Semantic Science: ontologies, data and probabilistic theories

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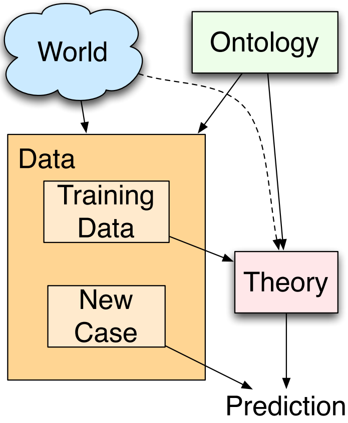
Outline

Notational Minefield

- Theory / hypothesis / model / law (Science)
- Variable (probability and logic and programming languages)
- Model (science, probability and logic)
- Parameter (mathematics and statistics)
- Domain (science and logic and probability and mathematics)
- Object/class (object-oriented programming and ontologies)
- $=$ (probability and logic)
- First-order (logic and dynamical systems)

Semantic Science



- Ontologies represent the meaning of symbols.
- Data that adheres to an ontology is published.
- Theories that make (probabilistic) predictions on data are published.
- Data can be used to evaluate theories.
- Theories make predictions on new cases.

AI Traditions

- Expert Systems of the 70's and 80's
  - Probabilistic models and machine learning.
    Bayesian networks, Bayesian X...
  - Ontologies and Knowledge Representations.
    Description logic, X logic...

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  - Ontologies and Knowledge Representations.
    Description logic, X logic...
- Machine Learning
  - Heterogeneous data sets with rich ontologies
  - Persistent theories built by humans and automatically

Science in Broadest Sense

I mean *science* in the broadest sense:

- where and when landslides occur
- where to find gold
- what errors students make
- disease symptoms, prognosis and treatment
- what companies will be good to invest in
- what apartment Mary would like

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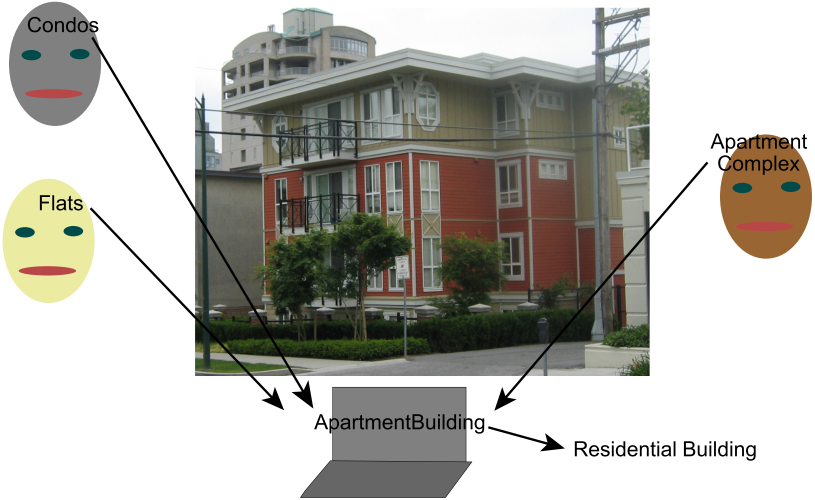
1. Semantic Science Overview
   - Ontologies
   - Data
   - Theories
2. Representing Probabilistic Theories
   - First-order probabilistic models
   - Probabilities with Ontologies
   - Existence and Identity Uncertainty
3. Pragmatics of Real Theories

Ontologies

- In philosophy, ontology the study of existence.
- In CS, an ontology is a (formal) specification of the meaning of the vocabulary used in an information system.
- Ontologies are needed so that information sources can inter-operate at a semantic level.

Ontologies


Condos
Flats
Apartment Complex
ApartmentBuilding
Residential Building

Choosing Individuals and Relations in Logic

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E.g., How to represent: "Pen #7 is red."

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- $color(pen_7, red)$. It's easy to ask "What's red?"
  It's easy to ask "What is the color of pen_7?"
  Can't ask "What property of pen_7 has value red?"

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$prop(Individual, Property, Value)$ is the only relation needed:
$\langle Individual, Property, Value\rangle$ triples, Semantic network, entity relationship model, ...

Reification

- To represent $scheduled(cs422, 2, 1030, cc208)$. "section 2 of course $cs422$ is scheduled at 10:30 in room $cc208$."
- Let $b123$ name the booking:

$$prop(b123, course, cs422).$$
$$prop(b123, section, 2).$$
$$prop(b123, time, 1030).$$
$$prop(b123, room, cc208).$$

- We have reified the booking.
- Reify means: to make into an individual.

Semantic Web Ontology Languages

- RDF — language for triples in XML. Everything is a resource (with URI)
- RDF Schema — define resources in terms of each other: class, type, subClassOf, subPropertyOf, collections...
- OWL — allows for equality statements, restricting domains and ranges of properties, transitivity, cardinality...
- OWL-Lite, OWL-DL, OWL-Full

Main Components of an Ontology

- Individuals: the objects in the world (not usually specified as part of the ontology)
- Classes: sets of (potential) individuals
- Properties: between individuals and their values

Aristotelian definitions

Aristotle [350 B.C.] suggested the definition if a class C in terms of:

- Genus: the super-class
- Differentia: the attributes that make members of the class C different from other members of the super-class

"If genera are different and co-ordinate, their differentiae are themselves different in kind. Take as an instance the genus 'animal' and the genus 'knowledge'. 'With feet', 'two-footed', 'winged', 'aquatic', are differentiae of 'animal'; the species of knowledge are not distinguished by the same differentiae. One species of knowledge does not differ from another in being 'two-footed'."

Aristotle, *Categories*, 350 B.C.

An Aristotelian definition

- An **apartment building** is a **residential building** with **multiple units** and **units are rented**.

$$\begin{aligned} ApartmentBuilding &\equiv ResidentialBuilding\& \\ &\quad NumUnits = many\& \\ &\quad Ownership = rental \end{aligned}$$

  NumUnits is a property with domain *ResidentialBuilding* and range $\{one, two, many\}$
  Ownership is a property with domain *Building* and range $\{owned, rental, coop\}$.
- All classes can be defined in terms of properties.

