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

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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
Motivation

Consider predicting the effect of a treatment on a particular patient in a GP’s office. Information is:

- heterogenous, provided from many sources at multiple points in time. E.g., from patient reports, nurse observation, doctor observation, lab tests, x-rays, . . .
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- Consider predicting whether a particular person will like a particular apartment
Example: Medicine

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- Can we do better than: data $\rightarrow$ hypotheses $\rightarrow$ research papers $\rightarrow$ (mis)reading $\rightarrow$ clinical practice?
- Wouldn’t it be better to have the research published in machine readable form?
Example: Geology

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- 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]
**Welcome to OneGeology**

OneGeology is an international initiative of the geological surveys of the world. This ground-breaking project was launched in 2007 and contributed to the 'International Year of Planet Earth', becoming one of their flagship projects.

Thanks to the enthusiasm and support of participating nations, the initiative has progressed rapidly towards its target - creating [dynamic geological map data of the world](#), available to everyone via the web. We invite you to explore the website and view the maps in the OneGeology Portal.

Fill in our [online form](#) to be kept informed of the OneGeology initiative progress and receive our regular newsletters.

Read our latest newsletter
Ontologies represent the meaning of symbols.

Observational data describes the world using symbols defined in ontology.

Hypotheses make predictions on data.

Data used to evaluate hypotheses.

Hypotheses used for predictions on new cases.

All evolve in time.
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In CS, an **ontology** is a (formal) specification of the meaning of the vocabulary used in an information system.

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

Motivation Semantic Science Models Domains Ontologies Data Hypotheses

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Probabilistic reasoning with complex heterogeneous observations
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
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\[ \langle \text{Individual}, \text{Property}, \text{Value} \rangle \] 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**.

  \[
  \text{ApartmentBuilding} \equiv \text{ResidentialBuilding} \& \\
  \text{NumUnits} = \text{many} \& \\
  \text{Ownership} = \text{rental}
  \]

  \text{NumUnits} is a property with domain \text{ResidentialBuilding} and range \{one, two, many\}

  \text{Ownership} is a property with domain \text{Building} and range \{owned, rental, coop\}.

- All classes are defined in terms of properties.
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- Multiple levels of detail
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- 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?
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- Errors, forgeries, …
Example Data, Geology

Input Layer: Slope

Howe Sound (sea)

[Clinton Smyth, Georeference Online.]
Example Data, Geology

**Input Layer: Structure**

[Map showing geologic contacts and faults with legend]

Map Sheet No: 92G065

Contacts & Faults

[Clinton Smyth, Georeference Online.]
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!)
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- 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.
  - → probabilistic programs
Example Prediction from a Hypothesis

**Test Results: Model SoilSlide02**

M92G065ABCD by SoilSlide2m65score_raw
- 80,000 to 85,000 (31)
- 79,000 to 80,000 (1002)
- 78,000 to 79,000 (1531)
- All others (10679)

JacksonOutlines01Type by LSType
- (21)
- Rockfall: (2)
- Rockslide: (6)
- Soil slide: (22)
- Talus source: (15)

Map Sheet No: 92G065

Observed Landslides (black outlines) plotted over Soilslide Model 2 Susceptibility Scores

[Clinton Smyth, Georeference Online.]
Random Variables and Triples

- Reconcile:
  - random variables (RVs) of probability theory
  - individuals, classes, properties of modern ontologies
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  $\langle x, R, y_1 \rangle$ and $\langle x, R, y_2 \rangle$ implies $y_1 = y_2$. 
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- For **non-functional properties**: 
  random variable for each $\langle individual, property \rangle$ pair,
  range of the RV is range of the property.
  E.g., if $Height$ is functional, $\langle building17, Height \rangle$ is a RV.
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- For **non-functional properties**:
  Boolean RV for each $\langle$individual, property, value$\rangle$ triple.
  E.g., if $YearRestored$ is non-functional
  $\langle building 17, YearRestored, 1988 \rangle$ is a Boolean RV.
# Ranges

<table>
<thead>
<tr>
<th>Datatype</th>
<th>OWL</th>
<th>Probability</th>
</tr>
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<tbody>
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ObjectProperty

- Discrete / Multinomial
- Relational

E.g., consider the ranges:

