Learning and reasoning about entities and relations under uncertainty: a story of romance and disappointment

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What is the real world made of?

A Features or random variables

B Words, pixels, phonemes . . .

C Entities and events (e.g., plants, people, diseases, lectures, university courses)

D Huh? There is a real world?

Outline

Motivation

- AI studies what agents should do.
  - Acting is gambling: agents who don't use probabilities will lose to those who do.
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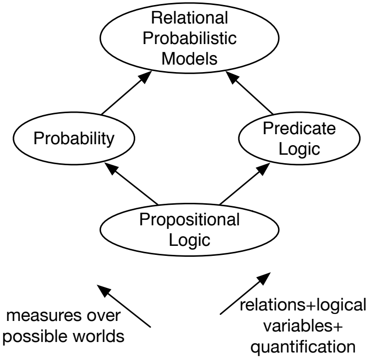

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What are relational models?

Introductions to AI and machine learning typically start with learning from relations, e.g.:

Example	*Author*	*Thread*	*Length*	*Where_read*	*User_action*
e_1	*known*	*new*	*long*	*home*	*skips*
e_2	*unknown*	*new*	*short*	*work*	*reads*
...	...	...	...	...	...

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What makes relational models in ML special is that the values include meaningless names. E.g., student number, product id, user id, movie id:

User	*Movie*	*Rating*	*Timestamp*
196	242	3	881250949
186	302	3	891717742
...	...	...	...

(Movielens 100k)

Names can be changed or exchanged with exactly same meaning.

Choosing Entities and Relations in Logic

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

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

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- $color(pen_7, red)$.
- $prop(pen_7, color, red)$.

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- $prop(pen_7, color, red)$.
- a single relation can be implicit $\longrightarrow$ triples: $(pen_7, color, red)$.

All relations can be represented in terms of triples:

	...	P_j	...
	...	...	...
r_i	...	v_{ij}	...
	...	...	...

can be represented as

Triples are universal representations of relations

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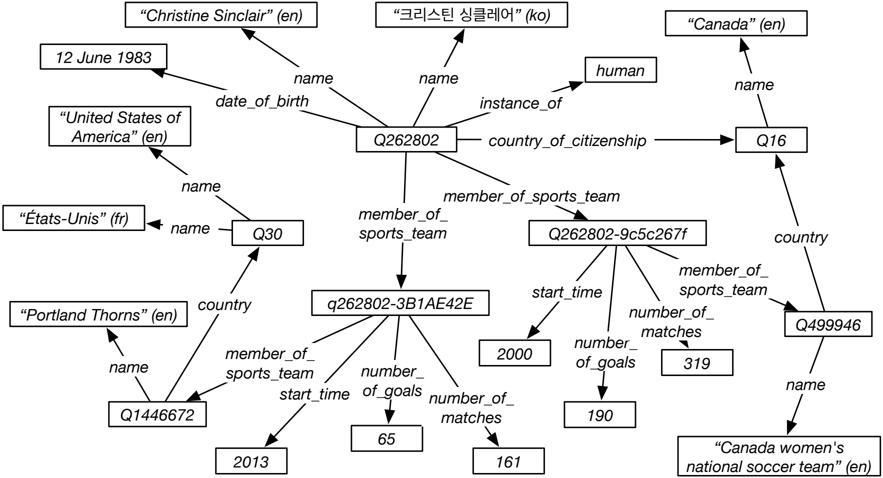
$prop(Entity, Property, Value)$ is the only relation needed:
$(Entity, Property, Value)$ triples, semantic network, entity relationship model, knowledge graphs, ...

Wikidata example: Christine Sinclair



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Projecting onto pairs loses information:

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- These are true triples:
  $(Air\ Canada, Flies\ From, New\ York)$
  $(Air\ Canada, Flies\ To, Los\ Angeles)$
- However, Air Canada does not fly from New York to Los Angeles.
  The information about flights is lost!

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FB15K, a knowledge base commonly used in research papers based on FreeBase, contains test triples:

- (Jade North,
  /sports/pro_athlete/teams./soccer/football_roster_position/position,
  Defender (association football))
  "*Jade North plays position defender.*"
- (Derby County F.C.,
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Please look at a knowledge graph before you use it!

