Lecture 34 of 42

Machine Learning: Decision Trees & Statistical Learning Discussion: Feedforward ANNs & Backprop

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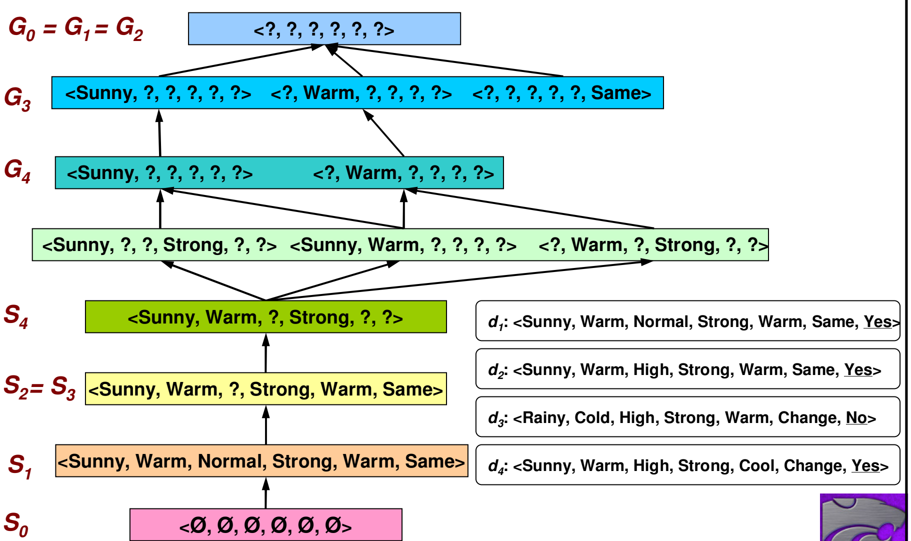
KSOL course page: http://snipurl.com/v9v3
Course web site: http://www.kddresearch.org/Courses/CIS730
Instructor home page: http://www.cis.ksu.edu/~bhsu

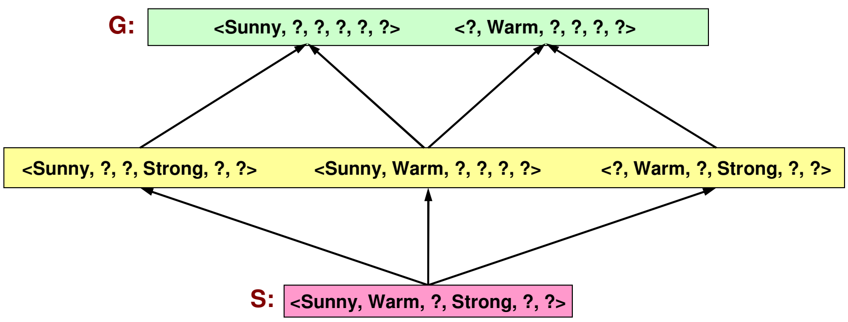
Reading for Next Class:

Chapter 20, Russell and Norvig

Example Trace



What Next Training Example?



- **Active Learning: What Query Should The Learner Make Next?**
- **How Should These Be Classified?**
  - **<Sunny, Warm, Normal, Strong, Cool, Change>**
  - **<Rainy, Cold, Normal, Light, Warm, Same>**
  - **<Sunny, Warm, Normal, Light, Warm, Same>**

What Justifies This Inductive Leap?

- **Example: Inductive Generalization**
  - **Positive example: <Sunny, Warm, Normal, Strong, Cool, Change, Yes>**
  - **Positive example: <Sunny, Warm, Normal, Light, Warm, Same, Yes>**
  - **Induced *S*: <Sunny, Warm, Normal, ?, ?, ?>**
- **Why Believe We Can Classify The Unseen?**
  - **e.g., <Sunny, Warm, Normal, Strong, Warm, Same>**
  - **When is there enough information (in a new case) to make a prediction?**

An Unbiased Learner

- **Inductive Bias**
  - Any preference for one hypothesis over another, *besides* consistency
  - Example: $H \equiv$ *conjunctive* concepts with don't cares
  - What concepts can H not express? (Hint: what are its syntactic limitations?)
- **Idea**
  - Choose unbiased H': expresses every teachable concept (i.e., power set of X)
  - Recall: $| A \rightarrow B | = | B |^{|A|}$ ($A = X$; B = {labels}; $H' = A \rightarrow B$)
  - {{Rainy, Sunny, Cloudy} × {Warm, Cold} × {Normal, High} × {None-Mild, Strong} × {Cool, Warm} × {Same, Change}} → {0, 1}
- **An Exhaustive Hypothesis Language**
  - Consider: H' = disjunctions ($\vee$), conjunctions ($\wedge$), negations ($\neg$) over H
  - $| H' | = 2^{(2 \cdot 2 \cdot 2 \cdot 3 \cdot 2 \cdot 2)} = 2^{96}$; $| H | = 1 + (3 \cdot 3 \cdot 3 \cdot 4 \cdot 3 \cdot 3) = 973$
- **What Are S, G For The Hypothesis Language H'?**
  - S ← *disjunction of all positive examples*
  - G ← *conjunction of all negated negative examples*

