## The Knowledge Contained in Similarity Measures

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## The Questions:

- Of which nature is the knowledge a similarity measure can contain?
- How to bring the knowledge into the measure?
- How to retrieve and use the knowledge for actual problems?


## The Relational Approach

## Basic Relations:

1) $R(x, y, u, v)$ :
" $x$ and $y$ are at least as similar as $u$ and $v$ are"

> 2) $\mathrm{S}(\mathrm{z}, \mathrm{x}, \mathrm{y}): \Leftrightarrow \mathrm{R}(\mathrm{z}, \mathrm{x}, \mathrm{z}, \mathrm{y})$
> " z and x are at least as similar as z and y are"

$$
\begin{aligned}
& \text { 3) } \mathrm{NN}(\mathrm{z}, \mathrm{x}): \Leftrightarrow \forall \mathrm{y} \mathrm{~S}(\mathrm{z}, \mathrm{x}, \mathrm{y}) \\
& \text { "x is a nearest neighbour of } \mathrm{z} \text { " }
\end{aligned}
$$

# On the Semantics of Similarity-Measures 

## Task: Classification $(a \in U, b \in C B)$

## A plausible request:

 $\operatorname{sim}(a, b)=\operatorname{Prob}(\operatorname{class}(a)=\operatorname{class}(b) \mid$ given observations)Conditional Probability!

## Advantage:

The Nearest-Neighbour-Principle is reduced to the Maximum-Likelihood-Principle

## Problem:

What to do if we have very few observations and no other (a priori) information?

## Two Possible Approaches:

(1)
The Evidence-Approach (Dempster - Shafer):
Determine an evidence measure $\mu$ on the case base $\mathrm{CB} \subseteq \mathrm{U}$,
(i.e. a probability on the power set of CB$)(\mathrm{a} \in \mathrm{U})$

$$
\mu_{a}: \wp(C B) \rightarrow[0,1]
$$

Evidence measures reflect ignorance!

## (2)

The Interval-Approach (Pöhlmann - Weichselberger):
Determine an interval for the (unknown) probability distribution:

$$
\begin{aligned}
& \text { I: } \mathrm{U} \times \mathrm{CB} \rightarrow[0,1] \times[0,1] \\
& \mathrm{I}(\mathrm{a}, \mathrm{~b})=(\mathrm{x}, \mathrm{y}) \Rightarrow \mathrm{x} \leq \mathrm{y} \\
& \mathrm{x} \leq \operatorname{Prob}(\text { class }(\mathrm{a})=\operatorname{class}(\mathrm{b}) \mid \text { given observations }) \leq \mathrm{y}
\end{aligned}
$$

The intervals also reflect ignorance!

## The Distribution of Knowledge in a CBR-System

## Knowledge Sources

## Vocabulary Attributes Predicates...

Similarity
Measure
Sim
Case Base CB
$\Downarrow$
To be
Interpreted at
Run Time
$\Downarrow$

Compile Time:
Every Time before Actual Problem Solving

## Distribution of Knowledge

## In principle, all knowledge could be

- in the case base:
pure interpreter approach
- all possible cases in $\mathrm{CB}=\mathrm{U}$
- in the measure: pure compiler approach


## A Simple View <br> on the Task of a CBR-System

Two simple tasks:
(1) Compute a function $f(x)$
(2) Decide for $a, b \in \operatorname{dom}(f): f(a)=f(b)$ ?

## Observations:

- The ability to solve task (1) is sufficient for solving task (2)
- Task (2) may be a lot easier than task(1) e.g. $f(x)=x^{2}$
- Task (2) suffices for task (1) if a table

$$
\left(a_{1}, f\left(a_{1}\right)\right),\left(a_{2}, f\left(a_{2}\right)\right), \ldots
$$

for many $\mathrm{a}_{\mathrm{i}}$ is available

## Issues

- The Semantical Issue:

What is the precise semantics of the parts of a CBR-system which can carry knowledge?

- The Software-(Knowledge-)Engineering Issue:
How is the transformation process Knowledge Sources $\rightarrow$ CBR-System best organized? In how far can existing techniques from knowledge engineering $b \in$ used?
- The Maintenance Issue:

How can one react to dynamic changes of the knowledge?

