Course 395: Machine Learning

- Lecturers: Maja Pantic (maja@doc.ic.ac.uk)
  Stavros Petridis (sp104@doc.ic.ac.uk)

- Goal (Lectures): To present basic theoretical concepts and key algorithms that form the core of machine learning

- Goal (CBC): To enable hands-on experience with implementing machine learning algorithms (developed using Matlab)

- Material: *Machine Learning* by Tom Mitchell (1997)
  Neural Networks & Deep Learning by Michael Nielsen (2017)
  Manual for completing the CBC
  Syllabus on CBR!!

- More Info: *https://www.ibug.doc.ic.ac.uk/courses*

Course 395: Machine Learning – Lectures

- Lecture 1-2: Concept Learning (*M. Pantic*)
- Lecture 3-4: Decision Trees & CBC Intro (*M. Pantic & S. Petridis*)
- Lecture 5-6: Evaluating Hypotheses (*S. Petridis*)
- Lecture 7-8: Artificial Neural Networks I (*S. Petridis*)
- Lecture 9-10: Artificial Neural Networks II (*S. Petridis*)
- Lecture 11-12: Instance Based Learning (*M. Pantic*)
- Lecture 13-14: Genetic Algorithms (*M. Pantic*)

Course 395: Machine Learning - CBC

- Lecture 1-2: Concept Learning
- Lecture 3-4: Decision Trees & CBC Intro
- Lecture 5-6: Evaluating Hypotheses
- Lecture 7-8: Artificial Neural Networks I
- Lecture 9-10: Artificial Neural Networks II
- Lecture 11-12: Instance Based Learning
- Lecture 13-14: Genetic Algorithms

Course 395: Machine Learning

NOTE

CBC accounts for 33% of the final grade for the Machine Learning Exam.

*final grade = 0.66*exam_grade + 0.33*CBC_grade*

Course 395: Machine Learning – Lectures

- Lecture 1-2: Concept Learning (*M. Pantic*)
- Lecture 3-4: Decision Trees & CBC Intro (*M. Pantic & S. Petridis*)
- Lecture 5-6: Evaluating Hypotheses (*S. Petridis*)
- Lecture 7-8: Artificial Neural Networks I (*S. Petridis*)
- Lecture 9-10: Artificial Neural Networks II (*S. Petridis*)
- Lecture 11-12: Instance Based Learning (*M. Pantic*)
- Lecture 13-14: Genetic Algorithms (*M. Pantic*)

Concept Learning – Lecture Overview

- Why machine learning?
- Well-posed learning problems
- Designing a machine learning system
- Concept learning task
- Concept learning as Search
- Find-S algorithm
- Candidate-Elimination algorithm

