Lecture 8: Instance based Learning

k-nearest neighbors, locally weighted linear regression, radial basis functions, lazy vs. eager learning, Case-based Reasoning and Analog

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Motivation

- all learning methods presented so far construct a general explicit description of the target function when examples are provided
- **Instance-based learning:**
  - examples are simply stored
  - generalization is postponed until a new instance must be classified
  - in order to assign a target function value, the example's relationship to the previously stored examples is examined
  - sometimes referred to as **lazy learning**

Motivation

- **advantages:**
  - instead of estimating f for the entire instance space, local approximations to the target function are possible
  - especially if target function is complex but still decomposable

- **disadvantages:**
  - classification costs are high

    efficient techniques for indexing examples are important to reduce computational effort

  - typically all attributes are considered when attempting to retrieve similar training examples

    if the concept depends only on a few attributes, the truly most similar instances may be far away ("curse of dimensionality")

Outline

- k-nearest Neighbor Learning
- Locally Weighted Regression
- Radial Basis Functions
- Lazy vs. eager learning
- Case-based reasoning (CBR) and Analogy
- Summary

k-nearest Neighbor Learning

- most basic instance-based method
- **assumption:**
  - instances correspond to a point in a n-dimensional space $\Re^n$
  - thus, nearest neighbors are defined in terms of the standard **Euclidean Distance**

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

  where an instance x is described by $\langle a_1(x), a_2(x), ..., a_n(x) \rangle$

- target function may be either discrete-valued or real-valued

k-nearest Neighbor Learning

- **discrete-valued target function:**
  - $f : \Re^n \rightarrow V$ where V is the finite set $\{v_1, v_2, ..., v_s\}$
  - the target function value is the most common value among the k nearest training examples

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

where

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

- **continuous-valued target function:**
  - algorithm has to calculate the mean value instead of the most common value
  - $f : \Re^n \rightarrow \Re$

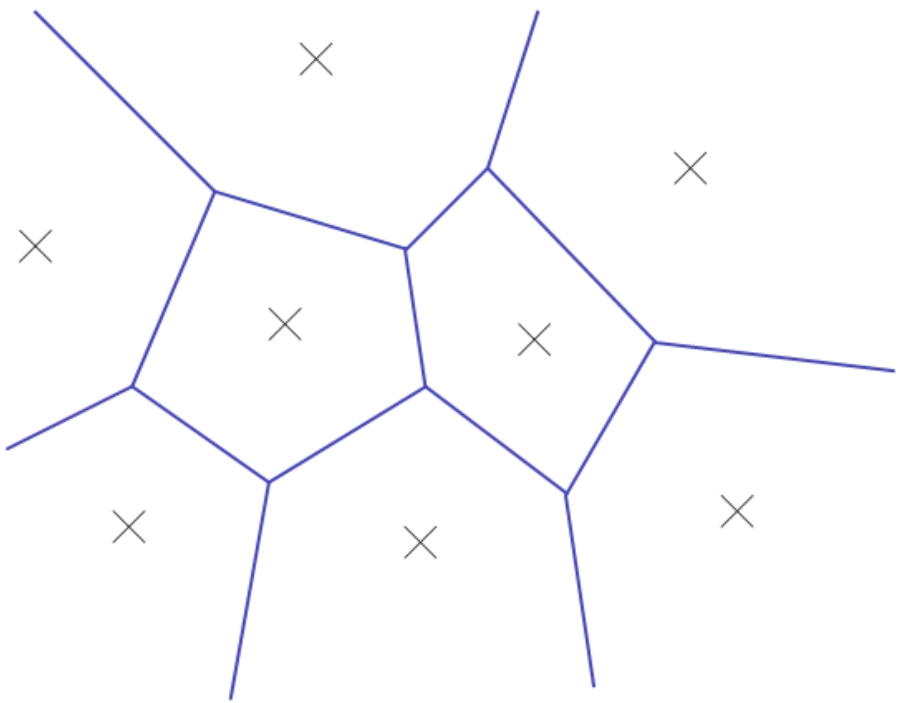
$$\hat{f}(x_q) \leftarrow \frac{\sum_{i=1}^{k} f(x_i)}{k}$$

k-nearest Neighbor Learning

- e.g. instances are points in a two-dimensional space where the target function is boolean-valued
  - 1-nearest neighbor: x_q is classified positive
  - 4-nearest neighbor: x_q is classified negative