Centrefor

## Further Generalizations:

- Mix task 1 and task 2:

Split dom(f) and find out which task to apply

- Mix task of type 2 with other tasks


## Example:

## Task Ind: Apply Inductive Reasoning

## The INRECA-Approach:

Mixing Task of Type 2 and Task Ind

## Problem Solving Knowledge

In

- classical (procedural) programs
- knowledge based systems
the knowledge is used to solve a certain problem, e.g. to solve task 1.
(A) In a CBR-system the knowledge is used to solve tasks of type 2.
(B) If a system has some CBR-part, then the knowledge is in addition used to select the part of the knowledge used in the CBR-part


## Consequence:

Methods for Knowledge Engineering should respect (A) and (B).

## Generalization:

## Task of Type 2: For any $a, b \in \operatorname{dom}(f)$

decide the question
"Is the solution $\mathrm{f}(\mathrm{b})$ "good enough" to replace $f(a)$ ?"
"Good enough" has many interpretations, e.g.:

- $f(b)$ is for further operations (almost) as good as $f(a)$
- $f(a)$ can be easily determined from $f(b)$ (adaption)
and others

The task of a CBR-system at compile time is essentially of type 2

Suppose $\mathrm{I}=\{1, \ldots, \mathrm{n}\}$; assume $\mathrm{J} \subseteq \mathrm{I}$ :

$$
\begin{aligned}
& X_{J}=\left\{x \in C B \mid x_{i}=a_{i}, i \in J\right\}, X_{i}=X_{\{i\}} \\
& m_{J}=\oplus\left(m_{i} \mid i \in J\right), m_{i}=m_{\{i\}}
\end{aligned}
$$

The sets $\mathrm{X}_{\mathrm{J}}$ are closed under intersections.
If $\mathrm{X}_{\mathrm{J} 1}=\mathrm{X}_{\mathrm{J} 2}$ for $\mathrm{J} 1 \neq \mathrm{J} 2$ we call it a multiplicity. Without multiplicities and conflicts, Dempster's rule simplifies and gives for $\mathrm{J}^{\prime} \subseteq \mathrm{J} \subseteq \mathrm{I}$

$$
\left.\begin{array}{rl} 
& m_{J}\left(X_{J^{\prime}}\right)=\prod_{i \in J^{\prime}} g_{i} * \prod_{i \in J \backslash J^{\prime}}\left(1-g_{i}\right) \\
= & \sum_{J^{\prime \prime}} \subseteq J \backslash J^{\prime} \\
i \in J^{\prime}
\end{array} \prod_{i}\right)^{*}(-1)^{\left|J^{\prime \prime}\right|} * \prod_{k \in J^{\prime \prime}} g_{k}{ }_{k}
$$

## Also:

$$
\mathrm{m}_{\mathrm{J}}(\mathrm{CB})=\prod_{\mathrm{i} \in \mathrm{~J} \backslash \mathrm{~J}^{\prime}}\left(1-\mathrm{g}_{\mathrm{i}}\right)=1-\sum_{\mathrm{J}^{\prime \prime}} \subseteq \mathrm{J} \backslash \mathrm{~J}^{\prime}(-1)^{\left|\mathrm{J}^{\prime \prime}\right|} * \prod_{\mathrm{k} \in \mathrm{~J}^{\prime \prime}} \mathrm{g}_{\mathrm{k}}
$$

Some $\mathrm{x} \in \mathrm{CB}$ may be elements of several focal sets X. Crucial assumption:
Each such membership contributes to the similarity of $x$ and a according to the evidence measure of each X .

Definition:
(i) $\quad v_{\mathrm{J}}(\mathrm{X})=\sum_{\mathrm{Y} \supseteq \mathrm{X}} \mathrm{m}_{\mathrm{J}}(\mathrm{Y}), \mathrm{Y}$ a focal set for $\mathrm{m}_{\mathrm{J}}$
(ii) $\quad \nu_{\mathrm{J}}(\mathrm{x})=\nu_{\mathrm{J}}(\mathrm{X}), \mathrm{X}$ the minimal focal set cor uniquely defined).
(iii) $\mu_{\mathrm{J}}^{\mathrm{D}}(\mathrm{a}, \mathrm{x})=\nu_{\mathrm{J}}(\mathrm{x})$, where a is the actual case.