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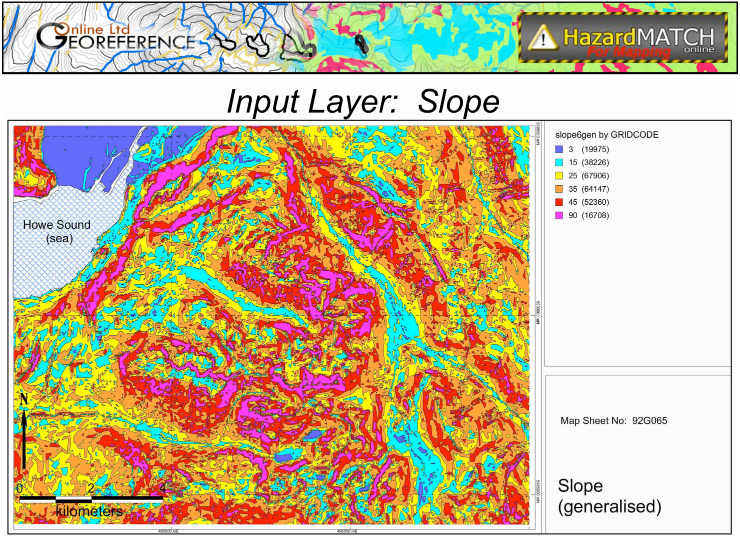
Data

Real data is messy!

- Multiple levels of abstraction
- Multiple levels of detail
- Uses the vocabulary from many ontologies: rocks, minerals, top-level ontology,...
- Rich meta-data:
  - Who collected each datum? (identity and credentials)
  - Who transcribed the information?
  - What was the protocol used to collect the data? (Chosen at random or chosen because interesting?)
  - What were the controls — what was manipulated, when?
  - What sensors were used? What is their reliability and operating range?

Example Data, Geology



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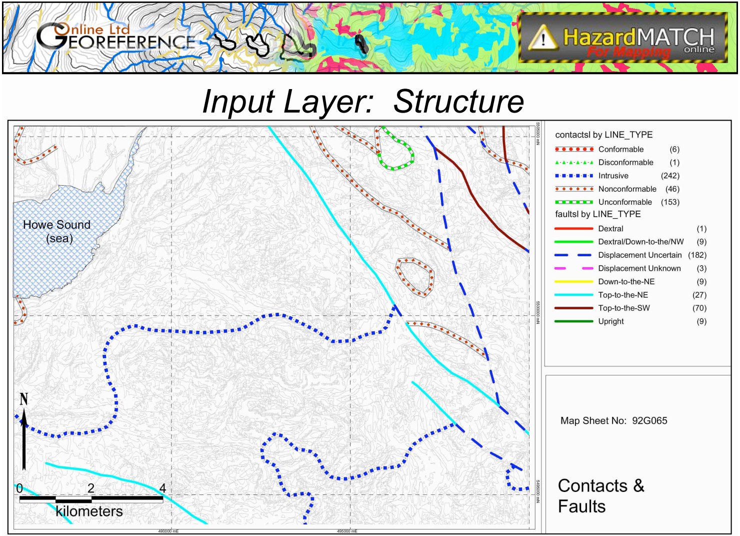


http://www.vsto.org/

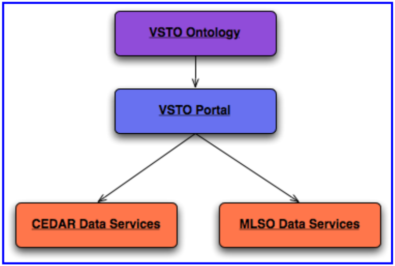
Welcome to the Virtual Solar Terrestrial Observatory

The Virtual Solar Terrestrial Observatory (VSTO) is a unified semantic environment serving data from diverse data archives in the fields of solar, solar-terrestrial, and space physics (SSTSP), currently:

- Upper atmosphere data from the **CEDAR** (Coupling, Energetics and Dynamics of Atmospheric Regions) archive
- Solar corona data from the **MLSO** (Mauna Loa Solar Observatory) archive

The VSTO portal uses an underlying ontology (i.e. an organized knowledge base of the SSTSP domain) to present a general interface that allows selection and retrieval of products (ascii and binary data files, images, plots) from heterogenous external data services.

VSTO Data Access



Data is theory-laden

- Sapir-Whorf Hypothesis [Sapir 1929, Whorf 1940]: people's perception and thought are determined by what can be described in their language. (Controversial in linguistics!)
- A stronger version for information systems:

  What is stored and communicated by an information system is constrained by the representation and the ontology used by the information system.

- Ontologies must come logically prior to the data.
- Data can't make distinctions that can't be expressed in the ontology.
- Different ontologies result in different data.

Outline

Theories make predictions on data

- Theories can make whatever predictions they like about data:
  - definitive predictions
  - point probabilities
  - probability ranges
  - ranges with confidence intervals
  - qualitative predictions
- For each prediction type, we need ways to judge predictions on data
- Users can use whatever criteria they like to evaluate theories (e.g., taking into account simplicity and elegance)

Theory Ensembles

- How can we compare theories that differ in their generality?
- Theory A makes predictions about all cancers.
  Theory B makes predictions about lung cancers.
  Should the comparison between A and B take into account A's predictions on non-lung cancer?

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- What about theory C: *if lung cancer, use B's prediction, else use A's prediction*?
- Proposal: make theory ensembles the norm.
  - Judge theories by how well they fit into ensembles.
  - Ensembles can be judged by simplicity.
  - Theory designers don't need to game the system by manipulating the generality of theories

Dynamics of Semantic Science

- Anyone can design their own ontologies.
  — People vote with their feet what ontology they use.
  — Need for semantic interoperability leads to ontologies with mappings between them.
- Ontologies evolve with theories:
  A theory hypothesizes unobserved features or useful distinctions
  $\longrightarrow$ add these to an ontology
  $\longrightarrow$ other researchers can refer to them
  $\longrightarrow$ reinterpretation of data
- Ontologies can be judged by the predictions of the theories that use them
  — the role of the vocabulary is to describe useful distinctions.