Hypothesis Space

- **no explicit** hypothesis is formed
- decision surface is a combination of convex polyhedra surrounding each of the training examples
- for each training example, the polyhedron indicates the set of possible query points x_q whose classification is completely determined by this training example (**Voronoi diagram**)



Distance-Weighted Nearest Neighbor

- contribution of each of the k nearest neighbors is weighted accorded to their distance to x_q
  - **discrete-valued target functions**

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

$$\text{where } w_i \equiv \frac{1}{d(x_q, x_i)^2} \text{ and } \hat{f}(x_q) = f(x_i) \text{ if } x_q = x_i$$

  - **continuous-valued target function:**

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

Locally Weighted Regression

- a note on terminology:
  - *Regression* means approximating a real-valued target function
  - *Residual* is the error $\hat{f}(x) - f(x)$ in approximating the target function
  - *Kernel function* is the function of distance that is used to determine the weight of each training example. In other words, the kernel function is the function K such that $w_i = K(d(x_i, x_q))$
- nearest neighbor approaches can be thought of as approximating the target function at the single query point x_q
- locally weighted regression is a generalization to this approach, because it constructs an explicit approximation of f over a local region surrounding x_q

Locally Weighted Linear Regression

- target function is approximated using a **linear function**

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

- methods like **gradient descent** can be used to calculate the coefficients $w_0, w_1, ..., w_n$ to minimize the error in fitting such linear functions
- ANNs require a global approximation to the target function
- here, just a local approximation is needed

$\Rightarrow$ the error function has to be redefined

Locally Weighted Linear Regression

- possibilities to redefine the error criterion E
  1. Minimize the squared error over just the k nearest neighbors

$$E_1(x_q) \equiv \frac{1}{2} \sum_{x \in k \text{ nearest neigbors}} (f(x) - \hat{f}(x))^2$$

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

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

  3. Combine 1 and 2

$$E_3(x_q) \equiv \frac{1}{2} \sum_{x \in k \text{ nearest neighbors}} (f(x) - \hat{f}(x))^2 \cdot K(d(x_q, x))$$

Locally Weighted Linear Regression

- choice of the error criterion
  - E_2 is the most esthetically criterion, because it allows every training example to have impact on the classification of x_q
  - however, computational effort grows with the number of training examples
  - E_3 is a good approximation to E_2 with constant effort
    Gradient descent rule

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

    with η as learning rate, a_j as attribute value

Locally Weighted Linear Regression

- Remarks on locally weighted linear regression:
  - in most cases, constant, linear or quadratic functions are used
  - costs for fitting more complex functions are prohibitively high
  - simple approximations are good enough over a sufficiently small subregion of X

Radial Basis Functions

- closely related to distance-weighted regression and to ANNs
- learned hypotheses have the form

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

  where
  - each x_u is an instance from X and
  - $K_u(d(x_u, x))$ decreases as $d(x_u, x)$ increases and
  - k is a user-provided constant