- \{very\_tall, tall, medium, short\}
- \{10 High St, 22 Smith St, 57 Jericho Ave\}
Aristotelian definition

\[
\text{ApartmentBuilding} \equiv \text{ResidentialBuilding} \& \\
\text{NumUnits} = \text{many} \& \\
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\]

leads to probability over class membership

\[
P(\langle A, \text{type}, \text{ApartmentBuilding} \rangle) \\
= P(\langle A, \text{type}, \text{ResidentialBuilding} \rangle) \times \\
\times P(\langle A, \text{NumUnits} \rangle = \text{many} \mid \langle A, \text{type}, \text{ResidentialBuilding} \rangle) \\
\times P(\langle A, \text{Ownership}, \text{rental} \rangle \mid \langle A, \text{NumUnits} \rangle = \text{many}, \\
\langle A, \text{type}, \text{ResidentialBuilding} \rangle)
\]

(Conjunction here is not commutative — like \(x \neq 0 \& y/x = z\))
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Governments are publishing data with rich ontologies. Journals are forcing authors to publish data.

Idea: also publish hypotheses that make (probabilistic) predictions
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.
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).
Dynamics of Semantic Science

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  - People vote with their feet what ontology they use.
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  A hypothesis invents useful distinctions (latent features)
  \[\rightarrow\] add these to an ontology
  \[\rightarrow\] other researchers can refer to them
  \[\rightarrow\] reinterpretation of data
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  A hypothesis invents useful distinctions (latent features)
  → add these to an ontology
  → other researchers can refer to them
  → reinterpretation of data
- Ontologies can be judged by the predictions of the hypotheses that use them
  — role of a vocabulary is to describe useful distinctions.
Zero Probabilities

What do the following have in common?

- Ozone hole over Antarctica (1976-1985)
- Robot kidnap problem
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  → don’t use zero probabilities for anything possible.
- International Astronomical Union (IAU) in 2006 defined “planet” so Pluto is not a planet.
- Is there a dataset that says “Justin is an Mammal”, “Justin is an animal” or “Justin is a holozoa”?
- What about “Justin is person but not an animal”?
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  \[\rightarrow\] all zero probabilities come from definitions.
  Ontologies give definitions — data that is inconsistent is rejected.
  Clarity principle. Clear definitions are useful!
More issues

- How can we stop people from publishing fictional data?
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- How can we get there?
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  Few hypotheses, published data....
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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.
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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

- How can we compare hypotheses that differ in their generality?

- Hypothesis $A$ makes predictions about all cancers. Hypothesis $B$ makes predictions about lung cancers. Should the comparison between $A$ and $B$ take into account $A$’s predictions on non-lung cancer?
Applying hypotheses to new cases

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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.
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” (⊥) to each range.
  - \( \text{range}(\text{isHuman}^+) = \{ \text{true}, \text{false}, \bot \} \).
  - \( \text{range}(\text{education}^+) = \{ \text{low}, \text{high}, \bot \} \).

- \( \text{education}^+ \) is like \( \text{education} \) but with an expanded range.

- Possible query: \( P(\text{education}^+ | \text{causeDamage}^+ = \text{true}) \)
Extended Belief Networks (EBNs)

However...

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

- OBBNs decouple the logical constraints (from the ontology) from the probabilistic dependencies.
- Don’t model undefined (⊥) in ranges.
- The probabilistic network does not contain any ontological information.
For each random variable, only specify (conditional) probabilities for well-defined contexts.
The query $P(education^+ | causeDamage = true)$ has a non-zero probability of $\perp$ — we can’t ignore the undefined values.
The following give the same answer for $P(Q^+ | \mathcal{E} = e)$:

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

$$P(Q^+ = \bot | \mathcal{E} = e) = 1 - \alpha$$
$$P(Q | \mathcal{E} = e) = \alpha \beta$$
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Conclusion

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  - 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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- Ontologies, hypotheses and observations interact in complex ways.
- Many formalisms will be developed and discarded before we converge on useful representations.
To Do

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- Representing, reasoning and learning complex (probabilistic) hypotheses. “probabilistic programming”
- Representations for observations that interacts with hypotheses.
- Build infrastructure to allow publishing and interaction of ontologies, data, hypotheses, models, evaluation criteria, meta-data.
To Do

- Representing, reasoning and learning complex (probabilistic) hypotheses. “probabilistic programming”
- 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
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.