Semantic Science: ontologies, data and probabilistic theories

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For when I am presented with a false theorem, I do not need to examine or even to know the demonstration, since I shall discover its falsity a posteriori by means of an easy experiment, that is, by a calculation, costing no more than paper and ink, which will show the error no matter how small it is...

And if someone would doubt my results, I should say to him: "Let us calculate, Sir," and thus by taking to pen and ink, we should soon settle the question.

—Gottfried Wilhelm Leibniz [1677]



Example: medical diagnosis

Example: people give symptoms and want to know what is wrong with them.

Current Practice (Google)	Semantic Science Alternative
— describe symptoms using	
keywords	
— results ranked by popu-	
larity (pagerank) and usually	
appeal to authority	
— text results	

Example: medical diagnosis

Example: people give symptoms and want to know what is wrong with them.

Current Practice (Google)	Semantic Science Alternative
— describe symptoms using	— use ontologies
keywords	
— results ranked by popu-	— predictions ranked by rele-
larity (pagerank) and usually	vance and fit to data
appeal to authority	
— text results	— probabilistic predictions with
	references to sources

Outline

- Semantic Science Overview
 - Ontologies
 - Data
 - Theories
- Representing Probabilistic Theories
 - Feature-based Theories
 - First-order probabilistic models
 - Probabilities with Ontologies
 - Existence and Identity Uncertainty
- Pragmatics of Real Theories

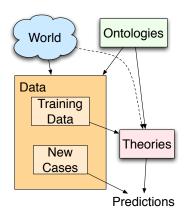


Notational Minefield

- 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.
- All evolve in time.



Al 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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- Expert Systems of the 70's and 80's
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 Bayesian networks, Bayesian X...
 - 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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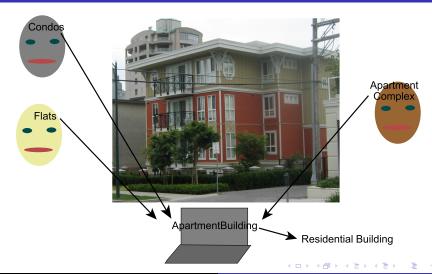


Semantic Science: ontologies, data and probabilistic theories

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



First-order logical languages allow many different ways of representing facts.

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

red(pen₇). It's easy to ask "What's red?"
 Can't ask "what is the color of pen₇?"

First-order logical languages allow many different ways of representing facts.

- red(pen₇). It's easy to ask "What's red?" Can't ask "what is the color of pen₇?"
- color(pen₇, red). It's easy to ask "What's red?"
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 Can't ask "What property of pen₇ has value red?"

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- prop(pen₇, color, red). It's easy to ask all these questions.

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- prop(pen₇, color, red). It's easy to ask all these questions. prop(Individual, Property, Value) is the only relation needed: (Individual, Property, Value) triples, Semantic network, entity relationship model, . . .

Reification

- To represent *scheduled*(*cs*422, 2, 1030, *cc*208). "section 2 of course *cs*422 is scheduled at 10:30 in room *cc*208."
- 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.

```
ApartmentBuilding \equiv ResidentialBuilding \& NumUnits = many \& Ownership = rental
```

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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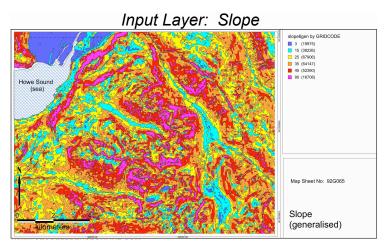


Data

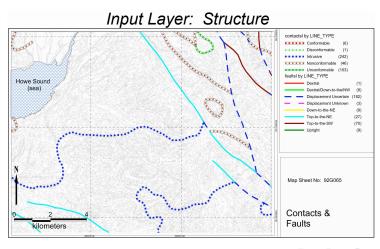
Real data is messy!

- 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



Example Data, Geology



http://www.vsto.org/

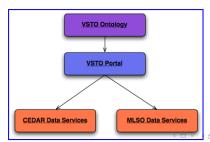
Welcome to the Virtual Solar Terrestrial Observatory

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 (ascil 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.