$$
\begin{aligned}
& \text { Noise } \\
& \mathrm{X}_{\mathrm{i}}{ }^{\mathrm{e}, \mathrm{~d}}=\left\{\mathrm{x} \in \mathrm{CB}\left|\mathrm{e} \leq\left|\mathrm{X}_{\mathrm{i}}-\mathrm{a}_{\mathrm{i}}\right| \leq \mathrm{d}\right\},\right. \\
& \mathrm{m}_{\mathrm{i}}{ }^{\mathrm{e}, \mathrm{~d}}\left(\mathrm{X}_{\mathrm{i}}{ }^{\mathrm{e}, \mathrm{~d}}\right)=\mathrm{g}^{\mathrm{e,d},}, \\
& \mathrm{~m}_{\mathrm{i}}{ }^{\mathrm{e}, \mathrm{~d}}(\mathrm{CB})=1-\sum\left(\mathrm{g}_{\mathrm{i}}{ }^{\mathrm{e}, \mathrm{~d}} \mid(\mathrm{e}, \mathrm{~d})\right) \\
& \text { for } 0 \leq \mathrm{e}<\mathrm{d} \leq 1 \text {; } \\
& \mathrm{g}_{\mathrm{i}}{ }^{\mathrm{e}, \mathrm{~d}} \text { are again real numbers. } \\
& \text { The rest is as above. }
\end{aligned}
$$

## Similarity and Utility

# Plans, Configurations (sometimes Diagnoses) are not only 

- Correct or incorrect but also
- more or less useful

Hence we have two parameters
$\alpha$ : measures degree of correctness
$\beta$ : measures utility
Also, we have to consider (Vocabulary, Similarity, Case Base)
plus
(Solution Transformation)

## Limitations of the

## Hamming Measure

$$
\begin{gathered}
g=\left(g_{1}, \ldots, g_{n}\right) \text { weight vector, } g_{i} \geq 0 \\
H_{g}(a, b)=\sum g_{i} \text { weighted H-distance } \\
a_{i} \neq b_{i}
\end{gathered}
$$

- The Hamming measure reflects importance
- The Hamming measure does not reflect dependencies
Why $\mathrm{g}_{\mathrm{i}} \geq 0$ ?
Otherwise there can be negative distances,
e.g. $d(a, b)<0 \leq d(a, a)$


## Hence: No unrestricted use of negative weights

## Consequences: Differences between attribute values cannot be expressed.

## One object - many cases

Often one connects
many problems with one object
i.e.
many cases with one object
Hence we need
all attributes for the problems considered

Each attribute needs

a justification<br>(for which problem is it useful?)

This allows the definition of a case class
(all possible attributes)
Each case description is obtained from the case class by the

## Objects versus Cases

- An object is defined by the primary attributes
- Each object gives rise to many problems an object may be
- classified in various ways
- planned
- constructed

Each problem defines a case Case description:

$$
\mathrm{C}=\left(\mathrm{A}_{1}, \ldots, \mathrm{~A}_{\mathrm{n}}, \mathrm{~B}_{1}, \ldots, \mathrm{~B}_{\mathrm{m}}\right)
$$

$\mathrm{A}_{\mathrm{i}}$ : Selected primary attributes $B_{k}$ : Defined secondary attributes

The selection and definition of attributes is an important knowledge engineering task

## Solution Transformation

If solution transformations are present knowledge is distributed over items:


Extreme: All knowledge in T<br>( T is the problem solver)

Assumption: T always checks for correctness

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## Semantics revisited

## Similarity measure sim and <br> solution transformation T have to be considered as a unit.

Now: a actual case, $x \in C B$

## Utility:

$\mu_{x, T}=f\left(\beta_{1}, \beta_{2}\right)$
where
$\beta_{1}$ measures cost of applying $T$ to the solution of $x$
$\beta_{2}$ measures degree of optimality of the solution

## How to find secondary attributes

This is a knowledge acquisition task.
Assumption: The expert can (intuitively) decide S ( $\mathrm{z}, \mathrm{x}, \mathrm{y}$ )

Scenario: - Present z , y to the expert

- Select i such that $\mathrm{z}_{\mathrm{i}} \neq \mathrm{y}_{\mathrm{i}}$
- Obtain $x$ from $y$ by changing $y_{i}$ to $z_{i}$
- Ask the expert: $\mathrm{S}(\mathrm{z}, \mathrm{x}, \mathrm{y})$ ?

