#### Al2 - Module 3

Task 5: Learning from Data Task 6: Coping with Incomplete Information

Lecturer: Mark Steedman e-mail: steedman@inf.ed.ac.uk Office: Room 2R.14, 2 Buccleuch Place Notes: Copies of the lecture slides. Activities: 18 lectures. Two practicals covering both tasks. Required Text: Russell & Norvig, 2nd Ed., Chaps. 13-16, 18-20. Further Reading: Tom Mitchell, *Machine Learning*, 1997.

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Introduction

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#### Task 5: Learning from Data Overview

- 1. Introduction
- 2. Learning with Decision Trees.
- 3. Learning as Search.
- 4. Neural Networks: the Perceptron, multi-layer networks, back-propagation.

Text: Chapters 18-20 of Russell & Norvig

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Introduction

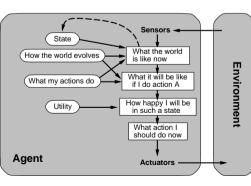
Learning from Data

Two related tasks in applying AI techniques to any task:

- 1. Represent relevant knowledge in a computationally tractable form.
- 2. *Design and implement algorithms* which effectively employ that knowledge so represented to achieve the desired processing.

Learning systems actually *change* and/or *augment* the represented knowledge on the basis of experience.

# A Performance Element (PE)



- PE selects external action
- New rules can be installed to modify PE
- What aspects of the PE can be changed by learning?

#### What components of PE can change?

Examples are:

- 1. A direct mapping from conditions on the current state to actions.
- 2. A means to infer relevant properties of the world from the percept sequence.
- 3. Information about the way the world evolves.
- 4. Information about the results of possible actions the agent can take.
- 5. Utility information indicating the desirability of world states.

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Introduction

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- 6. Action-value information indicating the desirability of particular actions in particular states.
- 7. Goals that describe classes of states whose achievement maximises the agent's utility.

Each of these components can be learned

- Have notion of performance standard
  - can be hardwired: e.g. hunger, pain etc.
  - provides feedback on quality of agent's behaviour

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Introduction

A Range of Applications

### Learning from Data

We will consider a slightly constrained setup known as

#### **Supervised Learning**

- The learning agent sees a set of *examples*.
- Each example is *labelled*, i.e. associated with some relevant information.
- The learning agent generalises by producing some *representation* that can be used *to predict* the associated value on unseen examples.
- The predictor is used either directly or in a larger system.

# Scientific research, control problems, engineering devices, game plaving, natural language applications, Internet tools, commerce.

- Diagnosing diseases in plants.
- Identifying useful drugs (pharmaceutical research).
- Predicting protein folds (Genome project).
- Cataloguing space images.
- Steering a car on highway (by mapping state to action).
- An automated pilot in a restricted environment (by mapping state to action).

- Playing Backgammon (by mapping state to its "value").
- Performing symbolic integration (by mapping expressions to integration operators).
- Controlling oil-gas separation.
- Generating the past tense of a verb.
- Context sensitive spelling correction ("I had a cake for *desert*").
- Filtering interesting articles from newsgroups.
- Identifying interesting web-sites.
- Fraud detection (on credit card activities).
- Identifying market properties for commerce.
- Stock market prediction.

| components. |  |
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- What *feedback* is available.
- What *representation* is used for the examples.
- What *prior knowledge* is available.

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Introduction

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Introduction

Major issues for learning problems

• What *components* of the performance element are to be improved.

• What *representation* is used for the knowledge in those

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### Sources and Types of Learning Systems

Is the system *passive* or *active*?

Is the system *taught* by someone else, or must it *learn for itself*?

Do we approach the system as a whole, or component by component?

Our setup of Supervised Learning implies a passive system that is taught through the selection of examples (though the "teacher" may not be helpful).

# **Other Types of Learning Problems**

*unsupervised* **learning** The system receives no external feedback, but has some internal utility function to maximise.

For example, a robot exploring a distant planet might be set to classify the forms of life it encounters there.

*reinforcement* **learning** The system is trained with post-hoc evaluation of every output.

For example, a system to play backgammon might be trained by letting it play some games, and at the end of each game telling it whether it won or lost. (There is no direct feedback on every action.)

#### **Supervised Learning**

- Some part of the performance element is modelled as a function *f* a mapping from possible descriptions into possible values.
- A *labelled example* is a pair (x, v) where x is the description and the intention is that the v = f(x).
- The learner is given some labelled examples.
- The learner is required to find a mapping *h* (for hypothesis) that can be used to compute the value of *f* on unseen descriptions: "*h* approximates *f*"

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Introduction

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#### Supervised Learning: Example

The first major practical application of machine learning techniques was indicated by Michalski and Chilausky's (1980) soybean experiment. They were presented with information about sick soya bean plants whose diseases had been diagnosed.

- Each plant was described by values of 35 attributes, such as leafspots halos and leafspot size, as well as by its actual disease.
- The plants had 1 of 4 types of diseases.

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Introduction

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- The learning system automatically inferred a set of rules which would predict the disease of a plant on the basis of its attribute values.
- When tested with new plants, the system predicted the correct disease 100% of the time. Rules constructed by human experts were only able to achieve 96.2%.
- However, the learned rules were much more complex than those extracted from the human experts.

#### Supervised Learning with Decision Trees Overview

- 1. Attribute-Value representation of examples
- 2. Decision tree representation
- 3. Supervised learning methodology
- 4. Decision tree learning algorithm
- 5. Was learning successful ?
- 6. Some applications

Text: Sections 18.2-18.3 of Russell & Norvig

#### Supervised Learning with Decision Trees

- Some part of the performance element is modelled as a function *f* a mapping from possible descriptions into possible values.
- A *labelled example* is a pair (x, v) where x is the description and the intention is that v = f(x).
- The learner is given some labelled examples.
- The learner is required to find a mapping *h* (for hypothesis) that can be used to compute the value of *f* on unseen descriptions.
- *h* is represented by a decision tree.

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Decision Trees

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# Attribute-Value Representation for Examples

The mapping f decides whether a credit card be granted to an applicant. What are the important *attributes* or *properties* ?

**Credit History** What is the applicant's credit history like? (values: *good, bad, unknown*)

**Debt** How much debt does the applicant have? (values: *low, high*)

**Collateral** Can the applicant put up any collateral? (values: *adequate, none*)

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Decision Trees - Representing Examples

**Income** How much does the applicant earn? (values: numerical)

**Dependents** Does the applicant have any Dependents ? (values: numerical)

The last two attributes are numerical. We may need to discretize them e.g. using (values: > 10000, < 10000) for Income and (values: *yes, no*) for Dependents.

### Example (cont.)

A set of examples (descriptions and labels) can be described as in the following table.

| ſ | Example | Attributes     |      |            | Goal   |            |        |
|---|---------|----------------|------|------------|--------|------------|--------|
|   |         | Credit History | Debt | Collateral | Income | Dependents | Yes/no |
| ſ | X1      | Good           | Low  | Adequate   | 20K    | 3          | yes    |
|   | X2      | Good           | High | None       | 15K    | 2          | yes    |
|   | X3      | Good           | High | None       | 7K     | 0          | no     |
|   | X4      | Bad            | Low  | Adequate   | 15K    | 0          | yes    |
|   | X5      | Bad            | High | None       | 10k    | 4          | no     |
|   | X6      | Unknown        | High | None       | 11K    | 1          | no     |
|   | X7      | Unknown        | Low  | None       | 9k     | 2          | no     |
|   | X8      | Unknown        | Low  | Adequate   | 9K     | 2          | yes    |
|   | X9      | Unknown        | Low  | None       | 19k    | 0          | yes    |

The learner is required to find a mapping h that can be used to compute the value of f on unseen descriptions.

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# Example (cont.)

Here the only possible values for h are  $\{yes, no\}$ .

Such mappings are called *Boolean functions*.

They can be used to model *concepts*, where yes means that the description refers to an object that belongs to the concept.

In our example the concept is "person who should be given credit".

Decision Trees - Representing Examples

### Supervised Learning: Terminology

- An **example** describes the value of each of the **attributes** and the value of the **goal predicate**.
- The value of the goal predicate is called the **classification** or the **label**.
- For boolean goal predicates we identify *positive examples* and *negative examples*:

If the classification is "yes" (or TRUE) the example is **positive**.

