent the more - general -than relation, with the arrow pointing toward the less general hypothesis.
- Note the subset of instances characterized by h_2 subsumes the subset characterized by h_1, hence h_2 is more - general– than h_1

FIND-S: FINDING A MAXIMALLY SPECIFIC HYPOTHESIS

FIND-S Algorithm

1. Initialize *h* to the most specific hypothesis in *H*
2. For each positive training instance *x*
For each attribute constraint a_i in *h*
If the constraint a_i is satisfied by *x*
Then do nothing
Else replace a_i in *h* by the next more general constraint that is satisfied by *x*
3. Output hypothesis *h*

To illustrate this algorithm, assume the learner is given the sequence of training examples from the ***EnjoySport*** task

Example	Sky	AirTemp	Humidity	Wind	Water	Forecast	EnjoySport
1	Sunny	Warm	Normal	Strong	Warm	Same	Yes
2	Sunny	Warm	High	Strong	Warm	Same	Yes
3	Rainy	Cold	High	Strong	Warm	Change	No
4	Sunny	Warm	High	Strong	Cool	Change	Yes

- The first step of FIND-S is to initialize h to the most specific hypothesis in H

  h - (Ø, Ø, Ø, Ø, Ø, Ø)

- Consider the first training example

  x_1 = <Sunny Warm Normal Strong Warm Same>, +

  Observing the first training example, it is clear that hypothesis *h* is too specific. None of the "Ø" constraints in h are satisfied by this example, so each is replaced by the next *more general constraint* that fits the example

  h_1 = <Sunny Warm Normal Strong Warm Same>

- Consider the second training example

  x_2 = <Sunny, Warm, High, Strong, Warm, Same>, +

  The second training example forces the algorithm to further generalize h, this time substituting a "?" in place of any attribute value in h that is not satisfied by the new example

  h_2 = <Sunny Warm ? Strong Warm Same>

- Consider the third training example

  x3 = <Rainy, Cold, High, Strong, Warm, Change>, -

  Upon encountering the third training the algorithm makes no change to h. The FIND-S algorithm simply ignores every negative example.

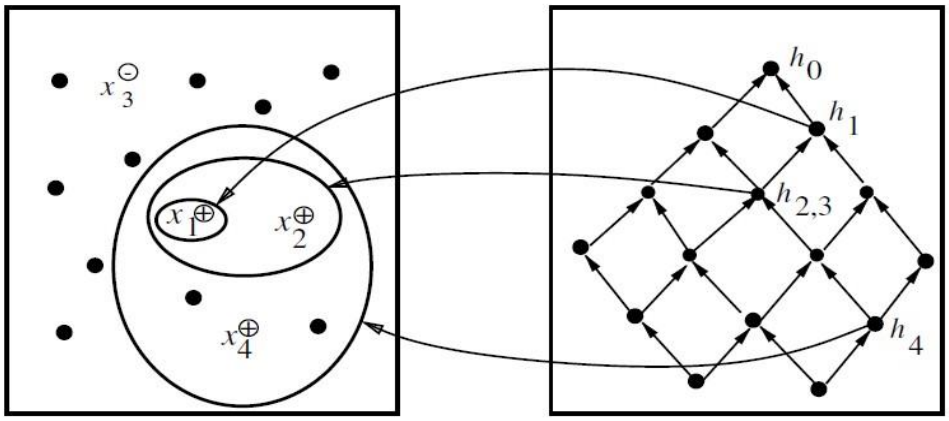
  h_3 = < Sunny Warm ? Strong Warm Same>

- Consider the fourth training example

  x_4 = <Sunny Warm High Strong Cool Change>, +

  The fourth example leads to a further generalization of h

  h_4 = < Sunny Warm ? Strong ? ? >



x_1 = <*Sunny Warm Normal Strong Warm Same*>, +
x_2 = <*Sunny Warm High Strong Warm Same*>, +
x_3 = <*Rainy Cold High Strong Warm Change*>, -
x_4 = <*Sunny Warm High Strong Cool Change*>, +

h_0 = <∅, ∅, ∅, ∅, ∅, ∅>
h_1 = <*Sunny Warm Normal Strong Warm Sam*
h_2 = <*Sunny Warm ? Strong Warm Same*>
h_3 = <*Sunny Warm ? Strong Warm Same*>
h_4 = <*Sunny Warm ? Strong ? ?* >

The key property of the FIND-S algorithm

- FIND-S is guaranteed to output the most specific hypothesis within H that is consistent with the positive training examples
- FIND-S algorithm's final hypothesis will also be consistent with the negative examples provided the correct target concept is contained in H, and provided the training examples are correct.

Unanswered by FIND-S

1. Has the learner converged to the correct target concept?
2. Why prefer the most specific hypothesis?
3. Are the training examples consistent?
4. What if there are several maximally specific consistent hypotheses?

VERSION SPACES AND THE CANDIDATE-ELIMINATION ALGORITHM

The key idea in the CANDIDATE-ELIMINATION algorithm is to output a description of the set of all ***hypotheses consistent with the training examples***

Representation

Definition: consistent- A hypothesis h is **consistent** with **a** set of training examples ***D*** if **and** only if ***h(x)*** = ***c(x)*** for each example ***(x, c(x))*** in ***D.***

$$Consistent\ (h, D) \equiv (\forall\ \langle x, c(x)\rangle \in D)\ h(x) = c(x))$$

Note difference between definitions of *consistent* and *satisfies*

- An example *x* is said to ***satisfy*** hypothesis ***h*** when ***h(x)*** = 1, regardless of whether *x* is a positive or negative example of the target concept.
- An example *x* is said to ***consistent*** with hypothesis ***h*** iff ***h(x)*** = ***c(x)***

Definition: version space- The **version space,** denoted $VS_{H, D}$ with respect to hypothesis space ***H*** and training examples D, is the subset of hypotheses from ***H*** consistent with the training examples in D

$$VS_{H, D} \equiv \{h \in H \mid Consistent\ (h, D)\}$$

The LIST-THEN-ELIMINATION algorithm

The LIST-THEN-ELIMINATE algorithm first initializes the version space to contain all hypotheses in H and then eliminates any hypothesis found inconsistent with any training example.

1. ***VersionSpace c*** a list containing every hypothesis in H
2. For each training example, (x, c(x))
   remove from ***VersionSpace*** any hypothesis h for which h(x) ≠ c(x)
3. Output the list of hypotheses in ***VersionSpace***

The LIST-THEN-ELIMINATE Algorithm

- List-Then-Eliminate works in principle, so long as version space is finite.
- However, since it requires exhaustive enumeration of all hypotheses in practice it is not feasible.

A More Compact Representation for Version Spaces

The version space is represented by its most general and least general members. These members form general and specific boundary sets that delimit the version space within the partially ordered hypothesis space.

Definition: The **general boundary** G, with respect to hypothesis space ***H*** and training data *D*, is the set of maximally general members of *H* consistent with *D*

$$G \equiv \{g \in H \mid Consistent(g, D) \wedge (\neg \exists g' \in H)[(g' >_g g) \wedge Consistent(g', D)]\}$$

Definition: The **specific boundary** S, with respect to hypothesis space *H* and training data *D*, is the set of minimally general (i.e., maximally specific) members of *H* consistent with *D*.

$$S \equiv \{s \in H \mid Consistent(s, D) \wedge (\neg \exists s' \in H)[(s >_g s') \wedge Consistent(s', D)]\}$$

Theorem: Version Space representation theorem

Theorem: Let X be an arbitrary set of instances and Let H be a set of Boolean-valued hypotheses defined over X. Let c: X $\rightarrow$ {O, 1} be an arbitrary target concept defined over X, and let D be an arbitrary set of training examples {(x, c(x))). For all X, H, c, and D such that S and G are well defined,

$$VS_{H,D} = \{ h \in H \mid (\exists s \in S)\ (\exists g \in G)\ (g \geq_g h \geq_g s) \}$$

To Prove:

1. Every h satisfying the right hand side of the above expression is in $\boldsymbol{VS_{H, D}}$

2. Every member of $\boldsymbol{VS_{H, D}}$ satisfies the right-hand side of the expression

Sketch of proof:

1. let g, h, s be arbitrary members of G, H, S respectively with $g \geq_g h \geq_g s$
   - By the definition of ***S,*** **s** must be satisfied by all positive examples in D. Because $h \geq_g s$, h must also be satisfied by all positive examples in D.
   - By the definition of ***G,*** g cannot be satisfied by any negative example in D, and because $g \geq_g h$ h cannot be satisfied by any negative example in D. Because h is satisfied by all positive examples in D and by no negative examples in D, h is consistent with D, and therefore h is a member of $VS_{H,D}$.
2. It can be proven by assuming some h in $VS_{H,D}$,that does not satisfy the right-hand side of the expression, then showing that this leads to an inconsistency

CANDIDATE-ELIMINATION Learning Algorithm

The CANDIDATE-ELIMINTION algorithm computes the version space containing all hypotheses from H that are consistent with an observed sequence of training examples.

Initialize G to the set of maximally general hypotheses in H
Initialize S to the set of maximally specific hypotheses in H
For each training example d, do

- If d is a positive example
  - Remove from G any hypothesis inconsistent with d
  - For each hypothesis s in S that is not consistent with d
    - Remove s from S
    - Add to S all minimal generalizations h of s such that
      - h is consistent with d, and some member of G is more general than h
    - Remove from S any hypothesis that is more general than another hypothesis in S

- If d is a negative example
  - Remove from S any hypothesis inconsistent with d
  - For each hypothesis g in G that is not consistent with d
    - Remove g from G
    - Add to G all minimal specializations h of g such that
      - h is consistent with d, and some member of S is more specific than h
    - Remove from G any hypothesis that is less general than another hypothesis in G

CANDIDATE- ELIMINTION algorithm using version spaces

An Illustrative Example

Example	Sky	AirTemp	Humidity	Wind	Water	Forecast	EnjoySport
1	Sunny	Warm	Normal	Strong	Warm	Same	Yes
2	Sunny	Warm	High	Strong	Warm	Same	Yes
3	Rainy	Cold	High	Strong	Warm	Change	No
4	Sunny	Warm	High	Strong	Cool	Change	Yes

CANDIDATE-ELIMINTION algorithm begins by initializing the version space to the set of all hypotheses in H;

Initializing the G boundary set to contain the most general hypothesis in H

$G_0 \langle ?, ?, ?, ?, ?, ? \rangle$

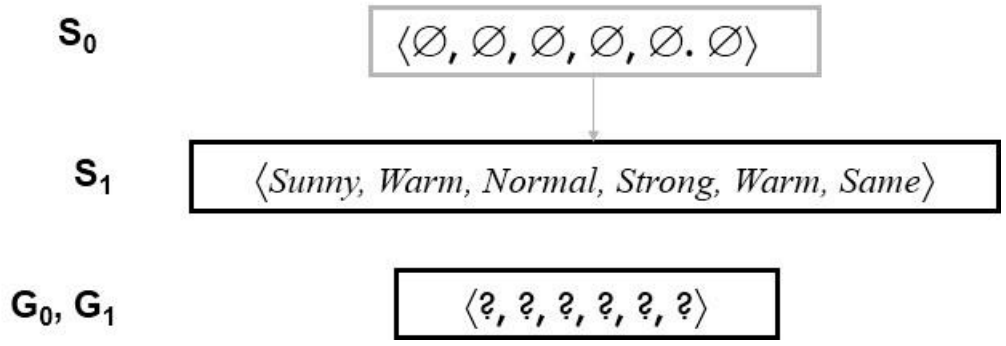
Initializing the S boundary set to contain the most specific (least general) hypothesis

$S_0 \langle \varnothing, \varnothing, \varnothing, \varnothing, \varnothing, \varnothing \rangle$

- When the first training example is presented, the CANDIDATE-ELIMINTION algorithm checks the S boundary and finds that it is overly specific and it fails to cover the positive example.
- The boundary is therefore revised by moving it to the least more general hypothesis that covers this new example
- No update of the G boundary is needed in response to this training example because G_o correctly covers this example

For training example d,

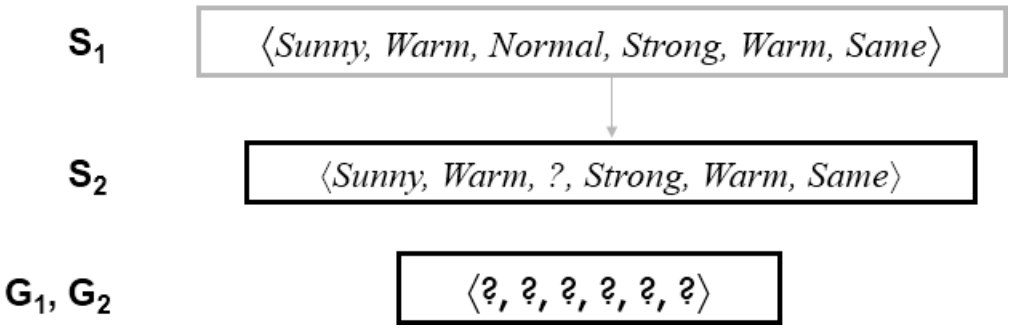
⟨Sunny, Warm, Normal, Strong, Warm, Same ⟩ +



- When the second training example is observed, it has a similar effect of generalizing S further to S_2, leaving G again unchanged i.e., $G_2 = G_1 = G_0$

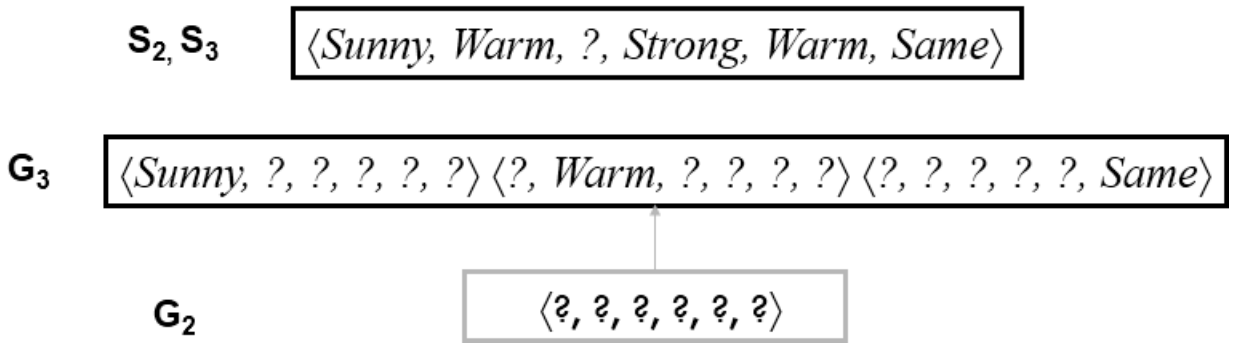
For training example d,

⟨Sunny, Warm, High, Strong, Warm, Same⟩ +



- Consider the third training example. This negative example reveals that the G boundary of the version space is overly general, that is, the hypothesis in G incorrectly predicts that this new example is a positive example.
- The hypothesis in the G boundary must therefore be specialized until it correctly classifies this new negative example

For training example d, ⟨Rainy, Cold, High, Strong, Warm, Change ⟩ –

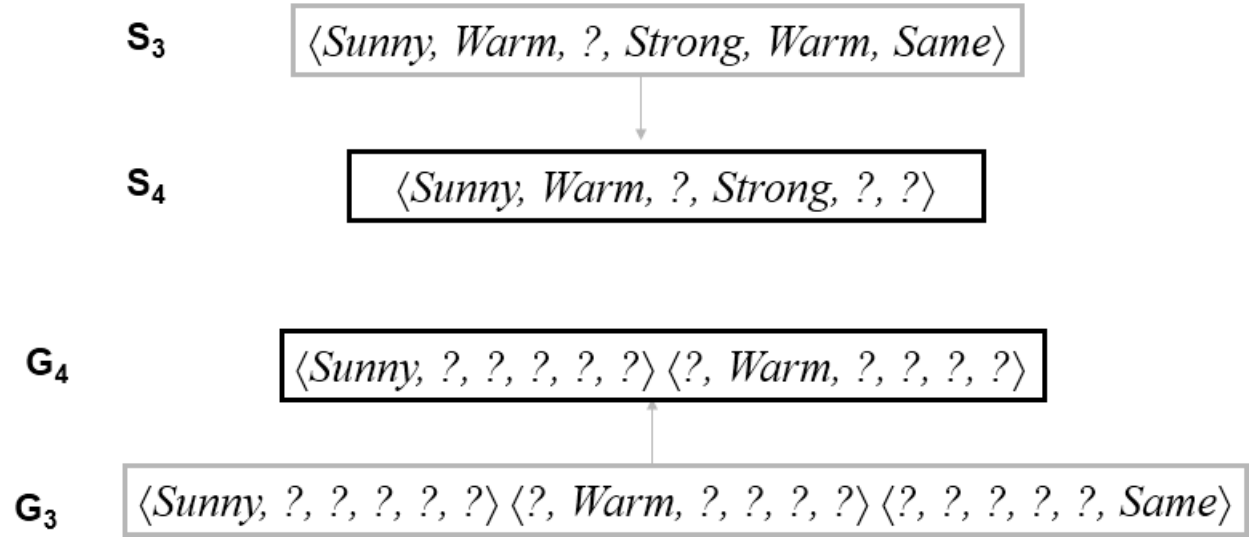


Given that there are six attributes that could be specified to specialize G_2, why are there only three new hypotheses in G_3?

For example, the hypothesis h = (?, ?, Normal, ?, ?, ?) is a minimal specialization of G_2 that correctly labels the new example as a negative example, but it is not included in G_3. The reason this hypothesis is excluded is that it is inconsistent with the previously encountered positive examples

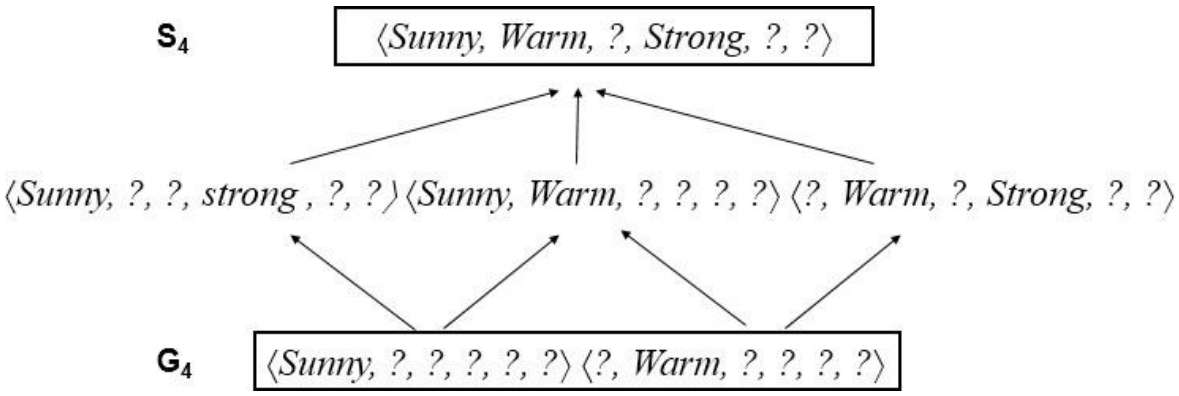
- Consider the fourth training example.

For training example d, ⟨Sunny, Warm, High, Strong, Cool Change ⟩ +



- This positive example further generalizes the S boundary of the version space. It also results in removing one member of the G boundary, because this member fails to cover the new positive example

After processing these four examples, the boundary sets S_4 and G_4 delimit the version space of all hypotheses consistent with the set of incrementally observed training examples.



INDUCTIVE BIAS

The fundamental questions for inductive inference

1. What if the target concept is not contained in the hypothesis space?
2. Can we avoid this difficulty by using a hypothesis space that includes every possible hypothesis?
3. How does the size of this hypothesis space influence the ability of the algorithm to generalize to unobserved instances?
4. How does the size of the hypothesis space influence the number of training examples that must be observed?

These fundamental questions are examined in the context of the CANDIDATE-ELIMINTION algorithm

A Biased Hypothesis Space

- Suppose the target concept is not contained in the hypothesis space *H*, then obvious solution is to enrich the hypothesis space to include every possible hypothesis.
  - Consider the ***EnjoySport*** example in which the hypothesis space is restricted to include only conjunctions of attribute values. Because of this restriction, the hypothesis space is unable to represent even simple disjunctive target concepts such as

    "Sky = Sunny or Sky = Cloudy."
  - The following three training examples of disjunctive hypothesis, the algorithm would find that there are zero hypotheses in the version space

⟨Sunny Warm Normal Strong Cool Change⟩	Y
⟨Cloudy Warm Normal Strong Cool Change⟩	Y
⟨Rainy Warm Normal Strong Cool Change⟩	N

  - If Candidate Elimination algorithm is applied, then it end up with empty Version Space. After first two training example

    S= ⟨? Warm Normal Strong Cool Change⟩

  - This new hypothesis is overly general and it incorrectly covers the third negative training example! So H does not include the appropriate c.
  - In this case, a more expressive hypothesis space is required.

An Unbiased Learner

- The solution to the problem of assuring that the target concept is in the hypothesis space H is to provide a hypothesis space capable of representing every teachable concept that is representing every possible subset of the instances X.
- The set of all subsets of a set X is called the power set of X

  - In the ***EnjoySport*** learning task the size of the instance space X of days described by the six attributes is 96 instances.
  - Thus, there are 2^{96} distinct target concepts that could be defined over this instance space and learner might be called upon to learn.
  - The conjunctive hypothesis space is able to represent only 973 of these - a biased hypothesis space indeed

  - Let us reformulate the ***EnjoySport*** learning task in an unbiased way by defining a new hypothesis space H' that can represent every subset of instances
  - The target concept "Sky = Sunny or Sky = Cloudy" could then be described as

(Sunny, ?, ?, ?, ?, ?) v (Cloudy, ?, ?, ?, ?, ?)

The Futility of Bias-Free Learning

Inductive learning requires some form of prior assumptions, or inductive bias

Definition:

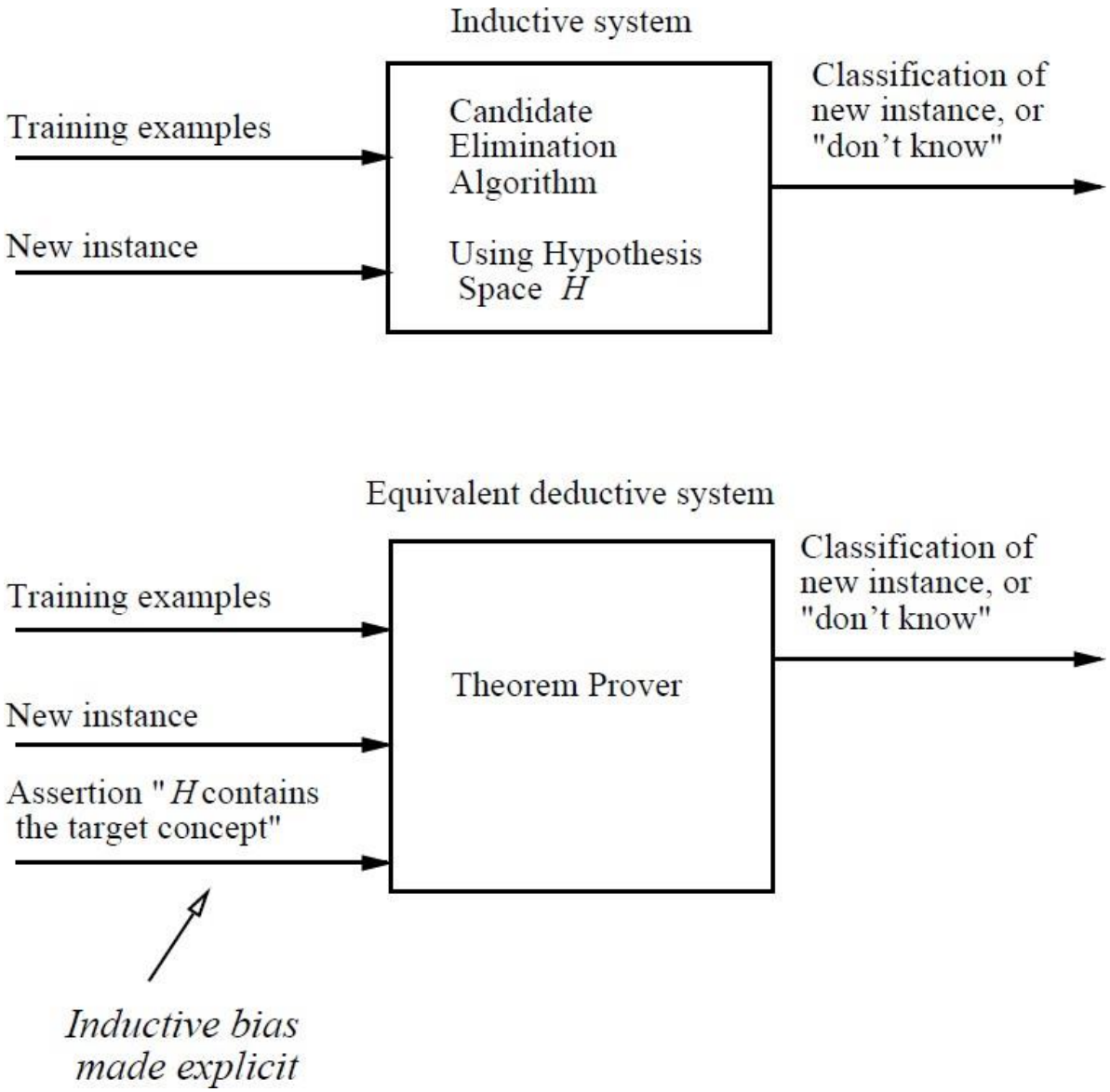
Consider a concept learning algorithm L for the set of instances X.

- Let c be an arbitrary concept defined over X
- Let $D_c = \{(x , c(x))\}$ be an arbitrary set of training examples of c.
- Let $L (x_i , D_c)$ denote the classification assigned to the instance x_i by L after training on the data D_c.
- The inductive bias of L is any minimal set of assertions B such that for any target concept c and corresponding training examples D_c

- $(\forall \langle x_i \in X) [(B \wedge D_c \wedge x_i) \vdash L (x_i, D_c)]$

The below figure explains

- Modelling inductive systems by equivalent deductive systems.
- The input-output behavior of the CANDIDATE-ELIMINATION algorithm using a hypothesis space H is identical to that of a deductive theorem prover utilizing the assertion "H contains the target concept." This assertion is therefore called the inductive bias of the CANDIDATE-ELIMINATION algorithm.
- Characterizing inductive systems by their inductive bias allows modelling them by their equivalent deductive systems. This provides a way to compare inductive systems according to their policies for generalizing beyond the observed training data.



Module-2

DECISION TREE LEARNING

INTRODUCTION

Decision tree learning is a method for approximating discrete-valued target functions, in which the learned function is represented by a decision tree. Learned trees can also be re-represented as sets of if-then rules to improve human readability. These learning methods are among the most popular of inductive inference algorithms and have been successfully applied to a broad range of tasks from learning to diagnose medical cases to learning to assess credit risk of loan applicants.

DECISION TREE REPRESENTATION

Decision trees classify instances by sorting them down the tree from the root to some leaf node, which provides the classification of the instance. Each node in the tree specifies a test of some attribute of the instance, and each branch descending from that node corresponds to one of the possible values for this attribute. An

instance is classified by starting at the root node of the tree, testing the attribute specified by this node, then moving down the tree branch corresponding to the value of the attribute in the given example. This process is then repeated for the subtree rooted at the new node.