If yes: Indication for attribute i independent from the rest of attributes

If no: $\quad$ Ask the expert: Why?
If the answer: "You have to change some $y_{J}$ too," then two dependent attributes
$\mathrm{A}_{\mathrm{i}}$ and $\mathrm{A}_{\mathrm{j}}$ are found.
Figure out the dependency $f(i, j)$ and create a new attribute

## The XOR Example

$$
\begin{aligned}
& \mathrm{U}=\{(0,0),(0,1),(1,0),(1,1)\} \\
& \mathrm{K}_{1}=\{(0,0),(1,1)\}, \mathrm{K}_{2}=\mathrm{U} \backslash \mathrm{~K}_{1}
\end{aligned}
$$

Observation: If $\mathrm{CB} \subseteq \mathrm{U},|\mathrm{CB}|=2$
then for no weighted Hamming measure Hg (C B, Hg ) can classify $\left(\mathrm{K}_{1}, \mathrm{~K}_{2}\right)$ correctly using NNP.

Two possibilities:
(1) Use other measures which can carry more knowledge
(2) Use a new secondary attibute $x_{3}$,

$$
\mathrm{x}_{3}=\mathrm{x}_{1} \oplus \mathrm{x}_{2}
$$

Example:

$$
\begin{aligned}
& \mathrm{f}\left(\mathrm{x}_{1}, \ldots, \mathrm{x}_{\mathrm{n}}, \mathrm{y}_{1}, \ldots \mathrm{y}_{\mathrm{n}}\right)= \begin{cases}1 & \text { if } \mathrm{x}_{\mathrm{i}}=\mathrm{y}_{\mathrm{i}} \text { all i } \\
0 & \text { else }\end{cases} \\
& \mathrm{X}=\left\{\mathrm{x}_{1}, \ldots, \mathrm{x}_{\mathrm{n}}\right\}, Y=\left\{\mathrm{y}_{1}, \ldots, \mathrm{y}_{\mathrm{n}}\right\} \\
& \mathrm{H}_{\mathrm{f}}(\mathrm{X})=\mathrm{H}_{\mathrm{f}}(Y)=0, \mathrm{H}_{\mathrm{f}}(\mathrm{X}, \mathrm{Y}) \approx \frac{\mathrm{n}}{2^{\mathrm{n}}} \\
& \underline{H}_{\mathrm{f}}(\mathrm{X})=\underline{H}_{\mathrm{f}}(Y)=\mathrm{n} \\
& \underline{H}_{\mathrm{f}}(X, Y)=1 \\
& \mathrm{I}_{1}(X, Y) \approx-\frac{\mathrm{n}}{2^{\mathrm{n}}} \approx 0 \\
& \mathrm{I}_{2}(X, Y)=2 \mathrm{n}-1
\end{aligned}
$$

## The Influence Measure

Def: The influence measure is the generalised Hamming measure given by the weights $\mathrm{g}_{\mathrm{J}}=\inf _{\mathrm{f}}(\mathrm{J})$

Observations:

- $g_{\mathrm{I}}=$ number of classes
- there may be $\mathrm{J} \subseteq \mathrm{I}$ with $\mathrm{g}_{\mathrm{J}}>\mathrm{g}_{\mathrm{I}}$ ( $\inf _{f}$ is not monotonic)
- f is difficult to compute

Task: Determine those J which

- are small
- have large influence


## Influence versus Entropy

$\underline{H}_{\mathrm{f}}(\mathrm{J})=\log \left(\inf _{\mathrm{f}}(\mathrm{J})\right)$
behaves like an entropy potential

$$
\mathrm{I}_{2}\left(\mathrm{~J}, \mathrm{~J}^{\prime}\right)=\underline{\mathrm{H}}_{\mathrm{f}}(\mathrm{~J})+\underline{\mathrm{H}}_{\mathrm{f}}\left(\mathrm{~J}^{\prime}\right)-\underline{\mathrm{H}}_{\mathrm{f}}\left(\mathrm{~J} \cup \mathrm{~J}^{\prime}\right)
$$