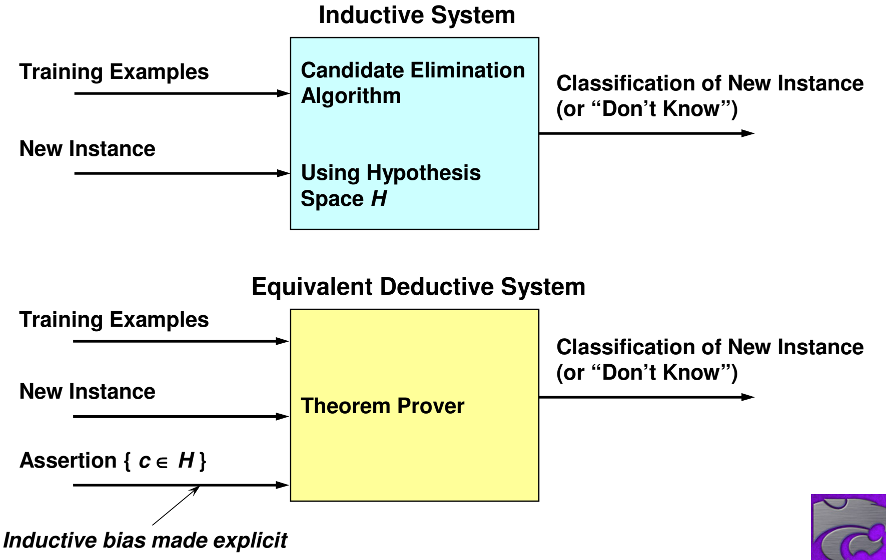
An Unbiased Learner

- **Components of An Inductive Bias Definition**
  - Concept learning algorithm L
  - Instances X, target concept c
  - Training examples $D_c = \{<x, c(x)>\}$
  - $L(x_i, D_c)$ = classification assigned to instance x_i by L after training on D_c
- **Definition**
  - 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,

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

    where A ⊢ B means A *logically entails* B
  - Informal idea: preference for (i.e., restriction to) certain hypotheses by structural (syntactic) means
- **Rationale**
  - Prior assumptions regarding target concept
  - Basis for inductive generalization

Inductive Systems & Equivalent Deductive Systems



Three Learners With Different Biases

- **Rote Learner**
  - Weakest bias: anything seen before, i.e., no bias
  - Store examples
  - Classify *x if and only if* it matches previously observed example
- **Version Space Candidate Elimination Algorithm**
  - Stronger bias: concepts belonging to conjunctive *H*
  - Store extremal generalizations and specializations
  - Classify *x if and only if* it "falls within" *S* and *G* boundaries (all members agree)
- **Find-S**
  - Even stronger bias: most specific hypothesis
  - Prior assumption: any instance *not observed to be positive* is negative
  - Classify *x* based on *S* set

Views of Learning

- **Removal of (Remaining) Uncertainty**
  - Suppose unknown function was *known* to be *m-of-n* Boolean function
  - Could use training data to infer the function
- **Learning and Hypothesis Languages**
  - Possible approach to *guess a good, small hypothesis language*:
    - Start with a very small language
    - Enlarge until it contains a hypothesis that fits the data
  - Inductive bias
    - Preference for certain languages
    - Analogous to data compression (removal of redundancy)
    - Later: coding the "model" versus coding the "uncertainty" (error)
- **We Could Be Wrong!**
  - Prior knowledge could be wrong (e.g., $y = x_4 \wedge$ one-of (x_1, x_3) consistent)
  - If guessed language was wrong, errors will occur on new cases

Approaches to Learning

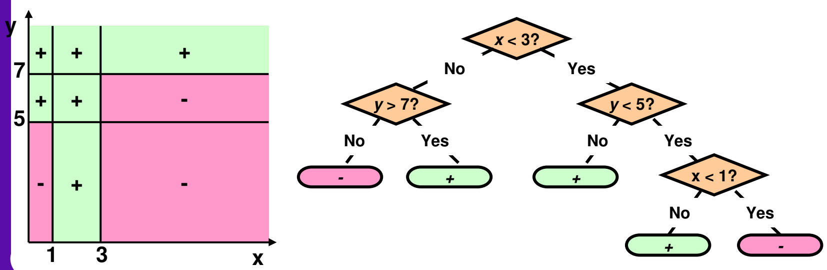
- **Develop Ways to Express Prior Knowledge**
  - Role of prior knowledge: guides search for hypotheses / hypothesis languages
  - Expression languages for prior knowledge
    - Rule grammars; stochastic models; etc.
    - Restrictions on computational models; other (formal) specification methods
- **Develop Flexible Hypothesis Spaces**
  - Structured collections of hypotheses
    - Agglomeration: nested collections (hierarchies)
    - Partitioning: decision trees, lists, rules
    - Neural networks; cases, etc.
  - Hypothesis spaces of adaptive size
- **Either Case: Develop Algorithms for Finding A Hypothesis That Fits Well**
  - Ideally, will generalize well
- **Later: Bias *Optimization* (Meta-Learning, Wrappers)**

When to Consider Using Decision Trees

- Instances Describable by Attribute-Value Pairs
- Target Function Is Discrete Valued
- Disjunctive Hypothesis May Be Required
- Possibly Noisy Training Data
- Examples
  - Equipment or medical diagnosis
  - Risk analysis
    - Credit, loans
    - Insurance
    - Consumer fraud
    - Employee fraud
  - Modeling calendar scheduling preferences (predicting quality of candidate time)

Decision Trees & Decision Boundaries

- Instances Usually Represented Using Discrete Valued Attributes
  - Typical types
    - Nominal ({red, yellow, green})
    - Quantized ({low, medium, high})
  - Handling numerical values
    - Discretization, a form of vector quantization (e.g., histogramming)
    - Using thresholds for splitting nodes
- Example: Dividing Instance Space into Axis-Parallel Rectangles



