Probabilistic reasoning with complex heterogeneous observations and applications in geology and medicine

David Poole

Department of Computer Science,
University of British Columbia

Work with: `http://georeferenceonline.com/`, `https://treatment.com/`

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Outline

1. Motivation
   - Ontologies
   - Data
   - Hypotheses
2. Semantic Science
3. Models: Ensembles of hypotheses
4. Property Domains and Undefined Random Variables

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- Consider predicting the effect of a treatment on a particular patient in a GP's office. Information is:
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- Consider predicting whether a particular person will like a particular apartment

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- Wouldn't it be better to have the research published in machine readable form?

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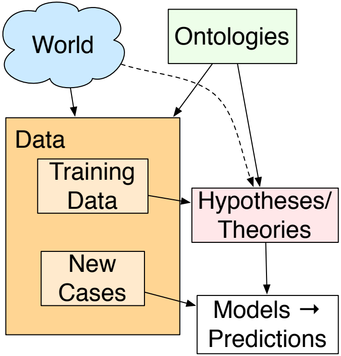
- Geological "observations" are published by the geological surveys of counties and states/provinces and globally (onegeology.org)
- Geological hypotheses are published in research journals.
- We built systems for mineral exploration and landslide prediction, represented the hypotheses of hundreds of research papers, and matched them on thousands of descriptions of interesting places

[Work with Clinton Smyth, Georeference Online]

OneGeology.org

OneGeology.org

Semantic Science



- Ontologies represent the meaning of symbols.
- Observational data describes world using symbols defined in ontology.
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- Data used to evaluate hypotheses.
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- All evolve in time.

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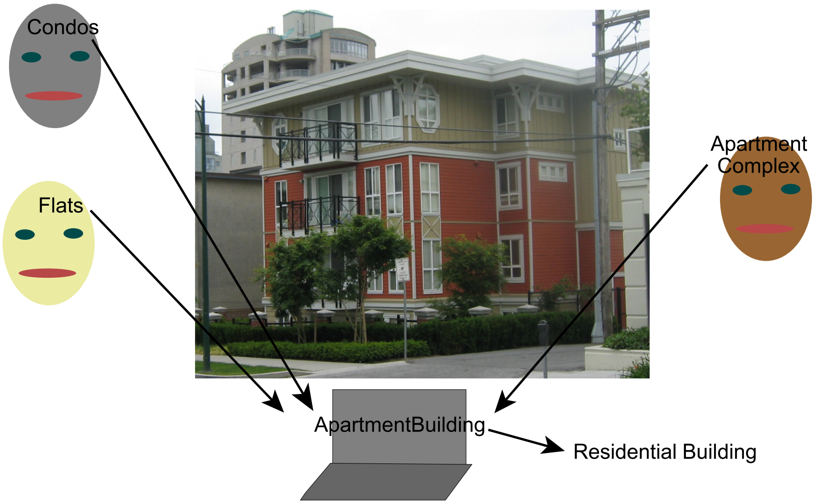
- Our geology ontology has 6022 minerals + 266 rocks in a "simplified" rock taxonomy + time + ...

Ontologies


Condos
Flats
Apartment Complex
ApartmentBuilding
Residential Building

Main Components of an Ontology

- Individuals: the objects in the world
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$\langle Individual, Property, Value\rangle$ triples are universal representations of relations.

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**.

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

  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 are defined in terms of properties.

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  - What was the protocol used to collect the data? (Chosen at random or chosen because interesting?)
  - What were the controls — what was manipulated, when?
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- Errors, forgeries, . . .

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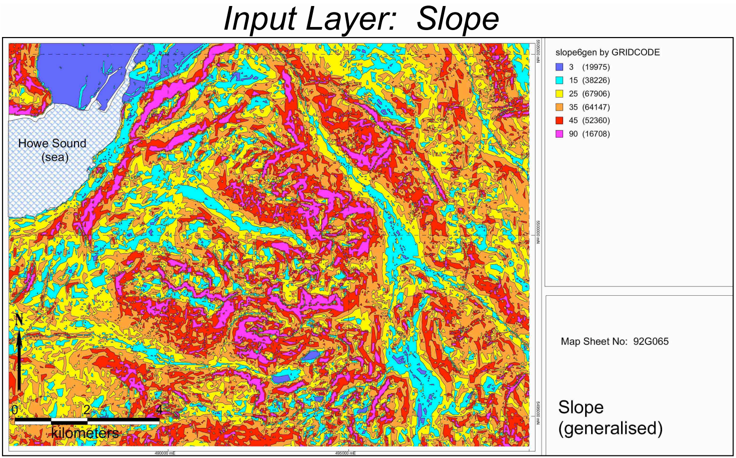

[Clinton Smyth, Georeference Online.]