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Probabilistic Prediction

- The role of models in prediction: Given a description of a new case,

$$P(prediction|description) = \sum_{m \in Models} \begin{pmatrix} P(prediction|m\&description) \times \\ P(m|description) \end{pmatrix}$$

Models is a set of mutually exclusive and covering set of hypotheses.

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  Models is a set of mutually exclusive and covering set of hypotheses.
- What features of the description are predictive?
- How do the features interact?
- What are the appropriate probabilities? (How can these be learned with limited data?)

Representing Uncertainty: Bayesian belief networks

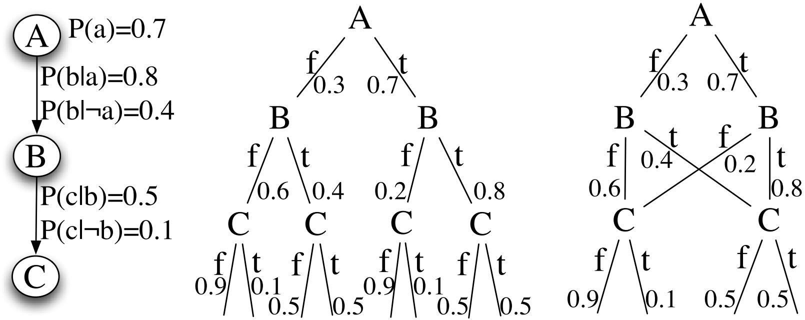
What:

- A belief network is a graphical representation of dependence amongst a set of random variables.

Why:

- Often the natural representation: independence represents causal structure
- Probabilities can be understood and learned locally
- We can exploit the structure for efficient inference

Semantic Tree



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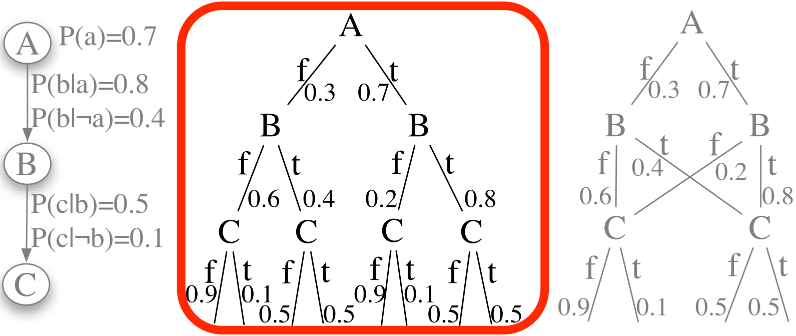


↑

semantic tree

event tree

decision tree...

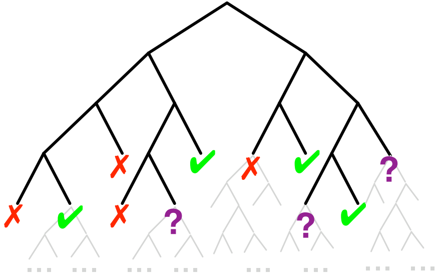
Semantic tree

- Nodes are propositions or discrete variables
- Child for each value in domain
- There is a probability distribution over the children of each node
- Each finite path from the root corresponds to a formula
- Each finite path from the root has a probability that is the product of the probabilities in the path

A generative model generates a semantic tree.

Infinite Semantic Tree

Given a proposition α:

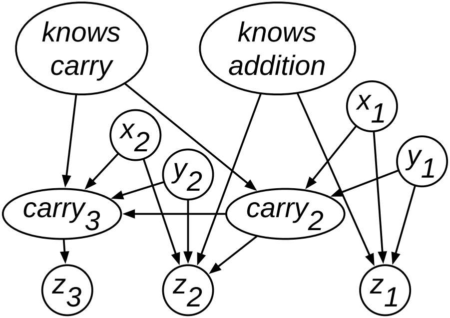


✔ *path* $\models \alpha$
✗ *path* $\models \neg\alpha$
? otherwise

The probability of α is well defined if for all $\epsilon > 0$ there is a finite sub-tree that can answer α in $> 1 - \epsilon$ of the probability mass.

Predicting students errors

$$\begin{array}{rrrr} & & x_2 & x_1 \\ + & & y_2 & y_1 \\ \hline & z_3 & z_2 & z_1 \end{array}$$



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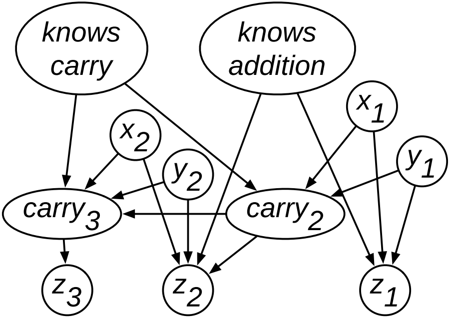

What if there were multiple digits

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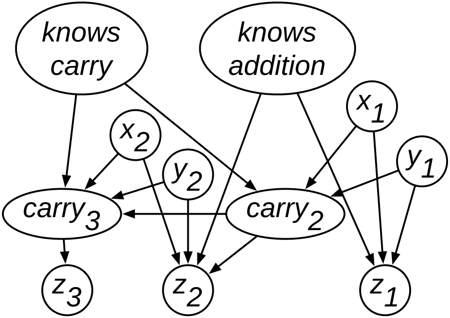

What if there were multiple digits, problems

Predicting students errors

$$
\begin{array}{cccc}
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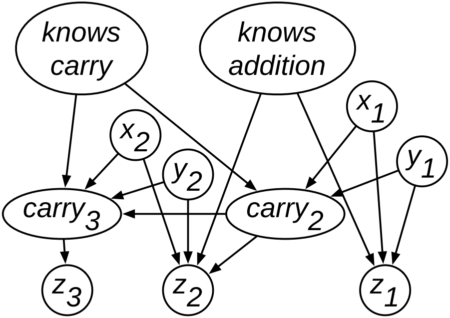

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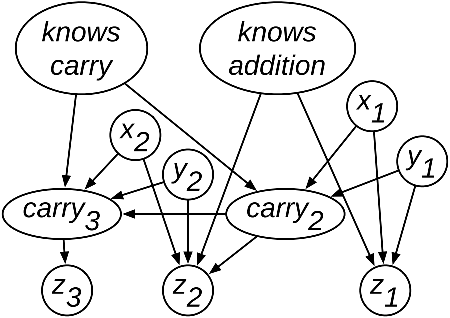

What if there were multiple digits, problems, students, times?