Machine Learning

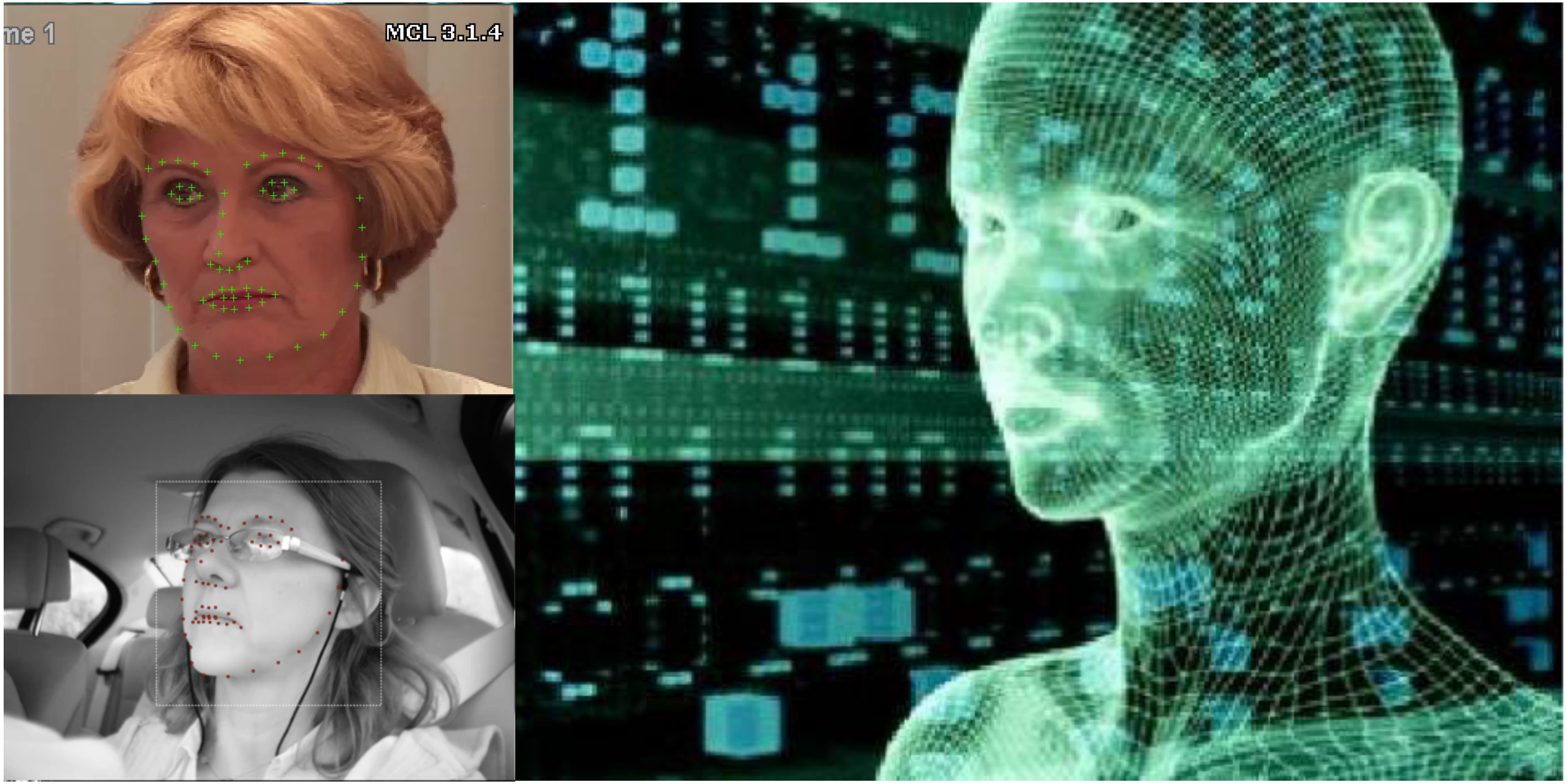
- Learning ↔ Intelligence

  (Def: *Intelligence is the ability to learn and use concepts to solve problems*.)

- Machine Learning ↔ Artificial Intelligence
  – Def: *AI is the science of making machines do things that require intelligence if done by men* (Minsky 1986)
  – Def: *Machine Learning is an area of AI concerned with development of techniques which allow machines to learn*

- Why Machine Learning? ↔ Why Artificial Intelligence?
  ≡ To build machines exhibiting intelligent behaviour (i.e., able to reason, predict, and adapt) while helping humans work, study, and entertain themselves

Machine Learning



Machine Learning

- Machine Learning ↔ Artificial Intelligence
- Machine Learning ← Biology (e.g., Neural Networks, Genetic Algorithms)
- Machine Learning ← Cognitive Sciences (e.g., Case-based Reasoning)
- Machine Learning ← Statistics (e.g., Support Vector Machines)
- Machine Learning ← Probability Theory (e.g., Bayesian Networks)
- Machine Learning ← Logic (e.g., Inductive Logic Programming)
- Machine Learning ← Information Theory (e.g., used by Decision Trees)

Machine Learning

- Human Learning ↔ Machine Learning
  - human-logic inspired problem solvers (e.g., rule-based reasoning)
  - biologically inspired problem solvers (e.g., Neural Networks)
    - supervised learning - generates a function that maps inputs to desired outputs
    - unsupervised learning - models a set of inputs, labelled examples are not available
  - learning by education (e.g., reinforcement learning, case-based reasoning)

- General Problem Solvers vs. Purposeful Problem Solvers
  - emulating general-purpose human-like problem solving is impractical
  - restricting the problem domain results in 'rational' problem solving
  - example of General Problem Solver: Turing Test
  - examples of Purposeful Problem Solvers: speech recognisers, face recognisers, facial expression recognisers, data mining, games, etc.

- Application domains: security, medicine, education, finances, genetics, etc.