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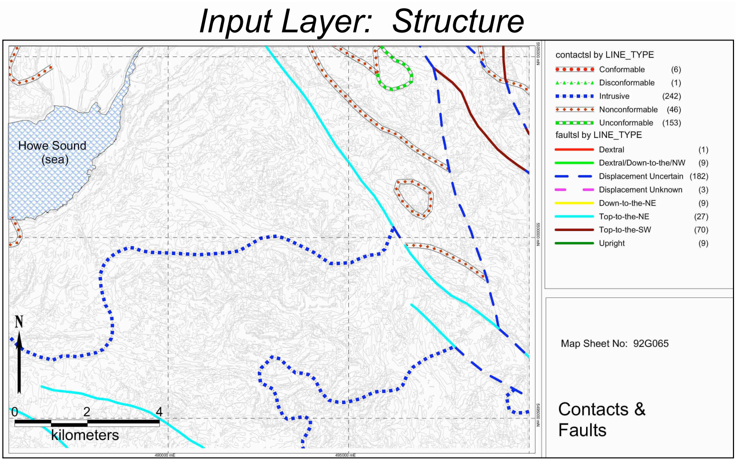

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- Data can't make distinctions that can't be expressed in the ontology.
- Different ontologies result in different data.

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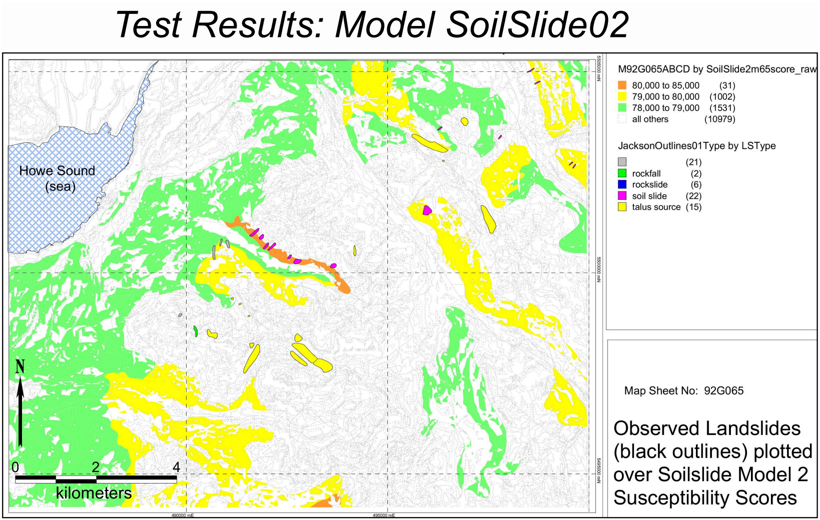
Hypotheses make predictions on data

- Hypotheses are programs that make predictions on data.
- To be useful for decision making, predictions should be probabilistic.
  $\longrightarrow$ probabilistic programs

Example Prediction from a Hypothesis



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  random variable for each $\langle \mathit{individual}, \mathit{property} \rangle$ pair,
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- For **non-functional properties**:
  Boolean RV for each $\langle \mathit{individual}, \mathit{property}, \mathit{value} \rangle$ triple.
  E.g., if *YearRestored* is non-functional
  $\langle \mathit{building}17, \mathit{YearRestored}, 1988 \rangle$ is a Boolean RV.

Ranges

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Datatype	Boolean, Real, Integer, String, DateTime...	Boolean, Real, Integer, String, DateTime...