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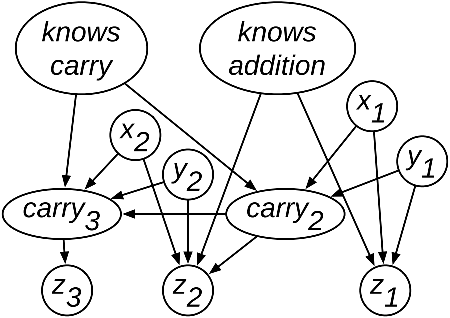
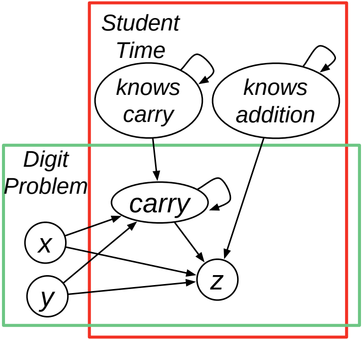


What if there were multiple digits, problems, students, times?
How can we build a model before we know the individuals?

Outline

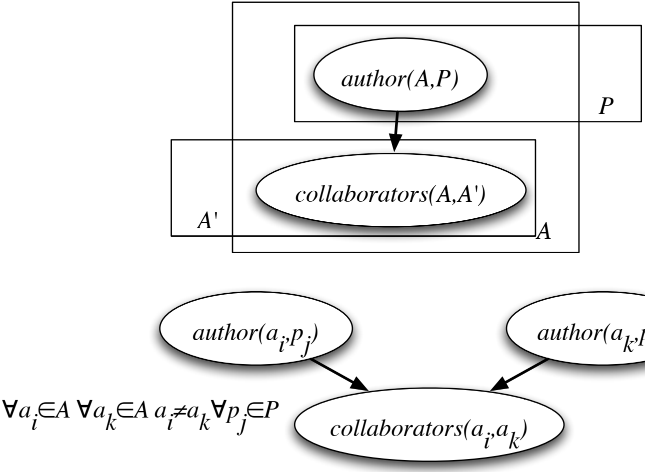
Multi-digit addition with parametrized BNs / plates

$$\begin{array}{rcccc} & x_{j_x} & \cdots & x_2 & x_1 \\ + & y_{j_z} & \cdots & y_2 & y_1 \\ \hline & z_{j_z} & \cdots & z_2 & z_1 \end{array}$$



Random Variables: $x(D,P)$, $y(D,P)$, $knowsCarry(S,T)$, $knowsAddition(S,T)$, $carry(D,P,S,T)$, $z(D,P,S,T)$
for each: digit D, problem P, student S, time T

Creating Dependencies: Relational Structure



Independent Choice Logic

- A language for first-order probabilistic models.
- Idea: combine logic and probability, where all uncertainty in handled in terms of Bayesian decision theory, and logic specifies consequences of choices.
- History: parametrized Bayesian networks, abduction and default reasoning $\longrightarrow$ probabilistic Horn abduction (IJCAI-91); richer language (negation as failure + choices by other agents $\longrightarrow$ independent choice logic (AIJ 1997).

Independent Choice Logic

- An alternative is a set of atomic formula.
  $\mathcal{C}$, the choice space is a set of disjoint alternatives.
- $\mathcal{F}$, the facts is a logic program that gives consequences of choices.
- P_0 a probability distribution over alternatives:

$$\forall A \in \mathcal{C} \; \sum_{a \in A} P_0(a) = 1.$$

Meaningless Example

$$\mathcal{C} = \{\{c_1, c_2, c_3\}, \{b_1, b_2\}\}$$

$$\begin{aligned}
\mathcal{F} = \{\ & f \leftarrow c_1 \wedge b_1, & f \leftarrow c_3 \wedge b_2, \\
& d \leftarrow c_1, & d \leftarrow \neg c_2 \wedge b_1, \\
& e \leftarrow f, & e \leftarrow \neg d\}
\end{aligned}$$

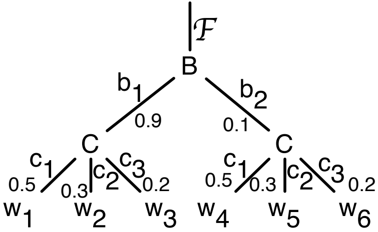
$$\begin{array}{lll}
P_0(c_1) = 0.5 & P_0(c_2) = 0.3 & P_0(c_3) = 0.2 \\
P_0(b_1) = 0.9 & P_0(b_2) = 0.1 &
\end{array}$$

Semantics of ICL

Probabilities are defined by a (possible infinite) semantic tree:

- Root has one choice corresponding to $\mathcal{F}$
- Each internal node corresponds to an alternative: child for each element of the alternative.