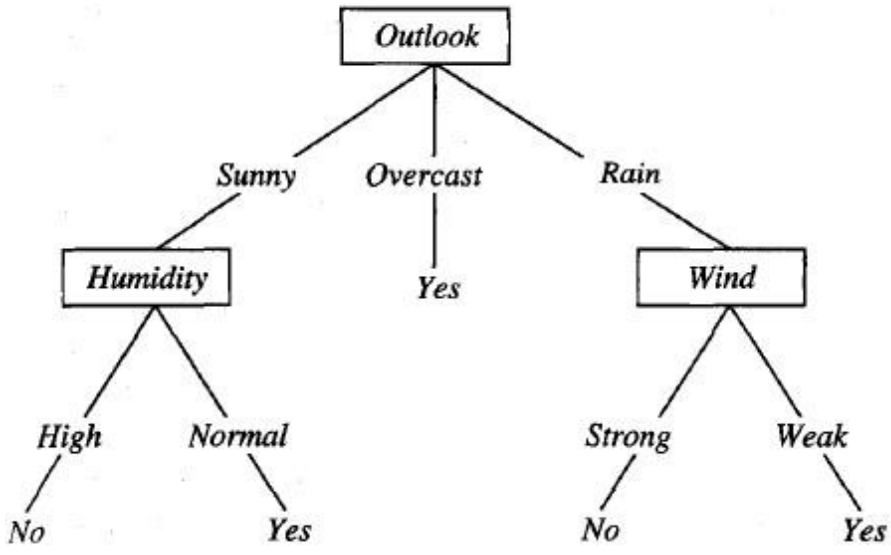


FIGURE 3.1
A decision tree for the concept *PlayTennis*. An example is classified by sorting it through the tree to the appropriate leaf node, then returning the classification associated with this leaf (in this case, *Yes* or *No*). This tree classifies Saturday mornings according to whether or not they are suitable for playing tennis.

Figure ***3.1*** illustrates a typical learned decision tree. This decision tree classifies Saturday mornings according to whether they are suitable for playing tennis. For example, the instance

(Outlook = ***Sunny, Temperature*** = ***Hot, Humidity*** = ***High, Wind*** = ***Strong)***

would be sorted down the leftmost branch of this decision tree and would therefore be classified as a negative instance (i.e., the tree predicts that ***PlayTennis*** = ***no).*** This tree and the example used in Table

to illustrate the ID3 learning algorithm are adapted from (Quinlan ***1986).*** In general, decision trees represent a disjunction of conjunctions of constraints on the attribute values of instances. Each path from the tree root to a leaf corresponds to a conjunction of attribute tests, and the tree itself to a disjunction of these conjunctions. For example, the decision tree shown in Figure 3.1 corresponds to the expression

(Outlook = ***Sunny*** **A** ***Humidity*** = ***Normal)***

V ***(Outlook*** = ***Overcast)***

v ***(Outlook*** = ***Rain A Wind*** = ***Weak)***

APPROPRIATE PROBLEMS FOR DECISION TREE LEARNING

Although a variety of decision tree learning methods have been developed with somewhat differing capabilities and requirements, decision tree learning is generally best suited to problems with the following characteristics:

- ***Instances are represented by attribute-value pairs.*** Instances are described by a fixed set of attributes (e.g., ***Temperature)*** and their values (e.g., ***Hot).*** The easiest situation for decision tree learning is when each attribute takes on small number of disjoint possible values (e.g., ***Hot, Mild, Cold).*** However, extensions to the basic algorithm (discussed in Section 3.7.2) allow handling real-valued attributes as well (e.g., representing ***Temperature*** numerically).
- ***The targetfunction has discrete output values.*** The decision tree in Figure 3.1assigns a boolean classification (e.g., ***yes*** or ***no)*** to each example. Decision tree methods easily extend to learning functions with more than two possible output values. A more substantial extension allows learning target functions with real-valued outputs, though the application of decision trees in this setting is less common.
- ***Disjunctive descriptions may be required.*** As noted above, decision trees naturally represent disjunctive expressions.
- ***The training data may contain errors.*** Decision tree learning methods are robust to errors, both errors in classifications of the training examples and errors in the attribute values that describe these examples.

- ***The training data may contain missing attribute values.*** Decision tree methods can be used even when some training examples have unknown values (e.g., if the ***Humidity*** of the day is known for only some of the training

  examples). This issue is discussed in Section 3.7.4.

Many practical problems have been found to fit these characteristics. Decision tree learning has therefore been applied to problems such as learning to classify medical patients by their disease, equipment malfunctions by their cause, and loan applicants by their likelihood of defaulting on payments. Such problems, in which the task is to classify examples into one of a discrete set of possible categories, are often referred to as ***classification problems.***

THE BASIC DECISION TREE LEARNING ALGORITHM

Most algorithms that have been developed for learning decision trees are variations on a core algorithm that employs a top-down, greedy search through the space of possible decision trees. This approach is exemplified by the ID3 algorithm

(Quinlan 1986) and its successor C4.5 (Quinlan 1993), which form the primary focus of our discussion here. In this section we present the basic algorithm for decision tree learning, corresponding approximately to the ID3 algorithm. In Section 3.7 we consider a number of extensions to this basic algorithm, including extensions incorporated into C4.5 and other more recent algorithms for decision tree learning. Our basic algorithm, ID3, learns decision trees by constructing them topdown, beginning with the question "which attribute should be tested at the root of the tree?"To answer this question, each instance attribute is evaluated using a statistical test to determine how well it alone classifies the training examples. The best attribute is selected and used as the test at the root node of the tree. A descendant of the root node is then created for each possible value of this attribute, and the training examples are sorted to the appropriate descendant node (i.e., down the branch corresponding to the example's value for this attribute). The entire process is then repeated using the training examples associated with each descendant node to select the best attribute to test at that point in the tree.This forms a greedy search for an acceptable decision tree, in which the algorithm never backtracks to reconsider earlier choices. **A** simplified version of the algorithm, specialized to learning boolean-valued functions (i.e., concept learning), is described in Table 3.1.

Which Attribute Is the Best Classifier?

The central choice in the ID3 algorithm is selecting which attribute to test at each node in the tree. We would like to select the attribute that is most useful for classifying examples. What is a good quantitative measure of the worth of an attribute? We will define a statistical property, called ***information gain,*** that measures how well a given attribute separates the training examples according to their target

classification. ID3 uses this information gain measure to select among the candidate attributes at each step while growing the tree.

$$Entropy(S) \equiv -p_{\oplus} \log_2 p_{\oplus} - p_{\ominus} \log_2 p_{\ominus} \qquad (3.1)$$

ID3(*Examples*, *Target_attribute*, *Attributes*)

Examples are the training examples. Target_attribute is the attribute whose value is to be predicted by the tree. Attributes is a list of other attributes that may be tested by the learned decision tree. Returns a decision tree that correctly classifies the given Examples.

- Create a *Root* node for the tree
- If all *Examples* are positive, Return the single-node tree *Root*, with label = +
- If all *Examples* are negative, Return the single-node tree *Root*, with label = −
- If *Attributes* is empty, Return the single-node tree *Root*, with label = most common value of *Target_attribute* in *Examples*
- Otherwise Begin
  - $A \leftarrow$ the attribute from *Attributes* that best* classifies *Examples*
  - The decision attribute for *Root* $\leftarrow A$
  - For each possible value, v_i, of A,
    - Add a new tree branch below *Root*, corresponding to the test $A = v_i$
    - Let $Examples_{v_i}$ be the subset of *Examples* that have value v_i for A
    - If $Examples_{v_i}$ is empty
      - Then below this new branch add a leaf node with label = most common value of *Target_attribute* in *Examples*
      - Else below this new branch add the subtree ID3($Examples_{v_i}$, *Target_attribute*, *Attributes* − {A}))
- End
- Return *Root*

---

* The best attribute is the one with highest *information gain*, as defined in Equation (3.4).

TABLE 3.1
Summary of the ID3 algorithm specialized to learning boolean-valued functions. ID3 is a greedy algorithm that grows the tree top-down, at each node selecting the attribute that best classifies the local training examples. This process continues until the tree perfectly classifies the training examples, or until all attributes have been used.

ENTROPY MEASURES HOMOGENEITY OF EXAMPLES

In order to define information gain precisely, we begin by defining a measure commonly used in information theory, called ***entropy.***

Definition of entropy:

It characterizes the (im)purity of an arbitrary collection of examples. Given a collection S(samples), containing positive and negative examples of some target concept, the entropy of S relative to this boolean classification is where p+, is the proportion of positive examples in S and p-, is the proportion of negative examples in S.

To illustrate, suppose S is a collection of 14 examples of some Boolean concept, including 9 positive and 5 negative examples (we adopt the notation [9+, 5-] to summarize such a sample of data). Then the entropy of S relative to this boolean classification is Notice that the entropy is 0 if all members of S belong to the same class. For example, if all members are positive (pe = I), then p, is 0, and Entropy(S) = $-1 \cdot \log_2(1) - 0 \cdot \log_2 0 = -1 \cdot 0 - 0 \cdot \log_2 0 = 0$. Note the entropy is 1 when the collection contains an equal number of positive and negative examples. If the collection contains unequal numbers of positive and negative examples, the entropy is between **0** and 1. Figure 3.2 shows the form of the entropy function relative to a boolean classification, as p+**,** varies between **0** and 1.

One interpretation of entropy from information theory is that it specifies the minimum number of bits of information needed to encode the classification of an arbitrary member of ***S*** (i.e., a member of ***S*** drawn at random with uniform probability). For example, if ***p,*** is 1, the receiver knows the drawn example will be positive, so no message need be sent, and the entropy is zero. On the other hand, if ***p+*** is 0.5, one bit is required to indicate whether the drawn example is positive or negative. If ***p+*** is 0.8, then a collection of messages can be encoded using on average less than 1 bit per message by assigning shorter codes to collections of positive examples and longer codes to less likely negative

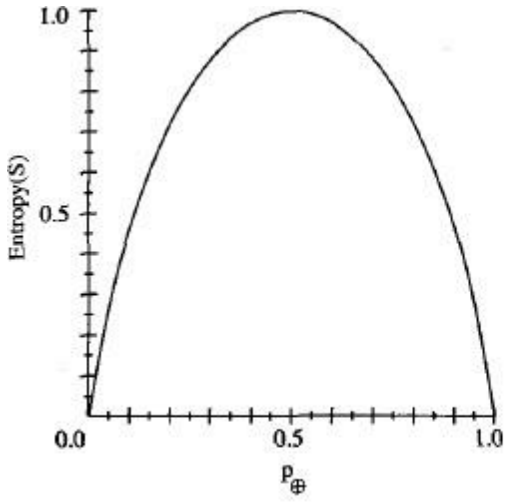


FIGURE 3.2
The entropy function relative to a boolean classification, as the proportion, $p_\oplus$, of positive examples varies between 0 and 1.

examples. Thus far we have discussed entropy in the special case where the target classification is boolean. More generally, if the target attribute can take on c different values, then the entropy of ***S*** relative to this c-wise classification is defined as

$$Entropy(S) \equiv \sum_{i=1}^{c} -p_i \log_2 p_i \qquad (3.3)$$

where ***pi*** is the proportion of ***S*** belonging to class ***i.*** Note the logarithm is still base 2 because entropy is a measure of the expected encoding length measured in ***bits.*** Note also that if the target attribute can take on c possible values, the entropy can be as large as log, ***c.***

INFORMATION GAIN MEASURES THE EXPECTED REDUCTION IN ENTROPY

Given entropy as a measure of the impurity in a collection of training examples, we can now define a measure of the effectiveness of an attribute in classifying the training data. The measure we will use, called ***information gain,*** is simply the expected reduction in entropy caused by partitioning the examples according to this attribute. More precisely, the information gain, ***Gain(S, A)*** of ***an*** attribute **A,** relative to a collection of examples ***S,*** is defined as

$$Gain(S, A) \equiv Entropy(S) - \sum_{v \in Values(A)} \frac{|S_v|}{|S|} Entropy(S_v) \qquad (3.4)$$

where ***Values(A)*** is the set of all possible values for attribute A, and ***S,*** is the subset of S for which attribute A has value v (i.e., $S_v = \{s \in S | A(s) = v\}$).

Note the first term in Equation ***(3.4)*** is just the entropy of the original collection ***S,*** and the second term is the expected value of the entropy after ***S*** is partitioned using attribute ***A.*** The expected entropy described by this second term is simply the sum of the entropies of each subset ***S,,*** weighted by the fraction of examples that belong to ***S,. Gain(S, A)*** is therefore the expected reduction in entropy caused by knowing the value of attribute A. Put another way, ***Gain(S, A)*** is the information provided about the ***target &action value,*** given the value of some other attribute ***A.*** The value of ***Gain(S, A)*** is the number of bits saved when encoding the target value of an arbitrary member of ***S,*** by knowing the value of attribute ***A.*** For example, suppose ***S*** is a collection of training-example days described by attributes including ***Wind,*** which can have the values ***Weak*** or ***Strong.*** As before, assume ***S*** is a collection containing ***14*** examples, [9+, 5-]. Of these 14 examples, suppose 6 of the positive and 2 of the negative examples have ***Wind*** = ***Weak,*** and the remainder have ***Wind*** = ***Strong.*** The information gain due to sorting the original ***14*** examples by the attribute ***Wind*** may then be calculated as

$$\begin{aligned}
Values(Wind) &= Weak, Strong \\
S &= [9+, 5-] \\
S_{Weak} &\leftarrow [6+, 2-] \\
S_{Strong} &\leftarrow [3+, 3-] \\
Gain(S, Wind) &= Entropy(S) - \sum_{v \in \{Weak, Strong\}} \frac{|S_v|}{|S|} Entropy(S_v) \\
&= Entropy(S) - (8/14) Entropy(S_{Weak}) \\
&\quad - (6/14) Entropy(S_{Strong}) \\
&= 0.940 - (8/14)0.811 - (6/14)1.00 \\
&= 0.048
\end{aligned}$$

Information gain is precisely the measure used by ID3 to select the best attribute at each step in growing the tree. The use of information gain to evaluate the relevance of attributes is summarized in Figure ***3.3.*** In this figure the information gain of two different attributes, ***Humidity*** and ***Wind,*** is computed in order to determine which is the better attribute for classifying the training examples shown in Table ***3.2.***

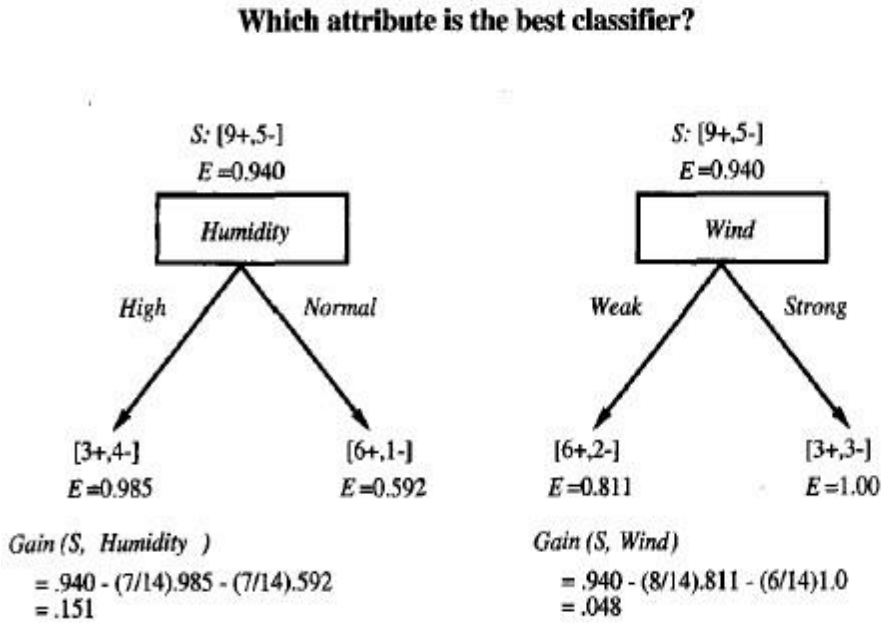


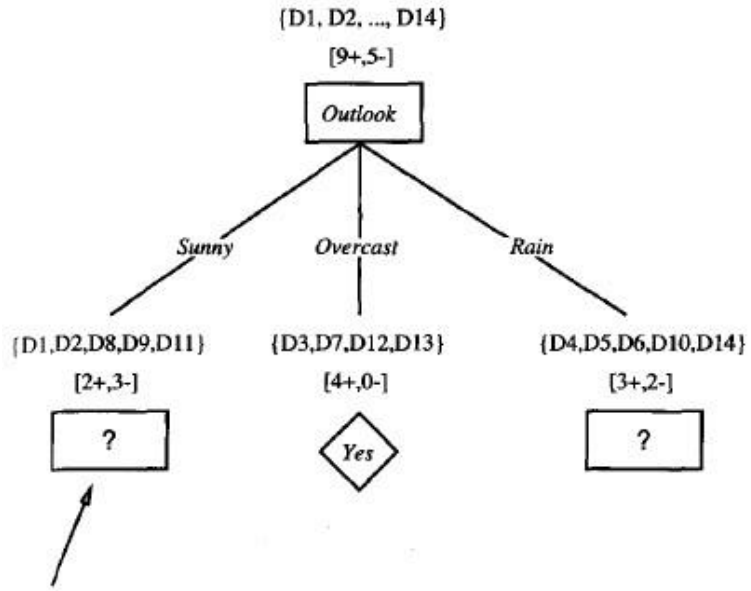
FIGURE 3.3
Humidity provides greater information gain than *Wind*, relative to the target classification. Here, *E* stands for entropy and *S* for the original collection of examples. Given an initial collection *S* of 9 positive and 5 negative examples, [9+, 5−], sorting these by their *Humidity* produces collections of [3+, 4−] (*Humidity* = *High*) and [6+, 1−] (*Humidity* = *Normal*). The information gained by this partitioning is .151, compared to a gain of only .048 for the attribute *Wind*.

An Illustrative Example

To illustrate the operation of ID3, consider the learning task represented by the training examples of Table 3.2. Here the target attribute ***PlayTennis,*** which can have values ***yes*** or ***no*** for different Saturday mornings, is to be predicted based on other attributes of the morning in question. Consider the first step through the algorithm, in which the topmost node of the decision tree is created. Which attribute should be tested first in the tree? ID3 determines the information gain for each candidate attribute (i.e., ***Outlook, Temperature, Humidity,*** and ***Wind),*** then gain for two of these attributes is shown in Figure 3.3.

Day	*Outlook*	*Temperature*	*Humidity*	*Wind*	*PlayTennis*
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

TABLE 3.2
Training examples for the target concept *PlayTennis*.



Which attribute should be tested here?

S_{sunny} = {D1,D2,D8,D9,D11}

Gain (S_{sunny}, *Humidity*) = .970 - (3/5) 0.0 - (2/5) 0.0 = .970

Gain (S_{sunny}, *Temperature*) = .970 - (2/5) 0.0 - (2/5) 1.0 - (1/5) 0.0 = .570

Gain (S_{sunny}, *Wind*) = .970 - (2/5) 1.0 - (3/5) .918 = .019

FIGURE 3.4
The partially learned decision tree resulting from the first step of ID3. The training examples are sorted to the corresponding descendant nodes. The *Overcast* descendant has only positive examples and therefore becomes a leaf node with classification *Yes*. The other two nodes will be further expanded, by selecting the attribute with highest information gain relative to the new subsets of examples.

The information gain values for all four attributes are

Gain(S, Outlook) = 0.246

Gain(S, Humidity) = 0.151

Gain(S, Wind) = 0.048

Gain(S, Temperature) = 0.029

where ***S*** denotes the collection of training examples from Table 3.2. According to the information gain measure, the ***Outlook*** attribute provides the best prediction of the target attribute, ***PlayTennis,*** over the training examples. Therefore, ***Outlook*** is selected as the decision attribute for the root node, and branches are created below the root for each of its possible values (i.e.***Sunny, Overcast,*** and ***Rain).*** The resulting partial decision tree is shown in Figure 3.4, along with the training examples sorted to each new descendant node. Note that every example for which ***Outlook*** = ***Overcast*** is also a positive example of ***PlayTennis.*** Therefore, this node of the tree becomes a leaf node with the classification ***PlayTennis*** = ***Yes.*** In contrast, the descendants corresponding to ***Outlook*** = ***Sunny*** and ***Outlook*** = ***Rain*** still have nonzero entropy, and the decision tree will be further elaborated below these nodes. The process of selecting a new attribute and partitioning the training examples is now repeated for each nontenninal descendant node, this time using only the training examples associated with that node. Attributes that have been incorporated higher in the tree are excluded, so that any given attribute can appear at most once along any path through the tree. This process continues for each new leaf node until either of two conditions is met: (1) every attribute has already been included along this path through the tree, or (2) the training examples associated with this leaf node all have the same target attribute value (i.e., their entropy is zero). Figure 3.4 illustrates the computations of information gain for the next step in growing the decision tree. The final decision tree learned by ID3 from the 14 training examples of Table 3.2 is shown in Figure 3.1.

HYPOTHESIS SPACE SEARCH IN DECISION TREE LEARNING

As with other inductive learning methods, ID3 can be characterized as searching a space of hypotheses for one that fits the training examples. The hypothesis space searched by ID3 is the set of possible decision trees. ID3 performs a simple-to complex, hill-climbing search through this hypothesis space, beginning with the empty tree, then considering progressively more elaborate hypotheses in search of a decision tree that correctly classifies the training data. The evaluation function that guides this hill-climbing search is the information gain measure. This search is depicted in Figure 3.5.

By viewing ID3 in terms of its search space and search strategy, we can get some insight into its capabilities and limitations.

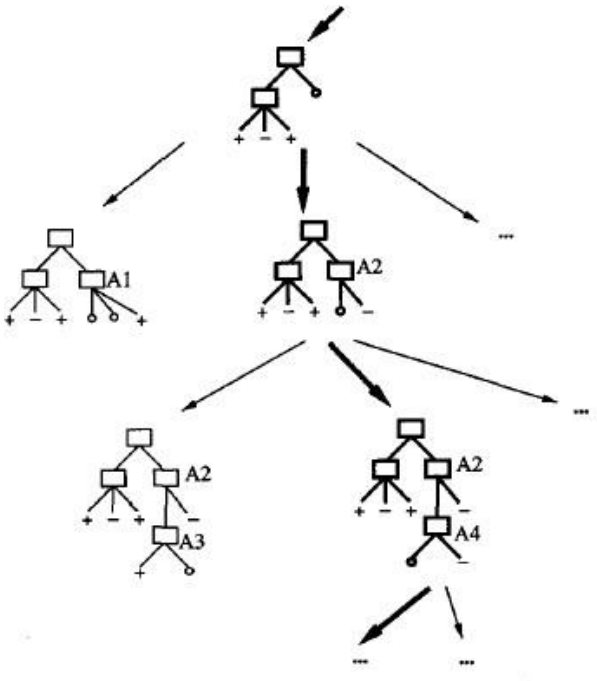


FIGURE 3.5
Hypothesis space search by ID3. ID3 searches through the space of possible decision trees from simplest to increasingly complex, guided by the information gain heuristic.

- **ID3's** hypothesis space of all decision trees is a ***complete*** space of finite discrete-valued functions, relative to the available attributes. Because every finite discrete-valued function can be represented by some decision tree, ID3

  avoids one of the major risks of methods that search incomplete hypothesis spaces (such as methods that consider only conjunctive hypotheses): that the hypothesis space might not contain the target function.
- **ID3** maintains only a single current hypothesis as it searches through the space of decision trees. This contrasts, for example, with the earlier version space candidate elimination method, which maintains the set of ***all*** hypotheses consistent with the available training examples. By determining only a single hypothesis, ID^ loses the capabilities that follow from explicitly representing all consistent hypotheses. For example, it does not have the ability to determine how many alternative decision trees are consistent with the available training data, or to pose new instance queries that optimally resolve among these competing hypotheses.
- **ID3** in its pure form performs no backtracking in its search. Once it, selects an attribute to test at a particular level in the tree, it never backtracks to reconsider this choice. Therefore, it is susceptible to the usual risks of hill-climbing search without backtracking: converging to locally optimal solutions that are not globally optimal. In the case of **ID3,** a locally optimal solution corresponds to the decision tree it selects along the single search path it explores. However, this locally optimal solution may be less desirable than trees that would have been encountered along a different branch of the search. Below we discuss an extension that adds a form of backtracking (post-pruning the decision tree).

- **ID3** uses all training examples at each step in the search to make statistically based decisions regarding how to refine its current hypothesis. This contrasts with methods that make decisions incrementally, based on individual training examples (e.g., FIND-S or CANDIDATE-ELIMINATOION).One advantage of using statistical properties of all the examples (e.g., information gain) is that the resulting search is much less sensitive to errors in individual training examples. **ID3** can be easily extended to handle noisy training data by modifying its termination criterion to accept hypotheses that imperfectly fit the training data.

INDUCTIVE BIAS IN DECISION TREE LEARNING

What is the policy by which ID3 generalizes from observed training examples to classify unseen instances? In other words, what is its inductive bias? Recall from Chapter 2 that inductive bias is the set of assumptions that, together with the training data, deductively justify the classifications assigned by the learner to future instances.

Given a collection of training examples, there are typically many decision trees consistent with these examples. Describing the inductive bias of ID3 therefore consists of describing the basis by which it chooses one of these consistent

hypotheses over the others. Which of these decision trees does ID3 choose? It chooses the first acceptable tree it encounters in its simple-to-complex, hill-climbing search through the space of possible trees. Roughly speaking, then, the ID3 search strategy (a) selects in favour of shorter trees over longer ones, and (b) selects trees that place the attributes with highest information gain closest to the root. Because of the subtle interaction between the attribute selection heuristic used by ID3 and the particular training examples it encounters, it is difficult to characterize precisely the inductive bias exhibited by ID3. However, we can approximately characterize its bias as a preference for short decision trees over complex trees.

Approximate inductive bias of ID3: Shorter trees are preferred over larger trees.

In fact, one could imagine an algorithm similar to ID3 that exhibits precisely this inductive bias. Consider an algorithm that begins with the empty tree and searches ***breadth First*** through progressively more complex trees, first considering

all trees of depth 1, then all trees of depth 2, etc. Once it finds a decision tree consistent with the training data, it returns the smallest consistent tree at that search depth (e.g., the tree with the fewest nodes). Let us call this breadth-first search algorithm BFS-ID3. BFS-ID3 finds a shortest decision tree and thus exhibits precisely the bias "shorter trees are preferred over longer trees." ID3 can be viewed as an efficient

approximation to BFS-ID3, using a greedy heuristic search to attempt to find the shortest tree without conducting the entire breadth-first search through the hypothesis space.

Because ID3 uses the information gain heuristic and a hill climbing strategy, it exhibits a more complex bias than BFS-ID3. In particular, it does not always find the shortest consistent tree, and it is biased to favor trees that place attributes with high information gain closest to the root.

A closer approximation to the inductive bias of ID3: Shorter trees are preferred over longer trees. Trees that place high information gain attributes close to the root are preferred over those that do not.

Restriction Biases and Preference Biases

There is an interesting difference between the types of inductive bias exhibited by ID3 and by the CANDIDATE-ELIMINATION algorithm discussed in Chapter 2.

Consider the difference between the hypothesis space search in these two approaches:

- ID3 searches a complete hypothesis space (i.e., one capable of expressing any finite discrete-valued function). It searches incompletely through this space, from simple to complex hypotheses, until its termination condition is met (e.g., until it finds a hypothesis consistent with the data). Its inductive bias is solely a consequence of the ordering of hypotheses by its search strategy. Its hypothesis space introduces no additional bias.
- The version space CANDIDATE-ELIMINATION algorithm searches an incomplete hypothesis space (i.e., one that can express only a subset of the potentially teachable concepts). It searches this space completely, finding every hypothesis consistent with the training data. Its inductive bias is solely a consequence of the expressive power of its hypothesis representation. Its search strategy introduces no additional bias.

In brief, the inductive bias of ID3 follows from its search strategy, whereas the inductive bias of the CANDIDATE-ELIMINATION algorithm follows from the definition of its search space.

The inductive bias of ID3 is thus a preference for certain hypotheses over others (e.g., for shorter hypotheses), with no hard restriction on the hypotheses that can be eventually enumerated. This form of bias is typically called a preference bias (or, alternatively, a search bias). In contrast, the bias of the CANDIDATEELIMINATION algorithm is in the form of a categorical restriction on the set of hypotheses considered. This form of bias is typically called a restriction bias (or, alternatively, a language bias).

Given that some form of inductive bias is required in order to generalize beyond the training data (see Chapter 2), which type of inductive bias shall we prefer; a preference bias or restriction bias?