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ObjectProperty		$\begin{cases}\text{Discrete / Multinomial}\\ \text{Relational}\end{cases}$

E.g., consider the ranges:

- {very_tall, tall, medium, short}
- {10 High St, 22 Smith St, 57 Jericho Ave}

Probabilities and Aristotelian Definitions

Aristotelian definition

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

leads to probability over class membership

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

(Conjunction here is not commutative — like $x \neq 0 \& y/x = z$)

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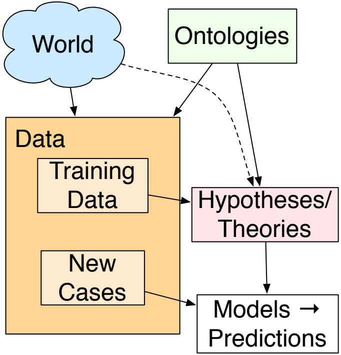
Semantic Science

- Governments are publishing data with rich ontologies. Journals are forcing authors to publish data.
- Idea: also publish hypotheses that make (probabilistic) predictions

Semantic Science



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Semantic Science Search Engine

Semantic Science Search Engine:

- Given a hypothesis, find data about which it makes predictions.
- Given a dataset, find hypotheses which make predictions on the dataset
- Given a new problem, find the best model (ensemble of hypotheses)

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- Ontologies can be judged by the predictions of the hypotheses that use them
  — role of a vocabulary is to describe useful distinctions.

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  $\longrightarrow$ all zero probabilities come from definitions.
  Ontologies give definitions — data that is inconsistent is rejected.
  Clarity principle. Clear definitions are useful!

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- How can we get there?
  Start in very narrow domains
  Few hypotheses, published data....
- Users should be able to express data and hypotheses in their own terms. They shouldn't have to be an expert in domain and statistics and (probabilistic) programming....
  They must see a value in representing data / hypotheses.

Outline

Hypotheses, Models and Predictions

- Hypotheses are often very narrow.
- We need to use many hypotheses to make a prediction.
- Hypotheses differ in
  - level of generality (high-level/low level)
    e.g., mammal vs poodle
  - level of detail (parts/subparts)
    e.g., mammal vs left eye

Applying hypotheses to new cases

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- What about C: *if lung cancer, use B's prediction, else use A's prediction*?
- A model is a set of hypotheses applied to a particular case. "ensemble"
  - Judge hypotheses by how well they fit into models.
  - Models can be judged by simplicity.
  - Hypothesis designers don't need to game the system by manipulating the generality of hypotheses

Programs and Meta-programs

Two sorts of probabilistic programs:

- Hypotheses are probabilistic programs that persist, are tuned to data. Often very narrow.
- Models are probabilistic programs that are adapted to particular cases. Transient. Use hypotheses as subroutines.

Science versus application.
Always ask: "Why should we believe this prediction?"

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Properties, Domains and Undefined Random Variables

- Properties have domains.
- A property is only defined for individuals in its domain.
- A property is almost always undefined:
  - *weight* is only defined for physical objects
  - *pitch* is only defined for sounds
  - *wavelength* is only defined for waves
  - *originality* is only defined for creative outputs
  - *hardness* (measured in Mohs scale) is only defined for minerals
  - *number_bedrooms* is only defined for buildings
- A dataset would not contain a triple with an undefined property

Domains and Undefined Random Variables (Example)

Example (Ontology)

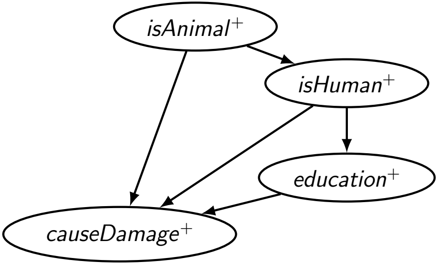
```
Classes:
  Thing
    Animal: Thing and isAnimal = true
      Human: Animal and isHuman = true

Properties:
  isAnimal:    domain: Thing   range: {true,false}
  isHuman:     domain: Animal  range: {true,false}
  education:   domain: Human   range: {low,high}
  causeDamage: domain: Thing   range: {true,false}
```

education is not defined when $isHuman = false$.

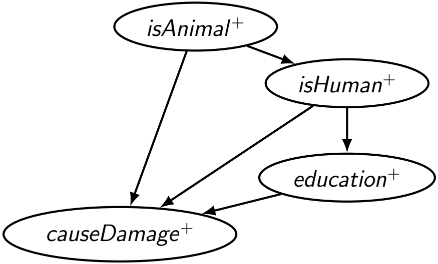
Extended Belief Networks (EBNs)

- Add "undefined" ($\perp$) to each range.
  - $range(isHuman^+) = \{true, false, \perp\}$.
  - $range(education^+) = \{low, high, \perp\}$.