Decision Tree Learning: Top-Down Induction

- **Algorithm *Build-DT* (*Examples*, *Attributes*)**

  IF all examples have the same label THEN RETURN (leaf node with *label*)

  ELSE

  IF set of attributes is empty THEN RETURN (leaf with *majority label*)

  ELSE

  Choose best attribute *A* as root

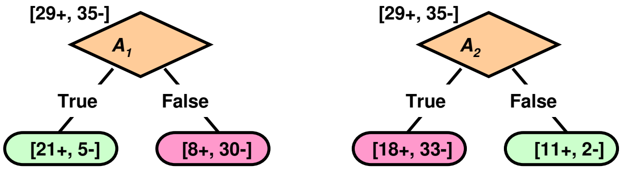
  FOR each value *v* of *A*

  Create a branch out of the root for the condition *A* = *v*

  IF {*x* ∈ *Examples*: *x.A* = *v*} = Ø THEN RETURN (leaf with *majority label*)

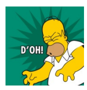
  ELSE *Build-DT* ({*x* ∈ *Examples*: *x.A* = *v*}, Attributes ~ {A})

- **But Which Attribute Is Best?**

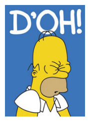


Choosing "Best" Root Attribute

- **Objective**
  - Construct a decision tree that is a small as possible (Occam's Razor)
  - Subject to: consistency with labels on training data
- **Obstacles**
  - Finding *minimal* consistent hypothesis (i.e., decision tree) is $\mathcal{NP}$-hard



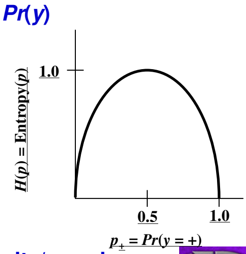
  - Recursive algorithm (*Build-DT*)



    - A greedy heuristic search for a simple tree
    - Cannot guarantee optimality
- **Main Decision: Next Attribute to Condition On**
  - Want: attributes that split examples into sets, each relatively pure in one label
  - Result: closer to a leaf node
  - Most popular heuristic
    - Developed by J. R. Quinlan
    - Based on information gain
    - Used in *ID3* algorithm

Entropy:
Intuitive Notion

- **A Measure of Uncertainty**
  - The Quantity
    - Purity: how close a set of instances is to having just one label
    - Impurity (disorder): how close it is to total uncertainty over labels
  - The Measure: Entropy
    - Directly proportional to impurity, uncertainty, irregularity, surprise
    - Inversely proportional to purity, certainty, regularity, redundancy
- **Example**
  - For simplicity, assume H = {0, 1}, distributed according to $Pr(y)$
    - Can have (more than 2) discrete class labels
    - Continuous random variables: differential entropy
  - Optimal purity for y: either
    - $Pr(y = 0) = 1$, $Pr(y = 1) = 0$
    - $Pr(y = 1) = 1$, $Pr(y = 0) = 0$
  - What is the least pure probability distribution?
    - $Pr(y = 0) = 0.5$, $Pr(y = 1) = 0.5$
    - Corresponds to maximum impurity/uncertainty/irregularity/surprise
    - Property of entropy: concave function ("concave downward")



Entropy:
Information Theoretic Definition [1]

- **Components**
  - D: set of examples $\{<x_1, c(x_1)>, <x_2, c(x_2)>, \ldots, <x_m, c(x_m)>\}$
  - $p_+ = Pr(c(x) = +)$, $p_- = Pr(c(x) = -)$
- **Definition**
  - H is defined over a probability density function p
  - D: examples whose frequency of + and - indicates p_+, p_- *for observed data*
  - The entropy of D relative to c is:

$$H(D) \equiv -p_+ \log_b (p_+) - p_- \log_b (p_-)$$

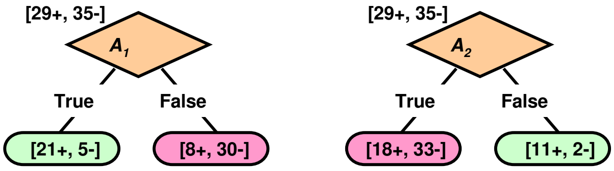
- **What Units is H Measured In?**
  - Depends on base b of log (bits for $b = 2$, nats for $b = e$, etc.)
  - Single bit required to encode each example in worst case ($p_+ = 0.5$)
  - If there is less uncertainty (e.g., $p_+ = 0.8$), we can use less than 1 bit each

Entropy: Information Theoretic Definition [2]

- **Partitioning on Attribute Values**
  - Recall: a partition of *D* is a collection of disjoint subsets whose union is *D*
  - Goal: ***measure the uncertainty removed*** by splitting on the value of attribute *A*
- **Definition**
  - The information gain of *D* relative to attribute A is the expected reduction in entropy due to splitting ("sorting") on A:

$$Gain(D, A) \equiv -H(D) - \sum_{v \in values(A)} \left[\frac{|D_v|}{|D|} \bullet H(D_v) \right]$$

    where D_v is $\{x \in D: x.A = v\}$, set of examples in *D* where attribute *A* has value *v*
  - Idea: partition on *A*; scale entropy to the size of each subset D_v
- **Which Attribute Is Best?**



Illustrative Example

- **Training Examples for Concept *PlayTennis***

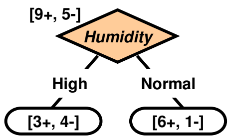
Day	Outlook	Temperature	Humidity	Wind	*PlayTennis*?
1	Sunny	Hot	High	Light	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Light	Yes
4	Rain	Mild	High	Light	Yes
5	Rain	Cool	Normal	Light	Yes
6	Rain	Cool	Normal	Strong	No
7	Overcast	Cool	Normal	Strong	Yes
8	Sunny	Mild	High	Light	No
9	Sunny	Cool	Normal	Light	Yes
10	Rain	Mild	Normal	Light	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Light	Yes
14	Rain	Mild	High	Strong	No