Typically, a preference bias is more desirable than a restriction bias, because it allows the learner to work within a complete hypothesis space that is assured to contain the unknown target function. In contrast, a restriction bias that strictly limits the set of potential hypotheses is generally less desirable, because it introduces the possibility of excluding the unknown target function altogether.

Whereas ID3 exhibits a purely preference bias and CANDIDATE-ELIMINATION a purely restriction bias, some learning systems combine both.

Why Prefer Short Hypotheses?

Is ID3's inductive bias favouring shorter decision trees a sound basis for generalizing beyond the training data? Philosophers and others have debated this question for centuries, and the debate remains unresolved to this day. William of Occam was one of the first to discuss the question, around the year 1320, so this bias often goes by the name of Occam's razor.

Occam's razor: Prefer the simplest hypothesis that fits the data.

Of course giving an inductive bias a name does not justify it. Why should one prefer simpler hypotheses? Notice that scientists sometimes appear to follow this inductive bias. Physicists, for example, prefer simple explanations for the motions of the planets, over more complex explanations. Why? One argument is that because there are fewer short hypotheses than long ones (based on straightforward combinatorial arguments), it is less likely that one will find a short hypothesis that coincidentally fits the training data. In contrast there are often many very complex hypotheses that fit the current training data but fail to generalize correctly to subsequent data. Consider decision tree hypotheses, for example. There are many more 500-node decision trees than 5-node decision trees. Given a small set of 20 training examples, we might expect to be able to find many 500-node decision trees consistent with these, whereas we would be more surprised if a 5-node decision tree could perfectly fit this data. We might therefore believe the 5-node tree is less likely to be a statistical coincidence and prefer this hypothesis over the 500-node hypothesis.

Upon closer examination, it turns out there is a major difficulty with the above argument. By the same reasoning we could have argued that one should prefer decision trees containing exactly 17 leaf nodes with 11 nonleaf nodes, that

use the decision attribute $\mathbf{A_1}$ at the root, and test attributes $\mathbf{A_2}$ through $\mathbf{A_{11}}$, in numerical order. There are relatively few such trees, and we might argue (by the same reasoning as above) that our a priori chance of finding one consistent with an arbitrary set of data is therefore small. The difficulty here is that there are very many small sets of hypotheses that one can define-most of them rather arcane. Why should we believe that the small set of hypotheses consisting of decision trees with ***short descriptions*** should be any more relevant than the multitude of other small sets of hypotheses that we might define?

A second problem with the above argument for Occam's razor is that the size of a hypothesis is determined by the particular representation used ***internally*** by the learner. Two learners using different internal representations could therefore arrive at different hypotheses, both justifying their contradictory conclusions by Occam's razor! For example, the function represented by the learned decision tree in Figure 3.1 could be represented as a tree with just one decision node, by a learner that uses the boolean attribute XYZ, where we define the attribute XYZ to be true for instances that are classified positive by the decision tree in Figure 3.1 and false otherwise. Thus, two learners, both applying Occam's razor, would generalize in different ways if one used the XYZ attribute to describe its examples and the other used only the attributes ***Outlook, Temperature, Humidity,*** and ***Wind.***

This last argument shows that Occam's razor will produce two different hypotheses from the same training examples when it is applied by two learners basis we might be tempted to reject Occam's razor altogether. However, consider the following scenario that examines the question of which internal representations might arise from a process of evolution and natural selection. Imagine a population of artificial learning agents created by a simulated evolutionary process involving reproduction, mutation, and natural selection of these agents. Let us assume that this evolutionary process can alter the perceptual systems of these agents from generation to generation, thereby changing the internal attributes by which they perceive their world. For the sake of argument, let us also assume that the learning agents employ a fixed learning algorithm (say ID3) that cannot be altered by evolution. It is reasonable to assume that over time evolution will produce internal representation that make these agents increasingly successful within their environment. Assuming that the success of an agent depends highly on its ability to generalize accurately, we would therefore expect evolution to develop internal representations that work well with whatever learning algorithm and inductive bias is present. If the species of agents employs a learning algorithm whose inductive bias is Occam's razor, then we expect evolution to produce internal representations for which Occam's razor is a successful strategy. The essence of the
argument here is that evolution will create internal representations that make the learning algorithm's inductive bias a self-fulfilling prophecy, simply because it can alter the representation easier than it can alter the learning algorithm.

ISSUES IN DECISION TREE LEARNING

Practical issues in learning decision trees include determining how deeply to grow the decision tree, handling continuous attributes, choosing an appropriate attribute selection measure, handling training data with missing attribute values, handling attributes with differing costs, and improving computational efficiency. Below we discuss each of these issues and extensions to the basic ID3 algorithm that address them. ID3 has itself been extended to address most of these issues, with the resulting system renamed C4.5 (Quinlan 1993).

Avoiding Overfitting the Data

The algorithm described in Table 3.1 grows each branch of the tree just deeply enough to perfectly classify the training examples. While this is sometimes a reasonable strategy, in fact it can lead to difficulties when there is noise in the data,

or when the number of training examples is too small to produce a representative sample of the true target function. In either of these cases, this simple algorithm can produce trees that ***overfit*** the training examples.

We will say that a hypothesis overfits the training examples if some other hypothesis that fits the training examples less well actually performs better over the entire distribution of instances (i.e., including instances beyond the training set).

Definition: **Given a hypothesis space H, a hypothesis *h* ε H is said to overlit the training data if there exists some alternative hypothesis *h'* ε H, such that *h* has smaller error than *h'* over the training examples, but *h'* has a smaller error than *h* over the entire distribution of instances.**

Figure 3.6 illustrates the impact of overfitting in a typical application of decision tree learning. In this case, the ID3 algorithm is applied to the task of learning which medical patients have a form of diabetes. The horizontal axis of this plot indicates the total number of nodes in the decision tree, as the tree is being constructed. The vertical axis indicates the accuracy of predictions made by the tree. The solid line shows the accuracy of the decision tree over the training examples, whereas the broken line shows accuracy measured over an independent set of test examples (not included in the training set). Predictably, the accuracy of the tree over the training examples increases monotonically as the tree is grown. However, the accuracy measured over the independent test examples first increases, then decreases. As can be seen, once the tree size exceeds approximately *25* nodes, further elaboration of the tree decreases its accuracy over the test examples despite increasing its accuracy on the training examples.

How can it be possible for tree h to fit the training examples better than h', but for it to perform more poorly over subsequent examples? One way this can occur is when the training examples contain random errors or noise. To illustrate, consider the effect of adding the following positive training example, incorrectly labeled as negative, to the (otherwise correct) examples in Table 3.2.

(Outlook = Sunny, Temperature = Hot, Humidity = Normal, Wind = Strong, PlayTennis = No)

Given the original error-free data, ID3 produces the decision tree shown in Figure 3.1. However, the addition of this incorrect example will now cause ID3 to construct a more complex tree. In particular, the new example will be sorted into the second leaf node from the left in the learned tree of Figure 3.1, along with the previous positive examples D9 and Dl 1. Because the new example is labeled as a negative

example, ID3 will search for further refinements to the tree below this node. Of course as long as the new erroneous example differs in some arbitrary way from the other examples affiliated with this node, ID3 will succeed in finding a new decision attribute to separate out this new example from the two previous positive examples at this tree node. The result is that ID3 will output a decision tree (h) that is more complex than the original tree from Figure 3.1 (h'). Of course h will fit the collection of training examples perfectly, whereas the simpler h' will not. However, given that the new decision node is simply a consequence of fitting the noisy training example, we expect h to outperform h' over subsequent data drawn from the same instance distribution.

The above example illustrates how random noise in the training examples can lead to overfitting. In fact, overfitting is possible even when the training data are noise-free, especially when small numbers of examples are associated with leaf nodes. In this case, it is quite possible for coincidental regularities to occur, in which some attribute happens to partition the examples very well, despite being unrelated to the actual target function. Whenever such coincidental regularities exist, there is a risk of overfitting.

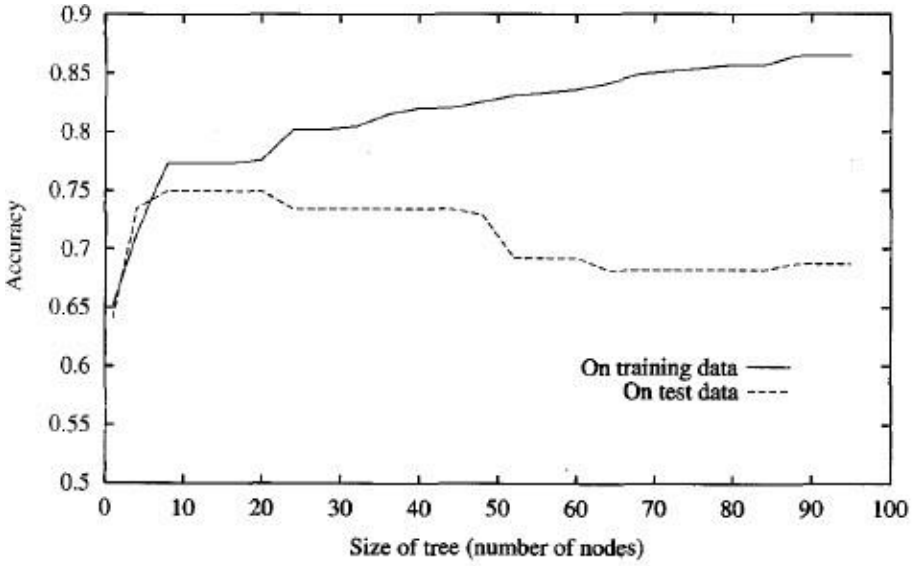


FIGURE 3.6
Overfitting in decision tree learning. As ID3 adds new nodes to grow the decision tree, the accuracy of the tree measured over the training examples increases monotonically. However, when measured over a set of test examples independent of the training examples, accuracy first increases, then decreases. Software and data for experimenting with variations on this plot are available on the World Wide Web at http://www.cs.cmu.edu/~tom/mlbook.html.

Overfitting is a significant practical difficulty for decision tree learning and many other learning methods. For example, in one experimental study of ID3 involving five different learning tasks with noisy, nondeterministic data (Mingers 1989b), overfitting was found to decrease the accuracy of learned decision trees by 10-25% on most problems.

There are several approaches to avoiding overfitting in decision tree learning.

These can be grouped into two classes:

- approaches that stop growing the tree earlier, before it reaches the point where it perfectly classifies the training data,
- approaches that allow the tree to overfit the data, and then post-prune the tree.

Although the first of these approaches might seem more direct, the second approach of post-pruning overfit trees has been found to be more successful in practice. This is due to the difficulty in the first approach of estimating precisely
when to stop growing the tree.

Regardless of whether the correct tree size is found by stopping early or by post-pruning, a key question is what criterion is to be used to determine the correct final tree size. Approaches include:

- Use a separate set of examples, distinct from the training examples, to evaluate the utility of post-pruning nodes from the tree.
- Use all the available data for training, but apply a statistical test to estimate whether expanding (or pruning) a particular node is likely to produce an improvement beyond the training set. For example, Quinlan (1986) uses a chi-square test to estimate whether further expanding a node is likely to improve performance over the entire instance distribution, or only on the current sample of training data.
- Use an explicit measure of the complexity for encoding the training examples and the decision tree, halting growth of the tree when this encoding size is minimized. This approach, based on a heuristic called the Minimum Description Length principle, is discussed further in Chapter 6, as well as in Quinlan and Rivest (1989) and Mehta et al. (1995).

The first of the above approaches is the most common and is often referred to as a training and validation set approach. We discuss the two main variants of this approach below. In this approach, the available data are separated into two sets of examples: a training set, which is used to form the learned hypothesis, and a separate validation set, which is used to evaluate the accuracy of this hypothesis over subsequent data and, in particular, to evaluate the impact of pruning this hypothesis. The motivation is this: Even though the learner may be misled by random errors and coincidental regularities within the training set, the validation set is unlikely to exhibit the same random fluctuations. Therefore, the validation set can be expected to provide a safety check against overfitting the spurious characteristics of the training set. Of course, it is important that the validation set be large enough to itself provide a statistically significant sample of the instances. One common heuristic is to withhold one-third of the available examples for the validation set, using the other two-thirds for training.

REDUCED ERROR PRUNING

How exactly might we use a validation set to prevent overfitting? One approach, called reduced-error pruning (Quinlan 1987), is to consider each of the decision nodes in the.tree to be candidates for pruning. Pruning a decision node consists of removing the subtree rooted at that node, making it a leaf node, and assigning it the most common classification of the training examples affiliated with that node. Nodes are removed only if the resulting pruned tree performs no worse than-the original over the validation set. This has the effect that any leaf node added due to coincidental regularities in the training set is likely to be pruned because these same coincidences are unlikely to occur in the validation set. Nodes are pruned iteratively, always choosing the node whose removal most increases the decision tree accuracy over the validation set. Pruning of nodes continues until further pruning is harmful (i.e., decreases accuracy of the tree over the validation set).

The impact of reduced-error pruning on the accuracy of the decision tree is illustrated in Figure **3.7.** As in Figure **3.6,** the accuracy of the tree is shown measured over both training examples and test examples. The additional line in Figure **3.7** shows accuracy over the test examples as the tree is pruned. When pruning begins, the tree is at its maximum size and lowest accuracy over the test set. As pruning proceeds, the number of nodes is reduced and accuracy over the test set increases. Here, the available data has been split into three subsets: the training examples, the validation examples used for pruning the tree, and a set of test examples used to provide an unbiased estimate of accuracy over future unseen examples. The plot shows accuracy over the training and test sets. Accuracy over the validation set used for pruning is not shown.

Using a separate set of data to guide pruning is an effective approach provided a large amount of data is available. The major drawback of this approach is that when data is limited, withholding part of it for the validation set reduces even further the number of examples available for training. The following section presents an alternative approach to pruning that has been found useful in many practical situations where data is limited. Many additional techniques have been proposed **as** well, involving partitioning the available data several different times in multiple ways, then averaging the results. Empirical evaluations of alternative tree pruning methods are reported by Mingers (1989b) and by Malerba et al. (1995).

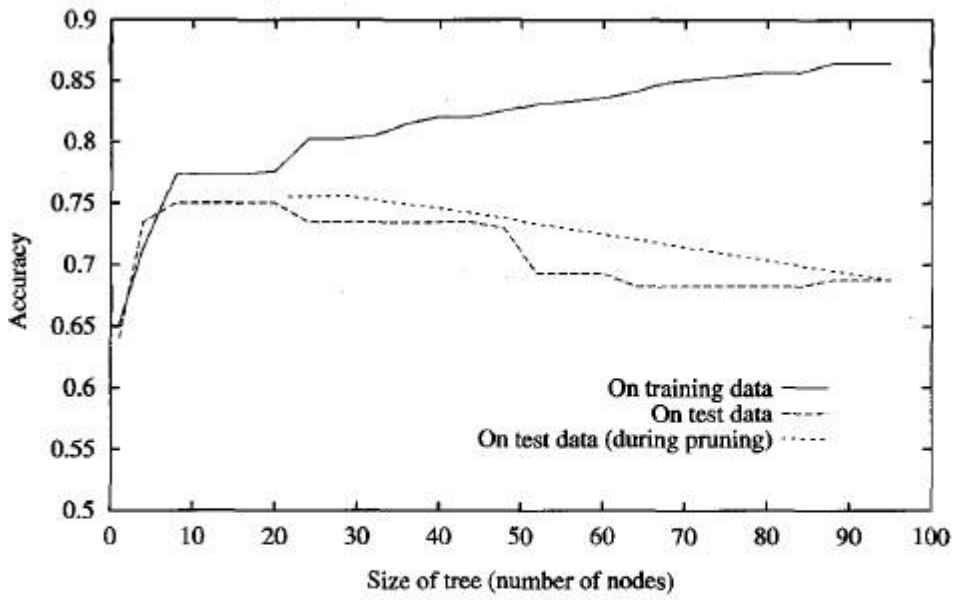


FIGURE 3.7
Effect of reduced-error pruning in decision tree learning. This plot shows the same curves of training and test set accuracy as in Figure 3.6. In addition, it shows the impact of reduced error pruning of the tree produced by ID3. Notice the increase in accuracy over the test set as nodes are pruned from the tree. Here, the validation set used for pruning is distinct from both the training and test sets.

RULE POST-PRUNING

In practice, one quite successful method for finding high accuracy hypotheses is a technique we shall call rule post-pruning. A variant of this pruning method is used by C4.5 (Quinlan 1993), which is an outgrowth of the original ID3 algorithm. Rule post-pruning involves the following steps:

1. Infer the decision tree from the training set, growing the tree until the training data is fit as well as possible and allowing overfitting to occur.

2. Convert the learned tree into an equivalent set of rules by creating one rule for each path from the root node to a leaf node.

3. Prune (generalize) each rule by removing any preconditions that result in improving its estimated accuracy.

4. Sort the pruned rules by their estimated accuracy, and consider them in this sequence when classifying subsequent instances.

To illustrate, consider again the decision tree in Figure 3.1. In rule postpruning, one rule is generated for each leaf node in the tree. Each attribute test along the path from the root to the leaf becomes a rule antecedent (precondition) and the classification at the leaf node becomes the rule consequent (postcondition). For example, the leftmost path of the tree in Figure 3.1 is translated into the rule

IF (Outlook = Sunny) A (Humidity = High) THEN PlayTennis = No

Next, each such rule is pruned by removing any antecedent, or precondition, whose removal does not worsen its estimated accuracy. Given the above rule, for example, rule post-pruning would consider removing the preconditions

(Outlook = Sunny) and (Humidity = High). It would select whichever of these pruning steps produced the greatest improvement in estimated rule accuracy, then consider pruning the second precondition as a further pruning step. No pruning step is performed if it reduces the estimated rule accuracy.

As noted above, one method to estimate rule accuracy is to use a validation set of examples disjoint from the training set. Another method, used by C4.5, is to evaluate performance based on the training set itself, using a pessimistic estimate to make up for the fact that the training data gives an estimate biased in favour of the rules. More precisely, C4.5 calculates its pessimistic estimate by calculating the rule accuracy over the training examples to which it applies, then calculating the standard deviation in this estimated accuracy assuming a binomial distribution. For a given confidence level, the lower-bound estimate is then taken as the measure of rule performance (e.g., for a 95% confidence interval, rule accuracy is pessimistically estimated by the observed accuracy over the training set, minus 1.96 times the estimated standard deviation). The net effect is that for large data sets, the pessimistic estimate is very close to the observed accuracy (e.g., the standard deviation is very small), whereas it grows further from the observed accuracy as the size of the data set decreases. Although this heuristic method is not statistically valid, it has nevertheless been found useful in practice. See Chapter 5 for a discussion of statistically valid approaches to estimating means and confidence intervals.

Why convert the decision tree to rules before pruning? There are three main advantages.

- Converting to rules allows distinguishing among the different contexts in which a decision node is used. Because each distinct path through the decision tree node produces a distinct rule, the pruning decision regarding that attribute test can be made differently for each path. In contrast, if the tree itself were pruned, the only two choices would be to remove the decision node completely, or to retain it in its original form.
- Converting to rules removes the distinction between attribute tests that occur near the root of the tree and those that occur near the leaves. Thus, we avoid messy bookkeeping issues such as how to reorganize the tree if the root node is pruned while retaining part of the subtree below this test.
- Converting to rules improves readability. Rules are often easier for people to understand.

Incorporating Continuous-Valued Attributes

Our initial definition of ID3 is restricted to attributes that take on a discrete set of values. First, the target attribute whose value is predicted by the learned tree must be discrete valued. Second, the attributes tested in the decision nodes of

the tree must also be discrete valued. This second restriction can easily be removed so that continuous-valued decision attributes can be incorporated into the learned tree. This can be accomplished by dynamically defining new discrete valued attributes that partition the continuous attribute value into a discrete set of intervals. In particular, for an attribute A that is continuous-valued, the algorithm can dynamically create a new boolean attribute A_c that is true if $A < c$
and false otherwise. The only question is how to select the best value for the threshold c.

As an example, suppose we wish to include the continuous-valued attribute ***Temperature*** in describing the training example days in the learning task of Table 3.2. Suppose further that the training examples associated with a particular node in the decision tree have the following values for ***Temperature*** and the target attribute ***PlayTennis.***

Temperature:	40	48	60	72	80	90
PlayTennis:	No	No	Yes	Yes	Yes	No

What threshold-based boolean attribute should be defined based on Temperature? Clearly, we would like to pick a threshold, ***c,*** that produces the greatest information gain. By sorting the examples according to the continuous attribute
A, then identifying adjacent examples that differ in their target classification, we can generate a set of candidate thresholds midway between the corresponding values of ***A.*** It can be shown that the value of ***c*** that maximizes information gain must always lie at such a boundary (Fayyad 1991). These candidate thresholds can then be evaluated by computing the information gain associated with each. In the current example, there are two candidate thresholds, corresponding to the values of Temperature at which the value of PlayTennis changes: (48 + 60)/2, and (80 + 90)/2.
The information gain can then be computed for each of the candidate attributes, Temperature>54 and Temperature>85 the best can be selected (Temperature>54). This dynamically created boolean attribute can then compete with the other discrete-valued candidate attributes available for growing the decision tree. Fayyad and Irani (1993) discuss an extension to this approach that splits the continuous attribute into multiple intervals rather than just two intervals based on a single threshold. Utgoff and Brodley (1991) and Murthy et al. (1994) discuss approaches that define features by thresholding linear combinations of several continuous-valued attributes.

Alternative Measures for Selecting Attributes

There is a natural bias in the information gain measure that favors attributes with many values over those with few values. As an extreme example, consider the attribute Date, which has a very large number of possible values (e.g., March 4, 1979). If we were to add this attribute to the data in Table 3.2, it would have the highest information gain of any of the attributes. This is because Date alone perfectly

predicts the target attribute over the training data. Thus, it would be selected as the decision attribute for the root node of the tree and lead to a (quite broad) tree of depth one, which perfectly classifies the training data. Of course, this decision tree would fare poorly on subsequent examples, because it is not a useful predictor despite the fact that it perfectly separates the training data.

What is wrong with the attribute Date? Simply put, it has so many possible values that it is bound to separate the training examples into very small subsets. Because of this, it will have a very high information gain relative to the training examples, despite being a very poor predictor of the target function over unseen instances.

One way to avoid this difficulty is to select decision attributes based on some measure other than information gain. One alternative measure that has been used successfully is the gain ratio (Quinlan 1986). The gain ratio measure penalizes attributes such as Date by incorporating a term, called split information, that is sensitive to how broadly and uniformly the attribute splits the data:

$$SplitInformation(S, A) \equiv -\sum_{i=1}^{c} \frac{|S_i|}{|S|} \log_2 \frac{|S_i|}{|S|} \qquad (3.5)$$

where S1 through S, are the ***c*** subsets of examples resulting from partitioning S by the c-valued attribute A. Note that Split Information is actually the entropy of S with respect to the values of attribute A. This is in contrast to our previous

uses of entropy, in which we considered only the entropy of S with respect to the target attribute whose value is to be predicted by the learned tree.

The Gain Ratio measure is defined in terms of the earlier Gain measure, as well as this Split information, as follows

$$GainRatio(S, A) \equiv \frac{Gain(S, A)}{Split\,Information(S, A)} \qquad (3.6)$$

Notice that the Split information term discourages the selection of attributes with many uniformly distributed values. For example, consider a collection of n examples that are completely separated by attribute A (e.g., Date). In this case, the Split information value will be log, n. In contrast, a boolean attribute B that splits the same n examples exactly in half will have Split information of 1. If attributes A and B produce the same information gain, then clearly B will score higher according to the Gain Ratio measure.

One practical issue that arises in using GainRatio in place of Gain to select attributes is that the denominator can be zero or very small when |Si | = |S | for one of the Si. This either makes the GainRatio undefined or very large for

attributes that happen to have the same value for nearly all members of S. To avoid selecting attributes purely on this basis, we can adopt some heuristic such as first calculating the Gain of each attribute, then applying the GainRatio test
only considering those attributes with above average Gain (Quinlan 1986).

An alternative to the GainRatio, designed to directly address the above difficulty, is a distance-based measure introduced by Lopez de Mantaras (1991). This measure is based on defining a distance metric between partitions of 'the data. Each attribute is evaluated based on the distance between the data partition it creates and the perfect partition (i.e., the partition that perfectly classifies the training data). The attribute whose partition is closest to the perfect partition is chosen. Lopez de Mantaras (1991) defines this distance measure, proves that it is not biased toward attributes with large numbers of values, and reports experimental studies indicating that the predictive accuracy of the induced trees is not significantly different from that obtained with the Gain and Gain Ratio measures. However, this distance measure avoids the practical difficulties associated with the GainRatio measure, and in his experiments it produces significantly smaller trees in the case of data sets whose attributes have very different numbers of values.

A variety of other selection measures have been proposed as well (e.g., see Breiman et al. 1984; Mingers 1989a; Kearns and Mansour 1996; Dietterich et al. 1996). Mingers (1989a) provides an experimental analysis of the relative
effectiveness of several selection measures over a variety of problems. He reports significant differences in the sizes of the unpruned trees produced by the different selection measures. However, in his experimental domains the choice of attribute selection measure appears to have a smaller impact on final accuracy than does the extent and method of post-pruning.

Handling Training Examples with Missing Attribute Values

In certain cases, the available data may be missing values for some attributes. For example, in a medical domain in which we wish to predict patient outcome based on various laboratory tests, it may be that the lab test Blood-Test-Result is available only for a subset of the patients. In such cases, it is common to estimate the missing attribute value based on other examples for which this attribute has a known value.

Consider the situation in which ***Gain(S, A)*** is to be calculated at node ***n*** in the decision tree to evaluate whether the attribute ***A*** is the best attribute to test at this decision node. Suppose that ***(x, c(x))*** is one of the training examples in ***S***
and that the value ***A(x)*** is unknown.

One strategy for dealing with the missing attribute value is to assign it the value that is most common among training examples at node ***n.*** Alternatively, we might assign it the most common value among examples at node ***n*** that have the classification ***c(x).*** The elaborated training example using this

estimated value for ***A(x)*** can then be used directly by the existing decision tree learning algorithm. This strategy is examined by Mingers (1989a).

A second, more complex procedure is to assign a probability to each of the possible values of ***A*** rather than simply assigning the most common value to ***A(x).*** These probabilities can be estimated again based on the observed frequencies of the various values for ***A*** among the examples at node ***n.*** For example, given a boolean attribute ***A,*** if node ***n*** contains six known examples with ***A*** = 1 and four with ***A*** = 0, then we would say the probability that ***A(x)*** = 1 is 0.6, and the probability that ***A(x)*** = 0 is 0.4. A fractional 0.6 of instance ***x*** is now distributed down the branch for ***A*** = 1, and a fractional 0.4 of ***x*** down the other tree branch. These fractional examples are used for the purpose of computing information ***Gain*** and can be further subdivided at subsequent branches of the tree if a second missing attribute value must be tested. This same fractioning of examples can also be applied after learning, to classify new instances whose attribute values are unknown. In this case, the classification of the new instance is simply the most probable classification, computed by summing the weights of the instance fragments classified in different ways at the leaf nodes of the tree. This method for handling missing attribute values is used in C4.5 (Quinlan 1993).

Handling Attributes with Differing Costs

In some learning tasks the instance attributes may have associated costs. For example, in learning to classify medical diseases we might describe patients in terms of attributes such **as** Temperature, BiopsyResult, Pulse, BloodTestResults, etc. These attributes vary significantly in their costs, both in terms of monetary cost and cost to patient comfort. In such tasks, we would prefer decision trees that use low-cost attributes where possible, relying on high-cost attributes only when needed to produce reliable classifications.

ID3 can be modified to take into account attribute costs by introducing a cost term into the attribute selection measure. For example, we might divide the ***Gain*** by the cost of the attribute, so that lower-cost attributes would be preferred. While such cost-sensitive measures do not guarantee finding an optimal cost-sensitive decision tree, they do bias the search in favor of low-cost attributes.

