Interoperability of probabilistic programs and data (probabilistic programs for representing scientific hypotheses)

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Research Agendas

- PubMed comprises over 24 million citations for biomedical literature. 10,000 added each week.
- IBM's Watson (and others) propose to read the literature to provide "evidence-based" advice for specific patients.
- Can we do better than data $\longrightarrow$ hypotheses $\longrightarrow$ research papers $\longrightarrow$ (mis)reading $\longrightarrow$ clinical practice?
- Wouldn't it be better to have the research published in machine readable form?

Example: Geology

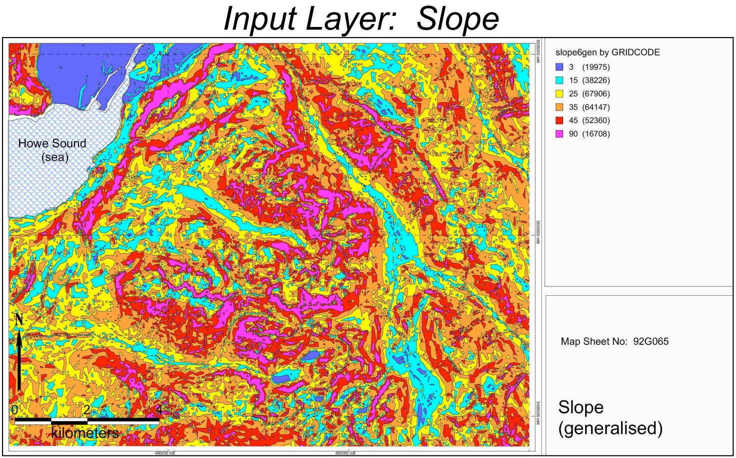
- Geologists know they need to make decisions under uncertainty
- Geologists know they need ontologies
- Geological "observations" are published by the geological surveys of counties and states/provinces and globally (onegeology.org)
- Geological hypotheses are published in research journals.
- We represented the hypotheses of hundreds of research papers, and matched them on thousands of descriptions of interesting places

[Research with Clinton Smyth, Georeference Online]

OneGeology.org

OneGeology.org

Example Data, Geology



[Clinton Smyth, Georeference Online.]

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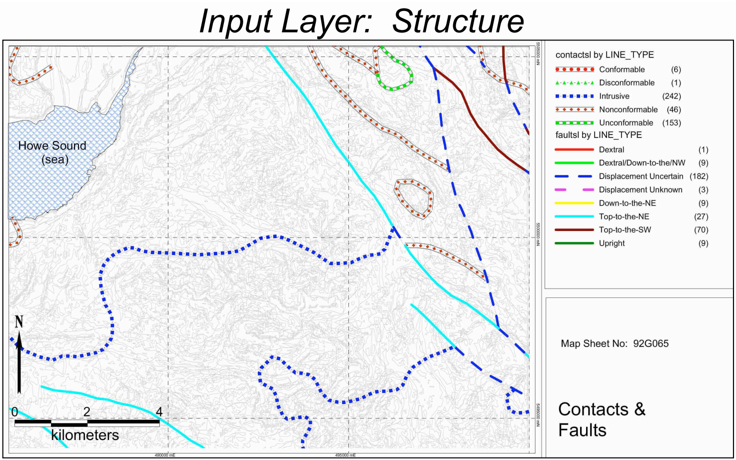

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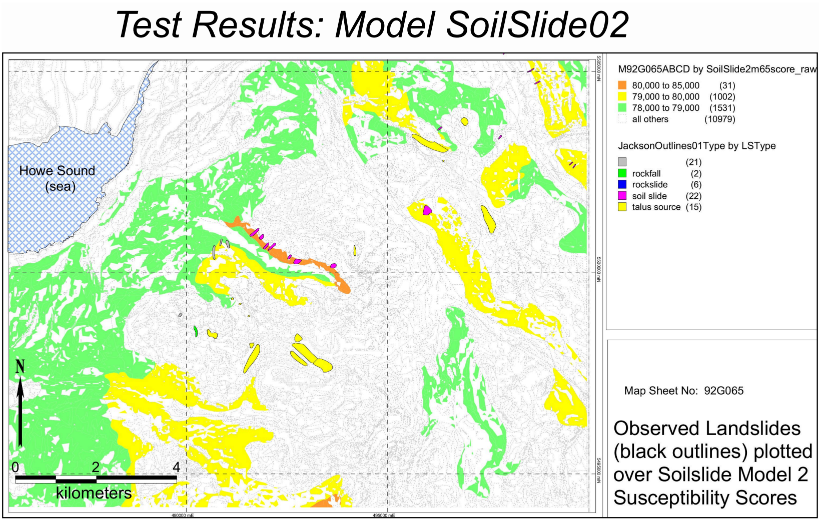
Example Prediction from a Hypothesis