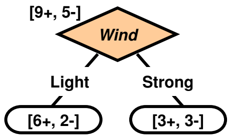
- ***ID3* ≡ *Build-DT* using *Gain*(•)**
- **How Will *ID3* Construct A Decision Tree?**

Constructing Decision Tree For *PlayTennis* using ID3 [1]

- **Selecting The Root Attribute**

Day	Outlook	Temperature	Humidity	Wind	*PlayTennis?*
1	Sunny	Hot	High	Light	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Light	Yes
4	Rain	Mild	High	Light	Yes
5	Rain	Cool	Normal	Light	Yes
6	Rain	Cool	Normal	Strong	No
7	Overcast	Cool	Normal	Strong	Yes
8	Sunny	Mild	High	Light	No
9	Sunny	Cool	Normal	Light	Yes
10	Rain	Mild	Normal	Light	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Light	Yes
14	Rain	Mild	High	Strong	No





- **Prior (unconditioned) distribution: 9+, 5-**
  - H(D) = -(9/14) lg (9/14) - (5/14) lg (5/14) bits = 0.94 bits
  - H(D, Humidity = High) = -(3/7) lg (3/7) - (4/7) lg (4/7) = 0.985 bits
  - H(D, Humidity = Normal) = -(6/7) lg (6/7) - (1/7) lg (1/7) = 0.592 bits
  - Gain(D, Humidity) = 0.94 - (7/14) * 0.985 + (7/14) * 0.592 = 0.151 bits
  - Similarly, Gain (D, Wind) = 0.94 - (8/14) * 0.811 + (6/14) * 1.0 = 0.048 bits

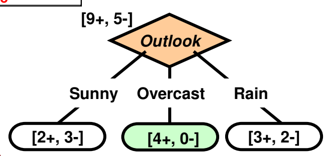
$$Gain(D, A) \equiv -H(D) - \sum_{v \in values(A)} \left[\frac{|D_v|}{|D|} \bullet H(D_v) \right]$$

Constructing Decision Tree For *PlayTennis* using ID3 [2]

- **Selecting The Root Attribute**

Day	Outlook	Temperature	Humidity	Wind	*PlayTennis?*
1	Sunny	Hot	High	Light	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Light	Yes
4	Rain	Mild	High	Light	Yes
5	Rain	Cool	Normal	Light	Yes
6	Rain	Cool	Normal	Strong	No
7	Overcast	Cool	Normal	Strong	Yes
8	Sunny	Mild	High	Light	No
9	Sunny	Cool	Normal	Light	Yes
10	Rain	Mild	Normal	Light	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Light	Yes
14	Rain	Mild	High	Strong	No

  - *Gain*(*D*, *Humidity*) = 0.151 bits
  - *Gain*(*D*, *Wind*) = 0.048 bits
  - *Gain*(*D*, *Temperature*) = 0.029 bits
  - *Gain*(*D*, *Outlook*) = 0.246 bits



- **Selecting The Next Attribute (Root of Subtree)**
  - Continue until every example is included in path or purity = 100%
  - What does purity = 100% mean?
  - Can *Gain*(*D*, *A*) < 0?

Constructing Decision Tree For *PlayTennis* using ID3 [3]

- **Selecting The Next Attribute (Root of Subtree)**

Day	Outlook	Temperature	Humidity	Wind	*PlayTennis?*
1	Sunny	Hot	High	Light	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Light	Yes
4	Rain	Mild	High	Light	Yes
5	Rain	Cool	Normal	Light	Yes
6	Rain	Cool	Normal	Strong	No
7	Overcast	Cool	Normal	Strong	Yes
8	Sunny	Mild	High	Light	No
9	Sunny	Cool	Normal	Light	Yes
10	Rain	Mild	Normal	Light	Yes
11	Sunny	Mild	Normal	Strong	Yes
12	Overcast	Mild	High	Strong	Yes
13	Overcast	Hot	Normal	Light	Yes
14	Rain	Mild	High	Strong	No

  – Convention: lg (0/a) = 0
  – *Gain*(D_{Sunny}, *Humidity*) = 0.97 - (3/5) * 0 - (2/5) * 0 = 0.97 bits
  – *Gain*(D_{Sunny}, *Wind*) = 0.97 - (2/5) * 1 - (3/5) * 0.92 = 0.02 bits
  – *Gain*(D_{Sunny}, *Temperature*) = 0.57 bits

- **Top-Down Induction**
  – For discrete-valued attributes, terminates in $O(n)$ splits
  – Makes at most one pass through data set at each level (why?)