Tan and Schlimmer (1990) and Tan (1993) describe one such approach and apply it to a robot perception task in which the robot must learn to classify different objects according to how they can be grasped by the robot's manipulator.

In this case the attributes correspond to different sensor readings obtained by movable sonar on the robot. Attribute cost is measured by the number of seconds required to obtain the attribute value by positioning and operating the sonar. They demonstrate that more efficient recognition strategies are learned, without sacrificing classification accuracy, by replacing the information gain attribute selection measure by the following measure

$$\frac{Gain^2(S, A)}{Cost(A)}$$

Nunez (1988) describes a related approach and its application to learning medical diagnosis rules. Here the attributes are different symptoms and laboratory tests with differing costs. His system uses a somewhat different attribute selection

Measure

$$\frac{2^{Gain(S,A)} - 1}{(Cost(A) + 1)^w}$$

where ***w*** **belongs** [0, 1] is a constant that determines the relative importance of cost versus information gain. Nunez (1991) presents an empirical comparison of these two approaches over a range of tasks.

MODULE 3

ARTIFICIAL NEURAL NETWORKS

INTRODUCTION

Artificial neural networks (ANNs) provide a general, practical method for learning real-valued, discrete-valued, and vector-valued target functions.

Biological Motivation

- The study of artificial neural networks (ANNs) has been inspired by the observation that biological learning systems are built of very complex webs of interconnected ***Neurons***
- Human information processing system consists of brain ***neuron***: basic building block cell that communicates information to and from various parts of body

Facts of Human Neurobiology

- Number of neurons ~ 10^{11}
- Connection per neuron ~ 10^{4-5}
- Neuron switching time ~ 0.001 second or 10^{-3}
- Scene recognition time ~ 0.1 second
- 100 inference steps doesn't seem like enough
- Highly parallel computation based on distributed representation

Properties of Neural Networks

- Many neuron-like threshold switching units
- Many weighted interconnections among units
- Highly parallel, distributed process
- Emphasis on tuning weights automatically
- Input is a high-dimensional discrete or real-valued (e.g, sensor input)

NEURAL NETWORK REPRESENTATIONS

- A prototypical example of ANN learning is provided by Pomerleau's system ALVINN, which uses a learned ANN to steer an autonomous vehicle driving at normal speeds on public highways
- The input to the neural network is a 30x32 grid of pixel intensities obtained from a forward-pointed camera mounted on the vehicle.
- The network output is the direction in which the vehicle is steered

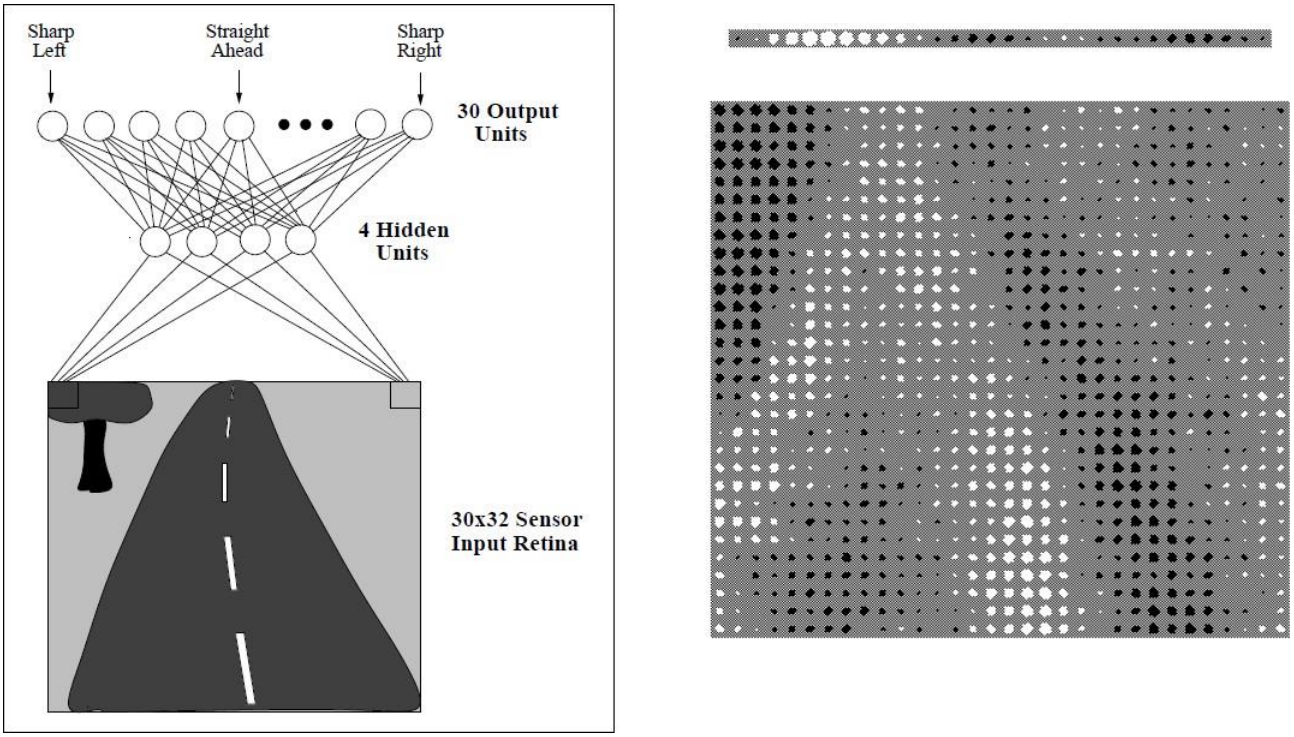


Figure: Neural network learning to steer an autonomous vehicle.

- Figure illustrates the neural network representation.
- The network is shown on the left side of the figure, with the input camera image depicted below it.
- Each node (i.e., circle) in the network diagram corresponds to the output of a single network unit, and the lines entering the node from below are its inputs.
- There are four units that receive inputs directly from all of the 30 x 32 pixels in the image. These are called "hidden" units because their output is available only within the network and is not available as part of the global network output. Each of these four hidden units computes a single real-valued output based on a weighted combination of its 960 inputs
- These hidden unit outputs are then used as inputs to a second layer of 30 "output" units.
- Each output unit corresponds to a particular steering direction, and the output values of these units determine which steering direction is recommended most strongly.
- The diagrams on the right side of the figure depict the learned weight values associated with one of the four hidden units in this ANN.
- The large matrix of black and white boxes on the lower right depicts the weights from the 30 x 32 pixel inputs into the hidden unit. Here, a white box indicates a positive weight, a black box a negative weight, and the size of the box indicates the weight magnitude.
- The smaller rectangular diagram directly above the large matrix shows the weights from this hidden unit to each of the 30 output units.

APPROPRIATE PROBLEMS FOR NEURAL NETWORK LEARNING

ANN learning is well-suited to problems in which the training data corresponds to noisy, complex sensor data, such as inputs from cameras and microphones.

ANN is appropriate for problems with the following characteristics:

1. Instances are represented by many attribute-value pairs.
2. The target function output may be discrete-valued, real-valued, or a vector of several real- or discrete-valued attributes.
3. The training examples may contain errors.
4. Long training times are acceptable.
5. Fast evaluation of the learned target function may be required
6. The ability of humans to understand the learned target function is not important

PERCEPTRON

- One type of ANN system is based on a unit called a perceptron. Perceptron is a single layer neural network.

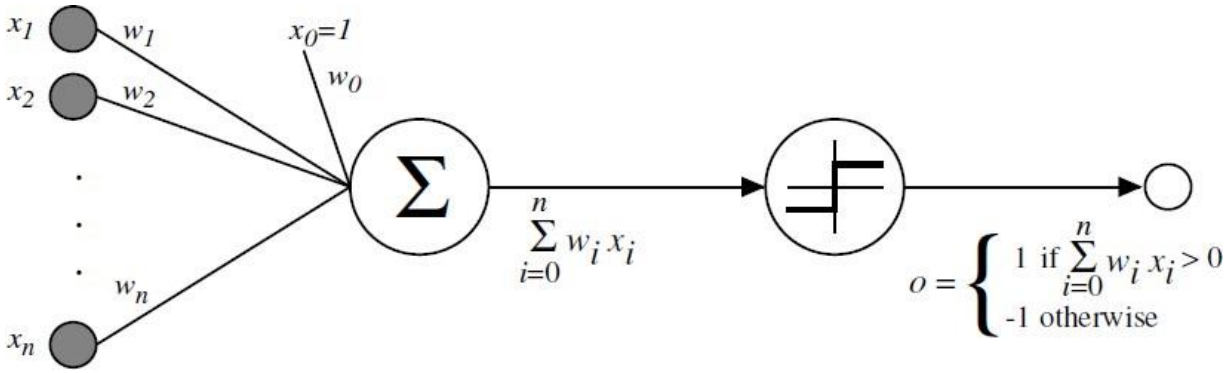


Figure: A perceptron

- A perceptron takes a vector of real-valued inputs, calculates a linear combination of these inputs, then outputs a 1 if the result is greater than some threshold and -1 otherwise.
- Given inputs ***x*** through ***x,*** the output **O*(x₁, . . . , xₙ)*** computed by the perceptron is

$$o(x_1, \ldots, x_n) = \begin{cases} 1 & \text{if } w_0 + w_1 x_1 + \cdots + w_n x_n > 0 \\ -1 & \text{otherwise.} \end{cases}$$

- Where, each w_i is a real-valued constant, or weight, that determines the contribution of input x_i to the perceptron output.
- $-w_0$ is a threshold that the weighted combination of inputs $w_1x_1 + \ldots + w_nx_n$ must surpass in order for the perceptron to output a 1.

Sometimes, the perceptron function is written as,

$$O(\vec{x}) = \text{sgn}\ (\vec{w} \,.\, \vec{x})$$

Where,

$$\text{sgn}(y) = \begin{cases} 1 & \text{if } y > 0 \\ -1 & \text{otherwise.} \end{cases}$$

Learning a perceptron involves choosing values for the weights $w_0, \ldots, w_n$. Therefore, the space H of candidate hypotheses considered in perceptron learning is the set of all possible real-valued weight vectors

$$H = \{\vec{w} \mid \vec{w} \in \Re^{(n+1)}\}$$

Representational Power of Perceptrons

- The perceptron can be viewed as representing a hyperplane decision surface in the n-dimensional space of instances (i.e., points)
- The perceptron outputs a 1 for instances lying on one side of the hyperplane and outputs a -1 for instances lying on the other side, as illustrated in below figure

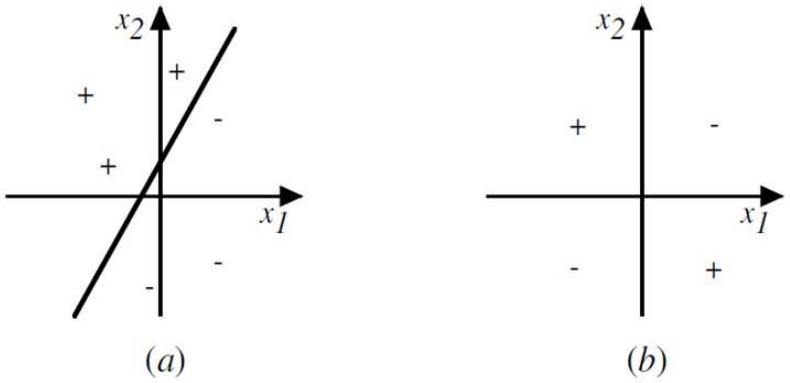
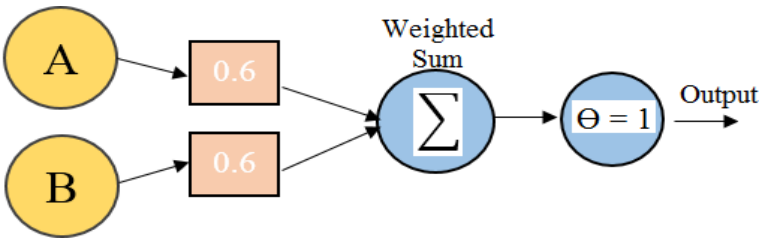


Figure : The decision surface represented by a two-input perceptron.
(a) A set of training examples and the decision surface of a perceptron that classifies them correctly. *(b)* A set of training examples that is not linearly separable.
x_1 and x_2 are the Perceptron inputs. Positive examples are indicated by "+", negative by "-".

Perceptrons can represent all of the primitive Boolean functions AND, OR, NAND (~ AND), and NOR (~OR)
Some Boolean functions cannot be represented by a single perceptron, such as the XOR function whose value is 1 if and only if $x_1 \neq x_2$

Example: Representation of AND functions

A	B	A ^ B
0	0	0
0	1	0
1	0	0
1	1	1



If A=0 & B=0 → 0*0.6 + 0*0.6 = 0.
This is not greater than the threshold of 1, so the output = 0.
If A=0 & B=1 → 0*0.6 + 1*0.6 = 0.6.
This is not greater than the threshold, so the output = 0.
If A=1 & B=0 → 1*0.6 + 0*0.6 = 0.6.
This is not greater than the threshold, so the output = 0.
If A=1 & B=1 → 1*0.6 + 1*0.6 = 1.2.
This exceeds the threshold, so the output = 1.

Drawback of perceptron

- The perceptron rule finds a successful weight vector when the training examples are linearly separable, it can fail to converge if the examples are not linearly separable

The Perceptron Training Rule

The learning problem is to determine a weight vector that causes the perceptron to produce the correct + 1 or - 1 output for each of the given training examples.

To learn an acceptable weight vector

- Begin with random weights, then iteratively apply the perceptron to each training example, modifying the perceptron weights whenever it misclassifies an example.
- This process is repeated, iterating through the training examples as many times as needed until the perceptron classifies all training examples correctly.
- Weights are modified at each step according to the perceptron training rule, which revises the weight w_i associated with input xi according to the rule.

$$w_i \leftarrow w_i + \Delta w_i$$

Where,

$$\Delta w_i = \eta(t - o)x_i$$

Here,
t is the target output for the current training example
o is the output generated by the perceptron
η is a positive constant called the ***learning rate***

- The role of the learning rate is to moderate the degree to which weights are changed at each step. It is usually set to some small value (e.g., 0.1) and is sometimes made to decay as the number of weight-tuning iterations increases

Drawback:
The perceptron rule finds a successful weight vector when the training examples are linearly separable, it can fail to converge if the examples are not linearly separable.

Gradient Descent and the Delta Rule

- If the training examples are not linearly separable, the delta rule converges toward a best-fit approximation to the target concept.
- The key idea behind the delta rule is to use ***gradient descent*** to search the hypothesis space of possible weight vectors to find the weights that best fit the training examples.

To understand the delta training rule, consider the task of training an unthresholded perceptron. That is, a linear unit for which the output ***O*** is given by

$$o = w_0 + w_1 x_1 + \cdots + w_n x_n$$

$$O(\vec{x}) = (\vec{w} \cdot \vec{x}) \qquad \text{equ. (1)}$$

To derive a weight learning rule for linear units, specify a measure for the ***training error*** of a hypothesis (weight vector), relative to the training examples.

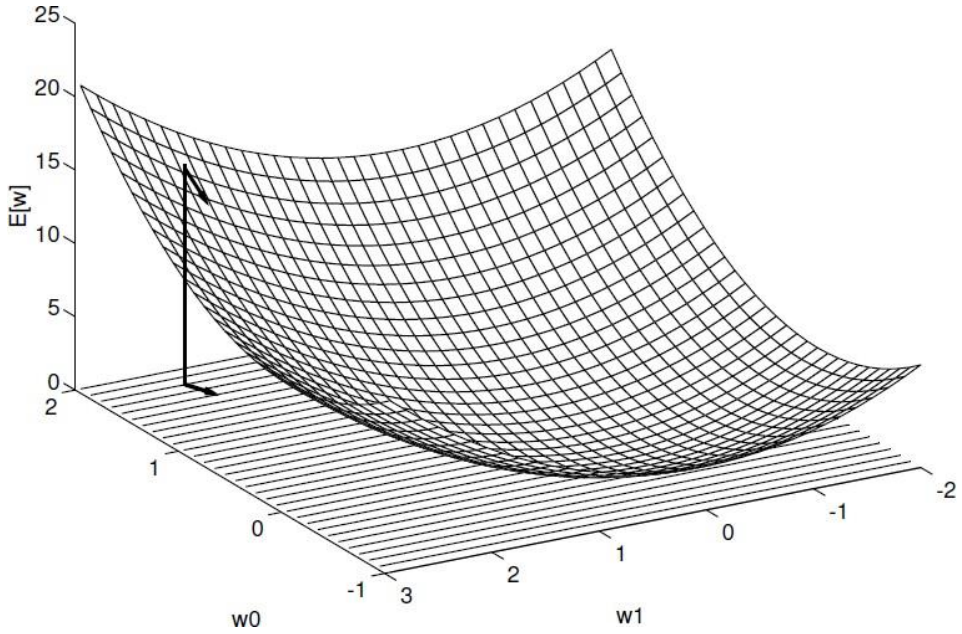
$$E[\vec{w}] \equiv \frac{1}{2} \sum_{d \in D} (t_d - o_d)^2 \qquad \text{equ. (2)}$$

Where,

- D is the set of training examples,
- t_d is the target output for training example d,
- o_d is the output of the linear unit for training example d
- E ($\vec{w}$) is simply half the squared difference between the target output t_d and the linear unit output o_d, summed over all training examples.

Visualizing the Hypothesis Space

- To understand the gradient descent algorithm, it is helpful to visualize the entire hypothesis space of possible weight vectors and their associated E values as shown in below figure.
- Here the axes w_0 and w_1 represent possible values for the two weights of a simple linear unit. The w_0, w_1 plane therefore represents the entire hypothesis space.
- The vertical axis indicates the error E relative to some fixed set of training examples.
- The arrow shows the negated gradient at one particular point, indicating the direction in the w_0, w_1 plane producing steepest descent along the error surface.
- The error surface shown in the figure thus summarizes the desirability of every weight vector in the hypothesis space



- Given the way in which we chose to define E, for linear units this error surface must always be parabolic with a single global minimum.

Gradient descent search determines a weight vector that minimizes E by starting with an arbitrary initial weight vector, then repeatedly modifying it in small steps.
At each step, the weight vector is altered in the direction that produces the steepest descent along the error surface depicted in above figure. This process continues until the global minimum error is reached.

Derivation of the Gradient Descent Rule

How to calculate the direction of steepest descent along the error surface?

The direction of steepest can be found by computing the derivative of E with respect to each component of the vector $\vec{w}$. This vector derivative is called the gradient of E with respect to $\vec{w}$, written as

$$\nabla E[\vec{w}] \equiv \left[\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \cdots \frac{\partial E}{\partial w_n}\right] \qquad \text{equ. (3)}$$

The gradient specifies the direction of steepest increase of E, the training rule for gradient descent is

$$\vec{w} \leftarrow \vec{w} + \Delta\vec{w}$$

Where,

$$\Delta\vec{w} = -\eta\nabla E(\vec{w}) \qquad \text{equ. (4)}$$

- Here η is a positive constant called the learning rate, which determines the step size in the gradient descent search.
- The negative sign is present because we want to move the weight vector in the direction that decreases E.

This training rule can also be written in its component form

$$w_i \leftarrow w_i + \Delta w_i$$

Where,

$$\Delta w_i = -\eta \frac{\partial E}{\partial w_i} \qquad \text{equ. (5)}$$

Calculate the gradient at each step. The vector of $\frac{\partial E}{\partial wi}$ derivatives that form the gradient can be obtained by differentiating E from Equation (2), as

$$\begin{aligned}
\frac{\partial E}{\partial w_i} &= \frac{\partial}{\partial w_i}\frac{1}{2}\sum_d (t_d - o_d)^2 \\
&= \frac{1}{2}\sum_d \frac{\partial}{\partial w_i}(t_d - o_d)^2 \\
&= \frac{1}{2}\sum_d 2(t_d - o_d)\frac{\partial}{\partial w_i}(t_d - o_d) \\
&= \sum_d (t_d - o_d)\frac{\partial}{\partial w_i}(t_d - \vec{w}\cdot\vec{x_d}) \\
\frac{\partial E}{\partial w_i} &= \sum_d (t_d - o_d)(-x_{i,d}) \qquad \text{equ. (6)}
\end{aligned}$$

Substituting Equation (6) into Equation (5) yields the weight update rule for gradient descent

$$\Delta w_i = \eta \sum_{d\in D} (t_d - o_d)\, x_{id} \qquad \text{equ. (7)}$$

GRADIENT DESCENT algorithm for training a linear unit

GRADIENT-DESCENT($training\_examples, \eta$)

Each training example is a pair of the form $\langle \vec{x}, t \rangle$*, where* $\vec{x}$ *is the vector of input values, and* t *is the target output value.* η *is the learning rate (e.g., .05).*

- Initialize each w_i to some small random value
- Until the termination condition is met, Do
  - Initialize each Δw_i to zero.
  - For each $\langle \vec{x}, t \rangle$ in $training\_examples$, Do
    - Input the instance $\vec{x}$ to the unit and compute the output o
    - For each linear unit weight w_i, Do

$$\Delta w_i \leftarrow \Delta w_i + \eta(t - o)x_i$$

  - For each linear unit weight w_i, Do

$$w_i \leftarrow w_i + \Delta w_i$$

To summarize, the gradient descent algorithm for training linear units is as follows:

- Pick an initial random weight vector.
- Apply the linear unit to all training examples, then compute Δw_i for each weight according to Equation (7).
- Update each weight w_i by adding Δw_i, then repeat this process

Issues in Gradient Descent Algorithm

Gradient descent is an important general paradigm for learning. It is a strategy for searching through a large or infinite hypothesis space that can be applied whenever

1. The hypothesis space contains continuously parameterized hypotheses
2. The error can be differentiated with respect to these hypothesis parameters

<u>The key practical difficulties in applying gradient descent are</u>

1. Converging to a local minimum can sometimes be quite slow
2. If there are multiple local minima in the error surface, then there is no guarantee that the procedure will find the global minimum

Stochastic Approximation to Gradient Descent

- The gradient descent training rule presented in Equation (7) computes weight updates after summing over all the training examples in D
- The idea behind stochastic gradient descent is to approximate this gradient descent search by updating weights incrementally, following the calculation of the error for each individual example

$$\Delta w_i = \eta\,(t - o)\,x_i$$

- where t, o, and x_i are the target value, unit output, and i^{th} input for the training example in question

---

GRADIENT-DESCENT(*training_examples*, η)

Each training example is a pair of the form $\langle \vec{x}, t \rangle$, *where* $\vec{x}$ *is the vector of input values, and* t *is the target output value.* η *is the learning rate (e.g., .05).*

- Initialize each w_i to some small random value
- Until the termination condition is met, Do
  - Initialize each Δw_i to zero.
  - For each $\langle \vec{x}, t \rangle$ in *training_examples*, Do
    - Input the instance $\vec{x}$ to the unit and compute the output o
    - For each linear unit weight w_i, Do

$$w_i \leftarrow w_i + \eta(t - o)\,x_i \qquad (1)$$

---

stochastic approximation to gradient descent

One way to view this stochastic gradient descent is to consider a distinct error function $E_d(\vec{w})$ for each individual training example d as follows

$$E_d(\vec{w}) = \frac{1}{2}(t_d - o_d)^2$$

- Where, t_d and o_d are the target value and the unit output value for training example d.
- Stochastic gradient descent iterates over the training examples d in D, at each iteration altering the weights according to the gradient with respect to $E_d(\vec{w})$
- The sequence of these weight updates, when iterated over all training examples, provides a reasonable approximation to descending the gradient with respect to our original error function $E_d(\vec{w})$
- By making the value of η sufficiently small, stochastic gradient descent can be made to approximate true gradient descent arbitrarily closely

The key differences between standard gradient descent and stochastic gradient descent are

- In standard gradient descent, the error is summed over all examples before updating weights, whereas in stochastic gradient descent weights are updated upon examining each training example.
- Summing over multiple examples in standard gradient descent requires more computation per weight update step. On the other hand, because it uses the true gradient, standard gradient descent is often used with a larger step size per weight update than stochastic gradient descent.
- In cases where there are multiple local minima with respect to stochastic gradient descent can sometimes avoid falling into these local minima because it uses the various $\nabla E_d(\vec{w})$ rather than $\nabla E(\vec{w})$ to guide its search

MULTILAYER NETWORKS AND THE BACKPROPAGATION ALGORITHM

Multilayer networks learned by the BACKPROPAGATION algorithm are capable of expressing a rich variety of nonlinear decision surfaces.

Consider the example:

- Here the speech recognition task involves distinguishing among 10 possible vowels, all spoken in the context of "h_d" (i.e., "hid," "had," "head," "hood," etc.).
- The network input consists of two parameters, F1 and F2, obtained from a spectral analysis of the sound. The 10 network outputs correspond to the 10 possible vowel sounds. The network prediction is the output whose value is highest.
- The plot on the right illustrates the highly nonlinear decision surface represented by the learned network. Points shown on the plot are test examples distinct from the examples used to train the network.

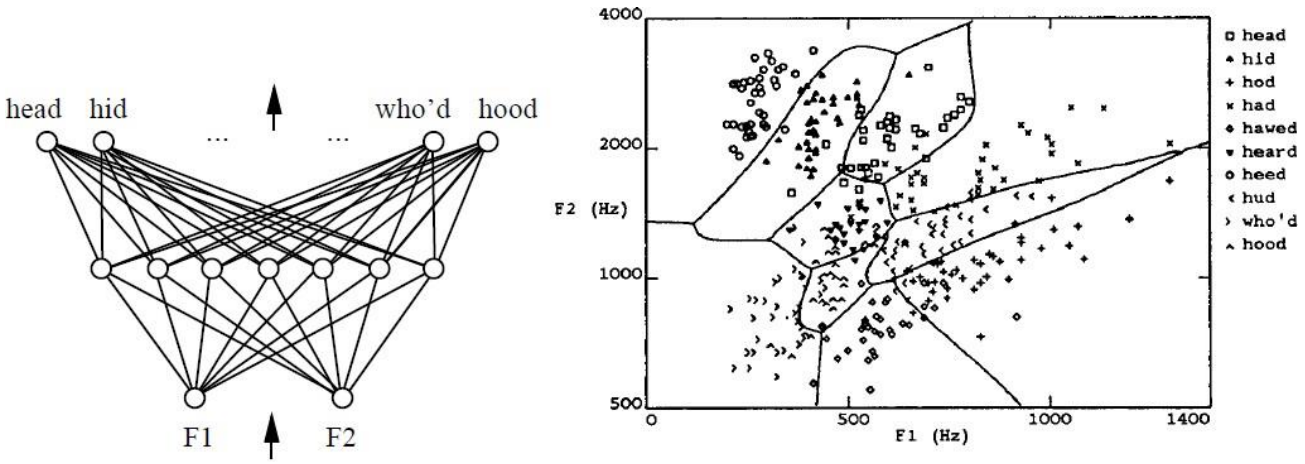


Figure: Decision regions of a multilayer feedforward network.

A Differentiable Threshold Unit (Sigmoid unit)

- Sigmoid unit-a unit very much like a perceptron, but based on a smoothed, differentiable threshold function.