$\mathrm{H}_{\mathrm{f}}(\mathrm{J})$ measures importance of J to y
$\underline{H}_{f}(\mathrm{~J})$ measures importance of J to y and $\mathrm{I} \backslash \mathrm{J}$

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## Entropy Potential

$$
\mathrm{f}\left(\mathrm{x}_{1}, \ldots, \mathrm{x}_{\mathrm{n}}\right) \longrightarrow \mathrm{y}
$$

Consider $\mathrm{x}_{1}, . ., \mathrm{x}_{\mathrm{n}}, \mathrm{y}$ as random variables
For $\mathrm{J} \subseteq\left\{\mathrm{x}_{1}, . ., \mathrm{x}_{\mathrm{n}}, \mathrm{y}\right\}: \mathrm{H}(\mathrm{J})$ entropy

## Cross - Entropy:

$$
\mathrm{H}_{\mathrm{f}}(\mathrm{~J})=\mathrm{H}(\mathrm{~J})+\mathrm{H}(\mathrm{y})-\mathrm{H}(\mathrm{~J} \cup\{\mathrm{y}\})
$$

## Dependencies:

$$
\mathrm{I}_{1}\left(\mathrm{~J}, \mathrm{~J}^{\prime}\right)=\mathrm{H}_{\mathrm{f}}(\mathrm{~J})+\mathrm{H}_{\mathrm{f}}\left(\mathrm{~J}^{\prime}\right)-\mathrm{H}_{\mathrm{f}}\left(\mathrm{~J} \cup \mathrm{~J}^{\prime}\right)
$$

## Semantics of Similarity

The meaning of the relations should be

For any z the choice of x such that NN( $\mathrm{z}, \mathrm{x}$ )
is the "best possible"

This is NNP : Nearest - Neighbor - Principle How can it be justified?

If the relations are obtained from a measure sim, what is the meaning of the numerical values of $\operatorname{sim}$ ?

## Evidences

Suppose we know the value $\mathrm{a}_{\mathrm{i}}$ of the actual case a.
This is a piece of information!
It gives some evidence that the NN of a is in

$$
X_{i}=\left\{x \in C B \mid a_{i}=x_{i}\right\}
$$

If no other information is present, elements of $\mathrm{X}_{\mathrm{i}}$ are not distinguished.

## The evidence

- may objective ( model based) or subjective
- comes from expert knowledge
- may be very small


## Evidences

## weight of the evidence:

$$
\mathrm{m}_{\mathrm{i}}\left(\mathrm{X}_{\mathrm{i}}\right)=\mathrm{g}_{\mathrm{i}}
$$

## Ignorance:

$$
\begin{aligned}
& m_{i}(C B)=1-g_{i} \\
& m_{i}(Y)=0 \text { for all other } Y \subseteq C B \\
& m_{i} \text { is a Dempster - measure on } \wp(C B)
\end{aligned}
$$

Two measures $m_{i}$ and $m_{j}$ can be accumulated to $\mathrm{m}_{\mathrm{i}} \oplus \mathrm{m}_{\mathrm{j}}$.
Dempster's rule computes this for independent observations.

## Summary

## Semantics:

- Correctness: Leads to the notion of approximate truth. One approach is according to evidence theory
- Optimality: Leads to preferences and utility
- A formal semantics should incorporate both.

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## Summary

## Knowledge Engineering:

- The knowledge sources should be investigated:
- Are there clearly described cases?
- Are the primary attributes collected?
- What kind of background knowledge is present and useful?
- How is the knowledge best distributed over (attributes, measure, case base, solution transformation)?
This is a pragmatic decision!
- Knowledge acquisition and information retrieval techniques should adapted to distribute knowledge
- Learning techniques should be applied


## Summary

## Maintenance:

- Compiled knowledge:
- Updating is difficult as in knowledge based systems
- If learning has been applied it could be continued
- Interpreted knowledge:
- Updating is easier; it results in the updating of the case base


## Moral: Compile

- as little knowledge as possible
- as much knowledge as absolutely necessary.