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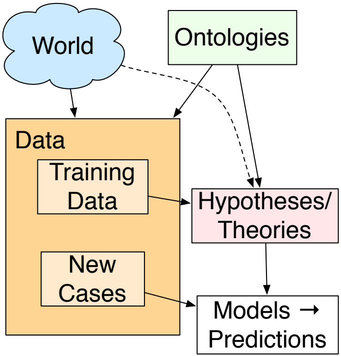
Outline

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

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.

Science as the foundation of world-wide mind

Observations and hypotheses can be about anything:

- 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
- which celebrities are having affairs

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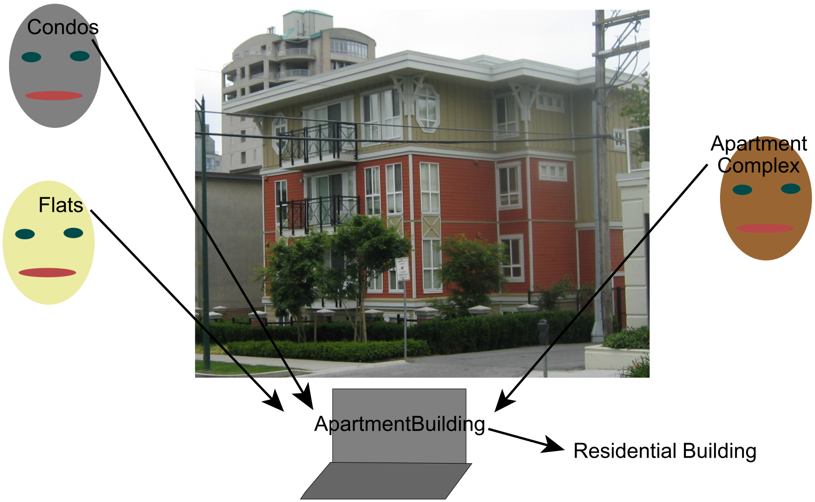
Ontologies

- 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

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

$\langle \mathit{Individual}, \mathit{Property}, \mathit{Value} \rangle$ 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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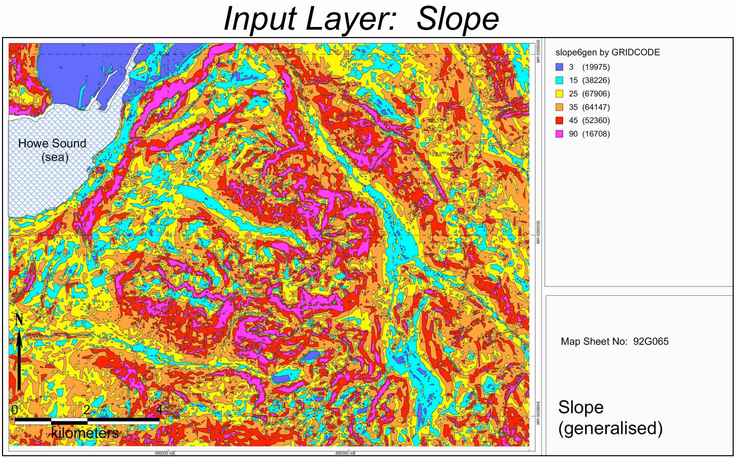
Data

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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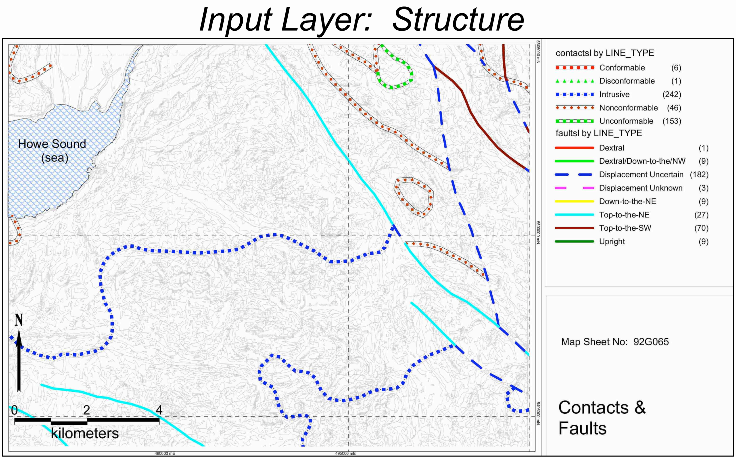

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Data is theory-laden

- 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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Hypotheses make predictions on data

Hypotheses are programs that make predictions on data.
Theories are hypotheses that best fit the observational data.