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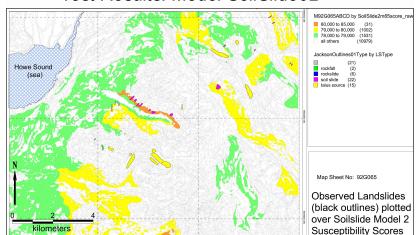
Theories make predictions on data

Hypotheses and theories are procedures that make prediction on data.

- Theories can make various predictions 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)
- We want to input hypotheses and output theories.

Example Prediction from a Theory

Test Results: Model SoilSlide02



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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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?
- 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
 - → other researchers can refer to them
 - → 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

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Levels of Semantic Science

- 0. Deterministic semantic science where all of the theories make definitive predictions.
- 1. Feature-based semantic science, with non-deterministic predictions about feature values of data.
- 2. Relational semantic science, with predictions about the properties of objects and relationships among objects.
- First-order semantic science, with predictions about the existence of objects, universally quantified statements and relations.

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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

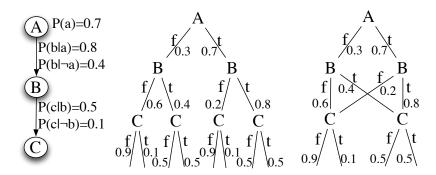
What:

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

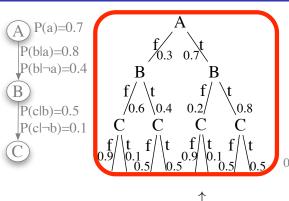
Why:

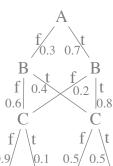
- Often the natural representation: independence represents causal structure
- Probabilities can be understood and learned locally
- We can exploit the structure for efficient inference

Semantic Tree



Semantic Tree





semantic tree event tree decision tree. . .

Semantic tree

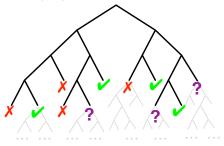
- Nodes are propositions or discrete variables
- Child for each value in domain
- There is a probability distribution over the children of each node
- Each finite path from the root corresponds to a formula
- Each finite path from the root has a probability that is the product of the probabilities in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

A generative model generates a semantic tree.



Infinite Semantic Tree

Given a proposition α :



✓
$$path \models \alpha$$

X $path \models \neg \alpha$
? 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.

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Data

Data is of observations of a world.

Meta-data about observations includes:

- The context in which the data was collected.
- The features that this data makes predictions about (the dependent variables).
- The features that were controlled for in the data (the independent variables).

Theories

A theory makes predictions about some feature values. A theory includes:

- A context in which specifies when it can be applied.
- A set of input features about which it does not make predictions.
- A set of output features to predict (as a function of the input features).

Example

Consider the following theories:

- T_1 predicts the prognosis of people with lung cancer.
- T₂ predicts the prognosis of people with cancer.
- T₃ is the null hypothesis that predicts the prognosis of people in general.
- T₄ predicts (probabilistically) whether people with cancer have lung cancer, as a function of coughing.
- \bullet T_5 predicts (probabilistically) whether people have cancer.

What should be used to predict the prognosis of a patient with observed symptoms?



Theory Ensembles

To make a prediction, multiple theories need to be used together—theory ensemble.

A theory ensemble T needs to satisfy the following properties:

- T is coherent: it does not rely on the value of a feature in a context where the features is not defined
- T is consistent: it does not make different predictions for any feature in any context.
- T is predictive: it makes a prediction in every context that is possible.
- T is minimal.



Prototype Feature-based Ensemble

- An (oversimplified) definition of theory ensembles is a set of $\langle c, t \rangle$ pairs, where t is a theory and c is a proposition.
- Pair $\langle c, t \rangle$ means theory t is used to predict in context c.