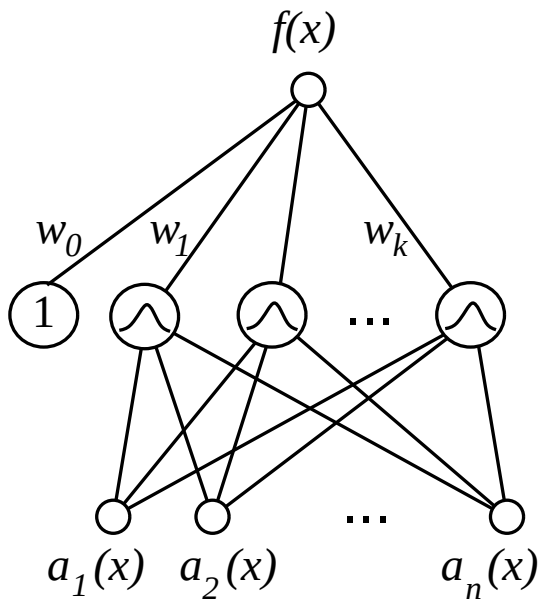
- though $\hat{f}(x)$ is a global approximation to $f(x)$, the contribution of each of the K_u terms is localized to a region nearby the point x_u

Radial Basis Functions

- it is common to choose each function $K_u(d(x_u, x))$ to be a Gaussian function centered at x_u with some variance σ_u^2

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

- the function of $\hat{f}(x)$ can be viewed as describing a two-layer network where the first layer of units computes the various $K_u(d(x_u, x))$ values and the second layer a linear combination of the results



Remarks

- highly effective inductive inference method for many practical problems provided a sufficiently large set of training examples
- robust to noisy data
- weighted average smoothes out the impact of isolated noisy training examples
- **inductive bias of k-nearest neighbors**
  - assumption that the classification of x_q will be similar to the classification of other instances that are nearby in the Euclidean Distance
- **curse of dimensionality**
  - distance is based on all attributes
  - in contrast to decision trees and inductive logic programming
  - solutions to this problem
    - attributes can be weighted differently
    - eliminate least relevant attributes from instance space

Remarks on Lazy Learning

- **lazy methods** defer the decision of how to generalize beyond the training data until a new query instance x_q is encountered
- **eager methods** generalize before any new query instance is encountered
- Lazy methods allow stepwise changes of hypotheses by taking into account new examples
  In contrast:
  in many eager methods hypotheses cannot be incrementally updated
- differences in computation time are obvious
- essential differences in the **inductive bias**
  - lazy methods are able to consider the query instance x_q when deciding how to generalize
  - eager methods already have committed to a global approximation of the target function before any x_q is encountered

  $\Rightarrow$ a lazy learner uses a richer H, because it uses many different local hypotheses to form a global approximation

Lazy Learning – Related Approaches

- Lazy Learning is an approach for modeling **exemplar based categorization** (see human learning)
- Similarity based approach is related to cluster analytical approaches (*k*-**means cluster analysis**)
- If *k*-means cluster are determined in the exemplar space, prototypes can be calculated as average cases (for metric features)
- For discrete-valued features (cp. family resemblance, human learning): contrast metric or Jaccard coefficient
- The *k*-nearest neighbor approach can also be used for **Case-based Reasoning** (CBR)
- Analogical inference is a powerful and cognitive plausible approach to example based reasoning and learning

Jaccard Coefficient:

$$J(A, B) = \frac{|A \cap B|}{|A \cup B|}$$

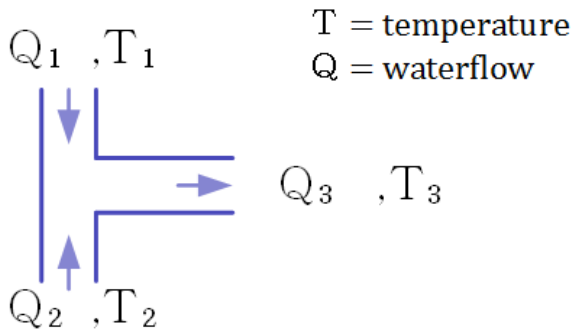
Case-based Reasoning

- If standard inference methods cannot be applied (no formalized domain knowledge, highly complex search space), CBR and analogical reasoning are helpful
- CBR: Find the case (the k cases) most similar to the current case and use information from the retrieved case for the new case
- Example: For some car offered for sale, the price might be determined by averaging the prices of the cars with the most similar features (brand, model, milage, etc.)
- Example: CADET system (Sycara et al., 1992), design of water faucets
- CBR/Analogy can also be used for problem solving: Find the case with the most similar problem specification and transfer the solution