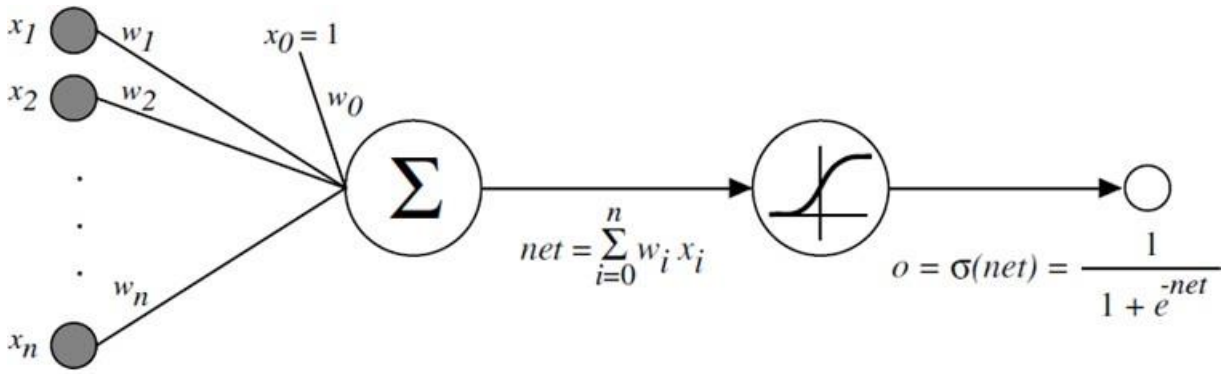


Figure: A Sigmoid Threshold Unit

- The sigmoid unit first computes a linear combination of its inputs, then applies a threshold to the result and the threshold output is a continuous function of its input.
- More precisely, the sigmoid unit computes its output O as

$$o = \sigma(\vec{w} \cdot \vec{x})$$

Where,

$$\sigma(y) = \frac{1}{1 + e^{-y}}$$

σ is the sigmoid function

The BACKPROPAGATION Algorithm

- The BACKPROPAGATION Algorithm learns the weights for a multilayer network, given a network with a fixed set of units and interconnections. It employs gradient descent to attempt to minimize the squared error between the network output values and the target values for these outputs.
- In BACKPROPAGATION algorithm, we consider networks with multiple output units rather than single units as before, so we redefine E to sum the errors over all of the network output units.

$$E(\vec{w}) \equiv \frac{1}{2} \sum_{d \in D} \sum_{k \in outputs} (t_{kd} - o_{kd})^2 \quad \text{.....equ. (1)}$$

where,

- ***outputs*** - is the set of output units in the network
- t_{kd} and O_{kd} - the target and output values associated with the k_{th} output unit
- ***d*** - training example

Algorithm:

BACKPROPAGATION (*training_example, η, n_{in}, n_{out}, n_{hidden})*

Each training example is a pair of the form $(\vec{x}, t)$, where (x) is the vector of network input values, (t) and is the vector of target network output values.
η is the learning rate (e.g., .05). n_i, is the number of network inputs, n_{hidden} the number of units in the hidden layer, and n_{out} the number of output units.
The input from unit i into unit j is denoted x_{ji}, and the weight from unit i to unit j is denoted w_{ji}

- Create a feed-forward network with n_i inputs, n_{hidden} hidden units, and n_{out} output units.
- Initialize all network weights to small random numbers
- Until the termination condition is met, Do
  - For each $(\vec{x}, t)$, in training examples, Do
    Propagate the input forward through the network:
  1. Input the instance $\vec{x}$, to the network and compute the output o_u of every unit u in the network.
     Propagate the errors backward through the network:
  2. For each network output unit k, calculate its error term δ_k

$$\delta_k \leftarrow o_k(1 - o_k)(t_k - o_k)$$

  3. For each hidden unit *h,* calculate its error term δ_h

$$\delta_h \leftarrow o_h(1 - o_h) \sum_{k \in outputs} w_{h,k}\delta_k$$

  4. Update each network weight w_{ji}

$$w_{ji} \leftarrow w_{ji} + \Delta w_{ji}$$

Where

$$\Delta w_{ji} = \eta \delta_j x_{i,j}$$

Adding Momentum

Because BACKPROPAGATION is such a widely used algorithm, many variations have been developed. The most common is to alter the weight-update rule the equation below

$$\Delta w_{ji} = \eta \, \delta_j \, x_{ji}$$

by making the weight update on the nth iteration depend partially on the update that occurred during the $(n - 1)^{th}$ iteration, as follows:

$$\Delta w_{ji}(n) = \eta \, \delta_j \, x_{ji} + \alpha \Delta w_{ji}(n-1)$$

Learning in arbitrary acyclic networks

- BACKPROPAGATION algorithm given there easily generalizes to feedforward networks of arbitrary depth. The weight update rule is retained, and the only change is to the procedure for computing δ values.
- In general, the ***δ***, value for a unit ***r*** in layer ***m*** is computed from the ***δ*** values at the next deeper layer m + 1 according to

$$\delta_r = o_r \, (1 - o_r) \sum_{s \in layer \, m+1} w_{sr} \, \delta_s$$

- The rule for calculating ***δ*** for any internal unit

$$\delta_r = o_r \, (1 - o_r) \sum_{s \in Downstream(r)} w_{sr} \, \delta_s$$

Where, Downstream(r) is the set of units immediately downstream from unit ***r*** in the network: that is, all units whose inputs include the output of unit ***r***

Derivation of the BACKPROPAGATION Rule

- Deriving the stochastic gradient descent rule: Stochastic gradient descent involves iterating through the training examples one at a time, for each training example d descending the gradient of the error E_d with respect to this single example
- For each training example d every weight w_{ji} is updated by adding to it Δw_{ji}

$$\Delta w_{ji} = -\eta \frac{\partial E_d}{\partial w_{ji}} \qquad \text{.....equ. (1)}$$

where, E_d is the error on training example d, summed over all output units in the network

$$E_d(\vec{w}) \equiv \frac{1}{2} \sum_{k \in output} (t_k - o_k)^2$$

Here outputs is the set of output units in the network, t_k is the target value of unit ***k*** for training example ***d***, and o_k is the output of unit ***k*** given training example ***d***.

The derivation of the stochastic gradient descent rule is conceptually straightforward, but requires keeping track of a number of subscripts and variables

- x_{ji} = the i^{th} input to unit j
- w_{ji} = the weight associated with the i^{th} input to unit j
- $net_j = \Sigma_i w_{ji} x_{ji}$ (the weighted sum of inputs for unit j)
- o_j = the output computed by unit j
- t_j = the target output for unit j
- σ = the sigmoid function
- outputs = the set of units in the final layer of the network
- Downstream(j) = the set of units whose immediate inputs include the output of unit j

derive an expression for $\frac{\partial E_d}{\partial w_{ji}}$ in order to implement the stochastic gradient descent rule

seen in Equation $\Delta w_{ji} = -\eta \frac{\partial E_d}{\partial w_{ji}}$

notice that weight w_{ji} can influence the rest of the network only through net_j.

Use chain rule to write

$$\frac{\partial E_d}{\partial w_{ji}} = \frac{\partial E_d}{\partial net_j} \frac{\partial net_j}{\partial w_{ji}}$$

$$= \frac{\partial E_d}{\partial net_j} x_{ji} \qquad \text{.....equ(2)}$$

Derive a convenient expression for $\frac{\partial E_d}{\partial net_j}$

Consider two cases: The case where unit j is an output unit for the network, and the case where j is an internal unit (hidden unit).

Case 1: Training Rule for Output Unit Weights.

w_{ji} can influence the rest of the network only through net_j, net_j can influence the network only through o_j. Therefore, we can invoke the chain rule again to write

$$\frac{\partial E_d}{\partial net_j} = \frac{\partial E_d}{\partial o_j}\frac{\partial o_j}{\partial net_j} \qquad \text{.....equ(3)}$$

To begin, consider just the first term in Equation (3)

$$\frac{\partial E_d}{\partial o_j} = \frac{\partial}{\partial o_j}\frac{1}{2}\sum_{k \in outputs}(t_k - o_k)^2$$

The derivatives $\frac{\partial}{\partial o_j}(t_k - o_k)^2$ will be zero for all output units k except when $k = j$. We therefore drop the summation over output units and simply set $k = j$.

$$\begin{aligned}\frac{\partial E_d}{\partial o_j} &= \frac{\partial}{\partial o_j}\frac{1}{2}(t_j - o_j)^2 \\ &= \frac{1}{2}2(t_j - o_j)\frac{\partial(t_j - o_j)}{\partial o_j} \\ &= -(t_j - o_j) \qquad \text{.....equ (4)}\end{aligned}$$

Next consider the second term in Equation (3). Since $o_j = \sigma(net_j)$, the derivative $\frac{\partial o_j}{\partial net_j}$ is just the derivative of the sigmoid function, which we have already noted is equal to $\sigma(net_j)(1 - \sigma(net_j))$. Therefore,

$$\begin{aligned}\frac{\partial o_j}{\partial net_j} &= \frac{\partial \sigma(net_j)}{\partial net_j} \\ &= o_j(1 - o_j) \qquad \text{.....equ(5)}\end{aligned}$$

Substituting expressions (4) and (5) into (3), we obtain

$$\frac{\partial E_d}{\partial net_j} = -(t_j - o_j)\, o_j(1 - o_j) \qquad \text{.....equ(6)}$$

and combining this with Equations (1) and (2), we have the stochastic gradient descent rule for output units

$$\Delta w_{ji} = -\eta\frac{\partial E_d}{\partial w_{ji}} = \eta\,(t_j - o_j)\, o_j(1 - o_j)x_{ji} \qquad \text{.....equ (7)}$$

Case 2: Training Rule for Hidden Unit Weights.

- In the case where j is an internal, or hidden unit in the network, the derivation of the training rule for w_{ji} must take into account the indirect ways in which w_{ji} can influence the network outputs and hence E_d.
- For this reason, we will find it useful to refer to the set of all units immediately downstream of unit j in the network and denoted this set of units by Downstream(j).
- net_j can influence the network outputs only through the units in Downstream(j). Therefore, we can write

$$\frac{\partial E_d}{\partial net_j} = \sum_{k \in Downstream(j)} \frac{\partial E_d}{\partial net_k} \frac{\partial net_k}{\partial net_j}$$

$$= \sum_{k \in Downstream(j)} -\delta_k \frac{\partial net_k}{\partial net_j}$$

$$= \sum_{k \in Downstream(j)} -\delta_k \frac{\partial net_k}{\partial o_j} \frac{\partial o_j}{\partial net_j}$$

$$= \sum_{k \in Downstream(j)} -\delta_k \, w_{kj} \frac{\partial o_j}{\partial net_j}$$

$$= \sum_{k \in Downstream(j)} -\delta_k \, w_{kj} \, o_j(1 - o_j) \qquad \text{.....equ (8)}$$

Rearranging terms and using δ_j to denote $-\frac{\partial E_d}{\partial net_j}$, we have

$$\delta_j = o_j(1 - o_j) \sum_{k \in Downstream(j)} \delta_k \, w_{kj}$$

and

$$\Delta w_{ji} = \eta \, \delta_j \, x_{ji}$$

REMARKS ON THE BACKPROPAGATION ALGORITHM

1. Convergence and Local Minima

- The BACKPROPAGATION multilayer networks is only guaranteed to converge toward some local minimum in E and not necessarily to the global minimum error.
- Despite the lack of assured convergence to the global minimum error, BACKPROPAGATION is a highly effective function approximation method in practice.
- Local minima can be gained by considering the manner in which network weights evolve as the number of training iterations increases.

Common heuristics to attempt to alleviate the problem of local minima include:

1. Add a momentum term to the weight-update rule. Momentum can sometimes carry the gradient descent procedure through narrow local minima
2. Use stochastic gradient descent rather than true gradient descent
3. Train multiple networks using the same data, but initializing each network with different random weights

2. Representational Power of Feedforward Networks

What set of functions can be represented by feed-forward networks?
The answer depends on the width and depth of the networks. There are three quite general results are known about which function classes can be described by which types of Networks

1. Boolean functions – Every boolean function can be represented exactly by some network with two layers of units, although the number of hidden units required grows exponentially in the worst case with the number of network inputs

2. Continuous functions – Every bounded continuous function can be approximated with arbitrarily small error by a network with two layers of units

3. Arbitrary functions – Any function can be approximated to arbitrary accuracy by a network with three layers of units.

3. Hypothesis Space Search and Inductive Bias

- Hypothesis space is the n-dimensional Euclidean space of the ***n*** network weights and hypothesis space is continuous.

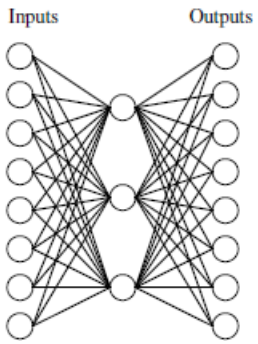
- As it is continuous, E is differentiable with respect to the continuous parameters of the hypothesis, results in a well-defined error gradient that provides a very useful structure for organizing the search for the best hypothesis.
- It is difficult to characterize precisely the inductive bias of BACKPROPAGATION algorithm, because it depends on the interplay between the gradient descent search and the way in which the weight space spans the space of representable functions. However, one can roughly characterize it as smooth interpolation between data points.

4. Hidden Layer Representations

BACKPROPAGATION can define new hidden layer features that are not explicit in the input representation, but which capture properties of the input instances that are most relevant to learning the target function.

Consider example, the network shown in below Figure

A network:



Learned hidden layer representation:

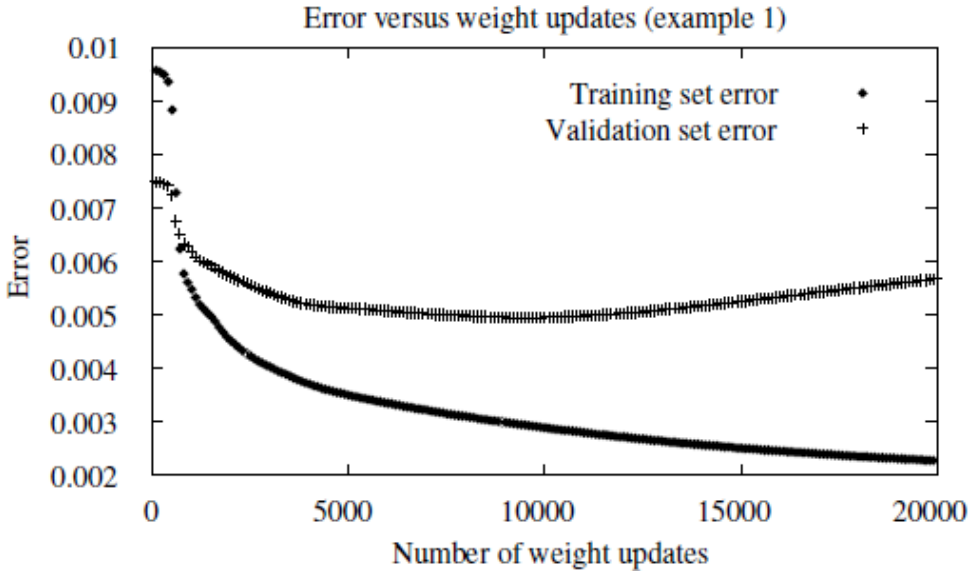
Input		Hidden Values				Output
10000000	→	.89	.04	.08	→	10000000
01000000	→	.01	.11	.88	→	01000000
00100000	→	.01	.97	.27	→	00100000
00010000	→	.99	.97	.71	→	00010000
00001000	→	.03	.05	.02	→	00001000
00000100	→	.22	.99	.99	→	00000100
00000010	→	.80	.01	.98	→	00000010
00000001	→	.60	.94	.01	→	00000001

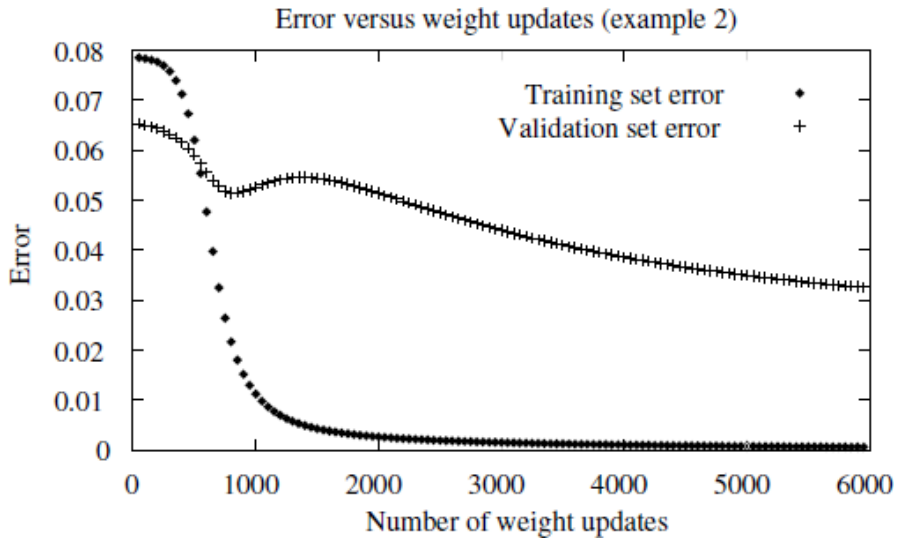
- Consider training the network shown in Figure to learn the simple target function f (x) = x, where x is a vector containing seven 0's and a single 1.
- The network must learn to reproduce the eight inputs at the corresponding eight output units. Although this is a simple function, the network in this case is constrained to use only three hidden units. Therefore, the essential information from all eight input units must be captured by the three learned hidden units.
- When BACKPROPAGATION applied to this task, using each of the eight possible vectors as training examples, it successfully learns the target function. By examining the hidden unit values generated by the learned network for each of the eight possible input vectors, it is easy to see that the learned encoding is similar to the familiar standard binary encoding of eight values using three bits (e.g., 000,001,010,. . . , 111). The exact values of the hidden units for one typical run of shown in Figure.
- This ability of multilayer networks to automatically discover useful representations at the hidden layers is a key feature of ANN learning

5. Generalization, Overfitting, and Stopping Criterion

What is an appropriate condition for terminating the weight update loop? One choice is to continue training until the error E on the training examples falls below some predetermined threshold.

To see the dangers of minimizing the error over the training data, consider how the error E varies with the number of weight iterations





- Consider first the top plot in this figure. The lower of the two lines shows the monotonically decreasing error E over the training set, as the number of gradient descent iterations grows. The upper line shows the error E measured over a different validation set of examples, distinct from the training examples. This line measures the generalization accuracy of the network-the accuracy with which it fits examples beyond the training data.

- The generalization accuracy measured over the validation examples first decreases, then increases, even as the error over the training examples continues to decrease. How can this occur? This occurs because the weights are being tuned to fit idiosyncrasies of the training examples that are not representative of the general distribution of examples. The large number of weight parameters in ANNs provides many degrees of freedom for fitting such idiosyncrasies

- Why does overfitting tend to occur during later iterations, but not during earlier iterations?
  By giving enough weight-tuning iterations, BACKPROPAGATION will often be able to create overly complex decision surfaces that fit noise in the training data or unrepresentative characteristics of the particular training sample.

MODULE 4

BAYESIAN LEARNING

Bayesian reasoning provides a probabilistic approach to inference. It is based on the assumption that the quantities of interest are governed by probability distributions and that optimal decisions can be made by reasoning about these probabilities together with observed data

INTRODUCTION

Bayesian learning methods are relevant to study of machine learning for two different reasons.

1. First, Bayesian learning algorithms that calculate explicit probabilities for hypotheses, such as the naive Bayes classifier, are among the most practical approaches to certain types of learning problems
2. The second reason is that they provide a useful perspective for understanding many learning algorithms that do not explicitly manipulate probabilities.

Features of Bayesian Learning Methods

- Each observed training example can incrementally decrease or increase the estimated probability that a hypothesis is correct. This provides a more flexible approach to learning than algorithms that completely eliminate a hypothesis if it is found to be inconsistent with any single example
- Prior knowledge can be combined with observed data to determine the final probability of a hypothesis. In Bayesian learning, prior knowledge is provided by asserting (1) a prior probability for each candidate hypothesis, and (2) a probability distribution over observed data for each possible hypothesis.
- Bayesian methods can accommodate hypotheses that make probabilistic predictions
- New instances can be classified by combining the predictions of multiple hypotheses, weighted by their probabilities.
- Even in cases where Bayesian methods prove computationally intractable, they can provide a standard of optimal decision making against which other practical methods can be measured.

Practical difficulty in applying Bayesian methods

1. One practical difficulty in applying Bayesian methods is that they typically require initial knowledge of many probabilities. When these probabilities are not known in advance they are often estimated based on background knowledge, previously available data, and assumptions about the form of the underlying distributions.
2. A second practical difficulty is the significant computational cost required to determine the Bayes optimal hypothesis in the general case. In certain specialized situations, this computational cost can be significantly reduced.

BAYES THEOREM

Bayes theorem provides a way to calculate the probability of a hypothesis based on its prior probability, the probabilities of observing various data given the hypothesis, and the observed data itself.

Notations

- P(h) prior probability of h, reflects any background knowledge about the chance that h is correct
- P(D) prior probability of D, probability that D will be observed
- P(D|h) probability of observing D given a world in which h holds
- P(h|D) posterior probability of h, reflects confidence that h holds after D has been observed

Bayes theorem is the cornerstone of Bayesian learning methods because it provides a way to calculate the posterior probability P(h|D), from the prior probability P(h), together with P(D) and P(D|h).

Bayes Theorem:

$$P(h|D) = \frac{P(D|h)P(h)}{P(D)}$$

- P(h|D) increases with P(h) and with P(D|h) according to Bayes theorem.
- P(h|D) decreases as P(D) increases, because the more probable it is that D will be observed independent of h, the less evidence D provides in support of h.

Maximum a Posteriori (MAP) Hypothesis

- In many learning scenarios, the learner considers some set of candidate hypotheses H and is interested in finding the most probable hypothesis h ∈ H given the observed data D. Any such maximally probable hypothesis is called a maximum a posteriori (MAP) hypothesis.
- Bayes theorem to calculate the posterior probability of each candidate hypothesis is h_{MAP} is a MAP hypothesis provided

$$\begin{aligned} h_{MAP} &= \underset{h \in H}{argmax}\ P(h|D) \\ &= \underset{h \in H}{argmax}\ \frac{P(D|h)P(h)}{P(D)} \\ &= \underset{h \in H}{argmax}\ P(D|h)P(h) \end{aligned}$$

- P(D) can be dropped, because it is a constant independent of h

Maximum Likelihood (ML) Hypothesis

- In some cases, it is assumed that every hypothesis in H is equally probable a priori ($P(h_i) = P(h_j)$ for all h_i and h_j in H).
- In this case the below equation can be simplified and need only consider the term P(D|h) to find the most probable hypothesis.

$$h_{MAP} = \underset{h \in H}{argmax}\ P(D|h)P(h)$$

the equation can be simplified

$$h_{ML} = \underset{h \in H}{argmax}\ P(D|h)$$

P(D|h) is often called the likelihood of the data D given h, and any hypothesis that maximizes P(D|h) is called a maximum likelihood (ML) hypothesis

Example

- Consider a medical diagnosis problem in which there are two alternative hypotheses: (1) that the patient has particular form of cancer, and (2) that the patient does not. The available data is from a particular laboratory test with two possible outcomes: + (positive) and - (negative).

- We have prior knowledge that over the entire population of people only .008 have this disease. Furthermore, the lab test is only an imperfect indicator of the disease.
- The test returns a correct positive result in only 98% of the cases in which the disease is actually present and a correct negative result in only 97% of the cases in which the disease is not present. In other cases, the test returns the opposite result.
- The above situation can be summarized by the following probabilities:

$$P(cancer) = .008 \qquad P(\neg cancer) = 0.992$$
$$P(\oplus|cancer) = .98 \qquad P(\ominus|cancer) = .02$$
$$P(\oplus|\neg cancer) = .03 \qquad P(\ominus|\neg cancer) = .97$$

Suppose a new patient is observed for whom the lab test returns a positive (+) result. Should we diagnose the patient as having cancer or not?

$$P(\oplus|cancer)P(cancer) = (.98).008 = .0078$$
$$P(\oplus|\neg cancer)P(\neg cancer) = (.03).992 = .0298$$
$$\Rightarrow h_{MAP} = \neg cancer$$

The exact posterior probabilities can also be determined by normalizing the above quantities so that they sum to 1

$$P(cancer|\oplus) = \frac{0.0078}{0.0078 + 0.0298} = 0.21$$

$$P(\neg cancer|\oplus) = \frac{0.0298}{0.0078 + 0.0298} = 0.79$$

Basic formulas for calculating probabilities are summarized in Table

---

- ***Product rule***: probability $P(A \wedge B)$ of a conjunction of two events A and B

$$P(A \wedge B) = P(A|B)P(B) = P(B|A)P(A)$$

- ***Sum rule***: probability of a disjunction of two events A and B

$$P(A \vee B) = P(A) + P(B) - P(A \wedge B)$$

- ***Bayes theorem***: the posterior probability $P(h|D)$ of h given D

$$P(h|D) = \frac{P(D|h)P(h)}{P(D)}$$

- ***Theorem of total probability***: if events $A_1, \ldots, A_n$ are mutually exclusive with $\sum_{i=1}^{n} P(A_i) = 1$, then

$$P(B) = \sum_{i=1}^{n} P(B|A_i)P(A_i)$$

BAYES THEOREM AND CONCEPT LEARNING

What is the relationship between Bayes theorem and the problem of concept learning?

Since Bayes theorem provides a principled way to calculate the posterior probability of each hypothesis given the training data, and can use it as the basis for a straightforward learning algorithm that calculates the probability for each possible hypothesis, then outputs the most probable.

Brute-Force Bayes Concept Learning

Consider the concept learning problem

- Assume the learner considers some finite hypothesis space H defined over the instance space X, in which the task is to learn some target concept $c : X \rightarrow \{0,1\}$.
- Learner is given some sequence of training examples $((x_1, d_1) \ldots (x_m, d_m))$ where x_i is some instance from X and where d_i is the target value of x_i (i.e., $d_i = c(x_i)$).
- The sequence of target values are written as $D = (d_1 \ldots d_m)$.

We can design a straightforward concept learning algorithm to output the maximum a posteriori hypothesis, based on Bayes theorem, as follows:

BRUTE-FORCE MAP LEARNING algorithm:

1. For each hypothesis h in H, calculate the posterior probability

$$P(h|D) = \frac{P(D|h)P(h)}{P(D)}$$

2. Output the hypothesis h_{MAP} with the highest posterior probability

$$h_{MAP} = \underset{h \in H}{argmax}\ P(h|D)$$

In order specify a learning problem for the BRUTE-FORCE MAP LEARNING algorithm we must specify what values are to be used for P(h) and for P(D|h) ?

Let's choose P(h) and for P(D|h) to be consistent with the following assumptions:

- The training data D is noise free (i.e., $d_i = c(x_i)$)
- The target concept c is contained in the hypothesis space H
- Do not have a priori reason to believe that any hypothesis is more probable than any other.

What values should we specify for P(h)?

- Given no prior knowledge that one hypothesis is more likely than another, it is reasonable to assign the same prior probability to every hypothesis h in H.
- Assume the target concept is contained in H and require that these prior probabilities sum to 1.

$$P(h) = \frac{1}{|H|} \text{ for all } h \in H$$

What choice shall we make for P(D|h)?

- P(D|h) is the probability of observing the target values D = ($d_1 \ldots d_m$) for the fixed set of instances ($x_1 \ldots x_m$), given a world in which hypothesis h holds
- Since we assume noise-free training data, the probability of observing classification d_i given h is just 1 if $d_i = h(x_i)$ and 0 if $d_i \neq h(x_i)$. Therefore,

$$P(D|h) = \begin{cases} 1 & \text{if } d_i = h(x_i) \text{ for all } d_i \in D \\ 0 & \text{otherwise} \end{cases}$$

Given these choices for P(h) and for P(D|h) we now have a fully-defined problem for the above BRUTE-FORCE MAP LEARNING algorithm.

