Model-theoretic embeddings

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  - formal definition of "truth" relies on "models"
  - universal algebra over formal languages (with signature Σ)

Description Logic EL++

Name	Syntax	Semantics
top	$\top$	$\Delta^{\mathcal{I}}$
bottom	$\bot$	$\emptyset$
nominal	$\{a\}$	$\{a^{\mathcal{I}}\}$
conjunction	$C \sqcap D$	$C^{\mathcal{I}} \cap D^{\mathcal{I}}$
existential restriction	$\exists r.C$	$\{x \in \Delta^{\mathcal{I}} \mid \exists y \in \Delta^{\mathcal{I}} : (x,y) \in r^{\mathcal{I}} \wedge y \in C^{\mathcal{I}}\}$
generalized concept inclusion	$C \sqsubseteq D$	$C^{\mathcal{I}} \subseteq D^{\mathcal{I}}$
role inclusion	$r_1 \circ \ldots \circ r_n \sqsubseteq r$	$r_1^{\mathcal{I}} \circ \ldots \circ r_n^{\mathcal{I}} \subseteq r^{\mathcal{I}}$

Models

- Interpretations and Σ-structures
- Model $\mathfrak{A}$ of a formula ϕ: ϕ is true in $\mathfrak{A}$ ($\mathfrak{A} \models \phi$)
- Theory T: set of formulas
- $\mathfrak{A}$ is a model of T if $\mathfrak{A}$ is a model of all formulas in T
- Ontologies are (special kinds of) theories

EL Embeddings

- given a theory/ontology T with signature $\Sigma(T)$
- aim: find $f_e : \Sigma(T) \mapsto \mathbb{R}^n$ s.t. $f_e(\Sigma(T))$ is a model of T ($f_e(\Sigma(T)) \models T$)

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- any consistent $\mathcal{EL}^{++}$theory has infinite models
- any consistent $\mathcal{EL}^{++}$theory has models in $\mathbb{R}^n$ (Loewenheim-Skolem, upwards; compactness)

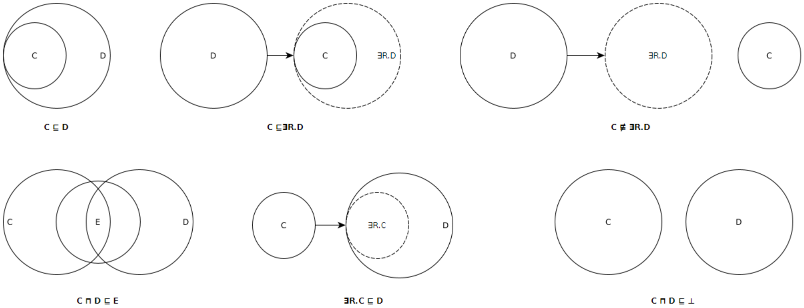
Key idea

- for all $r \in \Sigma(T)$ and $C \in \Sigma(T)$, define $f_e(r)$ and $f_e(C)$
- $f_e(C)$ maps to points in an open n-ball such that $f_e(C) = C^{\mathcal{I}}$: $C^{\mathcal{I}} = \{x \in \mathbb{R}^n | \, \|f_e(C) - x\| < r_e(C)\}$
  - these are the *extension* of a class in $\mathbb{R}^n$
- $f_e(r)$ maps a binary relation r to a vector such that $r^{\mathcal{I}} = \{(x, y) | x + f_e(r) = y\}$
  - that's the TransE property for *individuals*
- use the axioms in T as constraints

Algorithm

- normalize the theory:
  - every $\mathcal{EL}^{++}$theory can be expressed using four normal forms (Baader et al., 2005)
- eliminate the ABox: replace each individual symbol with a singleton class: a becomes $\{a\}$
- rewrite relation assertions $r(a, b)$ and class assertions $C(a)$ as $\{a\} \sqsubseteq \exists r.\{b\}$ and $\{a\} \sqsubseteq C$
  - something to remember for the next class-vs-instance discussion?
- normalization rules to generate:
  - $C \sqsubseteq D$
  - $C \sqcap D \sqsubseteq E$
  - $C \sqsubseteq \exists R.D$
  - $\exists R.C \sqsubseteq D$