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- Should we use the same sized vector for Canada as Q262802-3B1AE42E (the reified relation between Christine Sinclair and Portland Thorns)?

Outline

Aside: Probabilities $\leftrightarrow$ sigmoid

$$P(h \mid e) = \frac{P(h \land e)}{P(e)} = \frac{P(h \land e)}{P(h \land e) + P(\neg h \land e)}$$

Aside: Probabilities $\leftrightarrow$ sigmoid

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Typical: to learn probability of

- Boolean feature: sigmoid of a linear function
- discrete feature: softmax of a linear function

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— polyadic decomposition model (1927): two vector embeddings for each entity e ($E_0[e]$ and $E_2[e]$) and one for reach relation r ($E_1[r]$).

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- SimpleE^{+} = SimplE with non-negative entity embeddings
  - can represent arbitrary relations
  - point-wise $\leq$ corresponds to implication
  - easy to explain what it learns

What/how embedding-based models learn

PD^+:

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$E_0[h][f] \geq 0$ $E_2[h][f] \geq 0$.
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- Negative values of $E_1[r][i]$ provide exceptions.

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- Ideally we would try to do both; learn about specific entities and general knowledge.

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- Problem #1: is it not good for answers for which there is no answer or many answers:
  Who is the pope married to?

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- Challenge: design a good evaluation scheme. Log-likelihood seems reasonable, but requires knowledge of negations.

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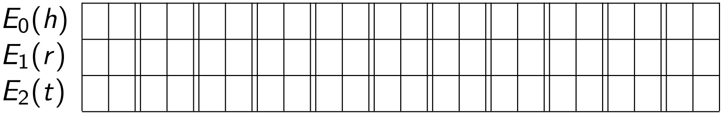
- We could convert them to triples by reifying . . . but the reified entities have very few data points (number of arguments of original relations)
- Design embedding-based model that work directly with original relations
- Allow them to be inferred from other relations

Beyond Triples

Distmult, Complex, Simple, Simple+... $P((h, r, t))$ is function of



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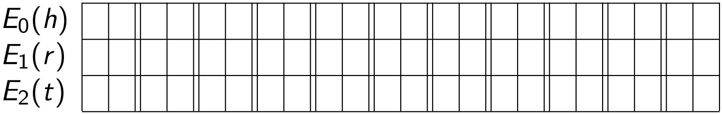

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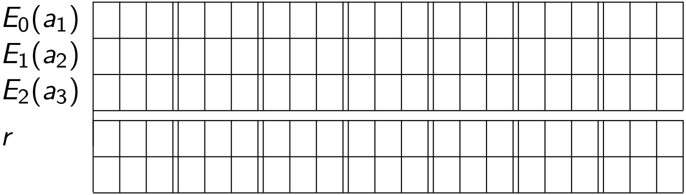
$P(r(a_1, a_2, a_3))$ is function of



window size varies; each window independent

Outline

What can't any of the previous models do?

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- Consider a flight with stopover:

$$\mathit{flight\_with\_stopover}(A, B) \leftrightarrow \exists C\ \mathit{flight}(A, C) \land \mathit{flight}(C, B)$$

The airport the second flight leaves from must be the same – not just similar – as the airport the first flight arrived at.

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  - Sam's mother
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- If we also specified that there was no one else: there are between 1 and 3 people.
- Aside: We need knowledge graphs to (be able to) state "there are no more . . ."

Identity $\neq$ similarity

Similar (same make, shape and color); not the same chair:

Not similar, but the same person:

Existence and Identity are tricky

- Is this reference to the same paper as this other reference?
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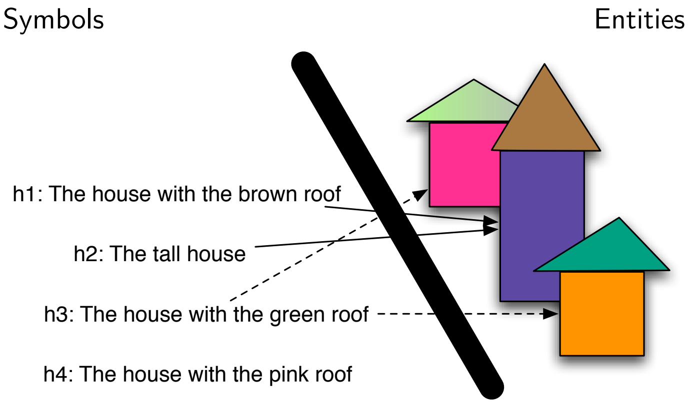
- Two entities cannot be equal (have same identity); otherwise there is only one object.
- Many methods (e.g., graph neural networks, Markov logic networks, probabilistic logic programs . . .) assume that this is already solved: we know what entities exist and what descriptions are equal.