Recalling Bayes theorem, we have

$$P(h|D) = \frac{P(D|h)P(h)}{P(D)}$$

Consider the case where h is inconsistent with the training data D

$$P(h|D) = \frac{0 \cdot P(h)}{P(D)} = 0$$

The posterior probability of a hypothesis inconsistent with D is zero

Consider the case where h is consistent with D

$$P(h|D) = \frac{1 \cdot \frac{1}{|H|}}{P(D)} = \frac{1 \cdot \frac{1}{|H|}}{\frac{|VS_{H,D}|}{|H|}} = \frac{1}{|VS_{H,D}|}$$

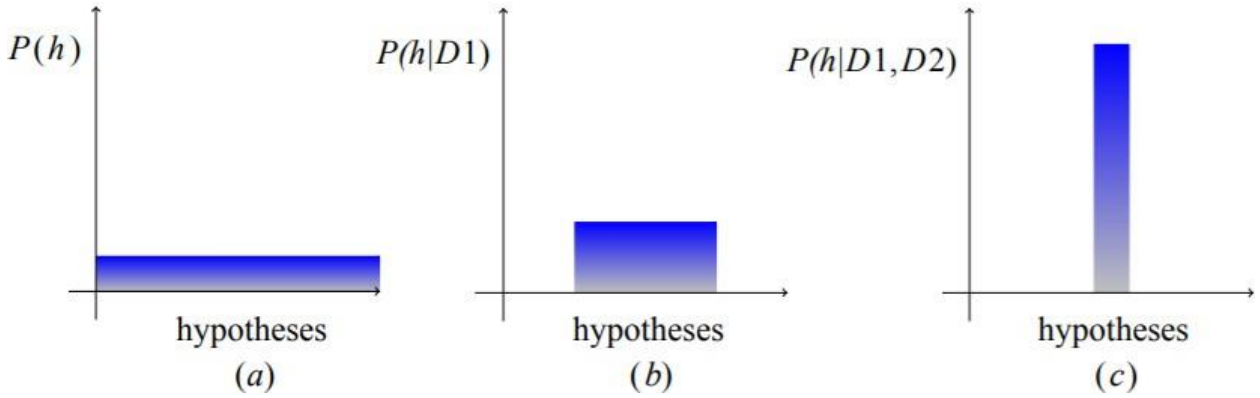
Where, $VS_{H,D}$ is the subset of hypotheses from H that are consistent with D

To summarize, Bayes theorem implies that the posterior probability P(h|D) under our assumed P(h) and P(D|h) is

$$P(D|h) = \begin{cases} \frac{1}{|V S_{H,D}|} & \text{if h is consistent with D} \\ 0 & \text{otherwise} \end{cases}$$

The Evolution of Probabilities Associated with Hypotheses

- Figure (a) all hypotheses have the same probability.
- Figures (b) and (c), As training data accumulates, the posterior probability for inconsistent hypotheses becomes zero while the total probability summing to 1 is shared equally among the remaining consistent hypotheses.



MAP Hypotheses and Consistent Learners

- A learning algorithm is a consistent learner if it outputs a hypothesis that commits zero errors over the training examples.
- Every consistent learner outputs a MAP hypothesis, if we assume a uniform prior probability distribution over H ($P(h_i) = P(h_j)$ for all i, j), and deterministic, noise free training data (P(D|h) =1 if D and h are consistent, and 0 otherwise).

Example:

- FIND-S outputs a consistent hypothesis, it will output a MAP hypothesis under the probability distributions P(h) and P(D|h) defined above.
- Are there other probability distributions for P(h) and P(D|h) under which FIND-S outputs MAP hypotheses? Yes.
- Because FIND-S outputs a maximally specific hypothesis from the version space, its output hypothesis will be a MAP hypothesis relative to any prior probability distribution that favours more specific hypotheses.

Note

- Bayesian framework is a way to characterize the behaviour of learning algorithms
- By identifying probability distributions P(h) and P(D|h) under which the output is a optimal hypothesis, implicit assumptions of the algorithm can be characterized (Inductive Bias)
- Inductive inference is modelled by an equivalent probabilistic reasoning system based on Bayes theorem

MAXIMUM LIKELIHOOD AND LEAST-SQUARED ERROR HYPOTHESES

Consider the problem of learning a *continuous-valued target function* such as neural network learning, linear regression, and polynomial curve fitting

A straightforward Bayesian analysis will show that under certain assumptions any learning algorithm that minimizes the squared error between the output hypothesis predictions and the training data will output a *maximum likelihood (ML) hypothesis*

- Learner L considers an instance space X and a hypothesis space H consisting of some class of real-valued functions defined over X, i.e., ($\forall$ h $\in$ H)[h : X $\rightarrow$ R] and training examples of the form $<x_i,d_i>$
- The problem faced by L is to learn an unknown target function f : X $\rightarrow$ R
- A set of m training examples is provided, where the target value of each example is corrupted by random noise drawn according to a Normal probability distribution with zero mean ($d_i = f(x_i) + e_i$)
- Each training example is a pair of the form (x_i ,d_i) where $d_i = f(x_i) + e_i$.
  - Here $f(x_i)$ is the noise-free value of the target function and e_i is a random variable representing the noise.
  - It is assumed that the values of the e_i are drawn independently and that they are distributed according to a Normal distribution with zero mean.
- The task of the learner is to *output a maximum likelihood hypothesis* or a *MAP hypothesis assuming all hypotheses are equally probable a priori.*

Using the definition of h_{ML} we have

$$h_{ML} = \underset{h \in H}{argmax}\ p(D|h)$$

Assuming training examples are mutually independent given h, we can write P(D|h) as the product of the various (d_i|h)

$$h_{ML} = \underset{h \in H}{argmax} \prod_{i=1}^{m} p(d_i|h)$$

Given the noise e_i obeys a Normal distribution with zero mean and unknown variance σ^2 , each d_i must also obey a Normal distribution around the true targetvalue $f(x_i)$. Because we are writing the expression for P(D|h), we assume h is the correct description of f.
Hence, $\mu = f(x_i) = h(x_i)$

$$h_{ML} = \underset{h \in H}{\text{argmax}} \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(d_i-\mu)^2}$$

$$h_{ML} = \underset{h \in H}{argmax} \prod_{i=1}^{m} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2\sigma^2}(d_i - h(x_i))^2}$$

Maximize the less complicated logarithm, which is justified because of the monotonicity of function p

$$h_{ML} = \underset{h \in H}{argmax} \sum_{i=1}^{m} \ln \frac{1}{\sqrt{2\pi\sigma^2}} - \frac{1}{2\sigma^2}(d_i - h(x_i))^2$$

The first term in this expression is a constant independent of h, and can therefore be discarded, yielding

$$h_{ML} = \underset{h \in H}{argmax} \sum_{i=1}^{m} -\frac{1}{2\sigma^2}(d_i - h(x_i))^2$$

Maximizing this negative quantity is equivalent to minimizing the corresponding positive quantity

$$h_{ML} = \underset{h \in H}{argmin} \sum_{i=1}^{m} \frac{1}{2\sigma^2}(d_i - h(x_i))^2$$

Finally, discard constants that are independent of h.

$$h_{ML} = \underset{h \in H}{argmin} \sum_{i=1}^{m} (d_i - h(x_i))^2$$

Thus, above equation shows that the maximum likelihood hypothesis h_{ML} is the one that minimizes the sum of the squared errors between the observed training values d_i and the hypothesis predictions $h(x_i)$

Note:

Why is it reasonable to choose the Normal distribution to characterize noise?

- Good approximation of many types of noise in physical systems
- Central Limit Theorem shows that the sum of a sufficiently large number of independent, identically distributed random variables itself obeys a Normal distribution

Only noise in the target value is considered, not in the attributes describing the instances themselves

MAXIMUM LIKELIHOOD HYPOTHESES FOR PREDICTING PROBABILITIES

- Consider the setting in which we wish to learn a nondeterministic (probabilistic) function f : X → {0, 1}, which has two discrete output values.
- We want a function approximator whose output is the probability that f(x) = 1. In other words, learn the target function f ` : X → [0, 1] such that f ` (x) = P(f(x) = 1)

How can we learn f ` using a neural network?

- Use of brute force way would be to first collect the observed frequencies of 1's and 0's for each possible value of x and to then train the neural network to output the target frequency for each x.

What criterion should we optimize in order to find a maximum likelihood hypothesis for f' in this setting?

- First obtain an expression for P(D|h)
- Assume the training data D is of the form D = {(x_1, d_1) . . . (x_m, d_m)}, where d_i is the observed 0 or 1 value for f (x_i).
- Both x_i and d_i as random variables, and assuming that each training example is drawn independently, we can write P(D|h) as

$$P(D \mid h) = \prod_{i=1}^{m} P(x_i, d_i \mid h) \qquad \text{equ (1)}$$

Applying the product rule

$$P(D \mid h) = \prod_{i=1}^{m} P(d_i \mid h, x_i) P(x_i) \qquad \text{equ (2)}$$

The probability $P(d_i|h, x_i)$

$$P(d_i|h, x_i) = \begin{cases} h(x_i) & \text{if } d_i = 1 \\ (1 - h(x_i)) & \text{if } d_i = 0 \end{cases} \qquad \text{equ (3)}$$

Re-express it in a more mathematically manipulable form, as

$$P(d_i|h, x_i) = h(x_i)^{d_i} (1 - h(x_i))^{1-d_i} \qquad \text{equ (4)}$$

Equation (4) to substitute for P(di |h, xi) in Equation (5) to obtain

$$P(D|h) = \prod_{i=1}^{m} h(x_i)^{d_i} (1 - h(x_i))^{1-d_i} P(x_i) \qquad \text{equ (5)}$$

We write an expression for the maximum likelihood hypothesis

$$h_{ML} = \underset{h \in H}{\operatorname{argmax}} \prod_{i=1}^{m} h(x_i)^{d_i} (1 - h(x_i))^{1-d_i} P(x_i)$$

The last term is a constant independent of h, so it can be dropped

$$h_{ML} = \underset{h \in H}{\operatorname{argmax}} \prod_{i=1}^{m} h(x_i)^{d_i} (1 - h(x_i))^{1-d_i} \qquad \text{equ (6)}$$

It easier to work with the log of the likelihood, yielding

$$h_{ML} = \underset{h \in H}{\operatorname{argmax}} \sum_{i=1}^{m} d_i \ln h(x_i) + (1 - d_i) \ln(1 - h(x_i)) \qquad \text{equ (7)}$$

Equation (7) describes the quantity that must be maximized in order to obtain the maximum likelihood hypothesis in our current problem setting

Gradient Search to Maximize Likelihood in a Neural Net

- Derive a weight-training rule for neural network learning that seeks to maximize G(h,D) using gradient ascent
- The gradient of G(h,D) is given by the vector of partial derivatives of G(h,D) with respect to the various network weights that define the hypothesis h represented by the learned network
- In this case, the partial derivative of G(h, D) with respect to weight w_{jk} from input k to unit j is

$$\begin{aligned} \frac{\partial G(h,D)}{\partial w_{jk}} &= \sum_{i=1}^{m} \frac{\partial G(h, D)}{\partial h(x_i)} \frac{\partial h(x_i)}{\partial w_{jk}} \\ &= \sum_{i=1}^{m} \frac{\partial (d_i \ln h(x_i) + (1 - d_i) \ln(1 - h(x_i)))}{\partial h(x_i)} \frac{\partial h(x_i)}{\partial w_{jk}} \\ &= \sum_{i=1}^{m} \frac{d_i - h(x_i)}{h(x_i)(1 - h(x_i))} \frac{\partial h(x_i)}{\partial w_{jk}} \qquad \text{equ (1)} \end{aligned}$$

- Suppose our neural network is constructed from a single layer of sigmoid units. Then,

$$\frac{\partial h(x_i)}{\partial w_{jk}} = \sigma'(x_i) x_{ijk} = h(x_i)(1 - h(x_i)) x_{ijk}$$

where x_{ijk} is the k^{th} input to unit j for the i^{th} training example, and d(x) is the derivative of the sigmoid squashing function.

- Finally, substituting this expression into Equation (1), we obtain a simple expression for the derivatives that constitute the gradient

$$\frac{\partial G(h, D)}{\partial w_{jk}} = \sum_{i=1}^{m} (d_i - h(x_i))\ x_{ijk}$$

Because we seek to maximize rather than minimize P(D|h), we perform gradient ascent rather than gradient descent search. On each iteration of the search the weight vector is adjusted in the direction of the gradient, using the weight update rule

$$w_{jk} \leftarrow w_{jk} + \Delta w_{jk}$$

Where,

$$\Delta w_{jk} = \eta \sum_{i=1}^{m} (d_i - h(x_i))\ x_{ijk} \qquad \text{equ (2)}$$

Where, η is a small positive constant that determines the step size of the i gradient ascent search

MINIMUM DESCRIPTION LENGTH PRINCIPLE

- A Bayesian perspective on Occam's razor
- Motivated by interpreting the definition of h_{MAP} in the light of basic concepts from information theory.

  $$h_{MAP} = \underset{h \in H}{argmax}\ P(D|h)P(h)$$

  which can be equivalently expressed in terms of maximizing the $\log_2$

  $$h_{MAP} = \underset{h \in H}{argmax}\ \log_2 P(D|h) + \log_2 P(h)$$

  or alternatively, minimizing the negative of this quantity

  $$h_{MAP} = \underset{h \in H}{argmin}\ -\log_2 P(D|h) - \log_2 P(h) \qquad \text{equ (1)}$$

This equation (1) can be interpreted as a statement that short hypotheses are preferred, assuming a particular representation scheme for encoding hypotheses and data

- $-\log_2 P(h)$: the description length of h under the optimal encoding for the hypothesis space H, $L_{CH}(h) = -\log_2 P(h)$, where C_H is the optimal code for hypothesis space H.
- $-\log_2 P(D \mid h)$: the description length of the training data D given hypothesis h, under the optimal encoding from the hypothesis space H: $L_{CH}(D|h) = -\log_2 P(D|\ h)$, where $C_{D|h}$ is the optimal code for describing data D assuming that both the sender and receiver know the hypothesis h.
- Rewrite Equation (1) to show that h_{MAP} is the hypothesis h that minimizes the sum given by the description length of the hypothesis plus the description length of the data given the hypothesis.

  $$h_{MAP} = \underset{h \in H}{argmin}\ L_{C_H}(h) + L_{C_{D|h}}(D|h)$$

  Where, C_H and $C_{D|h}$ are the optimal encodings for H and for D given h

The Minimum Description Length (MDL) principle recommends choosing the hypothesis that minimizes the sum of these two description lengths of equ.

$$h_{MAP} = \underset{h \in H}{argmin}\ L_{C_H}(h) + L_{C_{D|h}}(D|h)$$

Minimum Description Length principle:

$$h_{MDL} = \underset{h \in H}{\text{argmin}}\ L_{C_1}(h) + L_{C_2}(D \mid h)$$

Where, codes C_1 and C_2 to represent the hypothesis and the data given the hypothesis

The above analysis shows that if we choose C_1 to be the optimal encoding of hypotheses C_H, and if we choose C_2 to be the optimal encoding $C_{D|h}$, then $h_{MDL} = h_{MAP}$

Application to Decision Tree Learning

Apply the MDL principle to the problem of learning decision trees from some training data. *What should we choose for the representations C1 and C2 of hypotheses and data?*

- For C_1: C_1 might be some obvious encoding, in which the description length grows with the number of nodes and with the number of edges
- For C_2: Suppose that the sequence of instances (x_1 . . .x_m) is already known to both the transmitter and receiver, so that we need only transmit the classifications (f (x_1) . . . f (x_m)).
- Now if the training classifications (f (x_1) . . .f(x_m)) are identical to the predictions of the hypothesis, then there is no need to transmit any information about these examples. The description length of the classifications given the hypothesis ZERO
- If examples are misclassified by h, then for each misclassification we need to transmit a message that identifies which example is misclassified as well as its correct classification
- The hypothesis h_{MDL} under the encoding C_1 and C_2 is just the one that minimizes the sum of these description lengths.

NAIVE BAYES CLASSIFIER

- The naive Bayes classifier applies to learning tasks where each instance x is described by a conjunction of attribute values and where the target function f (x) can take on any value from some finite set V.
- A set of training examples of the target function is provided, and a new instance is presented, described by the tuple of attribute values (a_1, a_2.. .a_m).
- The learner is asked to predict the target value, or classification, for this new instance.

The Bayesian approach to classifying the new instance is to assign the most probable target value, V_{MAP}, given the attribute values (a_1, a_2.. .a_m) that describe the instance

$$v_{MAP} = \underset{v_j \in V}{\operatorname{argmax}} P(v_j | a_1, a_2 \ldots a_n)$$

Use Bayes theorem to rewrite this expression as

$$v_{MAP} = \underset{v_j \in V}{\operatorname{argmax}} \frac{P(a_1, a_2 \ldots a_n | v_j) P(v_j)}{P(a_1, a_2 \ldots a_n)}$$

$$= \underset{v_j \in V}{\operatorname{argmax}} P(a_1, a_2 \ldots a_n | v_j) P(v_j) \qquad \textbf{equ (1)}$$

- The naive Bayes classifier is based on the assumption that the attribute values are conditionally independent given the target value. Means, the assumption is that given the target value of the instance, the probability of observing the conjunction (a_1, a_2.. .a_m), is just the product of the probabilities for the individual attributes:

$$P(a_1, a_2 \ldots a_n | v_j) = \prod_i P(a_i | v_j)$$

Substituting this into Equation (1),

Naive Bayes classifier:

$$\mathbf{V_{NB} = \underset{v_j \in V}{\operatorname{argmax}} P(v_j) \prod_i P(a_i | v_j)} \qquad \text{equ (2)}$$

Where, V_{NB} denotes the target value output by the naive Bayes classifier

An Illustrative Example

- Let us apply the naive Bayes classifier to a concept learning problem i.e., classifying days according to whether someone will play tennis.
- The below table provides a set of 14 training examples of the target concept ***PlayTennis***, where each day is described by the attributes Outlook, Temperature, Humidity, and Wind

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

- Use the naive Bayes classifier and the training data from this table to classify the following novel instance:
  < Outlook = sunny, Temperature = cool, Humidity = high, Wind = strong >

- Our task is to predict the target value ***(yes or no)*** of the target concept ***PlayTennis*** for this new instance

$$V_{NB} = \underset{v_j \in \{yes, no\}}{\text{argmax}}\ P(v_j) \prod_i P(a_i | v_j)$$

$$V_{NB} = \underset{v_j \in \{yes, no\}}{\text{argmax}}\ P(v_j)\ P(\text{Outlook=sunny}|v_j)\ P(\text{Temperature=cool}|v_j)\ P(\text{Humidity=high}|v_j)\ P(\text{Wind=strong}|v_j)$$

The probabilities of the different target values can easily be estimated based on their frequencies over the 14 training examples

- P(P1ayTennis = yes) = 9/14 = 0.64
- P(P1ayTennis = no) = 5/14 = 0.36

Similarly, estimate the conditional probabilities. For example, those for Wind = strong

- P(Wind = strong | PlayTennis = yes) = 3/9 = 0.33
- P(Wind = strong | PlayTennis = no) = 3/5 = 0.60

Calculate V_{NB} according to Equation (1)

$$P(yes)\ P(sunny|yes)\ P(cool|yes)\ P(high|yes)\ P(strong|yes) = .0053$$
$$P(no)\ P(sunny|no)\ P(cool|no)\ P(high|no)\ P(strong|no) = .0206$$

Thus, the naive Bayes classifier assigns the target value ***PlayTennis = no*** to this new instance, based on the probability estimates learned from the training data.

By normalizing the above quantities to sum to one, calculate the conditional probability that the target value is ***no***, given the observed attribute values

$$\frac{.0206}{(.0206 + .0053)} = .795$$

Estimating Probabilities

- We have estimated probabilities by the fraction of times the event is observed to occur over the total number of opportunities.
- For example, in the above case we estimated P(Wind = strong | Play Tennis = no) by the fraction n_c /n where, n = 5 is the total number of training examples for which PlayTennis = no, and n_c = 3 is the number of these for which Wind = strong.
- When n_c = 0, then n_c /n will be zero and this probability term will dominate the quantity calculated in Equation (2) requires multiplying all the other probability terms by this zero value
- To avoid this difficulty we can adopt a Bayesian approach to estimating the probability, using the ***m-estimate*** defined as follows

m **-estimate of probability:**

$$\frac{n_c + mp}{n + m}$$

- p is our prior estimate of the probability we wish to determine, and m is a constant called the equivalent sample size, which determines how heavily to weight p relative to the observed data
- Method for choosing p in the absence of other information is to assume uniform priors; that is, if an attribute has k possible values we set p = 1 /k.

BAYESIAN BELIEF NETWORKS

- The naive Bayes classifier makes significant use of the assumption that the values of the attributes $a_1 \ldots a_n$ are conditionally independent given the target value v.
- This assumption dramatically reduces the complexity of learning the target function

A Bayesian belief network describes the probability distribution governing a set of variables by specifying a set of conditional independence assumptions along with a set of conditional probabilities
Bayesian belief networks allow stating conditional independence assumptions that apply to subsets of the variables

Notation

- Consider an arbitrary set of random variables $Y_1 \ldots Y_n$, where each variable Yi can take on the set of possible values $V(Y_i)$.
- The joint space of the set of variables Y to be the cross product $V(Y_1)$ x $V(Y_2)$ x. . . $V(Y_n)$.
- In other words, each item in the joint space corresponds to one of the possible assignments of values to the tuple of variables $(Y_1 \ldots Y_n)$. The probability distribution over this joint' space is called the joint probability distribution.
- The joint probability distribution specifies the probability for each of the possible variable bindings for the tuple $(Y_1 \ldots Y_n)$.
- A Bayesian belief network describes the joint probability distribution for a set of variables.

Conditional Independence

Let X, Y, and Z be three discrete-valued random variables. X is conditionally independent of Y given Z if the probability distribution governing X is independent of the value of Y given a value for Z, that is, if

$$(\forall x_i, y_j, z_k)\ P(X = x_i | Y = y_j, Z = z_k) = P(X = x_i | Z = z_k)$$

Where,

$$x_i \in V(X),\ y_j \in V(Y),\ \text{and}\ z_k \in V(Z).$$

The above expression is written in abbreviated form as

$$P(X \mid Y, Z) = P(X \mid Z)$$

Conditional independence can be extended to sets of variables. The set of variables $X_1 \ldots X_l$ is conditionally independent of the set of variables $Y_1 \ldots Y_m$ given the set of variables $Z_1 \ldots Z_n$ if

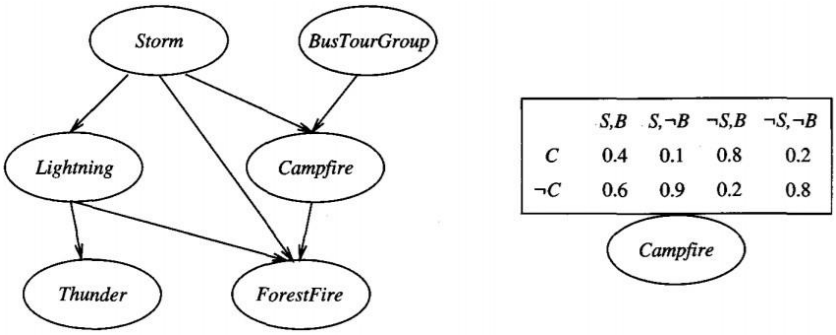
$$P(X_1 \ldots X_l | Y_1 \ldots Y_m, Z_1 \ldots Z_n) = P(X_1 \ldots X_l | Z_1 \ldots Z_n)$$

The naive Bayes classifier assumes that the instance attribute A_1 is conditionally independent of instance attribute A_2 given the target value V. This allows the naive Bayes classifier to calculate $P(A_1, A_2 \mid V)$ as follows,

$$\begin{aligned} P(A_1, A_2|V) &= P(A_1|A_2, V)P(A_2|V) \\ &= P(A_1|V)P(A_2|V) \end{aligned}$$

Representation

A Bayesian belief network represents the joint probability distribution for a set of variables. Bayesian networks (BN) are represented by directed acyclic graphs.



The Bayesian network in above figure represents the joint probability distribution over the boolean variables *Storm, Lightning, Thunder, ForestFire, Campfire,* and *BusTourGroup*

A Bayesian network (BN) represents the joint probability distribution by specifying a set of *conditional independence assumptions*

- BN represented by a directed acyclic graph, together with sets of local conditional probabilities
- Each variable in the joint space is represented by a node in the Bayesian network
- The network arcs represent the assertion that the variable is conditionally independent of its non-descendants in the network given its immediate predecessors in the network.
- A ***conditional probability table*** **(CPT)** is given for each variable, describing the probability distribution for that variable given the values of its immediate predecessors

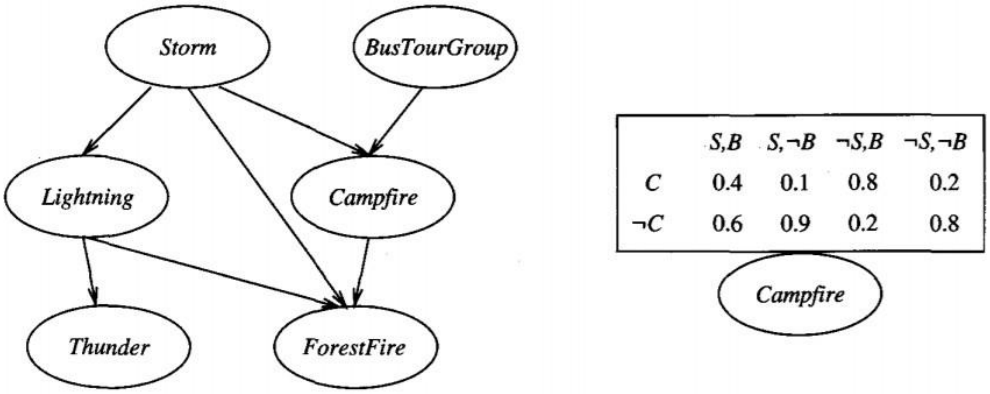
The joint probability for any desired assignment of values ($y_1, \ldots, y_n$) to the tuple of network variables ($Y_1 \ldots Y_m$) can be computed by the formula

$$P(y_1, \ldots, y_n) = \prod_{i=1}^{n} P(y_i | Parents(Y_i))$$

Where, Parents(Y_i) denotes the set of immediate predecessors of Y_i in the network.

Example:

Consider the node ***Campfire***. The network nodes and arcs represent the assertion that ***Campfire*** is conditionally independent of its non-descendants ***Lightning*** and ***Thunder***, given its immediate parents Storm and ***BusTourGroup***.



This means that once we know the value of the variables ***Storm*** and ***BusTourGroup***, the variables ***Lightning*** and ***Thunder*** provide no additional information about ***Campfire***

The conditional probability table associated with the variable ***Campfire.*** The assertion is

P(Campfire = True | Storm = True, BusTourGroup = True) = 0.4

Inference

- Use a Bayesian network to infer the value of some target variable (e.g., ForestFire) given the observed values of the other variables.
- Inference can be straightforward if values for all of the other variables in the network are known exactly.
- A Bayesian network can be used to compute the probability distribution for any subset of network variables given the values or distributions for any subset of the remaining variables.
- An arbitrary Bayesian network is known to be NP-hard

Learning Bayesian Belief Networks

Affective algorithms can be considered for learning Bayesian belief networks from training data by considering several different settings for learning problem

- First, the network structure might be given in advance, or it might have to be inferred from the training data.
- Second, all the network variables might be directly observable in each training example, or some might be unobservable.
  - In the case where the network structure is given in advance and the variables are fully observable in the training examples, learning the conditional probability tables is straightforward and estimate the conditional probability table entries
  - In the case where the network structure is given but only some of the variable values are observable in the training data, the learning problem is more difficult. The learning problem can be compared to learning weights for an ANN.

Gradient Ascent Training of Bayesian Network

The gradient ascent rule which maximizes P(D|h) by following the gradient of ***ln P(D|h)*** with respect to the parameters that define the conditional probability tables of the Bayesian network.

Let w_{ijk} denote a single entry in one of the conditional probability tables. In particular w_{ijk} denote the conditional probability that the network variable Y_i will take on the value y_i, given that its immediate parents U_i take on the values given by u_{ik}.

The gradient of ***ln P(D|h)*** is given by the derivatives $\frac{\partial \ln P(D|h)}{\partial w_{ijk}}$ for each of the w_{ijk}.
As shown below, each of these derivatives can be calculated as

$$\frac{\partial \ln P(D|h)}{\partial w_{ij}} = \sum_{d \in D} \frac{P(Y_i = y_{ij}, U_i = u_{ik}|d)}{w_{ijk}} \qquad \textbf{equ(1)}$$

Derive the gradient defined by the set of derivatives $\frac{\partial P_h(D)}{\partial w_{ijk}}$ for all ***i, j,*** and ***k***. Assuming the training examples ***d*** in the data set D are drawn independently, we write this derivative as

$$\begin{aligned}\frac{\partial \ln P_h(D)}{\partial w_{ijk}} &= \frac{\partial}{\partial w_{ijk}} \ln \prod_{d \in D} P_h(d) \\ &= \sum_{d \in D} \frac{\partial \ln P_h(d)}{\partial w_{ijk}} \\ &= \sum_{d \in D} \frac{1}{P_h(d)} \frac{\partial P_h(d)}{\partial w_{ijk}}\end{aligned}$$

We write the abbreviation $P_h(D)$ to represent $P(D|h)$.