Algorithm: loss functions



EL Embeddings

$$
\begin{align}
Male &\sqsubseteq Person \tag{1}\\
Female &\sqsubseteq Person \tag{2}\\
Father &\sqsubseteq Male \tag{3}\\
Mother &\sqsubseteq Female \tag{4}\\
Father &\sqsubseteq Parent \tag{5}\\
Mother &\sqsubseteq Parent \tag{6}\\
Female \sqcap Male &\sqsubseteq \bot \tag{7}\\
Female \sqcap Parent &\sqsubseteq Mother \tag{8}\\
Male \sqcap Parent &\sqsubseteq Father \tag{9}\\
\exists hasChild.Person &\sqsubseteq Parent \tag{10}\\
Parent &\sqsubseteq Person \tag{11}\\
Parent &\sqsubseteq \exists hasChild.\top \tag{12}
\end{align}
$$

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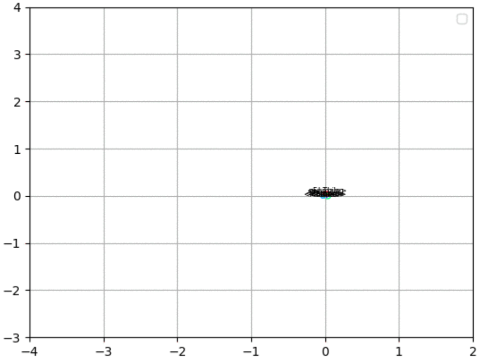
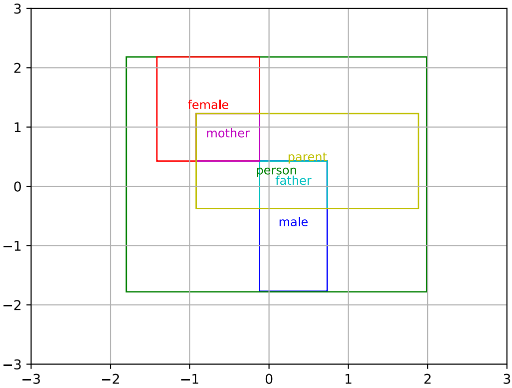
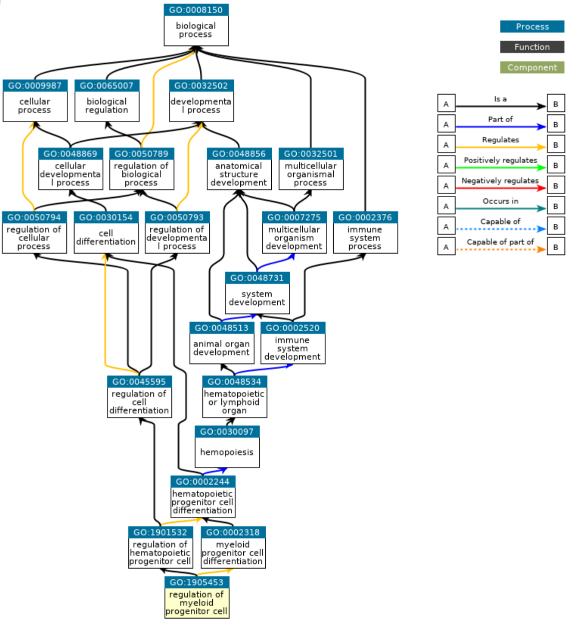


- model with $\Delta = R^n$
- support quantifiers, negation, conjunction,...

EL BOX Embeddings



Gene Ontology



QuickGO - https://www.ebi.ac.uk/QuickGO

DeepGOZero - function prediction