Constructing Decision Tree For *PlayTennis* using ID3 [4]

Day	Outlook	Temperature	Humidity	Wind	*PlayTennis?*
1	Sunny	Hot	High	Light	No
2	Sunny	Hot	High	Strong	No
3	Overcast	Hot	High	Light	Yes
4	Rain	Mild	High	Light	Yes
5	Rain	Cool	Normal	Light	Yes
6	Rain	Cool	Normal	Strong	No
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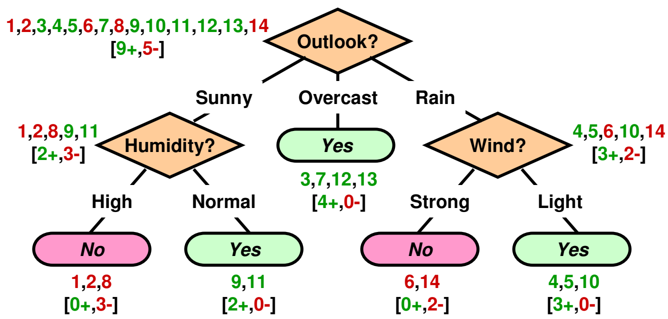
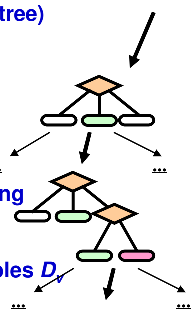


Hypothesis Space Search in ID3

- **Search Problem**
  - Conduct a search of the *space of decision trees*, which can represent all possible discrete functions
    - Pros: expressiveness; flexibility
    - Cons: computational complexity; large, incomprehensible trees (next time)
  - Objective: to find the best decision tree (minimal consistent tree)
  - Obstacle: finding this tree is NP-hard
  - Tradeoff
    - Use heuristic (figure of merit that guides search)
    - Use greedy algorithm
    - *Aka* hill-climbing (gradient "descent") without backtracking
- **Statistical Learning**
  - Decisions based on statistical descriptors p_+, p_- for subsamples D_v
  - In ID3, *all data used*
  - Robust to noisy data



Inductive Bias in ID3 (& C4.5 / J48)

- **Heuristic : Search :: Inductive Bias : Inductive Generalization**
  - *H* is the power set of instances in *X*
  - $\Rightarrow$ Unbiased? Not really…
    - Preference for short trees (termination condition)
    - Preference for trees with high information gain attributes near the root
    - *Gain*(•): a heuristic function that *captures the inductive bias of ID3*
  - Bias in *ID3*
    - Preference for some hypotheses is encoded in heuristic function
    - Compare: a restriction of hypothesis space *H* (previous discussion of propositional normal forms: *k*-CNF, etc.)
- **Preference for Shortest Tree**
  - Prefer shortest tree that fits the data
  - An Occam's Razor bias: shortest hypothesis that explains the observations

Terminology

- Decision Trees (DTs)
  - Boolean DTs: target concept is binary-valued (i.e., Boolean-valued)
  - Building DTs
    - Histogramming: method of vector quantization (encoding input using bins)
    - Discretization: continuous input into discrete (*e.g.*, histogramming)
- Entropy and Information Gain
  - Entropy *H*(*D*) for data set *D* relative to implicit concept *c*
  - Information gain *Gain* (*D*, *A*) for data set partitioned by attribute *A*
  - Impurity, uncertainty, irregularity, surprise *vs.*
    purity, certainty, regularity, redundancy
- Heuristic Search
  - Algorithm *Build-DT*: greedy search (hill-climbing without backtracking)
  - *ID3* as *Build-DT* using the heuristic *Gain*(•)
  - Heuristic : Search :: Inductive Bias : Inductive Generalization
- *MLC++* (Machine Learning Library in C++)
  - Data mining libraries (e.g., *MLC++*) and packages (e.g., *MineSet*)
  - Irvine Database: the Machine Learning Database Repository at UCI

Summary Points

- Decision Trees (DTs)
  - Can be boolean ($c(x) \in \{+, -\}$) or range over multiple classes
  - When to use DT-based models
- Generic Algorithm *Build-DT*: Top Down Induction
  - Calculating best attribute upon which to split
  - Recursive partitioning
- Entropy and Information Gain
  - Goal: to measure *uncertainty removed* by splitting on a candidate attribute *A*
    - Calculating information gain (change in entropy)
    - Using information gain in construction of tree
  - *ID3* ≡ *Build-DT* using *Gain*(•)
- ID3 as Hypothesis Space Search (in State Space of Decision Trees)
- Heuristic Search and Inductive Bias
- Data Mining using *MLC++* (Machine Learning Library in C++)
- Next: More Biases (Occam's Razor); Managing DT Induction

Connectionist (Neural Network) Models

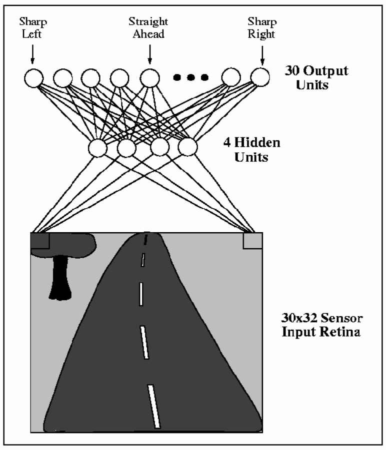
- **Human Brains**
  - Neuron switching time: ~ 0.001 (10^{-3}) second
  - Number of neurons: ~10-100 billion (10^{10} – 10^{11})
  - Connections per neuron: ~10-100 thousand (10^{4} – 10^{5})
  - Scene recognition time: ~0.1 second
  - 100 inference steps doesn't seem sufficient! → highly parallel computation
- **Definitions of Artificial Neural Networks (ANNs)**
  - "… a system composed of many simple processing elements operating in parallel whose function is determined by network structure, connection strengths, and the processing performed at computing elements or nodes." - DARPA (1988)
  - NN FAQ List: http://www.ci.tuwien.ac.at/docs/services/nnfaq/FAQ.html
- **Properties of ANNs**
  - Many neuron-like threshold switching units
  - Many weighted interconnections among units
  - Highly parallel, distributed process
  - Emphasis on tuning weights automatically