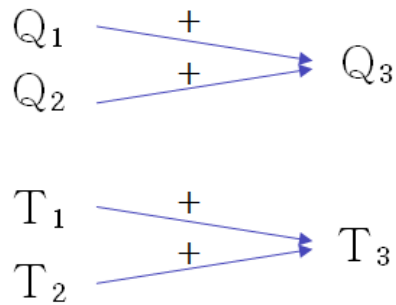
Design of Water Faucets

A stored case: T-junction pipe

Structure:



Function:

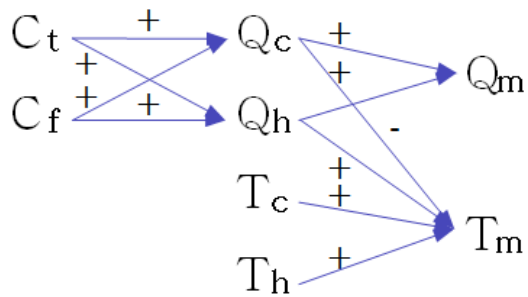


A problem specification: Water faucet

Structure:

?

Function:



Ubiquitousness of Analogical Thinking

Analogy is a powerful and often used cognitive skill:

> Exploiting experience from one domain (**base**) to explain/predict unknown aspects of or solve problems in a different domain (**target**).

Many computational models and psychological experiments (e.g. Gentner, 1983; Hummel & Holyoak, 1997; Wiese, Konerding & Schmid, 2008)

> *Analogy pervades all our thinking, our everyday speech and our trivial conclusions as well as artistic ways of expression and the highest scientific achievements.*
>
> *Polya, How to Solve It, 1945*

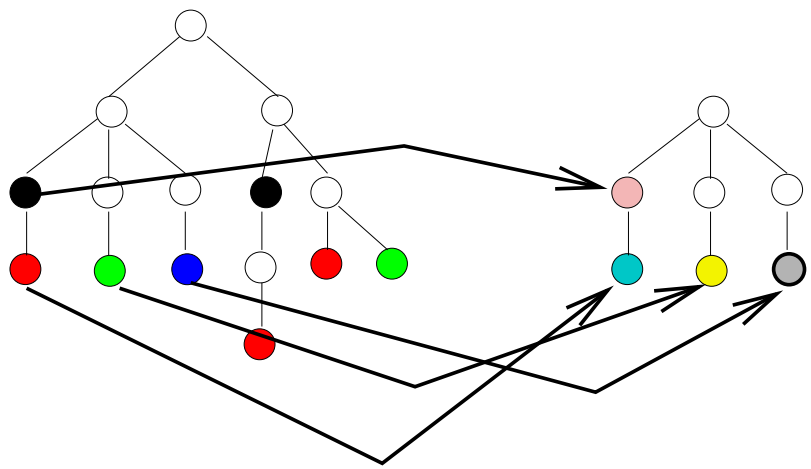
Example: Analogy in Literature

Analogy or proportion is when the second term is to the first as the fourth to the third. We may then use the fourth for the second, or the second for the fourth. Sometimes too we qualify the metaphor by adding the term to which the proper word is relative. [...] As old age is to life, so is evening to day. Evening may therefore be called, 'the old age of the day,' and old age, 'the evening of life,' or, in the phrase of Empedocles, 'life's setting sun.'