Example

- T₁ predicts the prognosis of people with lung cancer.
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A possible theory ensemble is:

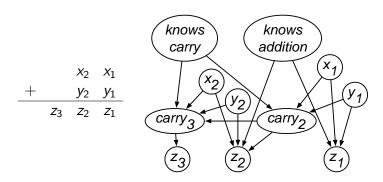
```
\{\langle person, T_5 \rangle, \langle \neg has\_cancer, T_3 \rangle, \langle has\_cancer, T_4 \rangle, \langle has\_lung\_cancer, T_1 \rangle, \langle has\_cancer \wedge \neg has\_lung\_cancer, T_2 \rangle\}
```

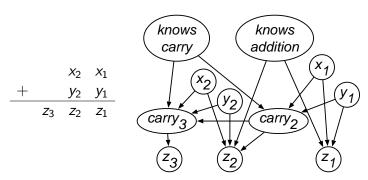


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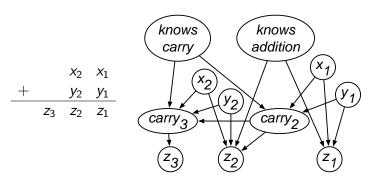
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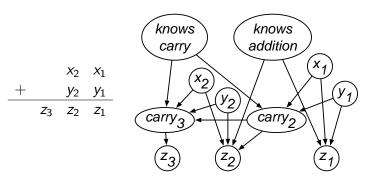




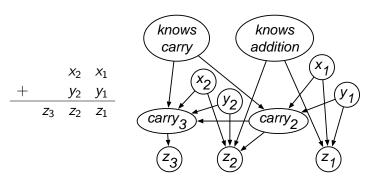
What if there were multiple digits



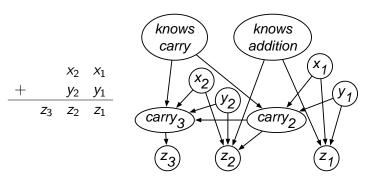
What if there were multiple digits, problems



What if there were multiple digits, problems, students

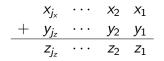


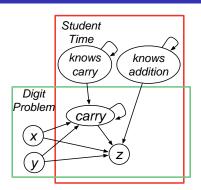
What if there were multiple digits, problems, students, times?



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

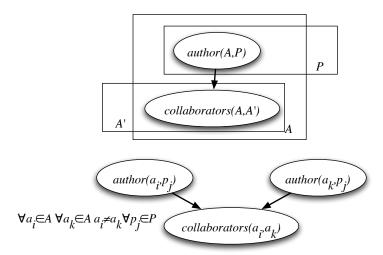
Multi-digit addition with parametrized BNs / plates





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 → probabilistic Horn abduction (IJCAI-91); richer language (negation as failure + choices by other agents → independent choice logic (AIJ 1997).

Independent Choice Logic

- An alternative is a set of atomic formula.
 C, the choice space is a set of disjoint alternatives.
- 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

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

$$F = \{f \leftarrow c_1 \land b_1, f \leftarrow c_3 \land b_2, d \leftarrow c_1, d \leftarrow \neg c_2 \land b_1, e \leftarrow f, e \leftarrow \neg d\}\$$

$$P_0(c_1) = 0.5 P_0(c_2) = 0.3 P_0(c_3) = 0.2$$

$$P_0(b_1) = 0.9 P_0(b_2) = 0.1$$

Semantics of ICL

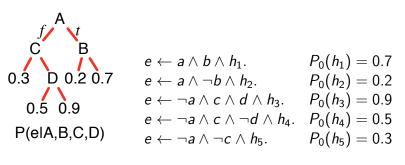
Probabilities are defined by a (possible infinite) semantic tree:

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

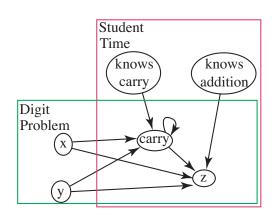
Meaningless Example: Semantics

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:



Example: Multi-digit addition



ICL rules for multi-digit addition

$$z(D, P, S, T) = V \leftarrow z(x(D, P) = Vx \land y(D, P) = Vy \land z(T, P) = Vx \land z(T, P) = Vx \land z(T, P) \land z($$

$$z(D, P, S, T) = V \leftarrow knowsAddition(S, T) \land mistake(D, P, S, T) \land selectDig(D, P, S, T) = V.$$

 $z(D, P, S, T) = V \leftarrow \neg knowsAddition(S, T) \land selectDig(D, P, S, T) = V.$

Alternatives:

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



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Feature-based Theories First-order probabilistic models Probabilities with Ontologies Existence and Identity Uncertainty

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 (individual, property) pair, where the domain of the random variable is the range of the property.
- For non-functional properties:
 Boolean random variable for each \(\ind \text{individual}, \text{property}, \text{value}\) triple.