Meaningless Example: Semantics

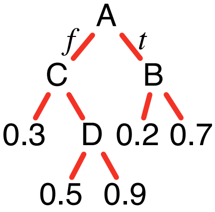


w_1	$\models$	c_1	b_1	f	d	e	$P(w_1) = 0.45$
w_2	$\models$	c_2	b_1	$\neg f$	$\neg d$	e	$P(w_2) = 0.27$
w_3	$\models$	c_3	b_1	$\neg f$	d	$\neg e$	$P(w_3) = 0.18$
w_4	$\models$	c_1	b_2	$\neg f$	d	$\neg e$	$P(w_4) = 0.05$
w_5	$\models$	c_2	b_2	$\neg f$	$\neg d$	e	$P(w_5) = 0.03$
w_6	$\models$	c_3	b_2	f	$\neg d$	e	$P(w_6) = 0.02$

$$P(e) = 0.45 + 0.27 + 0.03 + 0.02 = 0.77$$

Belief Networks, Decision trees and ICL rules

- There is a local mapping from belief networks into ICL.
- Rules can represent decision tree representation of conditional probabilities:



P(e|A,B,C,D)

$$
\begin{array}{ll}
e \leftarrow a \wedge b \wedge h_1. & P_0(h_1) = 0.7 \\
e \leftarrow a \wedge \neg b \wedge h_2. & P_0(h_2) = 0.2 \\
e \leftarrow \neg a \wedge c \wedge d \wedge h_3. & P_0(h_3) = 0.9 \\
e \leftarrow \neg a \wedge c \wedge \neg d \wedge h_4. & P_0(h_4) = 0.5 \\
e \leftarrow \neg a \wedge \neg c \wedge h_5. & P_0(h_5) = 0.3
\end{array}
$$

Example: Multi-digit addition

$$
\begin{array}{ccccc}
 & x_{j_x} & \cdots & x_2 & x_1 \\
+ & y_{j_z} & \cdots & y_2 & y_1 \\
\hline
 & z_{j_z} & \cdots & z_2 & z_1
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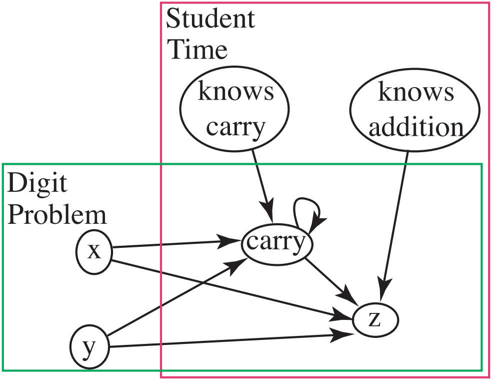
$$



ICL rules for multi-digit addition

$$\begin{aligned}
z(D,P,S,T) = V \leftarrow & \\
& x(D,P) = Vx \wedge \\
& y(D,P) = Vy \wedge \\
& carry(D,P,S,T) = Vc \wedge \\
& knowsAddition(S,T) \wedge \\
& \neg mistake(D,P,S,T) \wedge \\
& V \text{ is } (Vx + Vy + Vc) \text{ div } 10.
\end{aligned}$$

$$\begin{aligned}
z(D,P,S,T) = V \leftarrow & \\
& knowsAddition(S,T) \wedge \\
& mistake(D,P,S,T) \wedge \\
& selectDig(D,P,S,T) = V. \\
z(D,P,S,T) = V \leftarrow & \\
& \neg knowsAddition(S,T) \wedge \\
& selectDig(D,P,S,T) = V.
\end{aligned}$$

Alternatives:

$\forall DPST\{noMistake(D,P,S,T), mistake(D,P,S,T)\}$

$\forall DPST\{selectDig(D,P,S,T) = V \mid V \in \{0..9\}\}$

Outline

Random Variables and Triples

- Reconcile:
  - random variables of probability theory
  - individuals, classes, properties of modern ontologies

Random Variables and Triples

- Reconcile:
  - random variables of probability theory
  - individuals, classes, properties of modern ontologies
- For functional properties:
  random variable for each $\langle individual, property \rangle$ pair, where the domain of the random variable is the range of the property.
- For non-functional properties:
  Boolean random variable for each $\langle individual, property, value \rangle$ triple.

Triples and Probabilities

- $\langle individual, property, value\rangle$ triples are complete for representing relations
- $\langle individual, property, value, probability\rangle$ quadruples can represent probabilities of relations (or reify again)
- e.g., in addition $P(z(3, prob23, fred, t3) = 4) = 0.43$:

$$\left.\begin{array}{l}\langle z543, type, AdditionZValue\rangle\\ \langle z543, digit, 3\rangle\\ \langle z543, problem, prob23\rangle\\ \langle z543, student, fred\rangle\\ \langle z543, time, t3\rangle\end{array}\right\}\text{defines random variable}$$

$$\left.\begin{array}{l}\langle z543, valueWithProb, 4, 0.43\rangle\\ \langle z543, valueWithProb, 5, 0.03\rangle\\ \ldots\end{array}\right\}\text{defines distribution}$$

Probabilities and Aristotelian Definitions

Aristotelian definition

$$\begin{aligned} ApartmentBuilding &\equiv ResidentialBuilding\& \\ &\quad NumUnits = many\& \\ &\quad Ownership = rental \end{aligned}$$

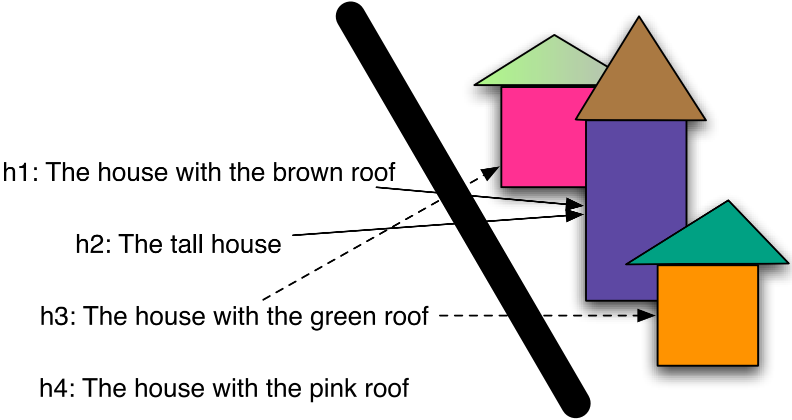
leads to probability over property values

$$\begin{aligned} &P(\langle A, type, ApartmentBuilding\rangle) \\ &\quad = P(\langle A, type, ResidentialBuilding\rangle) \times \\ &\qquad P(\langle A, NumUnits, many\rangle \mid \langle A, type, ResidentialBuilding\rangle) \times \\ &\qquad P(\langle A, Ownership, rental\rangle \mid \langle A, NumUnits, many\rangle , \\ &\qquad\quad \langle A, type, ResidentialBuilding\rangle) \end{aligned}$$

No need to consider undefined propositions.