Aristotle, Poetics, chap. 21, "Words"

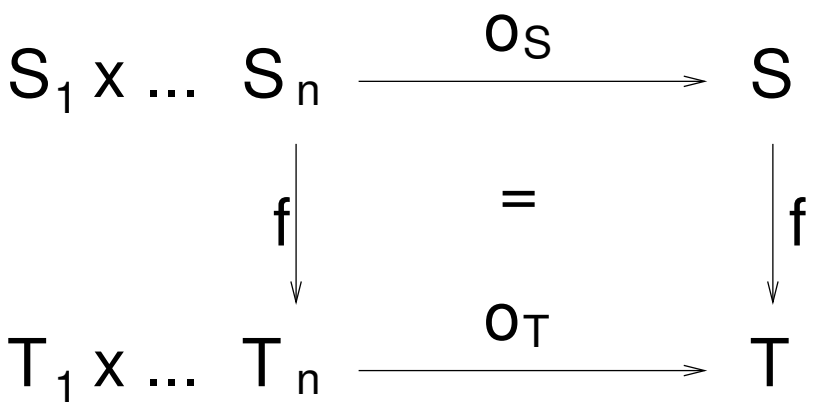
Mapping

- Core of analogy
- Structure preserving mapping
- First order (same relations/functions in both domains) or higher order
- In well-structured, formal domains: homomorphism



Homomorphism

- Structure preserving mapping $f : S \rightarrow T$
- such that $f(o_S(s_1, \ldots, s_n)) = o_T(f(s_1), \ldots, f(s_n))$



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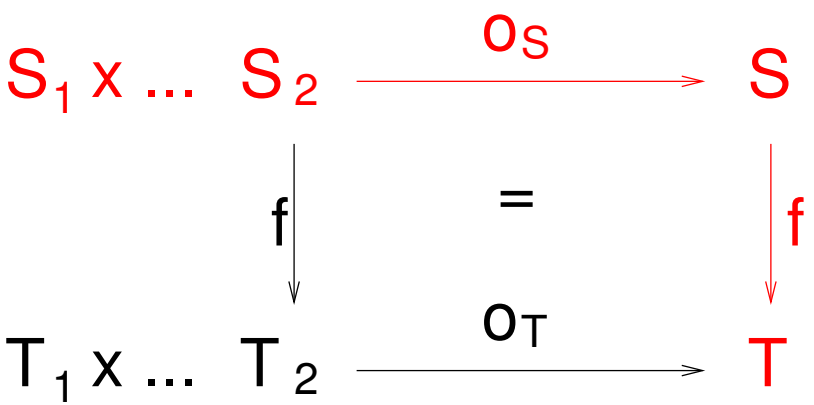