Correspondence Problem



Equality corresponds to partition of the symbols.

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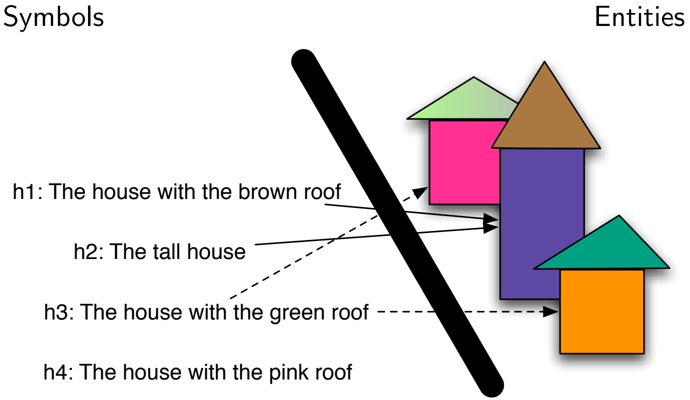

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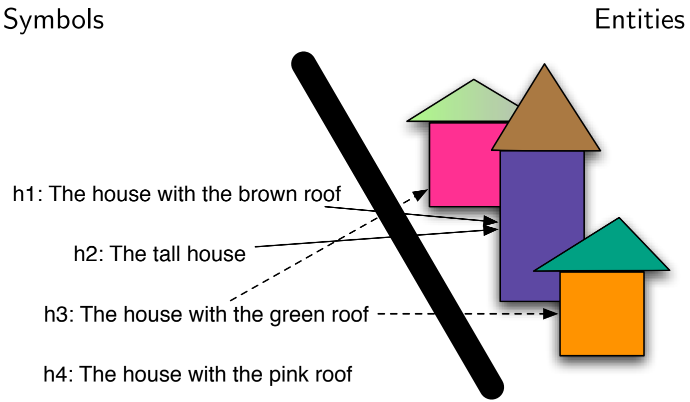

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Common to use MCMC.

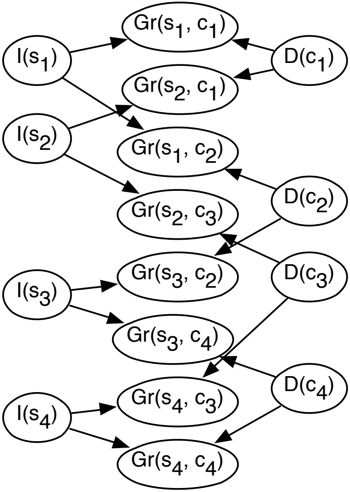
Outline

Example: Predicting Relations

Student	*Course*	*Grade*
s_1	c_1	A
s_2	c_1	C
s_1	c_2	B
s_2	c_3	B
s_3	c_2	B
s_4	c_3	B
s_3	c_4	?
s_4	c_4	?

- Students s_3 and s_4 have the same averages, on courses with the same averages.
- Which student would you expect to better on course c_4?