This last step makes use of the general equality $\frac{\partial \ln f(x)}{\partial x} = \frac{1}{f(x)} \frac{\partial f(x)}{\partial x}$. We can now introduce the values of the variables Y_i and $U_i = Parents(Y_i)$, by summing over their possible values $y_{ij'}$ and $u_{ik'}$.

$$\frac{\partial \ln P_h(D)}{\partial w_{ijk}} = \sum_{d \in D} \frac{1}{P_h(d)} \frac{\partial}{\partial w_{ijk}} \sum_{j',k'} P_h(d|y_{ij'}, u_{ik'}) P_h(y_{ij'}, u_{ik'})$$

$$= \sum_{d \in D} \frac{1}{P_h(d)} \frac{\partial}{\partial w_{ijk}} \sum_{j',k'} P_h(d|y_{ij'}, u_{ik'}) P_h(y_{ij'}|u_{ik'}) P_h(u_{ik'})$$

This last step follows from the product rule of probability . Now consider the rightmost sum in the final expression above. Given that $w_{ijk} \equiv P_h(y_{ij}|u_{ik})$, the only term in this sum for which $\frac{\partial}{\partial w_{ijk}}$ is nonzero is the term for which $j' = j$ and $i' = i$. Therefore

$$\frac{\partial \ln P_h(D)}{\partial w_{ijk}} = \sum_{d \in D} \frac{1}{P_h(d)} \frac{\partial}{\partial w_{ijk}} P_h(d|y_{ij}, u_{ik}) P_h(y_{ij}|u_{ik}) P_h(u_{ik})$$

$$= \sum_{d \in D} \frac{1}{P_h(d)} \frac{\partial}{\partial w_{ijk}} P_h(d|y_{ij}, u_{ik}) w_{ijk} P_h(u_{ik})$$

$$= \sum_{d \in D} \frac{1}{P_h(d)} P_h(d|y_{ij}, u_{ik}) P_h(u_{ik})$$

Applying Bayes theorem to rewrite $P_h(d|y_{ij}, u_{ik})$, we have

$$\frac{\partial \ln P_h(D)}{\partial w_{ijk}} = \sum_{d \in D} \frac{1}{P_h(d)} \frac{P_h(y_{ij}, u_{ik}|d) P_h(d) P_h(u_{ik})}{P_h(y_{ij}, u_{ik})}$$

$$= \sum_{d \in D} \frac{P_h(y_{ij}, u_{ik}|d) P_h(u_{ik})}{P_h(y_{ij}, u_{ik})}$$

$$= \sum_{d \in D} \frac{P_h(y_{ij}, u_{ik}|d)}{P_h(y_{ij}|u_{ik})}$$

$$= \sum_{d \in D} \frac{P_h(y_{ij}, u_{ik}|d)}{w_{ijk}} \qquad \textbf{equ (2)}$$

Thus, we have derived the gradient given in Equation (1). There is one more item that must be considered before we can state the gradient ascent training procedure. In particular, we require that as the weights w_{ijk} are updated they must remain valid probabilities in the interval [0,1]. We also require that the sum $\sum_j w_{ijk}$ remains 1 for all i, k. These constraints can be satisfied by updating weights in a two-step process. First we update each w_{ijk} by gradient ascent

$$w_{ijk} \leftarrow w_{ijk} + \eta \sum_{d \in D} \frac{P_h(y_{ij}, u_{ik}|d)}{w_{ijk}}$$

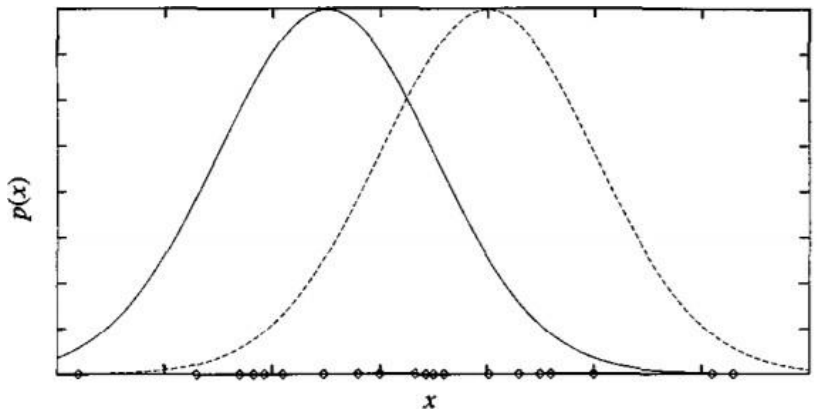
where η is a small constant called the learning rate. Second, we renormalize the weights w_{ijk} to assure that the above constraints are satisfied.
this process will converge to a locally maximum likelihood hypothesis for the conditional probabilities in the Bayesian network.

THE EM ALGORITHM

The EM algorithm can be used even for variables whose value is never directly observed, provided the general form of the probability distribution governing these variables is known.

Estimating Means of k Gaussians

- Consider a problem in which the data D is a set of instances generated by a probability distribution that is a mixture of k distinct Normal distributions.



- This problem setting is illustrated in Figure for the case where k = 2 and where the instances are the points shown along the x axis.
- Each instance is generated using a two-step process.
  - First, one of the k Normal distributions is selected at random.
  - Second, a single random instance x_i is generated according to this selected distribution.
- This process is repeated to generate a set of data points as shown in the figure.

- To simplify, consider the special case
  - The selection of the single Normal distribution at each step is based on choosing each with uniform probability
  - Each of the k Normal distributions has the same variance σ^2, known value.
- The learning task is to output a hypothesis h = (μ_1 , . . . ,μ_k) that describes the means of each of the k distributions.
- We would like to find a maximum likelihood hypothesis for these means; that is, a hypothesis ***h*** that maximizes p(D |h).

$$\mu_{ML} = \underset{\mu}{\operatorname{argmin}} \sum_{i=1}^{m} (x_i - \mu)^2 \qquad (1)$$

In this case, the sum of squared errors is minimized by the sample mean

$$\mu_{ML} = \frac{1}{m} \sum_{i=1}^{m} x_i \qquad (2)$$

- Our problem here, however, involves a mixture of k different Normal distributions, and we cannot observe which instances were generated by which distribution.
- Consider full description of each instance as the triple (x_i, z_{i1}, z_{i2}),
  - where x_i is the observed value of the ith instance and
  - where z_{i1} and z_{i2} indicate which of the two Normal distributions was used to generate the value x_i
- In particular, z_{ij} has the value 1 if x_i was created by the j^{th} Normal distribution and 0 otherwise.
- Here x_i is the observed variable in the description of the instance, and z_{il} and z_{i2} are hidden variables.
- If the values of z_{il} and z_{i2} were observed, we could use following Equation to solve for the means p_1 and p_2
- Because they are not, we will instead use the EM algorithm

EM algorithm

Step 1: Calculate the expected value $E[z_{ij}]$ of each hidden variable z_{ij}, assuming the current hypothesis $h = \langle \mu_1, \mu_2 \rangle$ holds.

Step 2: Calculate a new maximum likelihood hypothesis $h' = \langle \mu'_1, \mu'_2 \rangle$, assuming the value taken on by each hidden variable z_{ij} is its expected value $E[z_{ij}]$ calculated in Step 1. Then replace the hypothesis $h = \langle \mu_1, \mu_2 \rangle$ by the new hypothesis $h' = \langle \mu'_1, \mu'_2 \rangle$ and iterate.

Let us examine how both of these steps can be implemented in practice. Step 1 must calculate the expected value of each z_{ij}. This $E[z_{ij}]$ is just the probability that instance x_i was generated by the jth Normal distribution

$$E[z_{ij}] = \frac{p(x = x_i | \mu = \mu_j)}{\sum_{n=1}^{2} p(x = x_i | \mu = \mu_n)}$$

$$= \frac{e^{-\frac{1}{2\sigma^2}(x_i - \mu_j)^2}}{\sum_{n=1}^{2} e^{-\frac{1}{2\sigma^2}(x_i - \mu_n)^2}}$$

Thus the first step is implemented by substituting the current values $\langle \mu_1, \mu_2 \rangle$ and the observed x_i into the above expression.

In the second step we use the $E[z_{ij}]$ calculated during Step 1 to derive a new maximum likelihood hypothesis $h' = \langle \mu'_1, \mu'_2 \rangle$.
maximum likelihood hypothesis in this case is given by

$$\mu_j \leftarrow \frac{\sum_{i=1}^{m} E[z_{ij}] \; x_i}{\sum_{i=1}^{m} E[z_{ij}]}$$

MODULE 5

INSTANCE BASED LEARNING

INTRODUCTION

- Instance-based learning methods such as nearest neighbor and locally weighted regression are conceptually straightforward approaches to approximating real-valued or discrete-valued target functions.
- Learning in these algorithms consists of simply storing the presented training data. When a new query instance is encountered, a set of similar related instances is retrieved from memory and used to classify the new query instance
- Instance-based approaches can construct a different approximation to the target function for each distinct query instance that must be classified

Advantages of Instance-based learning

1. Training is very fast
2. Learn complex target function
3. Don’t lose information

Disadvantages of Instance-based learning

- The cost of classifying new instances can be high. This is due to the fact that nearly all computation takes place at classification time rather than when the training examples are first encountered.
- In many instance-based approaches, especially nearest-neighbor approaches, is that they typically consider all attributes of the instances when attempting to retrieve similar training examples from memory. If the target concept depends on only a few of the many available attributes, then the instances that are truly most "similar" may well be a large distance apart.

k- NEAREST NEIGHBOR LEARNING

- The most basic instance-based method is the K- Nearest Neighbor Learning. This algorithm assumes all instances correspond to points in the n-dimensional space R^n.
- The nearest neighbors of an instance are defined in terms of the standard Euclidean distance.
- Let an arbitrary instance x be described by the feature vector

  $$((a_1(x), a_2(x), \ldots\ldots, a_n(x))$$

  Where, $a_r(x)$ denotes the value of the r^{th} attribute of instance x.

- Then the distance between two instances x_i and x_j is defined to be $d(x_i , x_j)$
  Where,

  $$d(x_i, x_j) \equiv \sqrt{\sum_{r=1}^{n} (a_r(x_i) - a_r(x_j))^2}$$

- In nearest-neighbor learning the target function may be either discrete-valued or real-valued.

Let us first consider learning ***discrete-valued target functions*** of the form

$$f : \Re^n \rightarrow V.$$

Where, V is the finite set $\{v_1, \ldots v_s\}$

The k- Nearest Neighbor algorithm for approximation a **discrete-valued target function** is given below:

Training algorithm:

- For each training example $\langle x, f(x) \rangle$, add the example to the list *training_examples*

Classification algorithm:

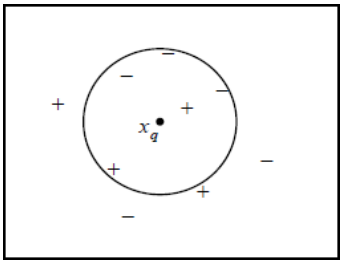
- Given a query instance x_q to be classified,
  - Let $x_1 \ldots x_k$ denote the k instances from *training_examples* that are nearest to x_q
  - Return

$$\hat{f}(x_q) \leftarrow \underset{v \in V}{\operatorname{argmax}} \sum_{i=1}^{k} \delta(v, f(x_i))$$

where $\delta(a, b) = 1$ if $a = b$ and where $\delta(a, b) = 0$ otherwise.

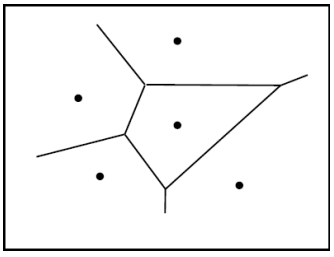
- The value $\hat{f}(x_q)$ returned by this algorithm as its estimate of $f(x_q)$ is just the most common value of f among the k training examples nearest to x_q.
- If k = 1, then the 1- Nearest Neighbor algorithm assigns to $\hat{f}(x_q)$ the value f(xi). Where x_i is the training instance nearest to x_q.
- For larger values of k, the algorithm assigns the most common value among the k nearest training examples.

- Below figure illustrates the operation of the k-Nearest Neighbor algorithm for the case where the instances are points in a two-dimensional space and where the target function is Boolean valued.



- The positive and negative training examples are shown by "+" and "-" respectively. A query point x_q is shown as well.
- The 1-Nearest Neighbor algorithm classifies x_q as a positive example in this figure, whereas the 5-Nearest Neighbor algorithm classifies it as a negative example.

- Below figure shows the shape of this **decision surface** induced by 1- Nearest Neighbor over the entire instance space. The decision surface is a combination of convex polyhedra surrounding each of the training examples.



- For every training example, the polyhedron indicates the set of query points whose classification will be completely determined by that training example. Query points outside the polyhedron are closer to some other training example. This kind of diagram is often called the ***Voronoi diagram*** of the set of training example

The K- Nearest Neighbor algorithm for approximation a **real-valued target function** is given belo $f : \Re^n \rightarrow \Re$

Training algorithm:

- For each training example $\langle x, f(x) \rangle$, add the example to the list *training_examples*

Classification algorithm:

- Given a query instance x_q to be classified,
  - Let $x_1 \ldots x_k$ denote the k instances from *training_examples* that are nearest to x_q
  - Return

$$\hat{f}(x_q) \leftarrow \frac{\sum_{i=1}^{k} f(x_i)}{k}$$

Distance-Weighted Nearest Neighbor Algorithm

- The refinement to the k-NEAREST NEIGHBOR Algorithm is to weight the contribution of each of the k neighbors according to their distance to the query point x_q, giving greater weight to closer neighbors.
- For example, in the k-Nearest Neighbor algorithm, which approximates discrete-valued target functions, we might weight the vote of each neighbor according to the inverse square of its distance from x_q

Distance-Weighted Nearest Neighbor Algorithm for approximation a discrete-valued target functions

---

Training algorithm:

- For each training example $\langle x, f(x) \rangle$, add the example to the list *training_examples*

Classification algorithm:

- Given a query instance x_q to be classified,
  - Let $x_1 \ldots x_k$ denote the k instances from *training_examples* that are nearest to x_q
  - Return

$$\hat{f}(x_q) \leftarrow \underset{v \in V}{\operatorname{argmax}} \sum_{i=1}^{k} w_i \delta(v, f(x_i))$$

where

$$w_i \equiv \frac{1}{d(x_q, x_i)^2}$$

Distance-Weighted Nearest Neighbor Algorithm for approximation a Real-valued target functions

---

Training algorithm:

- For each training example $\langle x, f(x) \rangle$, add the example to the list *training_examples*

Classification algorithm:

- Given a query instance x_q to be classified,
  - Let $x_1 \ldots x_k$ denote the k instances from *training_examples* that are nearest to x_q
  - Return

$$\hat{f}(x_q) \leftarrow \frac{\sum_{i=1}^{k} w_i f(x_i)}{\sum_{i=1}^{k} w_i}$$

where

$$w_i \equiv \frac{1}{d(x_q, x_i)^2}$$

Terminology

- **Regression** means approximating a real-valued target function.
- **Residual** is the error $\hat{f}(x) - f(x)$ in approximating the target function.
- **Kernel function** is the function of distance that is used to determine the weight of each training example. In other words, the kernel function is the function K such that $w_i = K(d(x_i, x_q))$

LOCALLY WEIGHTED REGRESSION

- The phrase "**locally weighted regression**" is called **local** because the function is approximated based only on data near the query point, **weighted** because the contribution of each training example is weighted by its distance from the query point, and **regression** because this is the term used widely in the statistical learning community for the problem of approximating real-valued functions.

- Given a new query instance x_q, the general approach in locally weighted regression is to construct an approximation $\hat{f}$ that fits the training examples in the neighborhood surrounding x_q. This approximation is then used to calculate the value $\hat{f}(x_q)$, which is output as the estimated target value for the query instance.

Locally Weighted Linear Regression

- Consider locally weighted regression in which the target function ***f*** is approximated near x_q using a linear function of the form

$$\hat{f}(x) = w_0 + w_1 a_1(x) + \cdots + w_n a_n(x)$$

Where, $a_i(x)$ denotes the value of the i^{th} attribute of the instance x

- Derived methods are used to choose weights that minimize the squared error summed over the set D of training examples using gradient descent

$$E \equiv \frac{1}{2} \sum_{x \in D} (f(x) - \hat{f}(x))^2$$

Which led us to the gradient descent training rule

$$\Delta w_j = \eta \sum_{x \in D} (f(x) - \hat{f}(x)) a_j(x)$$

Where, η is a constant learning rate

- Need to modify this procedure to derive a local approximation rather than a global one. The simple way is to redefine the error criterion E to emphasize fitting the local training examples. Three possible criteria are given below.

1. Minimize the squared error over just the k nearest neighbors:

$$E_1(x_q) \equiv \frac{1}{2} \sum_{x \in k \text{ nearest nbrs of } x_q} (f(x) - \hat{f}(x))^2 \qquad \textbf{equ(1)}$$

2. Minimize the squared error over the entire set D of training examples, while weighting the error of each training example by some decreasing function K of its distance from x_q :

$$E_2(x_q) \equiv \frac{1}{2} \sum_{x \in D} (f(x) - \hat{f}(x))^2 \; K(d(x_q, x)) \qquad \textbf{equ(2)}$$

3. Combine 1 and 2:

$$E_3(x_q) \equiv \frac{1}{2} \sum_{x \in k \text{ nearest nbrs of } x_q} (f(x) - \hat{f}(x))^2 \; K(d(x_q, x)) \qquad \textbf{equ(3)}$$

If we choose criterion three and re-derive the gradient descent rule, we obtain the following training rule

$$\Delta w_j = \eta \sum_{x \in \ k \ nearest \ nbrs \ of \ x_q} K(d(x_q, x)) \ (f(x) - \hat{f}(x)) \ a_j(x)$$

The differences between this new rule and the rule given by Equation (3) are that the contribution of instance x to the weight update is now multiplied by the distance penalty **$K(d(x_q, x))$,** and that the error is summed over only the k nearest training examples.

RADIAL BASIS FUNCTIONS

- One approach to function approximation that is closely related to distance-weighted regression and also to artificial neural networks is learning with radial basis functions
- In this approach, the learned hypothesis is a function of the form

$$\hat{f}(x) = w_0 + \sum_{u=1}^{k} w_u K_u(d(x_u, x)) \qquad \textbf{equ (1)}$$

- Where, each x_u is an instance from X and where the kernel function $K_u(d(x_u, x))$ is defined so that it decreases as the distance d(xu, x) increases.
- Here k is a user provided constant that specifies the number of kernel functions to be included.
- $\hat{f}$ is a global approximation to f (x), the contribution from each of the $K_u(d(x_u, x))$ terms is localized to a region nearby the point x_u.

Choose each function $K_u(d(x_u, x))$ to be a Gaussian function centred at the point x_u with some variance σ_u^2

$$K_u(d(x_u, x)) = e^{\frac{1}{2\sigma_u^2} d^2(x_u, x)}$$

- The functional form of equ(1) can approximate any function with arbitrarily small error, provided a sufficiently large number k of such Gaussian kernels and provided the width σ^2 of each kernel can be separately specified
- The function given by equ(1) can be viewed as describing a two layer network where the first layer of units computes the values of the various $K_u(d(x_u, x))$ and where the second layer computes a linear combination of these first-layer unit values

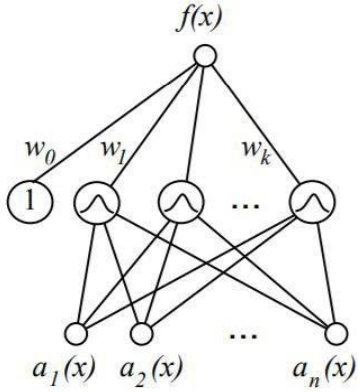
Example: Radial basis function (RBF) network

Given a set of training examples of the target function, RBF networks are typically trained in a two-stage process.

1. First, the number k of hidden units is determined and each hidden unit u is defined by choosing the values of x_u and σ_u^2 that define its kernel function $K_u(d(x_u, x))$
2. Second, the weights w, are trained to maximize the fit of the network to the training data, using the global error criterion given by

$$E \equiv \frac{1}{2} \sum_{x \in D} (f(x) - \hat{f}(x))^2$$

Because the kernel functions are held fixed during this second stage, the linear weight values w, can be trained very efficiently



Several alternative methods have been proposed for choosing an appropriate number of hidden units or, equivalently, kernel functions.

- One approach is to allocate a Gaussian kernel function for each training example $(x_i, f(x_i))$, centring this Gaussian at the point x_i.
  Each of these kernels may be assigned the same width σ^2. Given this approach, the RBF network learns a global approximation to the target function in which each training example $(x_i, f(x_i))$ can influence the value of $\hat{f}$ only in the neighbourhood of x_i.
- A second approach is to choose a set of kernel functions that is smaller than the number of training examples. This approach can be much more efficient than the first approach, especially when the number of training examples is large.

Summary

- Radial basis function networks provide a global approximation to the target function, represented by a linear combination of many local kernel functions.
- The value for any given kernel function is non-negligible only when the input x falls into the region defined by its particular centre and width. Thus, the network can be viewed as a smooth linear combination of many local approximations to the target function.
- One key advantage to RBF networks is that they can be trained much more efficiently than feedforward networks trained with BACKPROPAGATION.

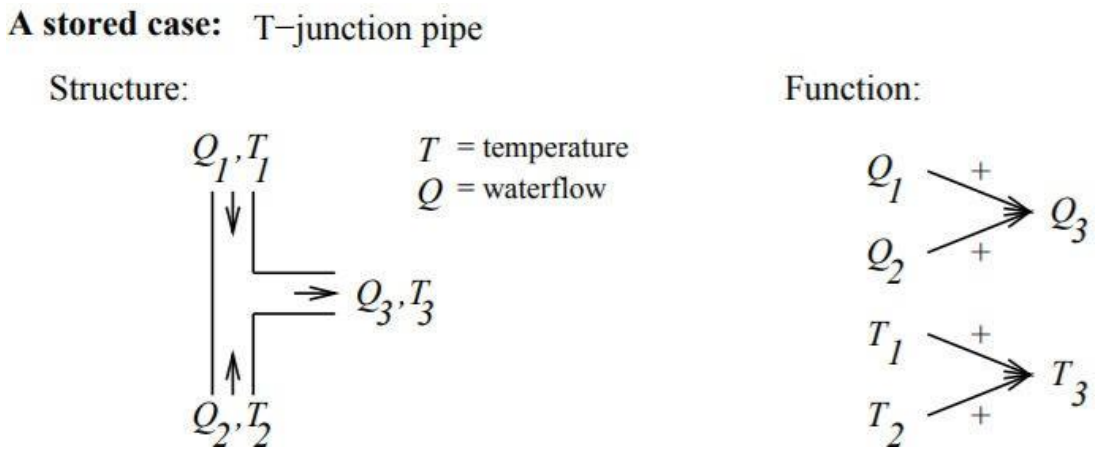
CASE-BASED REASONING

- Case-based reasoning (CBR) is a learning paradigm based on lazy learning methods and they classify new query instances by analysing similar instances while ignoring instances that are very different from the query.
- In CBR represent instances are not represented as real-valued points, but instead, they use a ***rich symbolic*** representation.
- CBR has been applied to problems such as conceptual design of mechanical devices based on a stored library of previous designs, reasoning about new legal cases based on previous rulings, and solving planning and scheduling problems by reusing and combining portions of previous solutions to similar problems

A prototypical example of a case-based reasoning

- The CADET system employs case-based reasoning to assist in the conceptual design of simple mechanical devices such as water faucets.
- It uses a library containing approximately 75 previous designs and design fragments to suggest conceptual designs to meet the specifications of new design problems.
- Each instance stored in memory (e.g., a water pipe) is represented by describing both its structure and its qualitative function.
- New design problems are then presented by specifying the desired function and requesting the corresponding structure.

The problem setting is illustrated in below figure



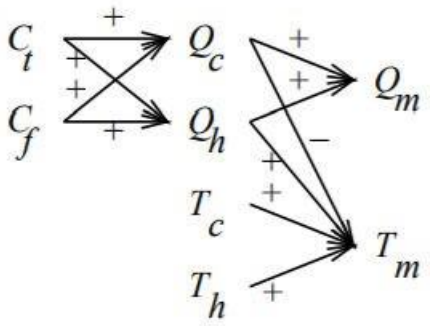
- The function is represented in terms of the qualitative relationships among the water-flow levels and temperatures at its inputs and outputs.
- In the functional description, an arrow with a "+" label indicates that the variable at the arrowhead increases with the variable at its tail. A "-" label indicates that the variable at the head decreases with the variable at the tail.
- Here Q_c refers to the flow of cold water into the faucet, Q_h to the input flow of hot water, and Q_m to the single mixed flow out of the faucet.
- T_c, T_h, and T_m refer to the temperatures of the cold water, hot water, and mixed water respectively.
- The variable C_t denotes the control signal for temperature that is input to the faucet, and C_f denotes the control signal for waterflow.
- The controls C_t and C_f are to influence the water flows Q_c and Q_h, thereby indirectly influencing the faucet output flow Q_m and temperature T_m.

A problem specification: Water faucet

Structure:

?

Function:



- CADET searches its library for stored cases whose functional descriptions match the design problem. If an exact match is found, indicating that some stored case implements exactly the desired function, then this case can be returned as a suggested solution to the design problem. If no exact match occurs, CADET may find cases that match various subgraphs of the desired functional specification.

REINFORCEMENT LEARNING

Reinforcement learning addresses the question of how an autonomous agent that senses and acts in its environment can learn to choose optimal actions to achieve its goals.

INTRODUCTION

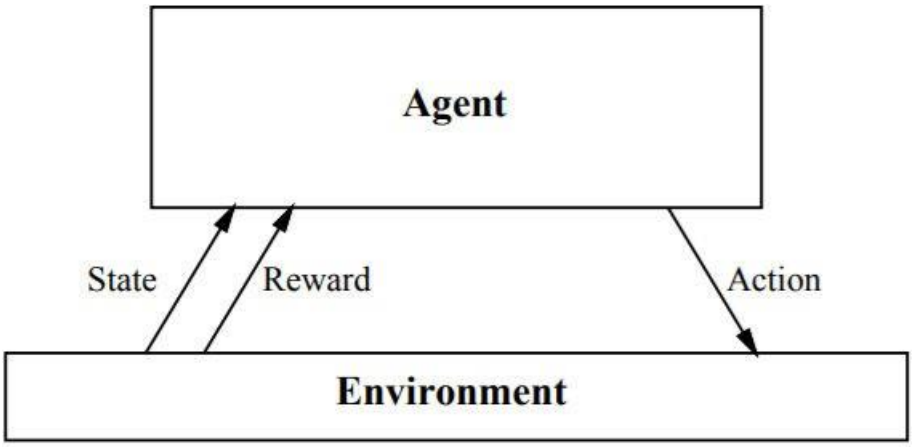
- Consider building a **learning robot**. The robot, or ***agent***, has a set of sensors to observe the state of its environment, and a set of actions it can perform to alter this state.
- Its task is to learn a control strategy, or ***policy***, for choosing actions that achieve its goals.
- The goals of the agent can be defined by a ***reward function*** that assigns a numerical value to each distinct action the agent may take from each distinct state.
- This reward function may be built into the robot, or known only to an external teacher who provides the reward value for each action performed by the robot.
- The **task** of the robot is to perform sequences of actions, observe their consequences, and learn a control policy.
- The control policy is one that, from any initial state, chooses actions that maximize the reward accumulated over time by the agent.

Example:

- A mobile robot may have sensors such as a camera and sonars, and actions such as "move forward" and "turn."
- The robot may have a goal of docking onto its battery charger whenever its battery level is low.
- The goal of docking to the battery charger can be captured by assigning a positive reward (Eg., +100) to state-action transitions that immediately result in a connection to the charger and a reward of zero to every other state-action transition.