When to Consider Neural Networks

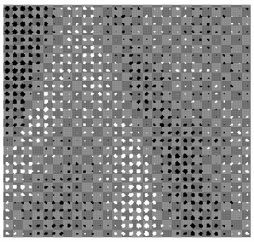
- **Input: High-Dimensional and Discrete or Real-Valued**
  - e.g., raw sensor input
  - Conversion of symbolic data to quantitative (numerical) representations possible
- **Output: Discrete or Real Vector-Valued**
  - e.g., low-level control policy for a robot actuator
  - Similar qualitative/quantitative (symbolic/numerical) conversions may apply
- **Data: Possibly Noisy**
- **Target Function: Unknown Form**
- **Result: Human Readability Less Important Than Performance**
  - Performance measured purely in terms of accuracy and efficiency
  - Readability: ability to explain inferences made using model; similar criteria
- **Examples**
  - Speech phoneme recognition [Waibel, Lee]
  - Image classification [Kanade, Baluja, Rowley, Frey]
  - Financial prediction

Autonomous Learning Vehicle in a Neural Net (ALVINN)

- **Pomerleau *et al***
  - http://www.cs.cmu.edu/afs/cs/project/alv/member/www/projects/ALVINN.html
  - Drives 70mph on highways

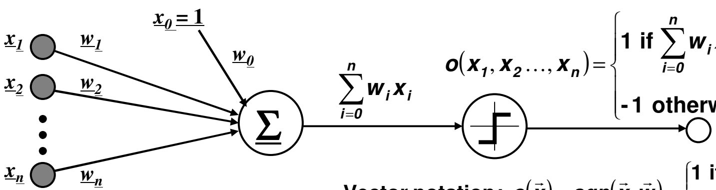


Hidden-to-Output Unit Weight Map (for one hidden unit)



Input-to-Hidden Unit Weight Map (for one hidden unit)

The Perceptron



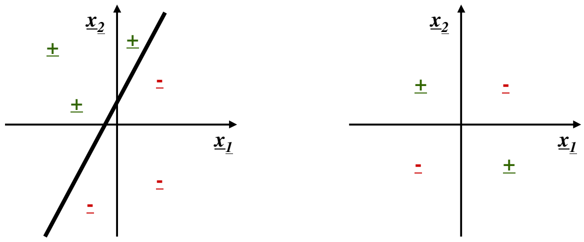
$$\sum_{i=0}^{n} w_i x_i$$

$$o(x_1, x_2 \ldots, x_n) = \begin{cases} 1 \text{ if } \sum_{i=0}^{n} w_i x_i > 0 \\ -1 \text{ otherwise} \end{cases}$$

Vector notation: $o(\vec{x}) = sgn(\vec{x}, \vec{w}) = \begin{cases} 1 \text{ if } \vec{w} \cdot \vec{x} > 0 \\ -1 \text{ otherwise} \end{cases}$

- **Perceptron: Single Neuron Model**
  - *aka* Linear Threshold Unit (LTU) or Linear Threshold Gate (LTG)
  - Net input to unit: defined as linear combination $net = \sum_{i=0}^{n} w_i x_i$
  - Output of unit: threshold (activation) function on net input (threshold $\theta = w_0$)
- **Perceptron Networks**
  - Neuron is modeled using a unit connected by weighted links w_i to other units
  - Multi-Layer Perceptron (MLP): next lecture

Decision Surface of a Perceptron



Example A   Example B

- **Perceptron: Can Represent *Some* Useful Functions**
  - LTU emulation of logic gates (McCulloch and Pitts, 1943)
  - e.g., What weights represent $g(x_1, x_2) = AND(x_1, x_2)$? $OR(x_1, x_2)$? $NOT(x)$?
- **Some Functions *Not* Representable**
  - e.g., not linearly separable
  - Solution: use networks of perceptrons (LTUs)

Learning Rules for Perceptrons

- **Learning Rule ≡ Training Rule**
  - Not specific to supervised learning
  - Context: updating a model
- **Hebbian Learning Rule (Hebb, 1949)**
  - Idea: if two units are both active ("firing"), weights between them should increase
  - $w_{ij} = w_{ij} + r\, o_i\, o_j$ where r is a learning rate constant
  - Supported by neuropsychological evidence
- **Perceptron Learning Rule (Rosenblatt, 1959)**
  - Idea: when a target output value is provided for a single neuron with fixed input, it can incrementally update weights to learn to produce the output
  - Assume binary (boolean-valued) input/output units; single LTU
  - $w_i \leftarrow w_i + \Delta w_i$

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

    where $t = c(x)$ is target output value, o is perceptron output, r is small learning rate constant (e.g., 0.1)
  - Can prove convergence if D linearly separable and r small enough

Perceptron Learning Algorithm

- **Simple Gradient Descent Algorithm**
  - Applicable to concept learning, symbolic learning (with proper representation)
- **Algorithm *Train-Perceptron* ($D \equiv \{<x, t(x) \equiv c(x)>\}$)**
  - Initialize all weights w_i to random values
  - WHILE not all examples correctly predicted DO

    FOR each training example $x \in D$

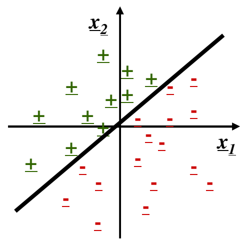
    Compute current output $o(x)$

    FOR i = 1 to n

    $w_i \leftarrow w_i + r(t - o)x_i$ // perceptron learning rule
- **Perceptron Learnability**
  - Recall: can only learn $h \in H$ - i.e., linearly separable (LS) functions
  - Minsky and Papert, 1969: demonstrated representational limitations
    - e.g., parity (n-attribute XOR: $x_1 \oplus x_2 \oplus \ldots \oplus x_n$)
    - e.g., symmetry, connectedness in visual pattern recognition
    - Influential book *Perceptrons* discouraged ANN research for ~10 years
  - NB: *$64K question* - "Can we transform learning problems into LS ones?"