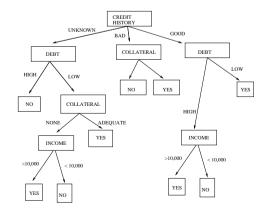
- If the classification is "no" (or FALSE), the example is **negative**.
- The complete set of examples is the **training set**.

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Decision Trees

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#### **Decision Trees: Example**



#### **Knowledge Representation**

A **Decision Tree** takes as input an object or situation described by a set of properties (attributes) and outputs a *yes/no* decision.

- Decision trees represent Boolean Functions.
- Each internal node in the tree corresponds to a test of a value of one of the properties.
- Each **branch** of the tree is labelled with the possible value of the test.
- Each **leaf-node** specifies the Boolean value to be returned if the leaf is reached.

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#### Knowledge Representation (cont.)

- Any path through a decision tree can be represented by a conjunction of logical tests.
- Can write an equivalent logical description of Yes leaves (or No leaves).
- Logically, a decision tree is a collection of individual implications corresponding to paths in tree ending in Yes nodes.
- Attributes correspond to propositions

 $\mathsf{E.g.} \ \forall m. \, credit\_story(m, good) \land debt(m, low) \Rightarrow given\_credit(m)$ 

| AI2-LFD | Decision Trees: the Representation | 2-10 |
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#### Expressive Power

#### **Expressive Power of Decision Trees**

• Despite the quantifier ∀, Decision Tree language is essentially propositional, limited to defining a new property over a single variable in terms of a logical combination of attributes of that variable—hence a decision tree cannot represent a test such as

IF credit-history(man, bad) AND income(man, < 10K) AND married-to(man, wife) AND income(wife, < 10K) THEN no credit

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Decision Trees: the Representation

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#### Expressive Power

• Any Boolean Function can be written as a tree but some such functions would require a very large tree.

The obvious translation:

- (1) at top level split on first attribute
- (2) at 2nd level split on 2nd attribute

. . .

may produce large trees (due to exponential growth).

• NB The ideas here can be generalised for situations where there are more than two outcomes.

#### Supervised Learning: How?

- The learner is required to find a mapping *h* that can be used to compute the value of *f* on unseen descriptions.
- In order to do that, machine learning programs normally *try to find a hypothesis h that gives correct classification to the training set.*

Is this reasonable?

#### **Decision Tree Induction: Quality**

(How to induce decision trees from examples)

- A trivial solution has one path to a leaf for each example.
- However, this just *memorises* the examples, and does not extract a pattern.
- A decision tree should be able to extrapolate from the given examples to examples it has not seen.
- A good decision tree should not only agree with the examples. It should also be *concise*.

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DTs: supervised learning methodology

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#### Supervised Learning: How? (cont.)

**Principle of Ockham's Razor** The most likely hypothesis is the simplest one consistent with all the observations.

This general argument has been given a rigorous quantitative treatment in *computational learning theory*.

**Can We Find the Smallest Decision Tree ?** There is no known efficient solution to this problem! What we can do is devise heuristics that will often give us fairly small trees.

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DTs: supervised learning methodology

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#### **Decision Tree Learning Algorithm**

- Choose a "good attribute" to put at the top level.
- Take this attribute and split up the examples into subsets, one for each value of the chosen attribute.
- For each subset that has only positive or only negative examples, attach a leaf with the corresponding value.
- Each subset that has *both* positive and negative examples, needs a new decision tree.

 $\Rightarrow$  Apply the *decision-tree-learning-algorithm* recursively. NB recursion has *fewer examples* and *one fewer attribute* 

#### Applying the Algorithm: Example

Choose Collateral:

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Value Adequate induces subset: {X1,X4,X8} Value None induces subset: {X2,X3,X5,X6,X7,X9}

 $\{X1, X4, X8\}$  all labelled yes - attach a leaf to this branch.

 $\{X2,X3,X5,X6,X7,X9\}$  has both positive and negative examples. Choose Income:

Value < 10K induces subset: {X3,X7}

Value  $\geq 10$ K induces subset: {X2,X5,X6,X9}

 $\{X3,X7\}$  all labelled no - attach a leaf to this branch.

 $\{X2, X5, X6, X9\}$  has both positive and negative examples. Choose Debt: Value Low induces subset:  $\{X9\}$  - attach a leaf to it

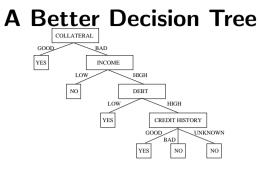
Value High induces subset: {X2,X5,X6}

 $\{X2, X5, X6\} \text{ has both positive and negative examples.} \\ Choose Credit History: \\ Value Good induces subset: \{X2\} - attach a leaf to it \\ Value Bad induces subset: \{X5\} - attach a leaf to it \\ Value Unknown induces subset: \{X6\} - attach a leaf to it \\ \end{tabular}$ 

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Decision Trees: Learning Algorithm

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- This is a better tree than Slide 2-8, with fewer nodes including leaf nodes
- Neither tree needs to use the Dependents property

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Decision Trees: Learning Algorithm

What if . . .

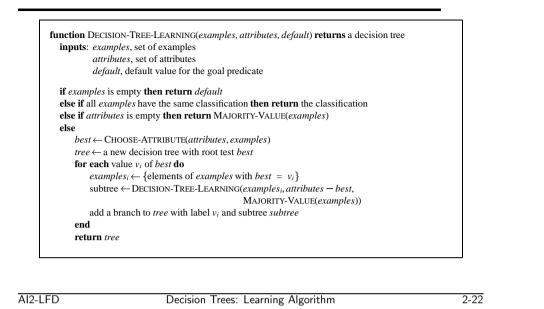
- If a value induces an empty subset {}, no such example has been observed: ⇒ return a default value using the majority classification of the parent set.
- If there are no attributes left, but still positive and negative examples, then there is a problem! The algorithm returns the majority classification of the remaining examples.

### **Noisy Training Set**

If there are no attributes left, but still positive and negative examples, then there is no decision tree that gives a correct classification to all the examples in the training set. What can be the reason?

- Some of the data may be incorrect—the data is said to be **noisy**.
- The attributes may not give enough information to fully describe the situation.
- The domain may be truly non-deterministic.

Algorithm returns the majority classification of remaining examples.



T. Mitchell, Machine Learning, Sec. 3.7.1

# Noise and Overfitting

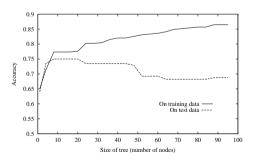
Noisy examples can also lead to growing the tree too much (so as to classify noisy examples correctly). Often, using a smaller part of the tree is better. How can we avoid overfitting ?

- Stop growing when data split not statistically significant (small number of examples). or
- Grow full tree, then post-prune.

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Decision Trees: Learning Algorithm

#### **Effect of Overfitting**



#### **Choosing attributes**

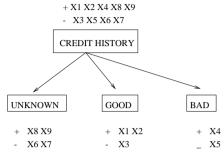
Imagine we have 100 positive and 100 negative examples. Use notation [100P, 100N] to describe this. Imagine we have 3 attributes generating the following splits:

- A1 generates [100P, 0N], [0P, 100N].
- A2 generates [70P, 30N], [30P, 70N].
- A3 generates [50P, 50N], [50P, 50N].

Which attribute is the best one? and the worst?

#### **Choosing attributes**

Credit History is NOT a good attribute to start with.

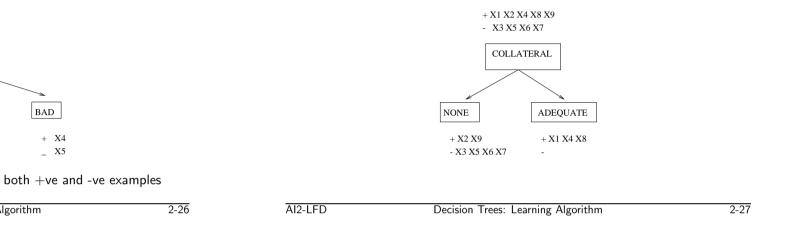


Has three possible outcomes, each of which has both +ve and -ve examples

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|         |                                    |      |

#### **Choosing attributes**

Collateral gives a definite response (Yes) for 3 cases.