Outline

Existence and Identity



Clarity Principle

Clarity principle: probabilities must be over well-defined propositions.

- What if an individual doesn't exist?
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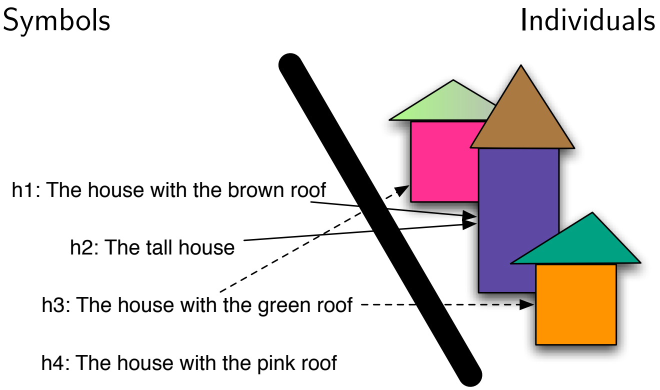
  —In a house with three bedrooms, which is the second bedroom?
- Reified individuals are special:
  — Non-existence means the relation is false.
  — Well defined what doesn't exist when existence is false.
  — Reified individuals with the same description are the same individual.

Correspondence Problem



c symbols and i individuals $\longrightarrow c^{i+1}$ correspondences

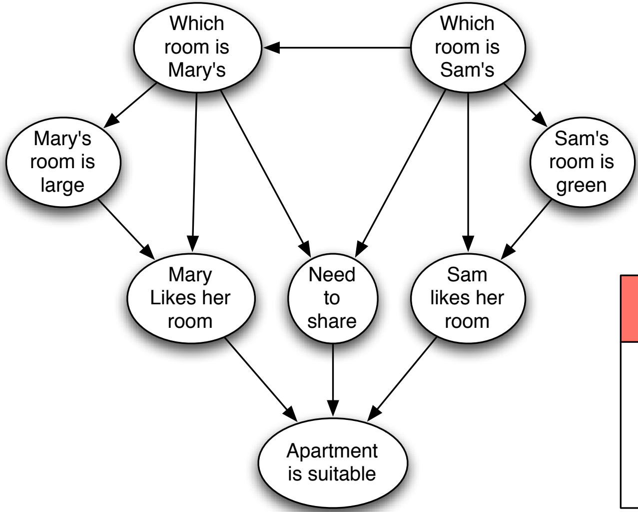
Role assignments

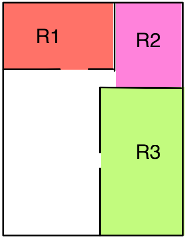
Theory about what apartment Mary would like.

Whether Mary likes an apartment depends on:

- Whether there is a bedroom for daughter Sam
- Whether Sam's room is green
- Whether there is a bedroom for Mary
- Whether Mary's room is large
- Whether they share

Role assignments

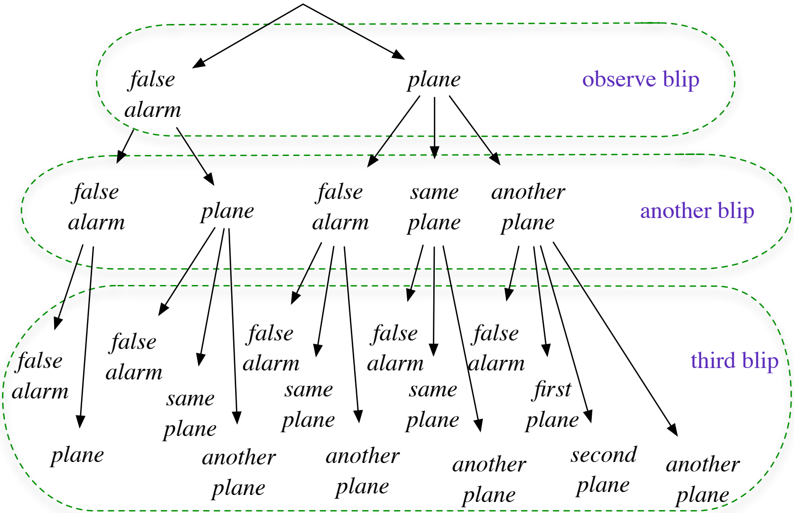




Number and Existence Uncertainty

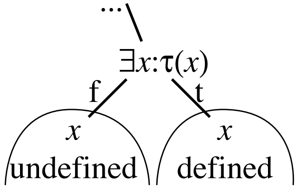
- PRMs (Pfeffer et al.), BLOG (Milch et al.): distribution over the number of individuals. For each number, reason about the correspondence.
- NP-BLOG (Carbonetto et al.): keep asking: is there one more?
  e.g., if you observe a radar blip, there are three hypotheses:
  - the blip was produced by plane you already hypothesized
  - the blip was produced by another plane
  - the blip wasn't produced by a plane

Existence Example



First-order Semantic Trees

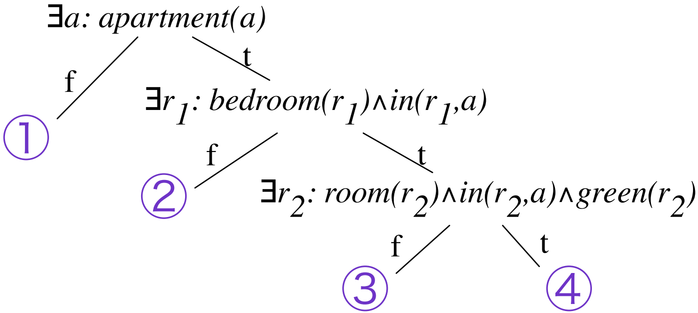
You can split on quantified first-order formulae:



- The "true" sub-tree is in the scope of x
- The "false" sub-tree is not in the scope of x

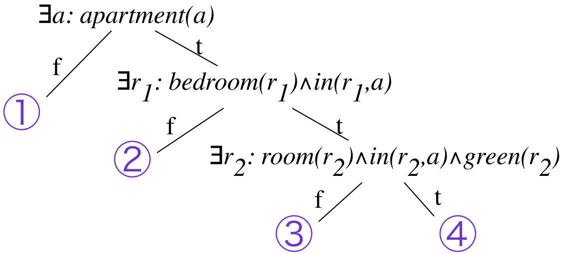
A logical generative model generates a first-order semantic tree.

First-order Semantic Tree (cont)



1. there is no apartment
2. there is no bedroom in the apartment
3. there is a bedroom but no green room
4. there is a bedroom and a green room

First-order Semantic Tree (cont)



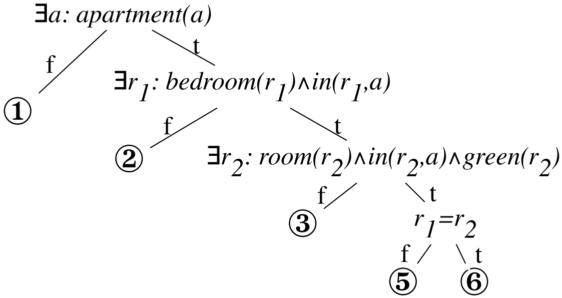
Path formulae:

① $(\neg \exists a\ apt(a))$

② $\exists a\ apt(a) \wedge \neg(\exists a\ apt(a) \wedge \exists r_1\ br(r_1) \wedge in(r_1, a))$

④ $\exists a\ apt(a) \wedge \exists r_1\ br(r_1) \wedge in(r_1, a) \wedge \exists r_2\ room(r_2) \wedge in(r_2, a) \wedge green(r_2)$

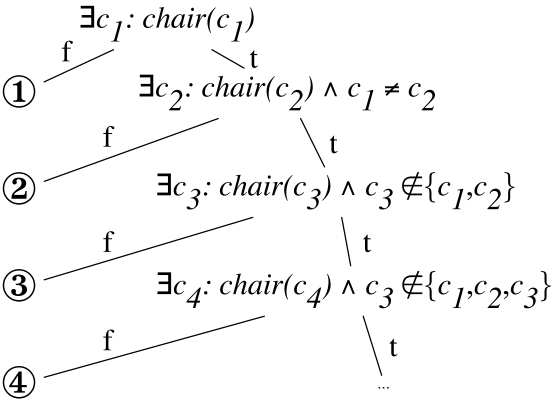
First-order Semantic Tree (cont)



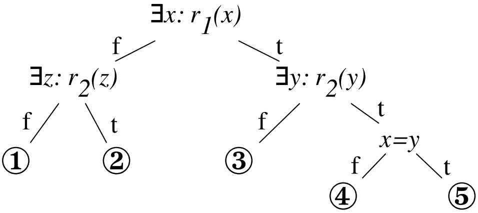
⑥ $\exists a\ apt(a) \land \exists r_1\ br(r_1) \land in(r_1, a) \land \exists r_2\ room(r_2) \land in(r_2, a) \land green(r_2) \land r_1 = r_2$
There is a green bedroom.

⑤ There is a bedroom and a green room, but no green bedroom.

Distributions over number



Roles and Identity (1)



① there no individual filling either role

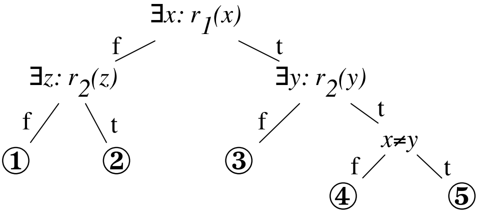
② there is an individual filling role r_2 but none filling r_1

③ there is an individual filling role r_1 but none filling r_2

④ only different individuals fill roles r_1 and r_2

⑤ some individual fills both roles r_1 and r_2

Roles and Identity (2)



① there no individual filling either role

② there is an individual filling role r_2 but none filling r_1

③ there is an individual filling role r_1 but none filling r_2

④ only the same individual fill roles r_1 and r_2

⑤ there are different individuals that fill roles r_1 and r_2

Exchangeability

- First-order semantic trees can represent existence uncertainty, but not how to draw balls out of urns!

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- Consider definition of conditional probability:

$$P(h|e) = \frac{P(h \wedge e)}{P(e)}$$

What if h refers to an individual in e?

Exchangeability

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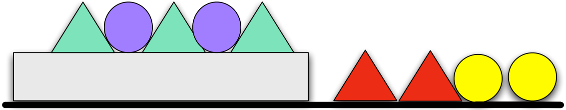
- Consider definition of conditional probability:

$$P(h|e) = \frac{P(h \land e)}{P(e)}$$

  What if h refers to an individual in e?

- Exchangeability: a priori each individual is equally likely to be chosen.

Exchangeability

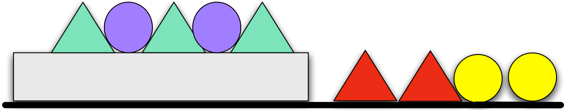


Consider the query:

$$P(green(x) \mid \exists x\ triangle(x) \land \exists y\ circle(y) \land touching(x, y))$$

The answer depends on how the x and y were chosen!