Linear Separators

- **Functional Definition**
  - $f(x) = 1$ if $w_1x_1 + w_2x_2 + \ldots + w_nx_n \geq \theta$, 0 otherwise
  - θ: threshold value
- **Linearly Separable Functions**
  - NB: D is LS does not necessarily imply $c(x) = f(x)$ is LS!
  - Disjunctions: $c(x) = x_1' \vee x_2' \vee \ldots \vee x_m'$
  - m of n: $c(x)$ = at least 3 of (x_1', x_2', …, x_m')
  - Exclusive *OR* (*XOR*): $c(x) = x_1 \oplus x_2$
  - General DNF: $c(x) = T_1 \vee T_2 \vee \ldots \vee T_m$; $T_i = l_1 \wedge l_1 \wedge \ldots \wedge l_k$
- **Change of Representation Problem**
  - Can we transform non-LS problems into LS ones?
  - Is this meaningful? Practical?
  - Does it represent a significant fraction of real-world problems?



Linearly Separable (LS) Data Set

Perceptron Convergence

- **Perceptron Convergence Theorem**
  - Claim: If there exist a set of weights that are consistent with the data (i.e., the data is linearly separable), the perceptron learning algorithm will converge
  - Proof: well-founded ordering on search region (“wedge width” is strictly decreasing) - see Minsky and Papert, 11.2-11.3
  - Caveat 1: How long will this take?
  - Caveat 2: What happens if the data is *not* LS?
- **Perceptron Cycling Theorem**
  - Claim: If the training data is not LS the perceptron learning algorithm will eventually repeat the same set of weights and thereby enter an infinite loop
  - Proof: bound on number of weight changes until repetition; induction on *n*, the dimension of the training example vector - MP, 11.10
- **How to Provide More Robustness, Expressivity?**
  - Objective 1: develop algorithm that will find closest approximation (today)
  - Objective 2: develop architecture to overcome representational limitation (next lecture)

Gradient Descent: Principle

- **Understanding Gradient Descent for Linear Units**
  - Consider simpler, unthresholded linear unit:

$$o(\vec{x}) = net(\vec{x}) = \sum_{i=0}^{n} w_i x_i$$

  - Objective: find “best fit” to *D*
- **Approximation Algorithm**
  - Quantitative objective: minimize error over training data set *D*
  - Error function: sum squared error (SSE)

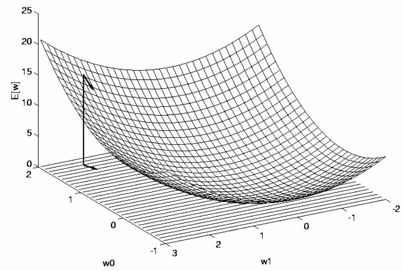
$$E[\vec{w}] = error_D[\vec{w}] = \frac{1}{2}\sum_{x \in D}(t(x) - o(x))^2$$

- **How to Minimize?**
  - Simple optimization
  - Move in direction of steepest gradient in weight-error space
    - Computed by finding tangent
    - i.e. partial derivatives (of *E*) with respect to weights (w_i)

Gradient Descent: Derivation of Delta/LMS (Widrow-Hoff) Rule

- **Definition: Gradient**

$$\nabla E[\vec{w}] \equiv \left[\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \ldots, \frac{\partial E}{\partial w_n}\right]$$



- **Modified Gradient Descent Training Rule**

$$\Delta\vec{w} = -r\nabla E[\vec{w}]$$

$$\Delta w_i = -r\frac{\partial E}{\partial w_i}$$

$$\frac{\partial E}{\partial w_i} = \frac{\partial}{\partial w_i}\left[\frac{1}{2}\sum_{x \in D}(t(x) - o(x))^2\right] = \frac{1}{2}\sum_{x \in D}\left[\frac{\partial}{\partial w_i}(t(x) - o(x))^2\right]$$

$$= \frac{1}{2}\sum_{x \in D}\left[2(t(x) - o(x))\frac{\partial}{\partial w_i}(t(x) - o(x))\right] = \sum_{x \in D}\left[(t(x) - o(x))\frac{\partial}{\partial w_i}(t(x) - \vec{w} \cdot \vec{x})\right]$$

$$\frac{\partial E}{\partial w_i} = \sum_{x \in D}\left[(t(x) - o(x))(-x_i)\right]$$

Gradient Descent: Algorithm using Delta/LMS Rule

- **Algorithm *Gradient-Descent* (*D*, *r*)**
  - Each training example is a pair of the form <*x*, *t*(*x*)>, where x is the vector of input values and *t*(*x*) is the output value. *r* is the learning rate (e.g., 0.05)
  - Initialize all weights w_i to (small) random values
  - UNTIL the termination condition is met, DO

    Initialize each Δw_i to zero

    FOR each <*x*, *t*(*x*)> in *D*, DO

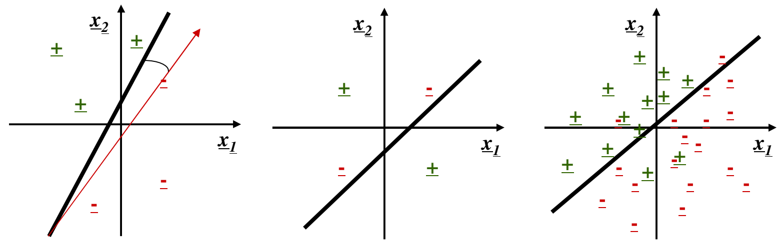
      Input the instance *x* to the unit and compute the output *o*