Well-posed Learning Problems

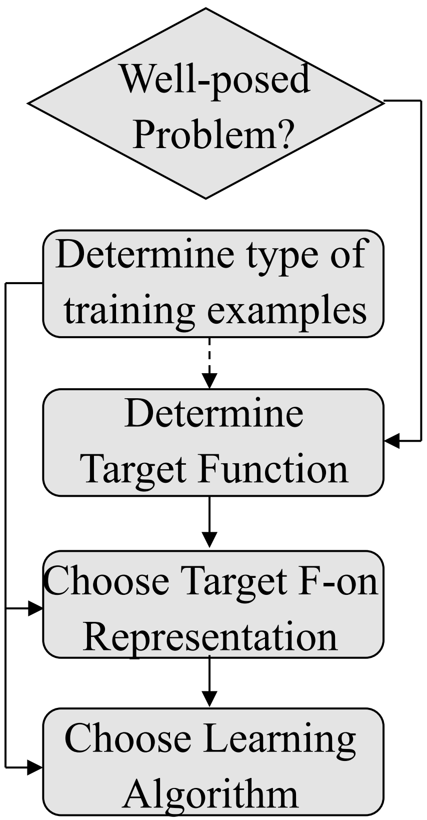
- Def 1 (*Mitchell 1997*):

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

- Def 2 (*Hadamard 1902*):

  A (machine learning) problem is well-posed if a solution to it exists, if that solution is unique, and if that solution depends on the data / experience but it is not sensitive to (reasonably small) changes in the data / experience.

Designing a Machine Learning System



- Target Function V represents the problem to be solved (e.g., choosing the best next move in chess, identifying people, classifying facial expressions into emotion categories)

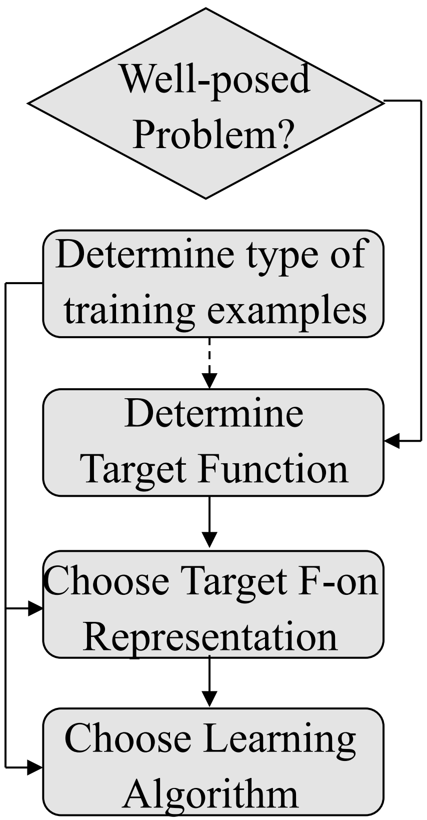
- $V: D \rightarrow C$ where D is the input state space and C is the set of classes
  $V: D \rightarrow [-1, 1]$ is a general target function of a binary classifier

- Ideal Target Function is usually not known; machine learning algorithms learn an approximation of V, say V'

- Representation of function V' to be learned should
  – be as close an approximation of V as possible
  – require (reasonably) small amount of training data to be learned

- $V'(d) = w_0 + w_1x_1 + \ldots + w_nx_n$ where $\langle x_1 \ldots x_n \rangle \equiv d \in D$ is an input state. This reduces the problem to learning (the most optimal) weights w.

Designing a Machine Learning System



- $V: D \rightarrow C$ where D is the input state and C is the set of classes
  $V: D \rightarrow [-1, 1]$ is a general target function of a binary classifier
- $V'(d) = w_0 + w_1x_1 + \ldots + w_nx_n$ where $\langle x_1 \ldots x_n \rangle \equiv d \in D$ is an input state. This reduces the problem to learning (the most optimal) weights w.
- Training examples suitable for the given target function representation V' are pairs $\langle d, c \rangle$ where $c \in C$ is the desired output (classification) of the input state $d \in D$.
- Learning algorithm learns the most optimal set of weights w (so-called *best hypothesis*), i.e., the set of weights that best fit the training examples $\langle d, c \rangle$.
- Learning algorithm is selected based on the availability of training examples (supervised vs. unsupervised), knowledge of the final set of classes C (offline vs. online, i.e., eager vs. lazy), availability of a tutor (reinforcement learning).
- The learned V' is then used to solve new instances of the problem.