Triples and Probabilities

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

```
 \left\langle z543, type, AdditionZValue \right\rangle \\ \left\langle z543, digit, 3 \right\rangle \\ \left\langle z543, problem, prob23 \right\rangle \\ \left\langle z543, student, fred \right\rangle \\ \left\langle z543, time, t3 \right\rangle \\ \left\langle z543, valueWithProb, 4, 0.43 \right\rangle \\ \left\langle z543, valueWithProb, 5, 0.03 \right\rangle \\ \vdots \\ \left\langle defines distribution \right\rangle
```

Probabilities and Aristotelian Definitions

```
Aristotelian definition
```

```
ApartmentBuilding \equiv ResidentialBuilding \& NumUnits = many \& Ownership = rental
```

leads to probability over property values

```
P(\langle A, type, ApartmentBuilding \rangle)
= P(\langle A, type, ResidentialBuilding \rangle) \times
P(\langle A, NumUnits, many \rangle | \langle A, type, ResidentialBuilding \rangle) \times
P(\langle A, Ownership, rental \rangle | \langle A, NumUnits, many \rangle,
\langle A, type, ResidentialBuilding \rangle)
```

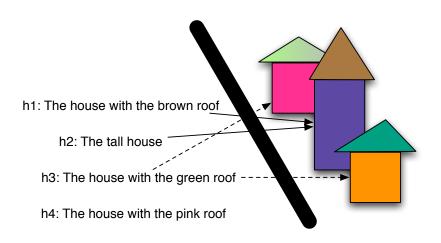
No need to consider undefined propositions.

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Existence and Identity



Clarity Principle

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

- What if an individual doesn't exist?
 - $house(h4) \land roof_colour(h4, pink) \land \neg exists(h4)$

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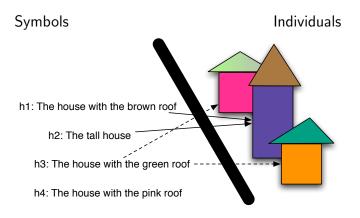
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 - —In a house with three bedrooms, which is the second bedroom?

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- What if more than one individual exists? Which one are we referring to?
 - —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

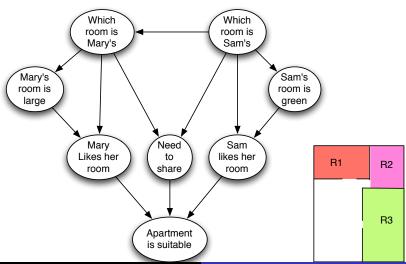
Theory about what apartment Mary would like.

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

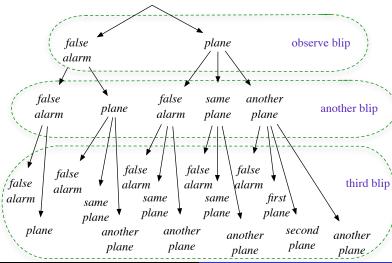


Number and Existence Uncertainty

- 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

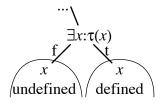


Existence Example



First-order Semantic Trees

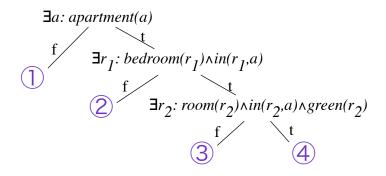
You can split on quantified first-order formulae:



- 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)

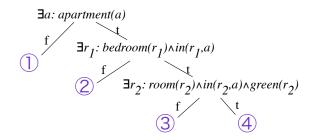


- 1 there is no apartment
- there is no bedroom in the apartment
- ③ there is a bedroom but no green room