- Hypotheses can make various predictions about data:
  - definitive predictions
  - point probabilities
  - probability ranges
  - ranges with confidence intervals
  - qualitative predictions
- Users can use whatever criteria they like to evaluate hypotheses (e.g., taking into account simplicity and elegance)
- Semantic science search engine: extract theories from published hypotheses.

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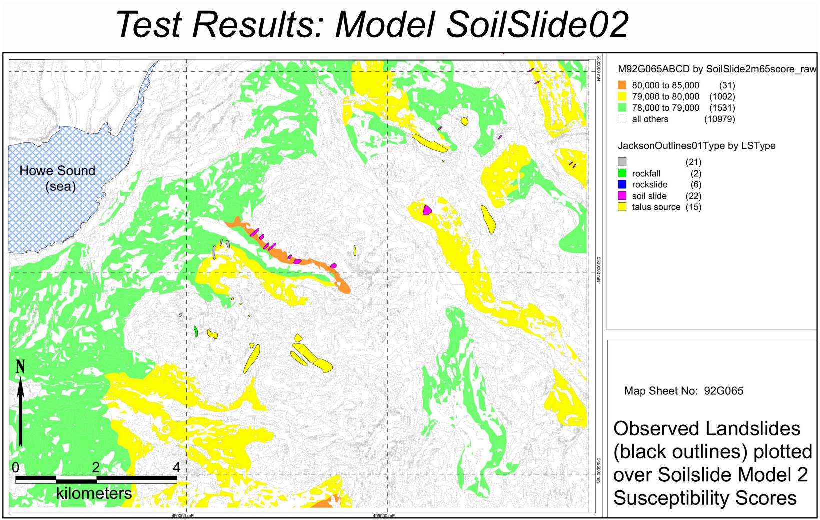

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Dynamics of Semantic Science

- New data and hypotheses are continually added.
- 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 hypotheses:
  A hypothesis 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 hypotheses that use them
  — role of a vocabulary is to describe useful distinctions.

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Random Variables and Triples

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

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- For **functional properties**:
  R is functional: $\langle x, R, y_1 \rangle$ and $\langle x, R, y_2 \rangle$ implies $y_1 = y_2$.
  random variable for each $\langle individual, property \rangle$ pair,
  range of the random variable is range of the property.
  E.g., if *Height* is functional, $\langle building17, Height \rangle$ is a random variable.

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  range of the random variable is range of the property.
  E.g., if *Height* is functional, $\langle \mathit{building}17, \mathit{Height} \rangle$ is a random variable.
- For **non-functional properties**:
  Boolean random variable 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 random var.

Ranges

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

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

No need to consider undefined propositions.

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Hypotheses, Models and Predictions

- Recall: a hypothesis is a program that makes predictions on data
- Hypotheses are often very narrow.
- We typically 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?

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- What about C: *if lung cancer, use B's prediction, else use A's prediction*?
- A model or hypothesis ensemble is a set of hypotheses applied to a particular case.
  - 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

Example Data

person visiting doctor:

Age	Sex	Coughs	HasLump
23	male	true	true
...	...	...	...

lump for person visiting doctor:

Location	LumpShape	Colour	CancerousLump
leg	oblong	red	false
...	...	...	...

person with cancer:

HasLungCancer	Treatment	Age	Outcome	Months
true	chemo	77	dies	7
...	...	...	...	...

Hypotheses

A hypothesis is of the form $\langle c, I, O, P \rangle$

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

Represents:

$$P(O \mid c, I)$$

or divide I into observation I_{obs} and intervention inputs I_{do}:

$$P(O \mid c, I_{obs}, do(I_{do}))$$

Example

Consider the following hypotheses:

- T_1 predicts the prognosis of people with lung cancer.
- T_2 predicts the prognosis of people with cancer.
- T_3 is the null hypothesis that predicts the prognosis of people in general.
- T_4 predicts whether people with cancer have lung cancer, as a function of coughing.
- T_5 predicts whether people have cancer.

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

Models

A model consists of multiple hypotheses, where each hypothesis can be used to predict a subset of its output features.