Concept Learning

- Concept learning
  - supervised, eager learning
  - target problem: whether something belongs to the target concept or not
  - target function: $V: D \rightarrow$ {true, false}
- Underlying idea: Humans acquire general concepts from specific examples (e.g., concepts: beauty, good friend, well-fitting-shoes)
  (note: each concept can be thought of as Boolean-valued function)
- Concept learning is inferring a Boolean-valued function from training data
  $\rightarrow$ concept learning is the prototype binary classification

Concept Learning as Search

- Concept learning task:
  - target concept: Girls who Simon likes
  - target function: c: $D \rightarrow \{0, 1\}$
  - data $d \in D$: Girls, each described in terms of the following attributes
    - $a_1 \equiv$ *Hair* (possible values: blond, brown, black)
    - $a_2 \equiv$ *Body* (possible values: thin, average, plump)
    - $a_3 \equiv$ *likesSimon* (possible values: yes, no)
    - $a_4 \equiv$ *Pose* (possible values: arrogant, natural, goofy)
    - $a_5 \equiv$ *Smile* (possible values: none, pleasant, toothy)
    - $a_6 \equiv$ *Smart* (possible values: yes, no)
  - target f-on representation: $h \equiv c'$: $\langle a_1, a_2, a_3, a_4, a_5, a_6 \rangle \rightarrow \{0, 1\}$
  - training examples D: positive and negative examples of target function c

instances

+ '?' + '?' + '?' + '?' + '?' + '?'

$|H| = 1 + 4 \cdot 4 \cdot 3 \cdot 4 \cdot 4 \cdot 3 = 2305$

$h \equiv \langle 0,0,0,0,0,0 \rangle$

error rate

- **Aim**: Find a hypothesis $h \in H$ such that $(\forall d \in D)\ h(d) - c(d) < \varepsilon \approx 0$, where H is the set of all possible hypotheses $h \equiv \langle a_1, a_2, a_3, a_4, a_5, a_6 \rangle$, where each a_k, $k = [1..6]$, may be '?' ($\equiv$ any value is acceptable), '0' ($\equiv$ no value is acceptable), or a specific value.

concept learning $\equiv$ searching through H

General-to-Specific Ordering

- Many concept learning algorithms utilize general-to-specific ordering of hypotheses
- General-to-Specific Ordering:
  - *h1* precedes (is more general than) *h2* $\Leftrightarrow$ $(\forall d \in D)\ (h1(d) = 1) \leftarrow (h2(d) = 1)$
    (e.g., $h1 \equiv \langle ?, ?, yes, ?, ?, ? \rangle$ and $h2 \equiv \langle ?, ?, yes, ?, ?, yes \rangle \Rightarrow h1 >_g h2$)
  - *h1* and *h2* are of equal generality $\Leftrightarrow$ $(\exists d \in D)$ { $[(h1(d) = 1) \rightarrow (h2(d) = 1)] \wedge$ $[(h2(d) = 1) \rightarrow (h1(d) = 1)] \wedge$ h1 and h2 have equal number of '?' }
    (e.g., $h1 \equiv \langle ?, ?, yes, ?, ?, ? \rangle$ and $h2 \equiv \langle ?, ?, ?, ?, ?, yes \rangle \Rightarrow h1 =_g h2$)
  - *h2* succeeds (is more specific than) *h1* $\Leftrightarrow$ $(\forall d \in D)\ (h1(d) = 1) \leftarrow (h2(d) = 1)$
    (e.g., $h1 \equiv \langle ?, ?, yes, ?, ?, ? \rangle$ and $h2 \equiv \langle ?, ?, yes, ?, ?, yes \rangle \Rightarrow h2 \not\geq_g h1$)

Find-S Algorithm – Example

1. Initialise $h \in H$ to the most specific hypothesis: $h \leftarrow \langle a_1,\ldots,a_n \rangle$, $(\forall i)\ a_i = 0$.
2. FOR each positive training instance $d \in D$, do:
   FOR each attribute a_i, $i = [1..n]$, in h, do:
   IF a_i is satisfied by d
   THEN do nothing
   ELSE replace a_i in h so that the resulting $h' >_g h$, $h \leftarrow h'$.
3. Output hypothesis h.

	c(d)	*hair*	*body*	*likesSimon*	*pose*	*smile*	*smart*
1	1	blond	thin	yes	arrogant	toothy	no
2	0	brown	thin	no	natural	pleasant	yes
3	1	blond	plump	yes	goofy	pleasant	no
4	0	black	thin	no	arrogant	none	no
5	0	blond	plump	no	natural	toothy	yes

$h \leftarrow \langle 0,0,0,0,0,0 \rangle$ → $h \equiv d1$ → $h \leftarrow \langle$blond, ?, yes, ?, ?, no$\rangle$

Find-S Algorithm

- Find-S is guaranteed to output the most specific hypothesis *h* that best fits positive training examples.
- The hypothesis h returned by Find-S will also fit negative examples as long as training examples are correct.