David Poole

4) there is a hedroom and a green room () () () () () () ()

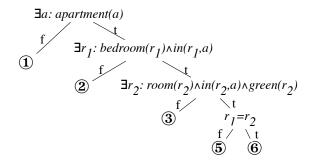
First-order Semantic Tree (cont)



Path formulae:

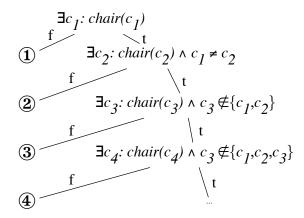
- ① $(\neg \exists a \ apt(a))$
- ② $\exists a \ apt(a) \land \neg(\exists a \ apt(a) \land \exists r_1 \ br(r_1) \land in(r_1, a))$
- $\exists a \ apt(a) \land \exists r_1 \ br(r_1) \land in(r_1, a) \land \exists r_2 \ room(r_2) \land in(r_2, a) \land green(r_2)$

First-order Semantic Tree (cont)

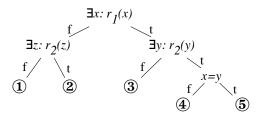


- ⑥ $\exists a \; apt(a) \land \exists r_1 \; br(r_1) \land in(r_1, a) \land \exists r_2 \; room(r_2) \land in(r_2, a) \land green(r_2) \land r_1 = r_2$ There is a green bedroom.
- (5) There is a bedroom and a green room, but no green bedroom.

Distributions over number

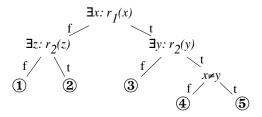


Roles and Identity (1)



- 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
- \bigcirc 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
- \circ there are different individuals that fill roles r_1 and r_2

Feature-based Theories First-order probabilistic models Probabilities with Ontologies Existence and Identity Uncertainty

Exchangeability

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

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

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Exchangeability

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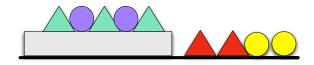
$$P(h|e) = \frac{P(h \wedge e)}{P(e)}$$

What if *h* refers to an individual in *e*?

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

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Exchangeability



Consider the query:

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

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



Protocol for Observing

P(green(x))



Outline

- Semantic Science Overview
 - Ontologies
 - Data
 - Theories
- 2 Representing Probabilistic Theories
 - Feature-based Theories
 - First-order probabilistic models
 - Probabilities with Ontologies
 - Existence and Identity Uncertainty
- 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:

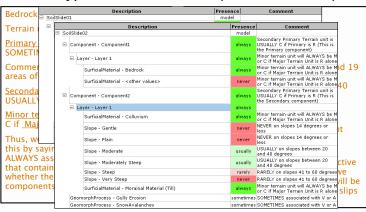
- No data from which to estimate them
- People who want to make decision use more information than provided in our theories
- Difficult to combine marginal probabilities with new information to make decisions
- It is not because decision theory is inappropriate. Decision makers use probabilities and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

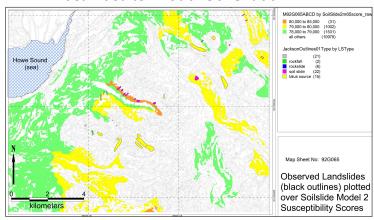
Example Model

Prototype SoilSlide Model (Jackson, 2007)



Example Model

Test Results: Model SoilSlide02



Conclusion

- Semantic science is a way to develop and deploy knowledge about how the world works.
- Scientists (and others) develop theories that refer to standardized ontologies and predict for new cases.
- Multiple theories—forming theory ensembles—are needed to make predictions in particular cases.
- For each prediction, we want to be able to ask, what theories it is based on.
- For each theory, we want to be able to ask what evidence it is based on.
- This talk is deliberately pre-theoretic. Many formalisms will be developed and discarded before we converge on useful representations.

To Do

- Theories of combining theories.
- Representing, reasoning and learning complex (probabilistic) theories.
- 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 that make predictions on the data
 - 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