## CBR

# CBR has many 

- applications
- aspects
- Classification, Diagnosis
- Configuration
- Planning
- Decision Support

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## Compilation versus Interpretation

## Compilation process comp ("Coding") Interpretation process Int



More Knowledge in Sim

## $\Rightarrow$

better classification, smaller CB, but application of Sim possibly more expensive

## Simple Cost Function:

$$
\begin{array}{ll}
\text { Costs } & =\mathrm{C}+\mathrm{n} \mathrm{P} \\
\mathrm{C} & =\text { Compilation Costs } \\
\mathrm{P} & =\text { Cost for one Solution } \\
\mathrm{n} & =\text { Number of Applications }
\end{array}
$$

## Attributes

## Two Sorts of attributes:

(1) Primary attributes: Values come from the available information sources.
(2) Secondary attributes: Are defined in terms of primary attributes.

- Primary attributes contain domain Knowledge
- Secondary attributes contain task knowledge

Example: Customers of a bank

## Primary attributes:

$\mathrm{A}_{1}:$ Income
$\mathrm{A}_{2}:$ Spending
$\mathrm{A}_{3}:$ Interest rate on savings account

## Secondary attributes:

$\mathrm{A}_{4}: \mathrm{A}_{1}-\mathrm{A}_{2}$
$\mathrm{A}_{5}$ : (maximal interest rate available today) - $\mathrm{A}_{3}$

Classification tasks:

1) Good customers : $\mathrm{A}_{4} \geq 0$
2) Customers that may change their bank :
$\mathrm{A}_{5}>0$

## Dependencies

Attributes $\mathrm{A}_{\mathrm{i}}, \mathrm{i} \in \mathrm{F}$;
Classification $\mathrm{f}: \mathrm{U} \rightarrow\{1, . ., \mathrm{n}\}$
k -ary dependencies between attributes subsets $\mathrm{J} \subseteq \mathrm{I},|\mathrm{J}|=\mathrm{k}$

Def: Generalized Hamming Distance : weights $g_{\mathrm{J}}$ for each $\mathrm{J} \subseteq \mathrm{I}$ $\mathrm{GH}(\mathrm{a}, \mathrm{b})=\sum\left(\mathrm{g}_{\mathrm{J}}|\mathrm{J} \subseteq \mathrm{I}, \mathrm{a}| \mathrm{J} \neq \mathrm{b} \mid \mathrm{J}\right)$

Specializations for 2-ary, 3-ary,... dependencies.

Question: How to choose the $\mathrm{g}_{\mathrm{J}}$ ?
This means: Which $\mathrm{J} \subseteq \mathrm{I}$ are important?
This is a - priori - knowledge, to be compiled
Again: - objective approach (model-based)

- subjective approach


## The Influence Potential

Notation: $\mathrm{U}_{\mathrm{J}}$ : Restriction to Attributes $\mathrm{A}_{\mathrm{i}}$, $i \in J$

Def:

(ii) The influence of J is $\inf _{f}(J):=\left|U_{J} / \equiv_{f}\right|$

The influence of $\mathrm{J} \subseteq \mathrm{I}$ is the number of different restrictions to $I \backslash J$ of the classifying function $f$.

## Observations:

- the influence potential reflects dependencies
- the influence potential is in general not known
- estimates are often subjective and reflect expert knowledge
- the Hamming distance corresponds to singletons $\{\mathrm{i}\} \subseteq \mathrm{I}$.
- one can approximate GH by knowing or estimating $\inf _{f}(\mathrm{~J})$ for $|\mathrm{J}|=2,3, \ldots$
- to estimate $\inf _{f}(\mathrm{~J})$ is often easier than to know the exact dependencies


## A suggestion for Semantics (sim,T)

Actual case: a

Observed attributes: indexed by $\mathbf{J}$
Minimal focal set: $\mathrm{X} \subseteq \mathrm{CB}$
Accumulated evidence: $\mathrm{v}_{\mathrm{J}}(\mathrm{X})$
Simplifying assumption: All cases in CB have optimal solutions

Reasonable definition for $\mathrm{x} \in \mathrm{X}$ :
$\mu_{\mathrm{J}}(\mathrm{a}, \mathrm{x}):=\mathrm{v}_{\mathrm{J}}(\mathrm{x}) \cdot \mu_{\mathrm{x}, \mathrm{T}}(\mathrm{a})$

## This grasps

- degree of correctness
- utility