- However,
  - Find-S is sensitive to noise that is (almost always) present in training examples.
  - there is no guarantee that *h* returned by Find-S is the *only h* that fits the data.
  - several maximally specific hypotheses may exist that fits the data but, Find-S will output only one.
  - Why we should prefer most specific hypotheses over, e.g., most general hypotheses?

Find-S Algorithm – Example

1. Initialise $h \in H$ to the most specific hypothesis: $h \leftarrow \langle a_1,\ldots,a_n \rangle$, $(\forall i)\ a_i = 0$.
2. FOR each positive training instance $d \in D$, do:
   FOR each attribute a_i, $i = [1..n]$, in h, do:
   IF a_i is satisfied by d
   THEN do nothing
   ELSE replace a_i in h so that the resulting $h' >_g h$, $h \leftarrow h'$.
3. Output hypothesis h.

	c(d)	*hair*	*body*	*likesSimon*	*pose*	*smile*	*smart*
1	1	blond	thin	yes	arrogant	toothy	no
2	0	brown	thin	no	natural	pleasant	yes
3	1	blond	plump	yes	goofy	pleasant	no
4	0	black	thin	no	arrogant	none	no
5	0	blond	plump	no	natural	toothy	yes

Find-S → $h = \langle$blond, ?, yes, ?, ?, no$\rangle$ BUT $h2 = \langle$blond,?, ?, ?, ?, no$>$ fits D as well

Find-S Algorithm – Example

1. Initialise $h \in H$ to the most specific hypothesis: $h \leftarrow \langle a_1,\dots,a_n \rangle$, $(\forall i)\ a_i = 0$.
2. FOR each positive training instance $d \in D$, do:

   FOR each attribute a_i, $i = [1..n]$, in h, do:

   IF a_i is satisfied by d

   THEN do nothing

   ELSE replace a_i in h so that the resulting $h' >_g h$, $h \leftarrow h'$.
3. Output hypothesis h.

	c(d)	*hair*	*body*	*likesSimon*	*pose*	*smile*	*smart*
1	1	blond	thin	yes	arrogant	toothy	no
2	0	brown	thin	no	natural	pleasant	yes
3	1	blond	plump	yes	goofy	pleasant	no
4	0	black	thin	no	arrogant	none	no
5	0	blond	plump	no	natural	toothy	yes

Find-S → $h1 = \langle$blond, ?, ?, ?, ?, no$\rangle$ YET $h2 = \langle$blond,?, yes, ?, ?, ?> fits D as well

Candidate-Elimination Algorithm

- Find-S is guaranteed to output the most specific hypothesis *h* that best fits positive training examples.
- The hypothesis h returned by Find-S will also fit negative examples as long as training examples are correct.

- However,
  1. Find-S is sensitive to noise that is (almost always) present in training examples.
  2. there is no guarantee that *h* returned by Find-S is the *only h* that fits the data.
  3. several maximally specific hypotheses may exist that fits the data but, Find-S will output only one.
  4. Why we should prefer most specific hypotheses over, e.g., most general hypotheses?

To address the last three drawbacks of Find-S, Candidate-Elimination was proposed

Candidate-Elimination (C-E) Algorithm

- Main idea: Output a set of hypothesis $VS \subseteq H$ that fit (are consistent) with data D
- Candidate-Elimination (C-E) Algorithm is based upon:
  - general-to-specific ordering of hypotheses
  - *Def:* h is consistent (fits) data $D \Leftrightarrow (\forall \langle d, c(d) \rangle)\ h(d) = c(d)$
  - *Def:* version space $VS \subseteq H$ is set of all $h \in H$ that are consistent with D
- C-E algorithm defines VS in terms of two boundaries:
  - general boundary $G \subseteq VS$ is a set of all $h \in VS$ that are the most general
  - specific boundary $S \subseteq VS$ is a set of all $h \in VS$ that are the most specific