#### **Revision: Information Content**

The *information content* (IC) of an event is the amount of new information communicated when we learn about the event. The information content of the event X = i, where X is a random variable and i is the outcome, is defined as

$$IC(X=i) = \log_2 \frac{1}{p(X=i)}.$$

The definition agrees with a number of common-sense ideas regarding 'information':

#### **Revision: Information Content**

1. More surprising events provide more information.

For example, if X is a random variable representing the current weather in Edinburgh, the information content of the event 'sunny', p(sunny = 0.001), IC = 11 bits, is higher than that of the event 'cloudy', p(cloudy = 0.8), IC = 0.322 bits.

2. Learning that an event that was bound to happen, did happen, provides no information.

Such an event has a probability 1. Since  $\log_2 1 = 0$ , IC = 0 bits.

#### **Revision: Information Content**

1. Learning the outcome of related random variables reduces the information content.

For example, the information provided by learning that a randomly selected English character is 'u' is lower when we already know that the previous letter was'q'.

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#### **Revision: Entropy**

The *entropy* of a random variable, I(X), is an average of the information content over the outcomes of the random variable. If a variable X has N possible outcomes,

$$I(X) = \sum_{i=1}^{N} p(X=i) \log_2 \frac{1}{p(X=i)}.$$

Entropy can be thought of as the average *uncertainty* of the random variable. Prediction is easier when the entropy is lower since we are less uncertain (on average).

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Decision Trees: Learning Algorithm

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#### **Revision: Entropy**

For example, the entropy of a coin is maximized when it is fair i.e. when p(heads = 0.5) and p(tail = 0.5),  $I(X) = 0.5 \cdot \log_2 \frac{1}{0.5} + 0.5 \cdot \log_2 \frac{1}{0.5} = \log_2 2 = 1$  bit. A fair coin is also most difficult to predict.

When the coin is biased, say, p(heads = 0.8) and p(tails = 0.2), the entropy will be lower i.e.  $0.8 \cdot \log_2 \frac{1}{0.8} + 0.2 \cdot \log_2 \frac{1}{0.2} = 0.722$  bits, and we can win money if we predict heads...

#### **Revision: Entropy**

Decision trees predict a class variable by asking questions about (hopefully correlated) attributes of an input example. The answers to these questions reduce the entropy (uncertainty) of the class assignment making prediction gradually easier at each node in the tree.

#### **Choosing attributes - the Details**

The current example set has p positive and n negative examples. A split on attribute A with v values generates v subsets with  $p_i, n_i$  examples respectively  $(i = 1 \dots v)$ .

$$I(p,n) = \frac{p}{p+n}\log(\frac{p+n}{p}) + \frac{n}{p+n}\log(\frac{p+n}{n})$$

measures the entropy of the current set.

Trying to measure how far we are from having a single label.

$$I(X, X) = 1$$
 and  $I(0, X) = I(X, 0) = 0$ 

for any value of X

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Decision Trees: Learning Algorithm
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$$Remainder(A) = \sum_{i=1}^{v} \frac{p_i + n_i}{p+n} I(p_i, n_i)$$

where A is an attribute, measures average entropy after split. Again, trying to measure how far we are from having a single label.

$$Gain(A) = I(p, n) - Remainder(A)$$

tries to measure the improvement obtained by the split.

 $\begin{array}{l} Gain(\texttt{Collateral}) = I(5,4) - \left(\frac{6}{9}I(2,4) + \frac{3}{9}I(3,0)\right) = \\ \frac{5}{9}\log\frac{9}{5} + \frac{4}{9}\log\frac{9}{4} - \frac{6}{9} \cdot \frac{2}{6}\log\frac{6}{2} - \frac{6}{9} \cdot \frac{4}{6}\log\frac{6}{4} - \frac{3}{9} \cdot \frac{3}{3}\log\frac{3}{3} - \frac{3}{9} \cdot \frac{0}{3}\log\frac{3}{0} = 0.38 \end{array}$ 

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Decision Trees: Learning Algorithm

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#### **Choosing attributes - the Details**

- 1. For each attribute A compute Gain(A)
- 2. Choose the attribute that has the maximum  ${\cal G}ain({\cal A})$

This is only a heuristic.

But it works well in practice.

Other criteria for choosing attributes were developed (including dealing with numerical attributes directly).

#### **Decision Tree Quality**

Having used a heuristic for finding a small decision tree, our hope was that this tree can be used to (correctly) compute the value of f on unseen instances.

- What if this tree is consistent with the training set but far from correct otherwise?
- Can we assess the quality of the tree?

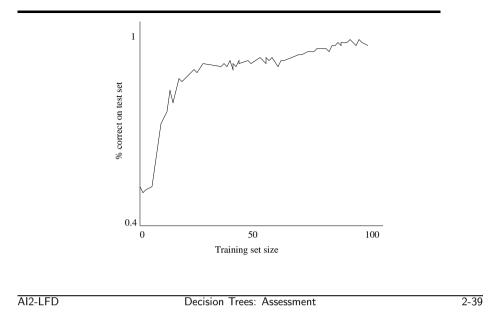
Some answers are provided by statistical analysis.

One approach, plotting learning curves, also gives some qualitative impression.

#### Assessing decision trees

- 1. Collect a large set of examples.
- 2. Divide into two disjoint sets: the training set and the test set.
- 3. Use the learning algorithm with the training set to generate a hypothesis H.
- 4. Measure the percentage of examples in the test set, correctly classified by H.
- 5. Repeat steps 1-4 with different sizes of training sets, and different randomly selected training sets of each size.
- 6. Plot the training set size against the average % correct on test sets —this is called the **learning curve**.

| AI2-LFD | Decision Trees: Assessment |
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#### **Designing Oil Platform Equipment**

- In 1986, BP used an expert system called GASOIL for designing oil-gas separation systems for offshore platforms.
- Separations are done by a system whose design depends on a large number of attributes—*relative proportions of oil, gas, water, flow-rate, pressure, density, viscosity, temperature....*
- GASOIL system contained 2500 rules!
- Building such a system by hand would have taken 10 person-years.
- Using decision-tree learning methods, the system was developed in 100 person days.

### Learning To Fly

- An automated controller can be constructed by learning the correct mapping from a state of the system to the correct action.
- Sammut et al. 1992 used this method for learning to fly a Cessna on a flight simulator, in a restricted environment.
- Data generated by watching human pilots perform a flight plan 30 times, each action taken resulted in a training examples being created.

- 90,000 examples were obtained, each described by 20 state values, and a resulting action.
- Decision tree created and converted into C code for use by the flight simulator (in a controlled manner).
- The program learns to fly, and at times flies *better* than its teachers.

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Decision Trees: Applications

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#### Learning as Search Overview

- 1. Learning can be done by searching for a good hypothesis
- 2. Learning Logical Descriptions
- 3. Current-Best-Search Learning
- 4. Version Space Learning

Text: Section 19.1 of Russell & Norvig

#### Sky Image Cataloguing and Analysis

System called SkyCat by (Fayad, Djorgovski, Weir, 1996).

- Task: catalogue entries for objects in images.
- Large amounts of data collected by astronomers; objects too "faint" need special methods.
- Images split to smaller parts; various features measured on each to generate examples.
- Relatively small number of examples classified by astronomers.
- Decision Tree methods used to learn classifiers.
- Performance: 94.1% correct on test data; results used by astronomers.

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Decision Trees: Applications

Artificial Intelligence 2Bh

### **Supervised Learning**

- **The Task:** The learner is required to find a mapping h that can be used to compute the value of f on unseen descriptions.
- **The Approach:** By Ockham's Razor, the learner tries to find a *concise* representation for h that is *consistent with all the examples.*
- **Hypothesis Space:** A *representation language* for the possible hypotheses must be fixed.
- **Bias:** Criteria for choosing between different hypotheses (such as conciseness) are employed; this shows an a-priori *bias* of the learner to prefer some hypotheses to others.

#### Learning as Search

Once the hypothesis space and preference criteria are fixed this approach to learning can be viewed as a kind of **search among a set of candidate concepts**, the hypothesis space.

This is useful since we can apply our general knowledge on search strategies to learning problems!

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Learning as Search

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#### Learning Logical Descriptions: Example

- **Task:** For instance, we could seek a definition of when it is worth waiting at a restaurant.
- **Language:** Logical expressions in the form of disjunctions of conjunctions, with negation only applying to individual predicates and with quantification only universal and over one variable.

**Vocabulary:** Unary predicates, corresponding to Boolean properties of a situation, e.g. Hungry(r), Fri/Sat(r).

Binary predicates, corresponding to other attributes, e.g. Patrons(r, Full), Type(r, French).