Protocol for Observing



$$P(green(x) \mid \exists x\ triangle(x) \land \exists y\ circle(y) \land touching(x,y))$$

$$\begin{array}{ccc}
| & | & | \\
commit(x) & commit(y) & commit(x,y) \\
| & | & | \\
commit(y) & commit(x) & \\
| & | & \\
3/4 & 2/3 & 4/5
\end{array}$$

Outline

1. Semantic Science Overview
   - Ontologies
   - Data
   - Theories
2. Representing Probabilistic Theories
   - First-order probabilistic models
   - Probabilities with Ontologies
   - Existence and Identity Uncertainty
3. Pragmatics of Real Theories

Expert Models

What if the models are provided by the experts in the field?

- not covering — only provide positive models
- not exclusive — they are often refinements of each other
- described at various levels of abstraction and detail
- often the experts don't know the probabilities and there is little data to estimate them

Providing Probabilities

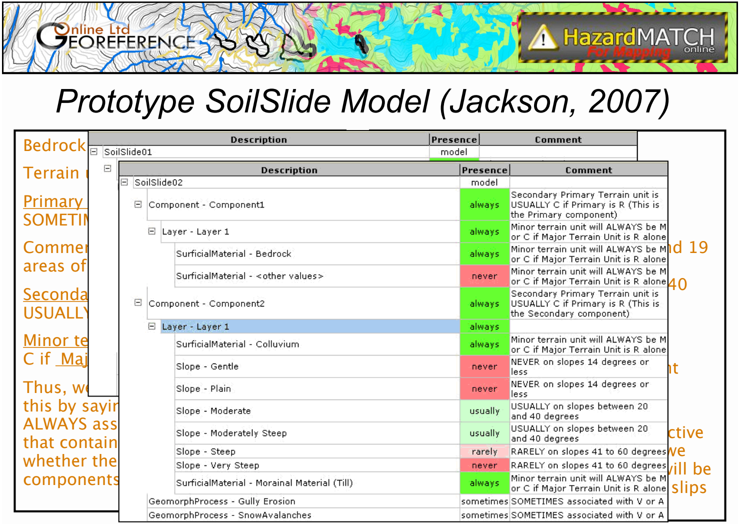
Experts are reluctant to give probabilities:

- No data from which to estimate them
- People who want to make decision use more information than provided in our theories
- Difficult to combine marginal probabilities with new information to make decisions
- It is *not* because decision theory is inappropriate. Decision makers use probabilities and utilities.

What we do

- Use qualitative probabilities: {*always*, *usually*, *sometimes*, *rarely*, *never*}.
- With thousands of instances and hundreds of models, find the most likely and the rationale.
- Independence assumptions.

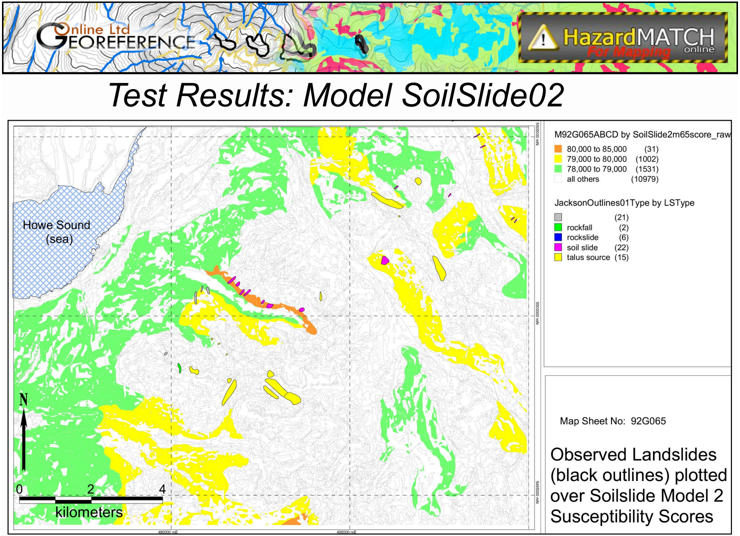
Example Model



Description	Presence	Comment
SoilSlide01	model	

Description	Presence	Comment
SoilSlide02	model	
Component - Component1	always	Secondary Primary Terrain unit is USUALLY C if Primary is R (This is the Primary component)
Layer - Layer 1	always	Minor terrain unit will ALWAYS be M or C if Major Terrain Unit is R alone
SurficialMaterial - Bedrock	always	Minor terrain unit will ALWAYS be M or C if Major Terrain Unit is R alone
SurficialMaterial - <other values>	never	Minor terrain unit will ALWAYS be M or C if Major Terrain Unit is R alone
Component - Component2	always	Secondary Primary Terrain unit is USUALLY C if Primary is R (This is the Secondary component)
Layer - Layer 1	always	
SurficialMaterial - Colluvium	always	Minor terrain unit will ALWAYS be M or C if Major Terrain Unit is R alone
Slope - Gentle	never	NEVER on slopes 14 degrees or less
Slope - Plain	never	NEVER on slopes 14 degrees or less
Slope - Moderate	usually	USUALLY on slopes between 20 and 40 degrees
Slope - Moderately Steep	usually	USUALLY on slopes between 20 and 40 degrees
Slope - Steep	rarely	RARELY on slopes 41 to 60 degrees
Slope - Very Steep	never	RARELY on slopes 41 to 60 degrees
SurficialMaterial - Morainal Material (Till)	always	Minor terrain unit will ALWAYS be M or C if Major Terrain Unit is R alone
GeomorphProcess - Gully Erosion	sometimes	SOMETIMES associated with V or A
GeomorphProcess - SnowAvalanches	sometimes	SOMETIMES associated with V or A

Example Model



Conclusion

- Demand from funders, scientists and users.
- Complementary to Semantic web.
- Representing, reasoning and learning complex probabilistic theories is largely unexplored.
- This may form the basis for a probabilistic mentalese.
- Still lots of work to be done!

To Do

- Fundamental research on complex probabilistic models.
- Build infrastructure to allow publishing and interaction of ontologies, data, theories, theory ensembles, evaluation criteria, meta-data.
- Build inverse semantic science web:
  - Given a theory, find relevant data
  - Given data, find theory ensembles
  - Given a new case, find relevant theory ensembles with explanations
- More complex models, e.g., for relational reinforcement learning where individuals are created and destroyed