- $education^+$ is like *education* but with an expanded range.
- Possible query: $P(education^+ \mid causeDamage^+ = true)$

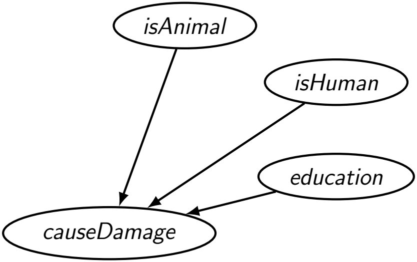
Extended Belief Networks (EBNs)



However...

- Expanding ranges is computationally expensive.
  - Exact inference has time complexity $\mathcal{O}(|range|^{treewidth})$.
- It may not be sensible to think about undefined values; no dataset would contain such values.
- Arcs $\langle isAnimal^+, isHuman^+\rangle$ and $\langle isHuman^+, education^+\rangle$ represent logical constraints

Ontologically-Based Belief Networks (OBBNs)



- OBBNs decouple the logical constraints (from the ontology) from the probabilistic dependencies.
- Don't model undefined ($\perp$) in ranges.
- The probabilistic network does not contain any ontological information.

Conditional Probabilities

isAmimal

true / \ *false*

isHuman (0.1, 0.9)

true / \ *false*

education (0.3, 0.7)

high / \ *low*

(0.9, 0.1) (0.5, 0.5)

$$P(causeDamage \mid isAnimal, isHuman, education)$$

- For each random variable, only specify (conditional) probabilities for well-defined contexts.

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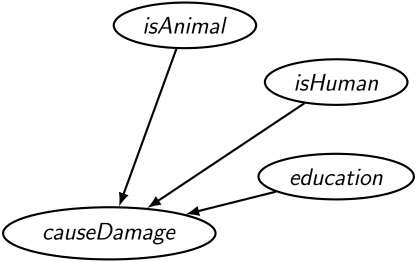

- The query $P(education^{+} \mid causeDamage = true)$ has a non-zero probability of $\perp$
  — we can't ignore the undefined values.

Ontologically-Based Belief Networks (Inference)

The following give the same answer for $P(Q^+ \mid \mathcal{E} = e)$:

- Compute $P(Q^+ \mid \mathcal{E}^+ = e)$ using the extended belief network.
- From the OGBN:
  - Query the ontology for $domain(Q)$
  - Let $\alpha = P(domain(Q) \mid \mathcal{E} = e)$
  - If $\alpha \neq 0$ let $\beta = P(Q \mid \mathcal{E} = e \wedge domain(Q))$
  - Return

$$P(Q^+ = \perp \mid \mathcal{E} = e) = 1 - \alpha$$
$$P(Q \mid \mathcal{E} = e) = \alpha\beta$$

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    - Scientists (and others) develop hypotheses that refer to standardized ontologies and predict for new cases.
    - Multiple hypotheses — forming models — are needed to make predictions in particular cases.
    - For each prediction, we can ask what hypotheses it is based on.
    - For each hypothesis, we can ask about the evidence on which it can be evaluated.

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  - Scientists (and others) develop hypotheses that refer to standardized ontologies and predict for new cases.
  - Multiple hypotheses — forming models — are needed to make predictions in particular cases.
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  - For each hypothesis, we can ask about the evidence on which it can be evaluated.
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- Ontologies, hypotheses and observations interact in complex ways.
- Many formalisms will be developed and discarded before we converge on useful representations.

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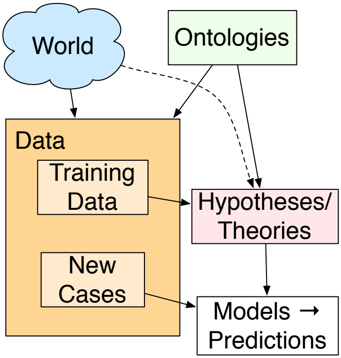
- Representations for observations that interacts with hypotheses.
- Build infrastructure to allow publishing and interaction of ontologies, data, hypotheses, models, evaluation criteria, meta-data.
- Build inverse semantic science web:
  - Given a hypothesis, find relevant data
  - Given data, find hypotheses that make predictions on the data
  - Given a new case, find relevant models with explanations

Semantic Science



- Ontologies represent the meaning of symbols.
- Observational data is published.
- Hypotheses make predictions on data.
- Data used to evaluate hypotheses.
- Hypotheses used for predictions on new cases.
- All evolve in time.