A model M needs to satisfy the following properties:

- M is coherent: it does not rely on the value of a feature in a context where the feature is not defined
- M is consistent: it does not make different predictions for any feature in any context.
- M is predictive: it makes a prediction in every context that is possible (probability > 0).
- M is minimal: no subset is also a model.

Model and Ensembles of Hypotheses

A hypothesis instance is a tuple of the form $\langle h, c, I, O \rangle$ such that:

- h is a hypothesis,
- c is a context in which the hypothesis will be used
- I is a set of inputs used by the hypothesis
- O is a set of outputs the hypothesis will be used to predict.

A model is a set of hypothesis instances that satisfy the previous conditions.

[Think of a model as a Bayesian belief network, but allowing for context-specific independence, avoiding undefined features, that interfaces with ontologies and used program to represent conditional probabilities.]

Example

- T_1 predicts the prognosis of people with lung cancer.
- T_2 predicts the prognosis of people with cancer.
- T_3 is the null hypothesis that predicts the prognosis of people in general.
- T_4 predicts (probabilistically) whether people with cancer have lung cancer, as a function of coughing.
- T_5 predicts (probabilistically) whether people have cancer.

A possible model for $P(Lives \mid person \wedge coughs)$:

- $\langle T_5, person, \{\}, \{HC\}\rangle$,
- $\langle T_3, person \wedge \neg hc, \{\}, \{Lives\}\rangle$,
- $\langle T_4, person \wedge hc, \{Coughs\}, \{HLC\}\rangle$,
- $\langle T_1, person \wedge hlc, \{\}, \{Lives\}\rangle$,
- $\langle T_2, person \wedge hc \wedge \neg hlc, \{\}, \{Lives\}\rangle$.

Programs and Meta-programs

Two sorts of probabilistic programs:

- Hypotheses are probabilistic programs that persist, are tuned to data.
- 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?"

Outline

Domains and Undefined Random Variables (Example)

Example (Ontology)

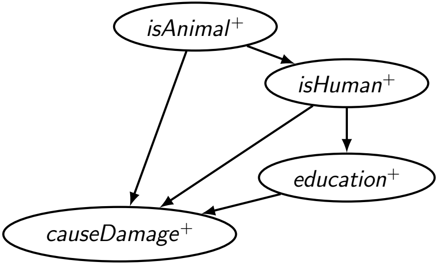
```
Classes:
  Thing
    Animal: Thing and isAnimal = true
      Human: Animal and isHuman = true

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}
```

A property is only defined for individuals in its domain.

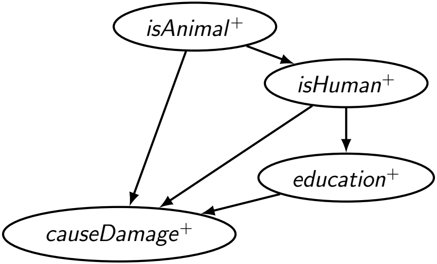
Extended Belief Networks (EBNs)

- 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: $P(education^{+} \mid causeDamage^{+} = true)$

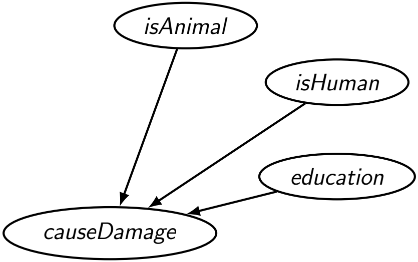
Extended Belief Networks (EBNs)



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

isAnimal

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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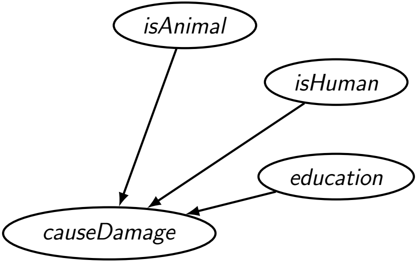

- The query $P(\mathit{education}^{+} \mid \mathit{causeDamage} = \mathit{true})$ has a non-zero probability of $\perp$
  — we can't ignore the undefined values.

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 $\beta = P(Q \mid \mathcal{E} = e \land domain(Q))$
    - Return

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

Some Objections

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- How can we test hypotheses if there is no "held-out" data? (Won't everyone cheat?)
- Why do you assume that probability is the right formalism?
- How can you convince people to use maximally informed priors rather than maximally uninformed priors?

Conclusion

- Semantic science is a way to develop and deploy knowledge about how the world works.
  - 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.
- Ontologies, hypotheses and observations interact in complex ways.
- Many formalisms will be developed and discarded before we converge on useful representations.

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