From Relations to Bayesian Belief Networks



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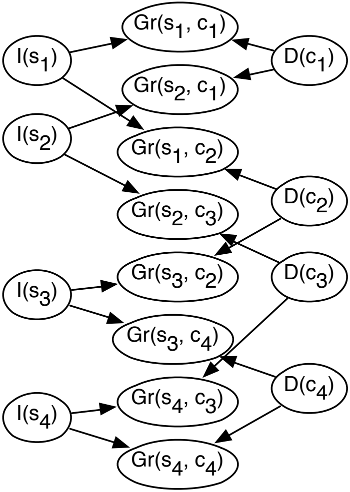
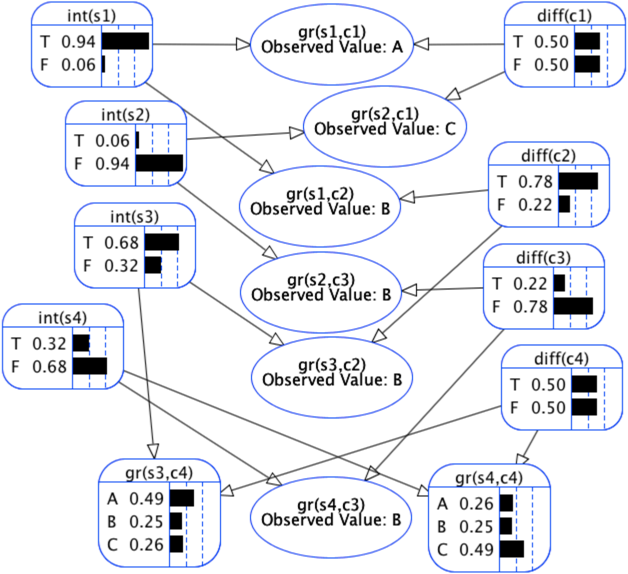


$I(S)$	$D(C)$	$Gr(S,C)$		
		A	B	C
true	*true*	0.5	0.4	0.1
true	*false*	0.9	0.09	0.01
false	*true*	0.01	0.09	0.9
false	*false*	0.1	0.4	0.5

$P(I(S)) = 0.5$
$P(D(C)) = 0.5$

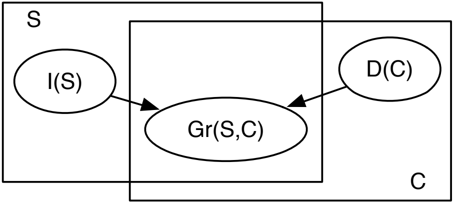
"parameter sharing"

Example: Predicting Relations



`http://artint.info/code/aispace/grades.xml`

Plate Notation



- S, C logical variable representing students, courses
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- $I(S)$, $Gr(S, C)$, $D(C)$ are parametrized random variables

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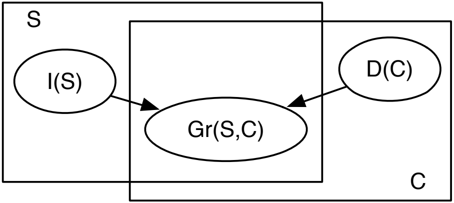

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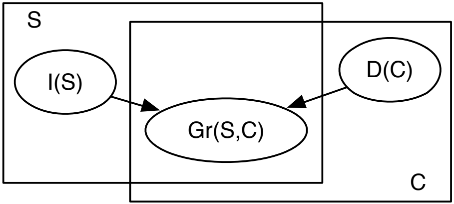

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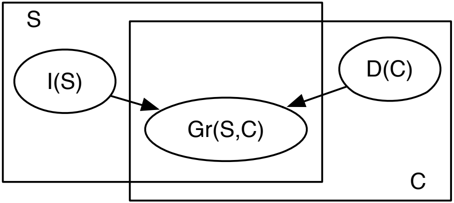

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- all instances share the same structure and parameters

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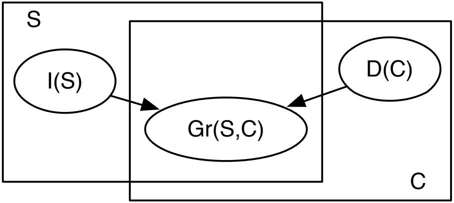

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  Grounding contains

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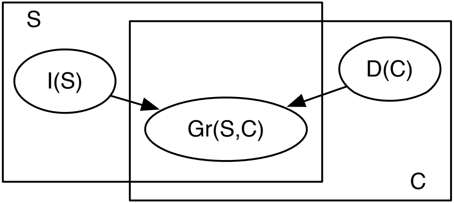

- If there were 1000 students and 100 courses:
  Grounding contains
  - 1000 $I(s)$ variables
  - 100 $D(c)$ variables
  - 100000 $Gr(s, c)$ variables

  total: 101100 variables
- To define the probabilities:
  1 for $I(S)$, 1 for $D(C)$, 8 for $Gr(S, C) = 10$ parameters.