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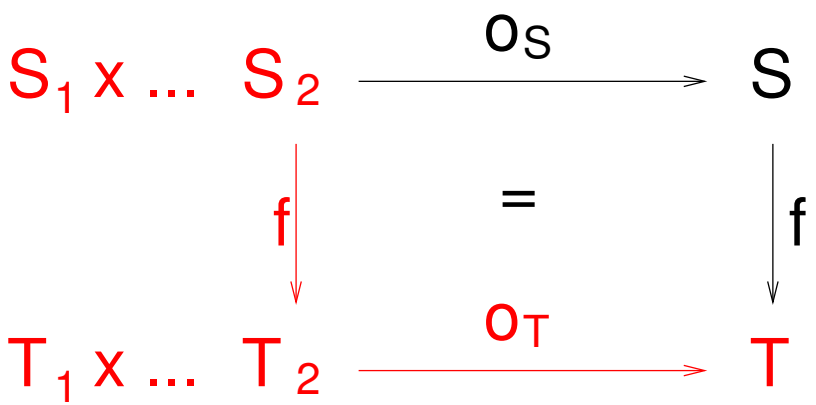
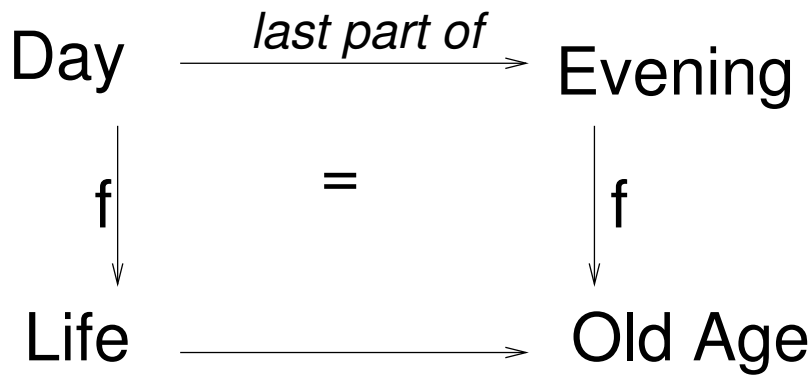
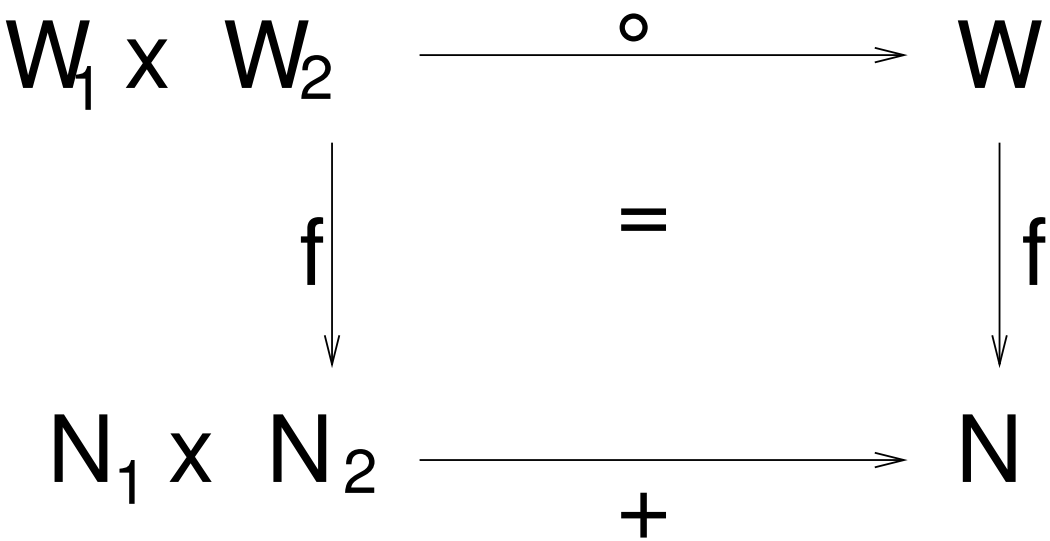


Example 1: Proportional Analogy



Example 2: Proportional Analogy

Relation between string concatenation and length of strings



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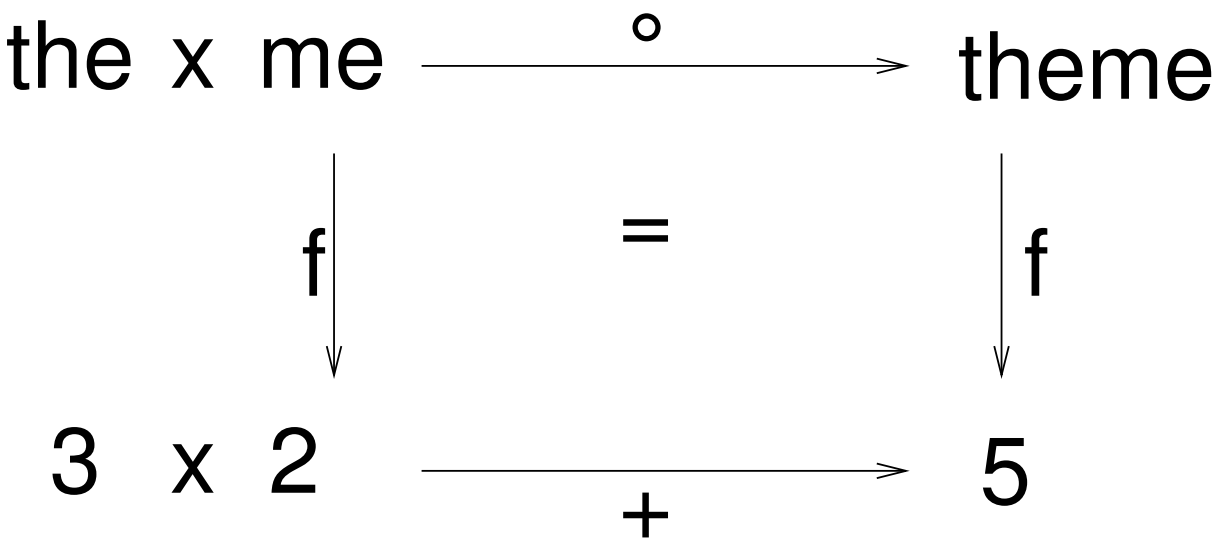