The goal predicate WillWait(r).

• Examples are again descriptions of objects.

The example  $X_1$  may be described using:

and the classification  $WillWait(X_1)$ .

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examples).

Learning as Search: logical descriptions

**Examples** 

The label indicates whether the goal predicate holds for the object.

"free" argument, referring to the object (like decision tree

• An object is described using a logical expression that has one

• Normally, a subset of the language used for hypotheses is used

3-4

#### Some possible hypotheses

 $h_1 =$ 

 $\forall r.WillWait(r) \Leftrightarrow$ 

Patrons(r, Some)

- $\lor Patrons(r, Full) \land \neg Hungry(r) \land Type(r, French)$
- $\lor Patrons(r, Full) \land \neg Hungry(r) \land Type(r, Burger)$

 $h_{2} =$ 

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 $\forall r.WillWait(r) \Leftrightarrow$ 

- $Patrons(r, Some) \land Hungry(r)$
- $\lor Patrons(r, Full) \land \neg Hungry(r) \land Type(r, French)$

Note that  $h_2$  is more restrictive than  $h_1$ .

Learning as Search: logical descriptions

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for examples. Here we do not allow disjunctions.

 $Patrons(X_1, Some) \land Hungry(X_1) \land Type(X_1, Thai) \land \dots$ 

Consistency

#### Consistency

When is an example consistent with a hypothesis? Except in the two cases:

False positive: If  $WillWait(X_1)$  follows from the hypothesis but  $X_1$  in fact is a negative example. Eg: Example:  $Patrons(X_1, Some) \land Hungry(X_1) \land \ldots$ Classification:  $\neg WillWait(X_1)$ Hypothesis:  $\forall r.WillWait(r) \Leftrightarrow Hungry(r)$ 

#### Consistency

**False negative:** If  $\neg WillWait(X_2)$  follows from the hypothesis but  $X_2$  in fact is a positive example. Eg: Example:  $Patrons(X_2, Full) \land \neg Hungry(X_2) \land \ldots$ Classification:  $WillWait(X_2)$ Hypothesis:  $\forall r.WillWait(r) \Leftrightarrow Hungry(r)$ 

| AI2-LFD | Learning as Search: logical descriptions | 3-7 | AI2-LFD | Learning as Search: logical descriptions | 3-8 |
|---------|--|-----|---------|--|-----|
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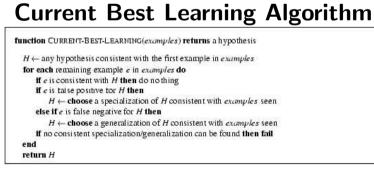
#### Dealing with inconsistent examples

| $\begin{bmatrix} - & - & - & - & - & - & - & - & - & - $ |  |  |  |  |
|--|--|--|--|--|
|--|--|--|--|--|

Coping with a false negative (b) requires generalisation (c).

Coping with a false positive (d) requires specialisation (e).

A learning algorithm results by performing a search over the hypothesis space using generalisation and specialisation operators.



The algorithm needs to choose generalisations and specialisations (there may be several). If it gets into trouble, it has to backtrack to an earlier decision or otherwise it fails.

#### Generalising a Description

- Remove a conjunct, e.g. change [Hungry(r) ∧ Patrons(r, Full)] to [Hungry(r)]
- Add a disjunct, e.g. change [Hungry(r)] to [Hungry(r) ∨ Patrons(r, Full)]
- Replace a predicate/value by a more general one, e.g. change [*Type*(*r*, *French*)] to [*Type*(*r*, *European*)]

Here we assumed that the learner knows the semantics of French and European.

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Learning as Search: current best learning

3-11

#### Specialising a Description

- Add a conjunct. e.g. change [Hungry(r)] to [Hungry(r) ∧ Patrons(r, Full)]
- Remove a disjunct, e.g. change [Hungry(r) ∨ Patrons(r, Full)] to [Hungry(r)]
- Replace a predicate/value by a more specific one, e.g. change [Hungry(r)] to [VeryHungry(r)]

Here we assumed that the learner knows the semantics of Hungry() and VeryHungry().

|--|

Learning as Search: current best learning

3-12

#### **CBL Example**

| Current Hypothesis                                   | Example              | Action          |
|--|----------------------|-----------------|
| $\forall r.WillWait(r) \Leftrightarrow false$        | $X_1$ false negative | Add disjunct    |
| $\forall r.WillWait(r) \Leftrightarrow Alternate(r)$ | $X_2$ false positive | Add conjunct    |
| $\forall r.WillWait(r) \Leftrightarrow$              | $X_3$ false negative | Remove conjunct |
| $[Alternate(r) \land Patrons(r, Some)]$              |                      |                 |
| $\forall r.WillWait(r) \Leftrightarrow$              | $X_4$ false negative | Add disjunct    |
| Patrons(r, Some)                                     |                      |                 |
| $\forall r.WillWait(r) \Leftrightarrow$              |                      |                 |
| $[Patrons(r, Some) \lor$                             |                      |                 |
| $(Patrons(r, Full) \land Fri/Sat(r))]$               |                      |                 |

There were, of course, many other possibilities.

AI2-LFD

3-13

#### **Problems with CBL**

Although CURRENT-BEST-LEARNING has been popular, it has a number of problems:

- It needs to store all encountered examples (to check that changes are consistent with all of them).
- Checking over all encountered examples when a change is made is expensive.
- It is difficult to find good heuristics.

Real hypothesis spaces are large or infinite.

Backtracking may not quickly reconsider the right decision and so may take a long time.

#### Least Commitment Search

- LCS Avoids making arbitrary decisions that might end up wrong.
- The set of hypotheses consistent with the examples seen so far is called the **version space**.
- The algorithm works by successively eliminating inconsistent hypotheses from the version space. Hence called the **candidate** elimination algorithm.

| 1                | e e in examples do  |
|------------------|---|
|                  | npty <b>then</b> $V \leftarrow \text{VERSION-SPACE-UPDATE}(V, e)$ |
| end              |   |
| return V         |   |
|                  |   |
| function VERSION | -SPACE-UPDATE(V, e) <b>returns</b> an updated version space       |
|                  |   |

function VERSION-SPACE-LEARNING(examples) returns a version space local variables: V, the version space: the set of all hypotheses

AI2-LFD

Boundary Representation

Learning as Search: version spaces

Candidate Elimination Algorithm (Version Space Learning)

AI2-LFD

Learning as Search: version spaces

3-15

#### Compact Representation of Version Spaces

Imagine you had to represent all the numbers between 1 and 2. You could represent this set just by specifying the boundaries [1,2]. This works because numbers are *ordered*.

Hypotheses are also ordered, in terms of *specificity*.

For instance, for hypotheses given on Slide 3-5,  $h_1$  is more general (less specific) than  $h_2$ .

Representation of a version space in terms of its boundaries uses two sets: S (most specific) and G (most general).

# This region all inconsistent $G_1$ $G_2$ $G_3$ $\cdots$ $G_m$ More general $S_1$ $S_2$ $\cdots$ $S_n$ this region all inconsistent

#### Updating the Version Space

Given the current version space (constructed from examples seen so far) and a new example, the sets S and G are updated to construct the new version space. Four cases arise:

- 1. False negative for  $S_i$ :  $\Rightarrow$  Further generalise  $S_i$ .
- 2. False positive for  $S_i$ :  $\Rightarrow$  Remove  $S_i$  from the S set.
- 3. False positive for  $G_j$ :  $\Rightarrow$  Further specialise  $G_j$ .
- 4. False negative for  $G_j$ :  $\Rightarrow$  Remove  $G_j$  from the G set.