Reinforcement Learning Problem

- An agent interacting with its environment. The agent exists in an environment described by some set of possible states S.
- Agent perform any of a set of possible actions A. Each time it performs an action a, in some state s_t the agent receives a real-valued reward r, that indicates the immediate value of this state-action transition. This produces a sequence of states s_i, actions a_i, and immediate rewards r_i as shown in the figure.
- The agent's task is to learn a control policy, $\boldsymbol{\pi}: \mathbf{S} \rightarrow \mathbf{A}$, that maximizes the expected sum of these rewards, with future rewards discounted exponentially by their delay.



$$s_0 \xrightarrow[r_0]{a_0} s_1 \xrightarrow[r_1]{a_1} s_2 \xrightarrow[r_2]{a_2} \dots$$

Goal: Learn to choose actions that maximize

$$r_0 + \gamma r_1 + \gamma^2 r_2 + \dots \text{ , where } 0 \leq \gamma < 1$$

Reinforcement learning problem characteristics

1. **Delayed reward**: The task of the agent is to learn a target function π that maps from the current state s to the optimal action a = π (s). In reinforcement learning, training information is not available in (s, π (s)). Instead, the trainer provides only a sequence of immediate reward values as the agent executes its sequence of actions. The agent, therefore, faces the problem of ***temporal credit assignment***: determining which of the actions in its sequence are to be credited with producing the eventual rewards.

2. **Exploration:** In reinforcement learning, the agent influences the distribution of training examples by the action sequence it chooses. This raises the question of which experimentation strategy produces most effective learning. The learner faces a trade-off in choosing whether to favor exploration of unknown states and actions, or exploitation of states and actions that it has already learned will yield high reward.

3. **Partially observable states:** The agent's sensors can perceive the entire state of the environment at each time step, in many practical situations sensors provide only partial information. In such cases, the agent needs to consider its previous observations together with its current sensor data when choosing actions, and the best policy may be one that chooses actions specifically to improve the observability of the environment.

4. **Life-long learning:** Robot requires to learn several related tasks within the same environment, using the same sensors. For example, a mobile robot may need to learn how to dock on its battery charger, how to navigate through narrow corridors, and how to pick up output from laser printers. This setting raises the possibility of using previously obtained experience or knowledge to reduce sample complexity when learning new tasks.

THE LEARNING TASK

- Consider Markov decision process (MDP) where the agent can perceive a set S of distinct states of its environment and has a set A of actions that it can perform.
- At each discrete time step t, the agent senses the current state s_t, chooses a current action a_t, and performs it.
- The environment responds by giving the agent a reward $r_t = r(s_t, a_t)$ and by producing the succeeding state $s_{t+1} = \delta(s_t, a_t)$. Here the functions $\delta(s_t, a_t)$ and $r(s_t, a_t)$ depend only on the current state and action, and not on earlier states or actions.

The task of the agent is to learn a policy, $\boldsymbol{\pi: S \rightarrow A}$, for selecting its next action a, based on the current observed state s_t; that is, $\boldsymbol{\pi(s_t) = a_t}$.

How shall we specify precisely which policy π we would like the agent to learn?

1. One approach is to require the policy that produces the greatest possible ***cumulative reward*** for the robot over time.

- To state this requirement more precisely, define the cumulative value $V^{\pi}(s_t)$ achieved by following an arbitrary policy π from an arbitrary initial state s_t as follows:

$$V^{\pi}(s_t) \equiv r_t + \gamma r_{t+1} + \gamma^2 r_{t+2} + \ldots$$

$$\equiv \sum_{i=0}^{\infty} \gamma^i r_{t+i} \qquad \textbf{equ (1)}$$

- Where, the sequence of rewards r_{t+i} is generated by beginning at state s_t and by repeatedly using the policy π to select actions.
- Here $0 \leq \gamma \leq 1$ is a constant that determines the relative value of delayed versus immediate rewards. if we set $\gamma = 0$, only the immediate reward is considered. As we set γ closer to 1, future rewards are given greater emphasis relative to the immediate reward.
- The quantity $V^{\pi}(s_t)$ is called the ***discounted cumulative reward*** achieved by policy π from initial state ***s***. It is reasonable to discount future rewards relative to immediate rewards because, in many cases, we prefer to obtain the reward sooner rather than later.

2. Other definitions of total reward is ***finite horizon reward,***

$$\sum_{i=0}^{h} r_{t+i}$$

Considers the undiscounted sum of rewards over a finite number ***h*** of steps

3. Another approach is ***average reward***

$$\lim_{h\to\infty} \frac{1}{h} \sum_{i=0}^{h} r_{t+i}$$

Considers the average reward per time step over the entire lifetime of the agent.

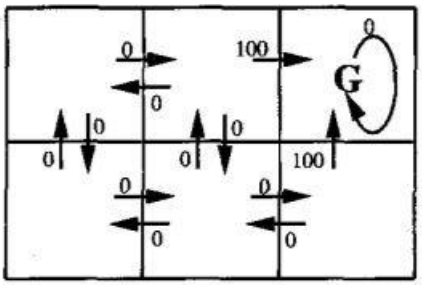
We require that the agent learn a policy π that maximizes $V^{\pi}(s_t)$ for all states s. such a policy is called an ***optimal policy*** and denote it by π*

$$\pi^* \equiv \underset{\pi}{\operatorname{argmax}}\, V^{\pi}(s), (\forall s) \qquad \textbf{equ (2)}$$

Refer the value function $V^{\pi*}(s)$ an optimal policy as V*(s). V*(s) gives the maximum discounted cumulative reward that the agent can obtain starting from state ***s***.

Example:

A simple grid-world environment is depicted in the diagram

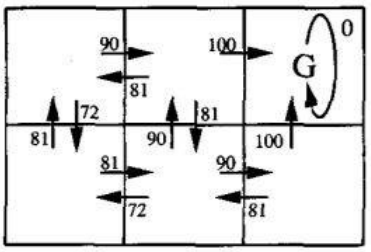


$r(s, a)$ (immediate reward) values

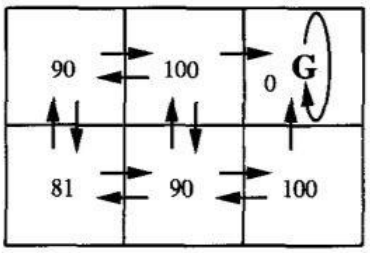
- The six grid squares in this diagram represent six possible states, or locations, for the agent.
- Each arrow in the diagram represents a possible action the agent can take to move from one state to another.
- The number associated with each arrow represents the immediate reward ***r(s, a)*** the agent receives if it executes the corresponding state-action transition
- The immediate reward in this environment is defined to be zero for all state-action transitions except for those leading into the state labelled G. The state G as the goal state, and the agent can receive reward by entering this state.

Once the states, actions, and immediate rewards are defined, choose a value for the discount factor γ, determine the optimal policy π * and its value function V*(s).

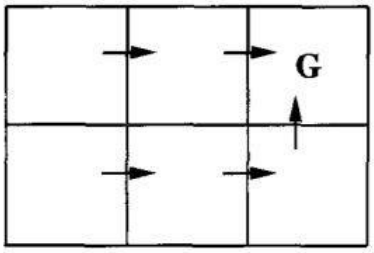
Let's choose γ = 0.9. The diagram at the bottom of the figure shows one optimal policy for this setting.



$Q(s, a)$ values



$V^*(s)$ values



One optimal policy

Values of V*(s) and Q(s, a) follow from r(s, a), and the discount factor γ = 0.9. An optimal policy, corresponding to actions with maximal Q values, is also shown.

The discounted future reward from the bottom centre state is

$$0+ \gamma\ 100+ \gamma^2\ 0+ \gamma^3\ 0+... = 90$$

Q LEARNING

How can an agent learn an optimal policy π * for an arbitrary environment?

The training information available to the learner is the sequence of immediate rewards $r(s_i,a_i)$ for i = 0, 1,2, ... Given this kind of training information it is easier to learn a numerical evaluation function defined over states and actions, then implement the optimal policy in terms of this evaluation function.

What evaluation function should the agent attempt to learn?

One obvious choice is V*. The agent should prefer state s_1 over state s_2 whenever $V^*(s_1) > V^*(s_2)$, because the cumulative future reward will be greater from s_1

The optimal action in state ***s*** is the action ***a*** that maximizes the sum of the immediate reward r(s, a) plus the value V* of the immediate successor state, discounted by γ.

$$\pi^*(s) = \underset{a}{\operatorname{argmax}}[r(s, a) + \gamma V^*(\delta(s, a))] \qquad \textbf{equ (3)}$$

The *Q* Function

The value of Evaluation function ***Q(s, a)*** is the reward received immediately upon executing action a from state ***s***, plus the value (discounted by γ) of following the optimal policy thereafter

$$Q(s,a) \equiv r(s,a) + \gamma V^*(\delta(s,a)) \qquad \textbf{equ (4)}$$

Rewrite Equation (3) in terms of ***Q(s, a)*** as

$$\pi^*(s) = \underset{a}{\operatorname{argmax}}\, Q(s,a) \qquad \textbf{equ (5)}$$

Equation (5) makes clear, it need only consider each available action ***a*** in its current state ***s*** and choose the action that maximizes ***Q(s, a)***.

An Algorithm for Learning *Q*

- Learning the Q function corresponds to learning the **optimal policy**.
- The key problem is finding a reliable way to estimate training values for ***Q***, given only a sequence of immediate rewards ***r*** spread out over time. This can be accomplished through ***iterative approximation***

$$V^*(s) = \max_{a'} Q(s,a')$$

Rewriting Equation

$$Q(s,a) = r(s,a) + \gamma \max_{a'} Q(\delta(s,a), a')$$

- **Q learning algorithm:**

Q learning algorithm

For each s, a initialize the table entry $\hat{Q}(s,a)$ to zero.
Observe the current state s
Do forever:

- Select an action a and execute it
- Receive immediate reward r
- Observe the new state s'
- Update the table entry for $\hat{Q}(s,a)$ as follows:

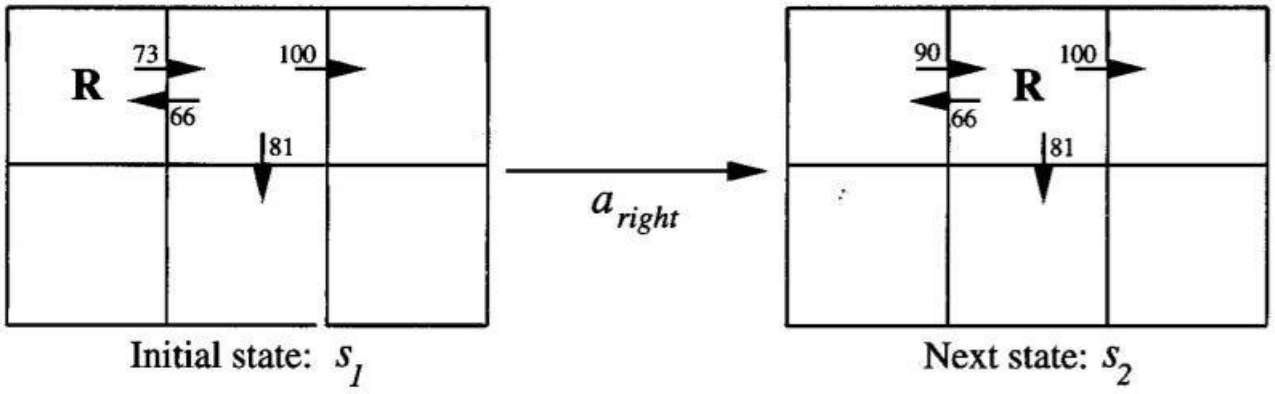
$$\hat{Q}(s,a) \leftarrow r + \gamma \max_{a'} \hat{Q}(s',a')$$

- $s \leftarrow s'$

- Q learning algorithm assuming deterministic rewards and actions. The discount factor γ may be any constant such that $0 \leq \gamma < 1$
- Q to refer to the learner's estimate, or hypothesis, of the actual Q function

An Illustrative Example

- To illustrate the operation of the Q learning algorithm, consider a single action taken by an agent, and the corresponding refinement to Q shown in below figure



- The agent moves one cell to the right in its grid world and receives an immediate reward of zero for this transition.
- Apply the training rule of Equation

$$\hat{Q}(s, a) \leftarrow r + \gamma \max_{a'} \hat{Q}(s', a')$$

to refine its estimate Q for the state-action transition it just executed.

- According to the training rule, the new Q estimate for this transition is the sum of the received reward (zero) and the highest Q value associated with the resulting state (100), discounted by γ (.9).

$$\begin{aligned} \hat{Q}(s_1, a_{right}) &\leftarrow r + \gamma \max_{a'} \hat{Q}(s_2, a') \\ &\leftarrow 0 + 0.9 \ \max\{66, 81, 100\} \\ &\leftarrow 90 \end{aligned}$$

Convergence

Will the Q Learning Algorithm converge toward a Q equal to the true Q function?

Yes, under certain conditions.

1. Assume the system is a deterministic MDP.
2. Assume the immediate reward values are bounded; that is, there exists some positive constant c such that for all states s and actions a, $|\mathbf{r(s, a)}| < \mathbf{c}$
3. Assume the agent selects actions in such a fashion that it visits every possible state-action pair infinitely often

Theorem Convergence of Q learning for deterministic Markov decision processes.

Consider a Q learning agent in a deterministic MDP with bounded rewards $(\forall s, a)|r(s, a)| \leq c$.

The Q learning agent uses the training rule of Equation $\hat{Q}(s, a) \leftarrow r + \gamma \max_{a'} \hat{Q}(s', a')$ initializes its table $\hat{Q}(s, a)$ to arbitrary finite values, and uses a discount factor γ such that $0 \leq \gamma < 1$. Let $\hat{Q}_n(s, a)$ denote the agent's hypothesis $\hat{Q}(s, a)$ following the nth update. If each state-action pair is visited infinitely often, then $\hat{Q}_n(s, a)$ converges to $Q(s, a)$ as $n \rightarrow \infty$, for all s, a.

Proof. Since each state-action transition occurs infinitely often, consider consecutive intervals during which each state-action transition occurs at least once. The proof consists of showing that the maximum error over all entries in the $\hat{Q}$ table is reduced by at least a factor of γ during each such interval. $\hat{Q}_n$ is the agent's table of estimated Q values after n updates. Let Δ_n be the maximum error in $\hat{Q}_n$; that is

$$\Delta_n \equiv \max_{s,a} |\hat{Q}_n(s, a) - Q(s, a)|$$

Below we use s' to denote $\delta(s, a)$. Now for any table entry $\hat{Q}_n(s, a)$ that is updated on iteration $n + 1$, the magnitude of the error in the revised estimate $\hat{Q}_{n+1}(s, a)$ is

$$\begin{aligned}
|\hat{Q}_{n+1}(s, a) - Q(s, a)| &= |(r + \gamma \max_{a'} \hat{Q}_n(s', a')) - (r + \gamma \max_{a'} Q(s', a'))| \\
&= \gamma |\max_{a'} \hat{Q}_n(s', a') - \max_{a'} Q(s', a')| \\
&\leq \gamma \max_{a'} |\hat{Q}_n(s', a') - Q(s', a')| \\
&\leq \gamma \max_{s'', a'} |\hat{Q}_n(s'', a') - Q(s'', a')| \\
|\hat{Q}_{n+1}(s, a) - Q(s, a)| &\leq \gamma \Delta_n
\end{aligned}$$

The third line above follows from the second line because for any two functions f_1 and f_2 the following inequality holds

$$|\max_a f_1(a) - \max_a f_2(a)| \leq \max_a |f_1(a) - f_2(a)|$$

In going from the third line to the fourth line above, note we introduce a new variable s'' over which the maximization is performed. This is legitimate because the maximum value will be at least as great when we allow this additional variable to vary. Note that by introducing this variable we obtain an expression that matches the definition of Δ_n.

Thus, the updated $Q_{n+1}(s, a)$ for any s, a is at most γ times the maximum error in the $\hat{Q}_n$ table, Δ_n. The largest error in the initial table, Δ_0, is bounded because values of $\hat{Q}_0(s, a)$ and $Q(s, a)$ are bounded for all s, a. Now after the first interval during which each s, a is visited, the largest error in the table will be at most $\gamma \Delta_0$. After k such intervals, the error will be at most $\gamma^k \Delta_0$. Since each state is visited infinitely often, the number of such intervals is infinite, and $\Delta_n \to 0$ as $n \to \infty$. This proves the theorem.

Experimentation Strategies

The Q learning algorithm does not specify how actions are chosen by the agent.

- One obvious strategy would be for the agent in state ***s*** to select the action ***a*** that maximizes $\hat{Q}(s, a)$, thereby exploiting its current approximation $\hat{Q}$
- However, with this strategy the agent runs the risk that it will overcommit to actions that are found during early training to have high Q values, while failing to explore other actions that have even higher values.
- For this reason, Q learning uses a probabilistic approach to selecting actions. Actions with higher $\hat{Q}$ values are assigned higher probabilities, but every action is assigned a nonzero probability.
- One way to assign such probabilities is

$$P(a_i|s) = \frac{k^{\hat{Q}(s,a_i)}}{\sum_j k^{\hat{Q}(s,a_j)}}$$

Where, $\mathbf{P(a_i|s)}$ is the probability of selecting action $\mathbf{a_i}$, given that the agent is in state **s**, and $\mathbf{k > 0}$ is a constant that determines how strongly the selection favors actions with high $\hat{Q}$ values

MODULE 5

EVALUATING HYPOTHESES

MOTIVATION

It is important to evaluate the performance of learned hypotheses as precisely as possible.

- One reason is simply to understand whether to use the hypothesis.
- A second reason is that evaluating hypotheses is an integral component of many learning methods.

Two key difficulties arise while learning a hypothesis and estimating its future accuracy given only a limited set of data:

1. **Bias in the estimate**. The observed accuracy of the learned hypothesis over the training examples is often a poor estimator of its accuracy over future examples. Because the learned hypothesis was derived from these examples, they will typically provide an optimistically biased estimate of hypothesis accuracy over future examples. This is especially likely when the learner considers a very rich hypothesis space, enabling it to overfit the training examples. To obtain an unbiased estimate of future accuracy, test the hypothesis on some set of test examples chosen independently of the training examples and the hypothesis.

2. **Variance in the estimate.** Even if the hypothesis accuracy is measured over an unbiased set of test examples independent of the training examples, the measured accuracy can still vary from the true accuracy, depending on the makeup of the particular set of test examples. The smaller the set of test examples, the greater the expected variance.

ESTIMATING HYPOTHESIS ACCURACY

Sample Error –
The sample error of a hypothesis with respect to some sample S of instances drawn from X is the fraction of S that it misclassifies.

Definition: The sample error (***$error_s(h)$***) of hypothesis h with respect to target function f and data sample S is

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

Where n is the number of examples in S, and the quantity $\delta(f(x), h(x))$ is 1 if $f(x) \neq h(x)$, and 0 otherwise.

True Error –
The true error of a hypothesis is the probability that it will misclassify a single randomly drawn instance from the distribution $\mathcal{D}$.

Definition: The true error ($error_{\mathcal{D}}(h)$) of hypothesis h with respect to target function f and distribution $\mathcal{D}$, is the probability that h will misclassify an instance drawn at random according to $\mathcal{D}$.

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

Confidence Intervals for Discrete-Valued Hypotheses

Suppose we wish to estimate the true error for some discrete valued hypothesis h, based on its observed sample error over a sample S, where

- The sample S contains n examples drawn independent of one another, and independent of h, according to the probability distribution $\mathcal{D}$
- $n \geq 30$
- Hypothesis h commits r errors over these n examples (i.e., $error_s(h) = r/n$).

Under these conditions, statistical theory allows to make the following assertions:

1. Given no other information, the most probable value of $error_{\mathcal{D}}(h)$ is $error_s(h)$
2. With approximately **95% probability**, the true error $error_{\mathcal{D}}(h)$ lies in the interval

$$error_S(h) \pm 1.96\sqrt{\frac{error_S(h)(1 - error_S(h))}{n}}$$

Example:

Suppose the data sample S contains n = 40 examples and that hypothesis h commits r = 12 errors over this data.

- The ***sample error*** is $error_s(h) = r/n = 12/40 = 0.30$
- Given no other information, ***true error*** is $error_{\mathcal{D}}(h) = error_s(h)$, i.e., $error_{\mathcal{D}}(h) = 0.30$
- With the 95% confidence interval estimate for $error_{\mathcal{D}}(h)$.

$$error_S(h) \pm 1.96\sqrt{\frac{error_S(h)(1 - error_S(h))}{n}}$$

$= 0.30 \pm (1.96 * 0.07)$ $= 0.30 \pm 0.14$

3. A different constant, ***ZN***, is used to calculate the **N% confidence interval**. The general expression for approximate N% confidence intervals for $error_{\mathcal{D}}(h)$ is

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

Where,

$N\%$:	50%	68%	80%	90%	95%	98%	99%
z_N:	0.67	1.00	1.28	1.64	1.96	2.33	2.58

The above equation describes how to calculate the confidence intervals, or error bars, for estimates of $error_{\mathcal{D}}(h)$ that are based on $error_s(h)$

Example:

Suppose the data sample S contains n = 40 examples and that hypothesis h commits r = 12 errors over this data.

- The ***sample error*** is $error_s(h) = r/n = 12/40 = 0.30$
- With the 68% confidence interval estimate for $error_{\mathcal{D}}(h)$.

$$error_S(h) \pm 1.00 \sqrt{\frac{error_S(h)(1 - error_S(h))}{n}}$$

$= 0.30 \pm (1.00 * 0.07)$

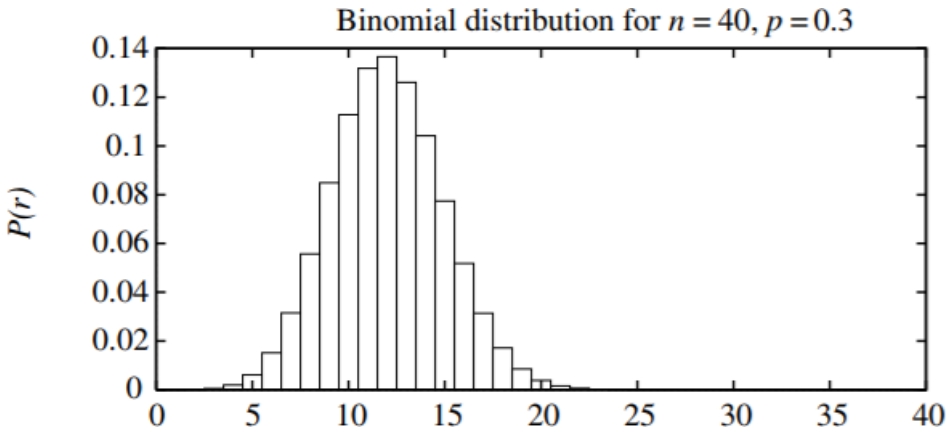
$= 0.30 \pm 0.07$

BASICS OF SAMPLING THEORY

Error Estimation and Estimating Binomial Proportions

- Collect a random sample S of *n* independently drawn instances from the distribution *D*, and then measure the sample error $error_s(h)$. Repeat this experiment many times, each time drawing a different random sample S_i of size *n*, we would expect to observe different values for the various $error_{si}(h)$, depending on random differences in the makeup of the various S_i. We say that $error_{si}(h)$, the outcome of the i^{th} such experiment, is a ***random variable***.

- Imagine that we were to run k random experiments, measuring the random variables $error_{s1}(h)$, $error_{s2}(h)$ . . . $errors_{sk}(h)$ and plotted a histogram displaying the frequency with which each possible error value is observed.
- As ***k*** grows, the histogram would approach a particular probability distribution called the ***Binomial distribution*** which is shown in below figure.



A Binomial distribution is defined by the probability function

$$P(r) = \frac{n!}{r!(n-r)!} p^r (1-p)^{n-r}$$

If the random variable ***X*** follows a Binomial distribution, then:

- The probability ***Pr(X = r)*** that ***X*** will take on the value ***r*** is given by ***P(r)***

- Expected, or mean value of X, $E[X]$, is

$$E[X] \equiv \sum_{i=0}^{n} iP(i) = np$$

- Variance of X is

$$Var(X) \equiv E[(X - E[X])^2] = np(1-p)$$

- Standard deviation of X, σ_X, is

$$\sigma_X \equiv \sqrt{E[(X - E[X])^2]} = \sqrt{np(1-p)}$$

The Binomial Distribution

Consider the following problem for better understanding of Binomial Distribution

- Given a worn and bent coin and estimate the probability that the coin will turn up heads when tossed.
- Unknown probability of heads ***p***. Toss the coin ***n*** times and record the number of times ***r*** that it turns up heads.

  Estimate of $p = r / n$
- If the experiment were *rerun*, generating a new set of ***n*** coin tosses, we might expect the number of heads ***r*** to vary somewhat from the value measured in the first experiment, yielding a somewhat different estimate for ***p***.
- The Binomial distribution describes for each possible value of ***r*** (i.e., from 0 to n), the probability of observing exactly ***r*** heads given a sample of ***n*** independent tosses of a coin whose true probability of heads is ***p***.

<u>The general setting to which the Binomial distribution applies is:</u>

1. There is a base experiment (e.g., toss of the coin) whose outcome can be described by a random variable 'Y'. The random variable Y can take on two possible values (e.g., Y = 1 if heads, Y = 0 if tails).
2. The probability that Y = 1 on any single trial of the base experiment is given by some constant p, independent of the outcome of any other experiment. The probability that Y = 0 is therefore (1 - p). Typically, p is not known in advance, and the problem is to estimate it.
3. A series of n independent trials of the underlying experiment is performed (e.g., n independent coin tosses), producing the sequence of independent, identically distributed random variables $Y_1, Y_2, \ldots, Y_n$. Let R denote the number of trials for which $Y_i = 1$ in this series of n experiments

$$R \equiv \sum_{i=1}^{n} Y_i$$

4. The probability that the random variable R will take on a specific value r (e.g., the probability of observing exactly r heads) is given by the Binomial distribution

$$\Pr(R = r) = \frac{n!}{r!(n-r)!} p^r (1-p)^{n-r} \qquad \textbf{equ (1)}$$

Mean, Variance and Standard Deviation

The Mean (expected value) is the average of the values taken on by repeatedly sampling the random variable

Definition: Consider a random variable Y that takes on the possible values $y_1, \ldots y_n$. The expected value (Mean) of Y, E[Y], is

$$E[Y] \equiv \sum_{i=1}^{n} y_i \Pr(Y = y_i)$$

The Variance captures how far the random variable is expected to vary from its mean value.

Definition: The variance of a random variable Y, Var[Y], is

$$Var[Y] \equiv E[(Y - E[Y])^2]$$

The variance describes the expected squared error in using a single observation of Y to estimate its mean E[Y].
The square root of the variance is called the standard deviation of Y, denoted σ_y

Definition: The standard deviation of a random variable Y, σ_y, is

$$\sigma_Y \equiv \sqrt{E[(Y - E[Y])^2]}$$

In case the ***random variable Y is governed by a Binomial distribution***, then the Mean, Variance and standard deviation are given by

$$E[Y] = np$$
$$Var[Y] = np(1 - p)$$
$$\sigma_Y = \sqrt{np(1 - p)}$$

Estimators, Bias, and Variance

Let us describe $error_s(h)$ and $error_D(h)$ using the terms in Equation (1) defining the Binomial distribution. We then have

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

$$error_D(h) = p$$

Where,

- n is the number of instances in the sample S,
- r is the number of instances from S misclassified by h
- p is the probability of misclassifying a single instance drawn from *D*

- Estimator:
  $error_s(h)$ an ***estimator*** for the true error $error_D(h)$: An estimator is any random variable used to estimate some parameter of the underlying population from which the sample is drawn

- Estimation bias: is the difference between the expected value of the estimator and the true value of the parameter.

  Definition: The estimation bias of an estimator Y for an arbitrary parameter p is

$$E[Y] - p$$