2nd Order Anti-Unification

Approach by Schmid et al.: AvA (Analogy via Abstraction), based on anti-unification

- 1st order AU of $10 + (15 \cdot 10)$ and $3.5 - (20.2 \cdot 3.5)$ is x
- The fact, that each term is built by an operation over a constant and a product got lost in generalization!
- 2nd order AU can be used to model generalization over function/predicate symbols

- Result: $x\ F\ (y \cdot x)$
  where x and y are object variables and F is a function variable
- Applied to programming by analogy (Wagner and Schmid) in context of our work on inductive program synthesis techniques

Programming by Analogy

Fac-Problem: If the factorial of 3 is calculated as $3 \cdot 2 \cdot 1 \cdot 1$ what is the factorial for a natural number n?

Fac-Solution: *fac(n) = if(n=0,1,n · fac(n-1))*.

NSum-Problem: If the neg. sum of 3 is calculated as $((0-1)-2)-3$ what is the neg. sum for a natural number n?

Fac-Unfolding:
if $n = 0$ then 1
else if $n = 1$ then $1 \cdot 1$
else if $n = 2$ then $2 \cdot (1 \cdot 1)$
else if $n = 3$ then $3 \cdot (2 \cdot (1 \cdot 1))$

NSum-Problem:
if $n = 0$ then 0
else if $n = 1$ then $0 - 1$
else if $n = 2$ then $(0 - 1) - 2$
else if $n = 3$ then $((0 - 1) - 2) - 3$

Fac-NSum-Generalization:
if n=0 then **x**
else if n=1 then 1 *F* **x**
else if n=2 then 2 *F* (1 *F* **x**)
else if n=3 then 3 *F* (2 *F* (1 *F* **x**))

$\sigma_{\text{fac}} = \{x \mapsto 1, F \mapsto (\cdot\ \pi_1, \pi_2)\}$
$\sigma_{\text{nsum}} = \{x \mapsto 0, F \mapsto (-\ \pi_2, \pi_1)\}$
Note that arguments of subtraction op are reversed!

Programming by Analogy

- The abstract term captures the role of 1 and 0 as neutral element and of $\cdot$ and $-$ as 'combination-operator' respectively.
- Obtaining the target solution: by applying the found substitutions to the recursive solution of the base problem
- Fac-Solution: *fac(n) = if(n=0,1,n* $\cdot$ *fac(n-1))*.
- NSum-Solution: *nsum(n) = if(n=0, 0, nsum(n-1)* $-$ *n)*.

Summary

- instance-based learning simply stores examples and postpones generalization until a new instance is encountered
- able to learn discrete- and continuous-valued concepts
- noise in the data is allowed (smoothed out by weighting distances)
- **Inductive Bias of k-nearest neighbors**: classification of an instance is similar to the classification of other instances nearby in the Euclidean Distance
- Locally Weighted Regression forms a local approximation of the target function
- Case-based reasoning (CBR) is a related approach to lazy learning
- Analogy is a process which can be used in CBR, analogy can incorporate (eager) generalization learning

Learning Terminology

Lazy Learning

Supervised Learning	**unsupervised learning**

Approaches:

Concept / Classification	Policy Learning
symbolic	**statistical** / neuronal network
inductive	analytical

Learning Strategy:	**learning from examples**
Data:	**arbitrary (features/struct., metric/symbolic)**
Target Values:	**arbitrary (concept, class, value, vector)**