Outline

Relational Learning in (Lifted) Graphs

A common framework:

- Nodes are entities (all existing, already disambiguated)
- (Hyper)- edges between entities that are related.
- Function of the dependency depends on the types of the entities. (E.g., whether one person likes another depends on the properties of entities, not their identity.)

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— main difference: in MLNs and PLPs, latent variables have a probabilistic interpretation. GNNs choose the function to maximize predictive performance.

Aggregation

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- Requires aggregation: some models provide built-in aggregation, and some you can use whatever aggregation you want.

Representations of Lifted Graphical models

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explicit: typically sum, average, or max	Graph Neural Networks	

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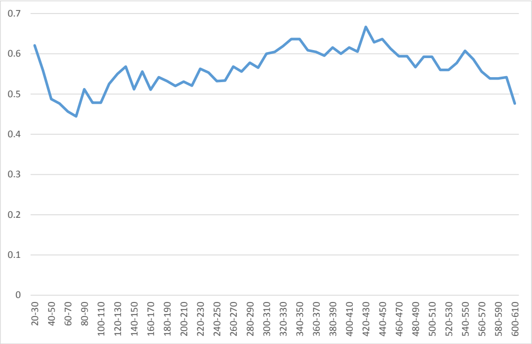
  E.g., one movie rated vs 1000 rated for a person.
- for sum aggregation in GNNs, and aggregation in Markov Logic networks and probabilistic logic programs, either
  - the prediction does not depend on neighbours, or
  - the prediction goes to 0 or 1 as the number of neighbours goes to infinity, or
  - the numbers cancel out in an unstable way

  for some models, this occurs even if there are no observations

Real Data



number of movies rated

Observed $P(25 < Age(u) < 45 \mid n)$, where n is number of movies watched from the Movielens 100k dataset.

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Both go from ≈ 1 at $n = 10$ to ≈ 0 at $n = 30$.
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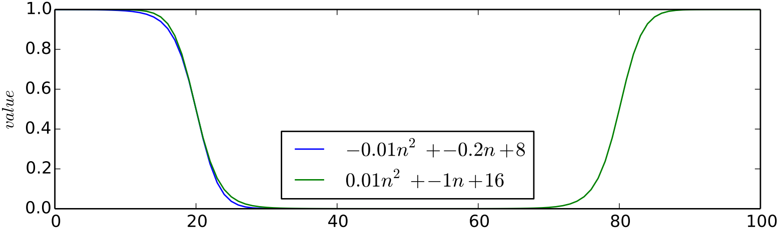

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- If people who drop out are ignored, it looks like the drug works: A larger proportion of those who took the drug are well.
- We need to go beyond the non-missing data to determine why data is missing.
- EM (and other methods) work, but produce nonsense!
- Almost all data in relational models is missing, but missingness is usually ignored

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  For all mined commodities combined, there are fewer than 10,000 known high-grade deposits. These are complex. Undiscovered deposits are (probably) unlike the known ones.
- Reified entities have very few facts about them.
- There is a long tail of entities about which we know very little

Outline

1. What are relational probabilistic models and relational learning?
   - Relational Models
   - Knowledge Graphs
2. Learning Knowledge Graphs
3. Existence and Identity Uncertainty
4. Lifted Graphical Models
5. Graph-based models
6. Missing data
7. Big Data
8. Bayesian $\Rightarrow$ Exchangeability $\Rightarrow$ Lifted Inference
9. Conclusion

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- See Van den Broeck, Kersting, Natarajan and Poole (Eds) *An Introduction to Lifted Inference*, MIT Press, 2021.

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- Predicting properties of entities and relationships among entities are (currently) different problems. Methods that work for one often don't work for other, but authors are often not explicit about what they do.

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- Will you step up to this challenge? There is still lots to do!

What is now required is to give the greatest possible development to mathematical logic, to allow to the full the importance of relations, and then to found upon this secure basis a new philosophical logic, which may hope to borrow some of the exactitude and certainty of its mathematical foundation. If this can be successfully accomplished, there is every reason to hope that the near future will be as great an epoch in pure philosophy as the immediate past has been in the principles of mathematics. Great triumphs inspire great hopes; and pure thought may achieve, within our generation, such results as will place our time, in this respect, on a level with the greatest age of Greece.

– Bertrand Russell, Mysticism and Logic and Other Essays (1917)