We initialize the version space as  $S_{\theta} = \{ \mathbf{false} \}$ ,  $G_0 = \{ \mathbf{true} \}$ 

```
Learning as Search: version spaces
```

#### VS Example

- Possible examples: a1, a2, a3, a4, a5.
   NB in order to simplify the description we are not giving the representation of examples here but just their names.
- All "good" hypotheses are marked as ala3 nodes on the graph.
- Each hypothesis description shows the <sup>1</sup>/<sub>ai</sub> examples that are positive for it.
- Edges represent generalisations and specialisations.

| LFD |  |  |
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Learning as Search: version spaces

Version Space

### Termination

Learning with version spaces can terminate in three ways:

- 1. We get to a single concept in the version space.  $\Rightarrow$  Return that as the answer.
- 2. The version space becomes empty, indicating that no hypotheses (in the given space) are consistent with all the examples.
   ⇒ version space "collapses"

#### **VS** Example

|       |             |             | Тдие        |
|-------|-------------|-------------|-------------|
| S     | G           | Example     |             |
| false | true        | a5 negative | a2a3a4      |
| false | a1a3,a2a3a4 | a1 negative |             |
| false | a2a3a4      | a4 positive | ala3 a3a4   |
| a4    | a2a3a4      | a2 negative |             |
| a4    | a3a4        | a3 positive | al a2 a3 a4 |
| a3a4  | a3a4        | CONVERGENCE |             |
| ι     |             |             | False       |

3-19

False

Version Space

AI2-LFD

- 3. We run out of examples, still with multiple elements in the version space. Not clear how to classify new examples. Several possibilities:
- (a) Select an element of the version space at random and use it.
- (b) Take the majority vote of all elements in the version space.
- (c) When classifying a new object, allow "maybe" as well as "yes" or "no" (in case not all hypotheses agree).

We must be able to perform this efficiently.

#### **Version Space Learning**

- + Is a *complete* search method (unlike heuristic methods for DTs).
- + Is an *incremental* method (no need to see all examples at once).
- + Has been shown by Gunter et al. (1997 AIJ) to be closely related to Assumption-Based Truth Maintenance (ATM)
- Is *not* tolerant to noise (version space will collapse).
- Will not work if arbitrary disjunctions are allowed in the concept language (generalisation then simply remembers the positive examples by rote).
- $-\,$  May not be efficient if the sets S and G are large.

Learning as Search: version spaces

3-24

#### Neural Networks — Overview

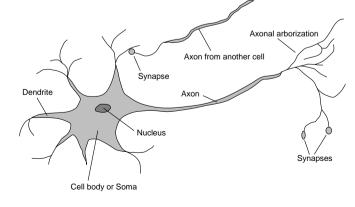
Learning as Search: version spaces

- 1. Overview, real neurons, basic neural computing units
- 2. Neural Networks as a Representation
- 3. Perceptrons and their learning algorithm
- 4. Useful mathematical concepts (gradient descent)
- 5. Multi-layer Perceptrons, back-propagation
- 6. Some Applications

Text: sections 20.5 of Russell & Norvig

#### **Real neurons**

The fundamental unit of all nervous system tissue is the neuron



#### A neuron consists of

- a soma, the cell body, which contains the cell nucleus
- dendrites: input fibres which branch out from the cell body
- an **axon**: a single long (output) fibre which branches out over a distance that can vary between 1cm and 1m
- synapse: a connecting junction between the axon and other cells

Neural Networks: introduction

#### **Real Neurons - Properties**

- $\bullet$  Each neuron can form synapses with anywhere between 10 and  $10^5 \ {\rm other} \ {\rm neurons}$
- Signals are propagated at the synapse through the release of chemical transmitters which raise or lower the electrical potential of the cell
- When the potential reaches a **threshold value**, an **action potential** is sent down the axon
- This eventually reaches the synapses and causes potentiation of the subsequent neurons

| A(2-1+1) |
|----------|
|----------|

Neural Networks: introduction

4-4

# • Synapses can be **inhibitory** (lower the post-synaptic potential) or **excitatory** (raise the post-synaptic potential)

• Synapses can also exhibit long term changes of strength in response to the pattern of stimulation

#### **Artificial Neural Networks**

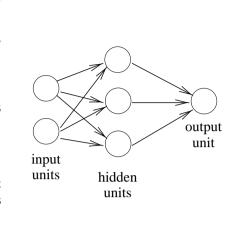
- A neural network is composed of a number of units connected together by links. Each link has an associated numeric weight
- Input and output units are connected to the environment
- Weights are the long term storage, learning involves changing the weights
- Learning modifies the weights so as to try to make the output value(s) correct given the input values.

AI2-LFD

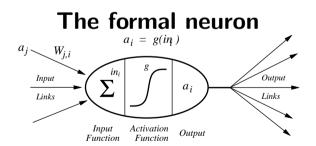
Recurrent networks allow cycles on directed graph i.e. links can form arbitrary topologies.

We will concentrate on acyclic networks, known as **feed-forward** networks.

- links are unidirectional
- network computes a function of the input values that depends on the weight settings
- no internal state other than weights themselves



| AI2-LFD | Neural Networks: introduction | 4-7 |
|---------|-------------------------------|-----|



• The neuron computes the total weighted input to the neuron

$$in_i = \sum_j W_{j,i}a_j = \mathbf{W}_i \cdot \mathbf{a}$$

- Each unit has input links from other neurons, and a current **activation** level.
- Each unit updates its activation (output) using a local computation based on its inputs without any need for global control over the set of units as a whole.
- This formal model is a gross simplification of the detailed function of a neuron.

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Neural Networks: introduction

4-8

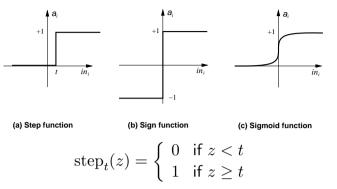
- $W_{j,i}$  is weight on link from neuron j to neuron i,  $\mathbf{W_i}$  is the vector of weights leading *into* unit i, and  $\mathbf{a}$  is the vector of input values.
- computing  $in_i$  is a *linear* operation
- A non-linear component called the activation function g transforms the sum of weighted inputs into the final output value  $a_i$

$$a_i \leftarrow g(in_i) = g(\mathbf{W}_i \cdot \mathbf{a})$$

Note: operation in  $\mathbf{W}_i \cdot \mathbf{a}$  is vector **dot product** 

- $\bullet$  We can use different mathematical functions for g
- Usually, all units (neurons) in network have the same activation function

#### **Activation Functions**



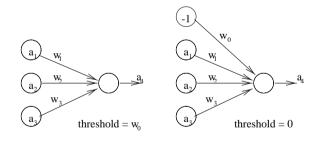
The step and sign functions are examples of the threshold activation function.

| AI2-I FD | Neural Networks: introduction | 4-11 |
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|          |                               |      |
|          |                               |      |

#### Thresholds

- For a step or sign function, with *threshold value* t: if  $in_i \ge t$  the unit fires. The threshold thus corresponds to the minimum total weighted input necessary to cause the neuron to fire.
- Convenient to replace the threshold with an extra weight W<sub>0</sub>, the bias weight, from unit 0 which always has activation a<sub>0</sub> = −1.
   Since in<sub>i</sub> ≥ t ⇔ in<sub>i</sub> − t ≥ 0

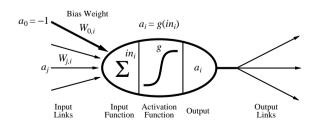
$$a_{i} = \operatorname{step}_{t} \left( \sum_{j=1}^{n} W_{j,i} a_{j} \right) = \operatorname{step}_{0} \left( \sum_{j=0}^{n} W_{j,i} a_{j} \right)$$
  
Al2-LFD Neural Networks: introduction 4-12



- Trick also useful for other activation functions, e.g. the sigmoid
- This makes the learning algorithm simpler as only weights need to be adjusted rather than weights *and* threshold

# Alternative Representation of Formal Neuron

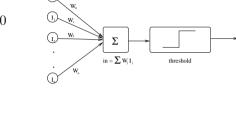
This leads to a modified mathematical model of the formal neuron where the bias weight  $W_{0,i}$  is connected to a fixed input  $a_0 = -1$ :



#### **The Perceptron**

A perceptron is a **single-layer feed-forward neural network**. Consider an example in which the activation function is a **step** function:

- Set  $I_0 = -1$
- Unit fires when  $\sum_{j=0}^{n} W_j I_j = \sum_{j=1}^{n} W_j I_j - W_0 \ge 0$



| AI2-LFD | Neural Networks: representation | 4-15 |
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#### AND-gate truth table

•  $W_0$  is the *threshold*:

the unit fires when

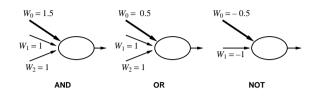
 $\sum_{i=1}^{n} W_i I_i \ge W_0$ 

| Bias | input<br>a1 |    | output |
|------|-------------|----|--------|
| a0   | a1          | a2 |        |
| -1   | 0           | 0  | 0      |
| -1   | 0           | 1  | 0      |
| -1   | 1           | 0  | 0      |
| -1   | 1           | 1  | 1      |

 $\mathsf{AND} = \mathrm{step}_{1.5}(1 \cdot a_1 + 1 \cdot a_2) = \mathrm{step}_0(1.5 \cdot -1 + 1 \cdot a_1 + 1 \cdot a_2)$ 

However, single-layer feed-forward nets (i.e. perceptrons) cannot represent *all* Boolean functions

#### **Computing Boolean Functions with Perceptrons**



Units with a (step) threshold activation function can act as logic gates, given appropriate input and bias weights.