Candidate-Elimination (C-E) Algorithm

1. Initialise $G \subseteq VS$ to the most general hypothesis: $h \leftarrow \langle a_1,\dots,a_n \rangle$, $(\forall i)\ a_i = ?$.
   Initialise $S \subseteq VS$ to the most specific hypothesis: $h \leftarrow \langle a1,\dots,an \rangle$, $(\forall i)\ ai = 0$.
2. FOR each training instance $d \in D$, do:
   - IF d is a positive example
     - Remove from G all h that are not consistent with d.
     - FOR each hypothesis $s \in S$ that is not consistent with d, do:
       - replace s with all h that are consistent with d, $h >_g s$, $\not{h} \geq_g g \in G$,
       - remove from S all s being more general than other s in S.
   - IF d is a negative example
     - Remove from S all h that are not consistent with d.
     - FOR each hypothesis $g \in G$ that is not consistent with d, do:
       - replace g with all h that are consistent with d, $g >_g h$, $h >_g s \in S$,
       - remove from G all g being less general than other g in G.
3. Output hypothesis *G and S*.

C-E Algorithm – Example

	c(d)	*hair*	*body*	*likesSimon*	*pose*	*smile*	*smart*
1	1	blond	thin	yes	arrogant	toothy	no
2	0	brown	thin	no	natural	pleasant	yes
3	1	blond	plump	yes	goofy	pleasant	no
4	0	black	thin	no	arrogant	none	no
5	0	blond	plump	no	natural	toothy	yes

$G_0 \leftarrow \{\langle ?, ?, ?, ?, ?, ? \rangle\}$, $S_0 \leftarrow \{\langle 0, 0, 0, 0, 0, 0 \rangle\}$

C-E Algorithm – Example

	c(d)	*hair*	*body*	*likesSimon*	*pose*	*smile*	*smart*
1	1	blond	thin	yes	arrogant	toothy	no
2	0	brown	thin	no	natural	pleasant	yes
3	1	blond	plump	yes	goofy	pleasant	no
4	0	black	thin	no	arrogant	none	no
5	0	blond	plump	no	natural	toothy	yes

d1 is positive $\rightarrow$ *refine S*

no $g \in G_0$ *is inconsistent with d1* $\rightarrow$ $G_1 \leftarrow G_0 \equiv \{\langle ?, ?, ?, ?, ?, ? \rangle\}$

add to S all minimal generalizations of $s \in S_0$ such that $s \in S_1$ is consistent with *d1*

$S_1 \leftarrow$ {‹blond, thin, yes, arrogant, toothy, no›}

C-E Algorithm – Example

	c(d)	*hair*	*body*	*likesSimon*	*pose*	*smile*	*smart*
1	1	blond	thin	yes	arrogant	toothy	no
2	0	brown	thin	no	natural	pleasant	yes
3	1	blond	plump	yes	goofy	pleasant	no
4	0	black	thin	no	arrogant	none	no
5	0	blond	plump	no	natural	toothy	yes

d2 is negative $\rightarrow$ *refine G*

no s $\in S_1$ *is inconsistent with d2* $\rightarrow$ $S_2 \leftarrow S_1 \equiv$ {‹blond, thin, yes, arrogant, toothy, no›}

add to G all minimal specializations of $g \in G_1$ such that $g \in G_2$ is consistent with *d2*

$G_1 \equiv$ {‹?, ?, ?, ?, ?, ?›}

$G_2 \leftarrow$ {‹blond, ?, ?, ?, ?, ?› , ‹?, ?, yes, ?, ?, ?› , ‹?, ?, ?, arrogant, ?, ?› ,
‹?, ?, ?, ?, toothy, ?›, ‹?, ?, ?, ?, ?, no› }

C-E Algorithm – Example

	c(d)	*hair*	*body*	*likesSimon*	*pose*	*smile*	*smart*
1	1	blond	thin	yes	arrogant	toothy	no
2	0	brown	thin	no	natural	pleasant	yes
3	1	blond	plump	yes	goofy	pleasant	no
4	0	black	thin	no	arrogant	none	no
5	0	blond	plump	no	natural	toothy	yes

d3 is positive $\rightarrow$ *refine S*

two $g \in G_2$ *are inconsistent with d3, i.e.,* ‹?, ?, ?, arrogant, ?, ?› *and* ‹?, ?, ?, ?, toothy, ?› $\rightarrow$