      FOR each linear unit weight w_i, DO

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

        $w_i \leftarrow w_i + \Delta w_i$
  - RETURN final *w*
- **Mechanics of Delta Rule**
  - Gradient is based on a derivative
  - Significance: later, will use nonlinear activation functions (*aka* transfer functions, squashing functions)

Gradient Descent: Perceptron Rule versus Delta/LMS Rule



Example A **Example B** **Example C**

- **LS Concepts: Can Achieve Perfect Classification**
  - Example A: perceptron training rule converges
- **Non-LS Concepts: Can Only Approximate**
  - Example B: not LS; delta rule converges, but can't do better than 3 correct
  - Example C: not LS; better results from delta rule
- **Weight Vector w = Sum of Misclassified $x \in D$**
  - Perceptron: minimize w
  - Delta Rule: minimize *error* ≡ distance from separator (I.e., maximize $\frac{\partial E}{\partial \vec{w}}$)

Review: Backprop, Feedforward

- **Intuitive Idea: Distribute *Blame* for Error to Previous Layers**
- **Algorithm *Train-by-Backprop* (*D*, *r*)**
  - Each training example is a pair of the form <*x*, *t*(*x*)>, where x is the vector of input values and *t*(*x*) is the output value. *r* is the learning rate (e.g., 0.05)
  - Initialize all weights w_i to (small) random values
  - UNTIL the termination condition is met, DO

    FOR each <*x*, *t*(*x*)> in *D*, DO

    Input the instance *x* to the unit and compute the output $o(x) = \sigma(net(x))$

    FOR each output unit *k*, DO

    $$\delta_k = o_k(x)(1 - o_k(x))(t_k(x) - o_k(x))$$

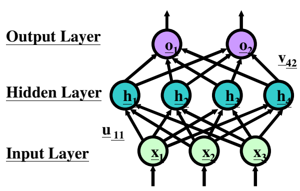
    FOR each hidden unit *j*, DO

    $$\delta_j = h_j(x)(1 - h_j(x)) \sum_{k \in outputs} v_{j,k}\delta_j$$

    Update each $w = u_{i,j}$ $(a = h_j)$ or $w = v_{j,k}$ $(a = o_k)$

    $w_{start\text{-}layer,\, end\text{-}layer} \leftarrow w_{start\text{-}layer,\, end\text{-}layer} + \Delta w_{start\text{-}layer,\, end\text{-}layer}$

    $\Delta w_{start\text{-}layer,\, end\text{-}layer} \leftarrow r\, \delta_{end\text{-}layer}\, a_{end\text{-}layer}$
  - RETURN final *u*, *v*



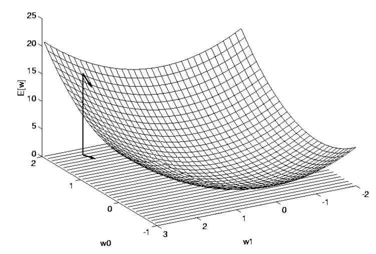
Review: Derivation of Backprop

- **Recall: Gradient of Error Function** $\nabla E[\vec{w}] \equiv \left[\frac{\partial E}{\partial w_0}, \frac{\partial E}{\partial w_1}, \ldots, \frac{\partial E}{\partial w_n}\right]$
- **Gradient of Sigmoid Activation Function**

$$\frac{\partial E}{\partial w_i} = \frac{\partial}{\partial w_i}\left[\frac{1}{2}\sum_{\langle \vec{x}, t(\vec{x})\rangle \in D}(t(\vec{x}) - o(\vec{x}))^2\right] = \frac{1}{2}\sum_{\langle \vec{x}, t(\vec{x})\rangle \in D}\left[\frac{\partial}{\partial w_i}(t(\vec{x}) - o(\vec{x}))^2\right]$$

$$= \frac{1}{2}\sum_{\langle \vec{x}, t(\vec{x})\rangle \in D}\left[2(t(\vec{x}) - o(\vec{x}))\frac{\partial}{\partial w_i}(t(\vec{x}) - o(\vec{x}))\right] = \sum_{\langle \vec{x}, t(\vec{x})\rangle \in D}\left[(t(\vec{x}) - o(\vec{x}))\left(-\frac{\partial o(\vec{x})}{\partial w_i}\right)\right]$$

$$= -\sum_{\langle \vec{x}, t(\vec{x})\rangle \in D}\left[(t(\vec{x}) - o(\vec{x}))\frac{\partial o(\vec{x})}{\partial net(\vec{x})}\frac{\partial net(\vec{x})}{\partial w_i}\right]$$



- **But We Know:**

$$\frac{\partial o(\vec{x})}{\partial net(\vec{x})} = \frac{\partial \sigma(net(\vec{x}))}{\partial net(\vec{x})} = o(\vec{x})(1 - o(\vec{x}))$$

$$\frac{\partial net(\vec{x})}{\partial w_i} = \frac{\partial(\vec{w} \cdot \vec{x})}{\partial w_i} = x_i$$

- **So:** $\frac{\partial E}{\partial w_i} = -\sum_{\langle \vec{x}, t(\vec{x})\rangle \in D}\left[(t(\vec{x}) - o(\vec{x})) \cdot (o(\vec{x})(1 - o(\vec{x}))) \cdot x_i\right]$