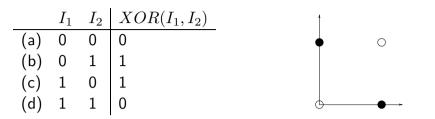
AI2-LFD

Neural Networks: representation

#### Some Geometry

- In 2 dimensions  $w_1x_1 + w_2x_2 w_0 = 0$  defines a line in the plane.
- In higher dimensions  $\sum_{i=1}^{n} w_i x_i w_0 = 0$  defines a hyperplane.
- The decision boundary of a perceptron is a hyperplane.
- If a hyperplane can separate all outputs of one type from outputs of the other type, the problem is said to be **linearly separable**.

#### XOR is not linearly separable



- Function as 2-dimensional plot based on values of 2 inputs
- black dot:  $XOR(I_1, I_2) = 1$  and white dot:  $XOR(I_1, I_2) = 0$
- Cannot draw a line that separates black dots from white ones

| AI2-LFD |  |
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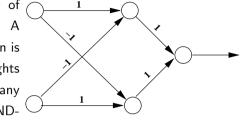
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Neural Networks: representation
```

4-19

#### **Multilayer Neural Network**

Can represent XOR using a network

with two inputs, a hidden layer of ( two units, and one output. A step (threshold) activation function is used at each unit (threshold weights (not shown) are all zero). Many architectures possible, this is an AND-NOT OR AND-NOT network.



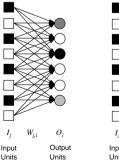
In fact, any Boolean function can be represented, and any bounded continuous function can be approximated.

| AI2-LFD | Neural Networks: | representation |
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4-20

#### Single Layer — Multiple Outputs

- Each output unit is independent of the others; each weight only affects one output unit.
- We can limit our study to singleoutput Perceptrons.
- Use several of them to make a multi-output perceptron.



Perceptron Network

#### Single Perceptron

Output

Unit

#### Supervised Learning: How?

- The learner sees labelled examples  $e = (I_e, T_e)$  such that  $f(I_e) = T_e$ .
- The learner is required to find a mapping *h* that can be used to compute the value of *f* on unseen descriptions.
- In order to do that, machine learning programs normally try to find a hypothesis *h* that gives correct classification to the training set (or otherwise minimises the number of errors).

#### Learning Perceptrons — Basic Idea

- **Important Note:** We assume a threshold activation function, namely a step function, in the next few slides.
- Start by assigning arbitrary weights to W.
- On each example e = (I, T): classify e with current network: O ← step<sub>0</sub>(W ⋅ I) = step<sub>0</sub>(∑W<sub>i</sub>I<sub>i</sub>) if O = T (correct prediction) do nothing.
  - if  $O \neq T$  change  $\mathbf{W}$  "in the right direction".

#### But what is "the right direction" ?

| _    |     |
|------|-----|
| Al2- | LFD |

Neural Networks: learning Perceptrons

The Right Direction

- if T = 1 and O = 0 we want to increase  $\mathbf{W} \cdot \mathbf{I} = \sum W_i I_i$ Can do this by assigning  $\mathbf{W}^{new} = \mathbf{W} + \eta \mathbf{I}$ since  $\mathbf{W}^{new} \cdot \mathbf{I} = \sum W_i^{new} I_i = \sum W_i I_i + \eta \sum I_i I_i > \sum W_i I_i$
- $\bullet$  Amount of increase controlled by parameter  $0<\eta<1$
- if T = 0 and O = 1 we want to decrease  $\mathbf{W} \cdot \mathbf{I} = \sum W_i I_i$ Can do this by assigning  $\mathbf{W}^{new} = \mathbf{W} - \eta \mathbf{I}$ since  $\mathbf{W}^{new} \cdot \mathbf{I} = \sum W_i^{new} I_i = \sum W_i I_i - \eta \sum I_i I_i < \sum W_i I_i$
- In both cases we can assign  $\mathbf{W}^{new} = \mathbf{W} + \eta \mathbf{I}(T O)$

```
Al2-LFD
```

Neural Networks: learning Perceptrons

4-24

Perceptron Learning Algorithm (Version 1)

function perceptron-learning(examples) returns a perceptron hyp.

 $network \leftarrow a \ network \ with \ randomly \ assigned \ weights$ 

#### repeat

#### for each e in examples do

```
O \leftarrow \mathsf{perceptron-output}(\mathsf{network}, \mathbf{I}_e)
```

```
T \leftarrow \text{required output for } \mathbf{I}_e
```

update weights in network based on  $\mathbf{I}_{e}\text{, }O$  and T

$$\mathbf{W} \leftarrow \mathbf{W} + \eta \mathbf{I}_e (T - O)$$

#### end

**until** all examples correctly predicted or other stopping criterion **return** NEURAL-NET-HYPOTHESIS(network)

Perceptron algorithm with step (threshold) activation function.

4-23

#### **Perceptron Learning Algorithm**

- $0<\eta<1$  is known as the learning rate, other symbols e.g.  $\alpha,\,\epsilon$  used by different authors
- $\bullet$  Rosenblatt (1960) showed that the PLA converges to  ${\bf W}$  that classifies the examples correctly (if this is possible).
- PLA behaves well with noisy examples.
- Note that PLA given above is an *incremental* algorithm; *batch* version also possible.

#### **PLA:Example**

- Assume that output O=1, and target is T=0,  $\Rightarrow$  T-O=-1
- $W_0 \leftarrow W_0 + \eta * (-1) * (-1)$
- $W_1 \leftarrow W_1 + \eta * I_1 * (-1)$

•  $W_2 \leftarrow W_2 + \eta * I_2 * (-1)$ 

(-1) (1) (1) (1) (1)

 $\times$ 

-2 -1

#### Understanding the PLA

- Will look at a simpler problem: *learning a linear model* y = W · I = ∑W<sub>i</sub>I<sub>i</sub>.
- For example:  $y = w_0 + w_1 x$ the model has unknown parameters  $w_0, w_1$ .
- We want to determine these on the basis of some training data.
- We can then use the model to *generalize*, i.e. to predict outputs for new inputs.

Neural Networks: gradient descent

- Trivial without noise but not so with noise.
- Al2-LFDNeural Networks: learning Perceptrons4-27

#### Weight space

- Any linear model has a particular number of weights (parameters).
- Particular values for these parameters can be thought of as a point in weight space.
- Can measure the cumulative error as function of parameters.

#### 4-29

AI2-LFD

4-28

#### **Error Function**

- Use an error function,  $E=\frac{1}{2}{\sum}_e(T_e-O_e)^2$
- Has desirable property that E = 0 if  $T_e = O_e$  for all e.
- $\bullet$  So, E=0 can be obtained if there is no noise.
- Otherwise E > 0 but we can try to minimise it.
- Each value of W generates a value of E, call it E(W). We are looking for W that minimises E(W).

AI2-LFD

#### **Error Function** — **Example**

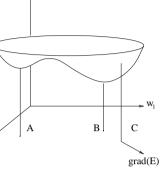
- Fit  $y = w_0 + w_1 x$  with 3 examples (the form is (x, y)): (1,9), (2,7), (3,4).
- Error is

AI2-LFD

$$E(\mathbf{W}) = \frac{1}{2} \left\{ (9 - w_1 - w_0)^2 + (7 - 2w_1 - w_0)^2 + (4 - 3w_1 - w_0)^2 \right\}$$
$$= 1.5w_0^2 + 7w_1^2 - 20w_0 - 35w_1 + 6w_0w_1 + 73$$



- lowest point on the error surface.
  Our problem has a single minimum (can be obtained analytically).
- General, non-linear problems, have a difficulty with local minima.
- → Search using methods that "go downhill" on the error surface.



AI2-LFD

Neural Networks: gradient descent

w,

#### **Gradient descent**

Neural Networks: gradient descent

- If  $E(\mathbf{W})$  is the error function, then the derivative  $\frac{\partial E}{\partial W_i}$  measures the slope of the error surface in the  $W_i$  direction.
- This is summarised in vector notation as:  $\mathbf{g} = \frac{\partial E}{\partial \mathbf{W}} =$
- $= \begin{pmatrix} \frac{\partial E}{\partial W_0} \\ \vdots \\ \frac{\partial E}{\partial W_n} \end{pmatrix}$
- Locally, if we are at point W, the quickest way to decrease E is to take a step in the direction -g.
- Given a formula for E,  $\frac{\partial E}{\partial W_i}$  can often be derived with straightforward algebra.

#### **Gradient Descent Algorithm**