$G_3 \leftarrow$ {‹blond, ?, ?, ?, ?, ?› , ‹?, ?, yes, ?, ?, ?› , ‹?, ?, ?, ?, ?, no› }

add to S all minimal generalizations of $s \in S_2$ such that $s \in S_3$ is consistent with *d3*

$S_2 \equiv$ {‹blond, thin, yes, arrogant, toothy, no›}

$S_3 \leftarrow$ {‹blond, ?, yes, ?, ?, no›}

C-E Algorithm – Example

	c(d)	*hair*	*body*	*likesSimon*	*pose*	*smile*	*smart*
1	1	blond	thin	yes	arrogant	toothy	no
2	0	brown	thin	no	natural	pleasant	yes
3	1	blond	plump	yes	goofy	pleasant	no
4	0	black	thin	no	arrogant	none	no
5	0	blond	plump	no	natural	toothy	yes

d4 is negative → *refine G*

no $s \in S_3$ *is inconsistent with d4* → $S_4 \leftarrow S_3 \equiv$ {‹blond, ?, yes, ?, ?, no›}

add to G all minimal specializations of $g \in G_3$ such that $g \in G_4$ is consistent with *d4*

$G_3 \equiv$ {‹blond, ?, ?, ?, ?, ?› , ‹?, ?, yes, ?, ?, ?› , ‹?, ?, ?, ?, ?, no› }

$G_4 \leftarrow$ {‹blond, ?, ?, ?, ?, ?› , ‹?, ?, yes, ?, ?, ?› }

C-E Algorithm – Example

	c(d)	*hair*	*body*	*likesSimon*	*pose*	*smile*	*smart*
1	1	blond	thin	yes	arrogant	toothy	no
2	0	brown	thin	no	natural	pleasant	yes
3	1	blond	plump	yes	goofy	pleasant	no
4	0	black	thin	no	arrogant	none	no
5	0	blond	plump	no	natural	toothy	yes

d5 is negative → *refine G*

no s $\in S_4$ *is inconsistent with d4* → $S_5 \leftarrow S_4 \equiv$ {‹blond, ?, yes, ?, ?, no›}

add to G all minimal specializations of $g \in G_4$ such that $g \in G_5$ is consistent with *d5*

$G_4 \equiv$ {‹blond, ?, ?, ?, ?, ?› , ‹?, ?, yes, ?, ?, ?›}

$G_5 \leftarrow$ {‹blond, ?, ?, ?, ?, no› , ‹?, ?, yes, ?, ?, ?›}

C-E Algorithm – Example

	c(d)	*hair*	*body*	*likesSimon*	*pose*	*smile*	*smart*
1	1	blond	thin	yes	arrogant	toothy	no
2	0	brown	thin	no	natural	pleasant	yes
3	1	blond	plump	yes	goofy	pleasant	no
4	0	black	thin	no	arrogant	none	no
5	0	blond	plump	no	natural	toothy	yes

Output of C-E:

version space of hypotheses $VS \subseteq H$ *bound with*
specific boundary $S \equiv$ {‹blond, ?, yes, ?, ?, no›} *and*
general boundary $G \equiv$ {‹?, ?, yes, ?, ?, ?› }

$VS \equiv$ {‹?, ?, yes, ?, ?, ?› , ‹blond, ?, yes, ?, ?, ?› ,
‹?, ?, yes, ?, ?, no› , ‹blond, ?, yes, ?, ?, no›}

Concept Learning – Practice

- Tom Mitchell's book – chapter 1 and chapter 2
- Relevant exercises from chapter 1: 1.1, 1.2, 1.3, 1.5
- Relevant exercises from chapter 2: 2.1, 2.2, 2.3, 2.4, 2.5

Course 395: Machine Learning – Lectures

- Lecture 1-2: Concept Learning (*M. Pantic*)
- Lecture 3-4: Decision Trees & CBC Intro (*M. Pantic & S. Petridis*)
- Lecture 5-6: Evaluating Hypotheses (*S. Petridis*)
- Lecture 7-8: Artificial Neural Networks I (*S. Petridis*)
- Lecture 9-10: Artificial Neural Networks II (*S. Petridis*)
- Lecture 11-12: Instance Based Learning (*M. Pantic*)
- Lecture 13-14: Genetic Algorithms (*M. Pantic*)