```
Initialize W

while E(\mathbf{W}) is unacceptably high

calculate \mathbf{g} = \frac{\partial E}{\partial \mathbf{W}}

\mathbf{W} \leftarrow \mathbf{W} - \eta \mathbf{g}

end while

return W
```

As in the PLA  $\eta$  is the learning rate.

Here updates are in batch (error computed on all examples); incremental version as in PLA also possible.

4-31

#### Example (continued)

- Fit  $y = w_0 + w_1 x$  with 3 examples (the form is (x, y)): (1,9), (2,7), (3,4).
- Error is  $E(\mathbf{W}) = 1.5w_0^2 + 7w_1^2 20w_0 35w_1 + 6w_0w_1 + 73$
- Partial derivatives:

 $\frac{\partial E}{\partial w_0} = 3w_0 - 20 + 6w_1 \\ \frac{\partial E}{\partial w_1} = 14w_1 - 35 + 6w_0$ 

• Initial guess:  $w_0 = 0, w_1 = 0; \eta = 0.1$ 

AI2-LFD

Neural Networks: gradient descent

4-35

- Iteration:
  - $w_0 \leftarrow w_0 0.1(3w_0 20 + 6w_1)$  $w_1 \leftarrow w_1 - 0.1(14w_1 - 35 + 6w_0)$
- $w_0 \leftarrow -0.1 \cdot -20 = 2; w_1 \leftarrow -0.1 \cdot -35 = 3.5$
- $w_0 \leftarrow 2 0.1(6 20 + 21) = 1.3$  $w_1 \leftarrow 3.5 - 0.1(49 - 35 + 12) = 0.9$
- . . .
- Convergence  $w_0 = 11.66$ ;  $w_1 = -2.50$ changes to weights  $< 10^{-4}$  after 226 iterations

```
AI2-LFD
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Neural Networks: gradient descent

#### Linear Models Again

- $O = \mathbf{W} \cdot \mathbf{I} = \sum W_i I_i$
- Use an error function,  $E = \frac{1}{2} \sum_{e} (T_e O_e)^2$
- $\frac{\partial E}{\partial W_i} = -(T_e O_e) \frac{\partial O_e}{\partial W_i} = -(T_e O_e) I_i$  So the update is:  $W_i \leftarrow W_i + \eta (T_e O_e) I_i$ .
- PLA uses the same update!

The formula however does not correspond to its O function (the derivative of step is not very useful).

NB This just says that it does not correspond to our analysis not that it is a bad algorithm.

### **Problems with Gradient Descent**

- Need to choose  $\eta$  (Too small  $\Rightarrow$  too slow; Too big, unstable).
- Local minima.
- Plateaux.
- Gradient descent is a "hill-climbing" (actually "hill-descending") search: An iterative improvement approach that always moves in the direction that is most promising *locally*.

No memory, no global perspective, no ability to backtrack.

• But it works well in many cases.

Perceptron Learning Algorithm (Version 2)

function perceptron-learning(examples) returns a perceptron hypothesis

inputs: examples, a set of examples, each with input  $\mathbf{x} = x_1, ..., x_n$  and output y. network, a perceptron with weights  $W_j$ , j = 0...n, and activation func. g

#### repeat

for each e in examples do

$$in \leftarrow \sum_{j=0}^{n} W_j x_j [e]$$
  

$$Err \leftarrow y[e] - g(in)$$
  

$$W_j \leftarrow W_j + \eta \times Err \times g'(in) \times x_j [e]$$
  
end

**until** all examples correctly predicted or other stopping criterion **return** NEURAL-NET-HYPOTHESIS(*network*)

**Gradient descent learning** algorithm for perceptrons, with differentiable activation function g. For threshold perceptrons, g'(in) is omitted from the weight update leading to previously seen algorithm (version 1).

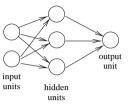
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AI2-LFD
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Neural Networks: gradient descent
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#### **Multi-Layer Neural Networks**

- More expressive than Perceptrons.
- Two issues for learning:
  - (1) what size and structure to use
  - (2) how to update the weights
- For (2) we can use the same scheme as before.
- But we need a differentiable activation function, in order to use the mathematical tools.



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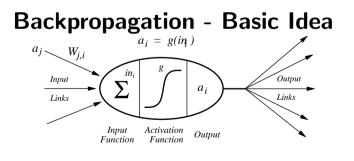
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Neural Networks: multi-layer networks

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#### Training a MLP using Gradient Descent

- Assume network structure chosen.
- Weights are adjusted to reduce the error W ← W − η∂E/∂W or for individual weights W<sub>ji</sub> ← W<sub>ji</sub> − η∂E/∂W<sub>ji</sub>
   NB change in notation: W<sub>ji</sub> connects unit j to unit i
- Need differentiable activation function (so step will not do).
- Calculation like before for the output layer but we do not have the output value for hidden layers.



- Calculate  $\Delta_i = -\frac{\partial E}{\partial i n_i}$  for each unit in the network
- Then  $\frac{\partial E}{\partial W_{ji}} = \frac{\partial E}{\partial in_i} \frac{\partial in_i}{\partial W_{ji}} = -\Delta_i a_j$ because  $\frac{\partial in_i}{\partial W_{ji}} = \frac{\partial [\sum_k W_{ki} a_k]}{\partial W_{ji}} = a_j$

#### The Update Rule

- Threshold Perceptron  $W_{ji} \leftarrow W_{ji} + \eta I_j (T_i O_i)$
- Backpropagation  $W_{ji} \leftarrow W_{ji} + \eta a_j \Delta_i$
- Q: How do we compute the  $\Delta s$  ?
- A: Compute them first for the output units, and then propagate them backwards through the net, from outputs to inputs
- Hence the name **backpropagation**

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# Computing $\Delta_i$ for Output Unit

- Here error refers to a single example.
- $\bullet$  For an output unit indexed by i

$$\Delta_i = -\frac{\partial E}{\partial i n_i} = -\frac{\partial [\frac{1}{2}(T_e - O_e)^2]}{\partial i n_i} = g'(in_i)(T_i - O_i)$$

where g' is the derivative of g and  $O_i = g(in_i)$ 

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Neural Networks: multi-layer networks

#### Computing $\Delta_i$ for Hidden Unit

•  $in_i$  contributes to E only through the outputs  $\Rightarrow$  only through nodes connected to the output of node i. Let k range over these nodes.

$$\Delta_i = -\frac{\partial E}{\partial i n_i} = -\sum_k \frac{\partial E}{\partial i n_k} \frac{\partial i n_k}{\partial a_i} \frac{\partial a_i}{\partial i n_i} = \sum_k \Delta_k W_{ik} g'(in_i)$$

- Reorganising:  $\Delta_i = g'(in_i) \sum_k W_{ik} \Delta_k$
- $\bullet$  Calculating a  $\Delta$  value only requires  $\Delta s$  from further forward in the network.

#### Backpropagation: summary

- Compute  $\Delta$  values for the output units:  $\Delta_i = g'(in_i)(T_i O_i)$
- $\bullet$  Starting with the output layer, keep propagating the  $\Delta$  values back to the previous layer, until the input layer is reached.
- This is computed by  $\Delta_i = g'(in_i) \sum_k W_{ik} \Delta_k$
- Update each weight using gradient descent  $W_{ji} \leftarrow W_{ji} + \eta a_j \Delta_i$

| Backpropagation: p    | oseudocode   |
|-----------------------|--|
| function backpr       | opagation-learning(examples) returns network             |
| network ←             | - a network with randomly assigned weights               |
| repeat                |  |
| for                   | each e in examples do                                    |
|                       | $\mathbf{O} \leftarrow neural-network-output(network,e)$ |
|                       | $\mathbf{T} \leftarrow required$ output for e            |
|                       | compute error and $\Delta s$ for unit in output layer    |
|                       | for each subsequent layer in the network                 |
|                       | compute the $\Delta s$ for units in the layer            |
|                       | end  |
|                       | update all weights                                       |
| end                   |  |
| <b>until</b> netw     | ork has converged  |
| <b>return</b> network | -  |
|                       |  |
|                       |  |
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#### Activation functions

- The activation function should be differentiable everywhere.
- This rules out the *sign* or *step* functions.
- The sigmoid function  $g(z) = \frac{1}{1+e^{-z}}$  is a common choice for multilaver networks
- It "approximates" a step function.
- Also has nice property that q'(z) = q(z)(1 q(z))so the computations are simple.

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Neural Networks: multi-layer networks

**Back Propagation - Example**  $\left(a_{1}\right)$ an output unit hidden units input units Assume  $\eta = 0.1$  $w_{21} = w_{31} = 1$ ,  $w_{42} = w_{43} = w_{52} = w_{53} = 0.6$  $w_{64} = w_{65} = w_{74} = w_{75} = 1$ Neural Networks: multi-layer networks

- Example  $(I_1, I_2) = (2,3)$  and T = 0• First Step: compute  $in_i$ ,  $a_i$ ,  $g'(in_i)$
- $-in_4 = 1 \cdot 2 + 1 \cdot 3 = 5;$   $a_4 = \frac{1}{1+e^{-5}} = 0.993;$   $g'(in_4) =$  $0.993 \cdot 0.007 = 0.007$
- $-in_5 = 5; a_5 = 0.993; q'(in_5) = 0.007$
- $-in_2 = 0.6 \cdot 0.993 + 0.6 \cdot 0.993 = 1.192; a_2 = 0.767; q'(in_2) =$ 0.179
- $-in_3 = in_2 = 1.192; a_3 = a_2 = 0.767; g'(in_3) = 0.179$
- $-in_1 = 1 \cdot 0.767 + 1 \cdot 0.767 = 1.534;$   $a_1 = \frac{1}{1+e^{-1.534}} =$ 0.823;  $q'(in_1) = 0.823 \cdot 0.177 = 0.146$

The output of the network,  $a_1 = 0.823$ , is far from the true

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output T = 0.  $-w_{21} \leftarrow w_{21} + \eta a_2 \Delta_1 = 1 + 0.1 \cdot 0.767 \cdot (-0.120) = 0.9908$ • Second step: compute  $\Delta$  $-\Delta_1 = q'(in_1)(T - a_1) = 0.146(0 - 0.823) = -0.120$ • We are now ready to handle the next example  $-\Delta_2 = q'(in_2)w_{21}\Delta_1 = 0.179 \cdot 1 \cdot -0.120 = -0.021$  $-\Delta_3 = \Delta_2$  $-\Delta_4 = q'(in_4) \cdot [w_{42}\Delta_2 + w_{43}\Delta_3] = -0.000176$  $-\Delta_5 = \Delta_4$ • Third Step: update weights  $-w_{64} \leftarrow w_{64} + \eta a_6 \Delta_4 = 1 + 0.1 \cdot 2 \cdot (-.000176) = 0.9999648$ — . . .  $-w_{42} \leftarrow w_{42} + \eta a_4 \Delta_2 = 0.6 + 0.1 \cdot 0.993 \cdot (-0.021) = 0.5579$ — . . . Neural Networks: multi-layer networks AI2-LFD 4-51 AI2-LFD Neural Networks: multi-layer networks 4-52

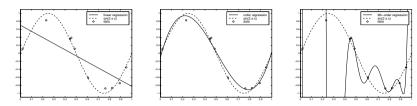
#### Using backprop to train a MLP

- Each pass over all examples is called an **epoch**.
- With m examples and  $|\mathbf{W}|$  weights, each epoch takes  $O(m|\mathbf{W}|)$  time.
- How many epochs are needed? Perhaps lots! Have to choose a good  $\eta$
- Local optima can be a problem; use different starting points in weight space and (?) find the best performance
- How do you choose a network architecture (i.e. number of layers, number of units in each layer)?

### Generalization

- We care about the **generalization** performance of a network, i.e. its predictions on *new* inputs.
- Use strategy similar to decision trees.
- $\bullet$  Divide into two disjoint sets: the training set and the test set.
- $\bullet$  Use the learning algorithm with the training set.
- Estimate generalization error using the test set.

#### **Choosing the Right Model**



Choice is crucial for getting good generalisation. Model too complex: "overfitting" Model too simple: "underfitting"

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Neural Networks: multi-layer networks
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#### Choosing a model

- Pick a number of different models and find out which one has the best test error.
- Different models may include:
  - (1) different architectures,

(2) networks with the same architecture but different starting weight vectors.

• The above method is the standard one, but this is an active research area ...

Neural Networks: multi-layer networks

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#### ALVINN

Autonomous Land Vehicle in a Neural Network (Pomerleau, 1993)

- Task: steer a vehicle along a single lane on a highway by observing the performance of a human driver
- The vehicle (Chevy van) is fitted with computer controlled steering, acceleration and braking
- On-board sensors include colour stereo video, laser rangefinder, radar, inertial navigation system
- Researchers ride along inside the vehicle to monitor the progress of the vehicle and network.

# The ALVINN Architecture

- Input:  $30 \times 32$  pixel array
- Output: 30 units, each corresponding to a steering direction.
- $\bullet$  5 hidden units, fully connected to inputs and outputs
- Method: Map single video frames to steering direction (pure reactive agent)
  - collect data from human drivers (5 minutes)
  - Train network, then ready to drive
  - problem: human drivers are too good!
  - solution: synthesize data from slightly off course

#### **ALVINN: Results**

- $+\,$  Has driven at up to 70 mph for 90 miles on public highways near Pittsburgh
- $+\,$  Has driven at normal speeds on single lane dirt roads, paved bike paths and two lane suburban streets
- Not able to drive on a road type for which it has not been trained

Neural Networks: applications

- Not very robust with respect to changes in lighting conditions.

#### **Playing Backgammon**

Tesauro (1990, 1995)

- A conventional program generates possible moves and presents them to the network for assessment
- Network evaluates moves by outputting a score for any (board position, dice values, possible move) combination
- $\bullet$  Training set of 3000 instances; there are  $\sim 10^{20}$  legal board positions in backgammon
- Each possible move is rate on a scale of -100 to 100
- "higher level" features such as "degree of trapping" turned out to be a necessary part of the input.

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Neural Networks: applications

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#### Playing Backgammon: Results

- Neurogammon convincingly won the computer backgammon championship at the 1989 International Computer Olympiad
- Can train with supervised learning, but better with reinforcement learning
- RL trained program is at, or near to, playing strength of best humans

### **Optical Character Recognition**

(LeCun et al, 1989)

- Task: read ZIP codes
- $\bullet$  Input: segmented, normalized,  $16\times16$  images
- Output: Decision  $0, 1, 2, \dots, 9$
- Architecture: complex, layers of trainable feature detectors (weight sharing)
- Performance: very good.

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### **Context Sensitive Spelling**

System called WinSpell, by Golding and Roth (1995).

- Mistakes like "I had a cake for *desert*" cannot be corrected by conventional spell checkers.
- Learn a classifier that for each occurrence decides which word of a "confusion set" it should be.
- Extract Boolean features from a sentence using given patterns. E.g. "in the \*", "arid within  $\pm 10$  words".
- Features extracted automatically from patterns.

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|---------|-------------------------------|

# • Use one layer of "selection nodes" to combine output of predictors for each word.

Use algorithm *Weighted Majority* (Littlestone and Warmuth, 1994) suitable for combining predictions.

- Use one node to make final decision.
- Performance: gets 96.4% correct on test set (currently best).

# WinSpell Architecture and Performance

- Several layers, but each layer is trained directly and separately.
- Use one layer of Perceptrons to learn many predictors for each word (vary parameters).

Learning algorithm is *Winnow* (Littlestone 1989), a variant of the PLA which is suitable for handling many irrelevant features (as is the case here).

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Neural Networks: applications

# Learning from Data

- We have looked at techniques for supervised learning: **given** a set of examples with associated labels **find** a function h that can be used to predict label values for unseen examples.
- Decision Trees, Logical Descriptions, Neural Networks.
- Representation matters.
- Large number and various kinds of applications.
- Much more exists: both theory and practical aspects. See modules LFD1, LFD2, CLT, GA, PMR

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