UNIVERSITÄT ZU LÜBECK
INSTITUT FÜR INFORMATIONSSYSTEME

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Knowledge Graph Embeddings

KI Kolloqium
December 2, 2019

Motivation

- Past talk of Ralf: tour from numbers to logic
- Today: tour from logic to numbers
  - Logic as a useful method/tool for machine learning (ML)

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- Today: tour from logic to numbers
  - Logic as a useful method/tool for machine learning (ML)
  - Maybe it is more: foundations of ML
  - But not easy ...*)

*)The Burden of Logical Foundations

For all that, PM is not widely used today: probably the foremost reason for this is its reputation for typographical complexity. Somewhat infamously, several hundred pages of PM precede the proof of the validity of the proposition 1+1=2.

Wikipedia entry for Principia Mathematica (accessed November 25, 2019)

Expressivity of Embeddings

Knowledge Graph (KG)

- Set of assertions in triple form $KG = \{ \ (subj \ pred \ obj) \ \}$
- Convenient logical notation $KG = \{ \ pred(subj, obj) \ \}$

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  W3C RDF

- Analytical philosophy
  Bernard Bolzano (1781-1848)

Knowledge Graph (KG)

Usually KGs highly incomplete $\Longrightarrow$ "Learn" new triples assuming regularities

Example

$$KG_2 = \{\mathit{worksIn(alice,AI)}, \mathit{subfield(AI,CS)}, \mathit{manyPubls(alice,bob)} \\ \underline{\mathit{worksIn(bob,AI)}}\}\}$$

Knowledge Graph Embeddings

- Capture regularities by embedding KG into continuous space $E = \mathbb{R}^n$
- Various recent approaches
  - TRansE, TransR, STransH
  - DistMult
  - ComplEx
  - SimplE
  - RESCAL ...

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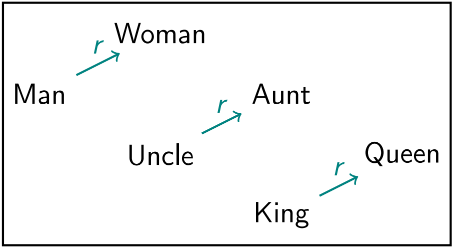
  - SimplE
  - RESCAL ...
- Can be described uniformly by scoring functions for relations R

$$s_R : E \times E \longrightarrow \mathbb{R}$$

Convention:
$s_R(u, v)$ small means probability of $R(u, v)$ is high.

TransE (Bordes et al. 13)



- $s_R(u, v) = \|u + r - v\|$ ($\|\cdot\|$: Euclidean Norm)

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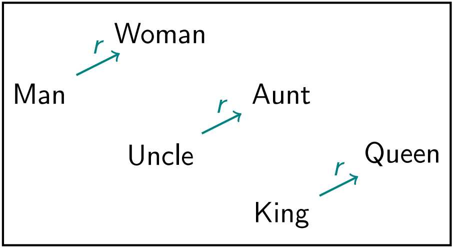

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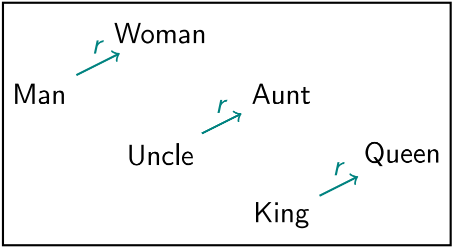

- $s_R(u, v) = \|u + r - v\|$ ($\|\cdot\|$: Euclidean Norm)
- Limitation: Relations r = vector translations, hence functional
- Generalizations
  - TransR (map in R-specific space before translation)

    $$s_R(u, v) = \|M_r u + r - M_r v\|$$

  - STransE (different matrices for subject (s) and object (o))

    $$s_R(u, v) = \|M_r^s u + r - M_r^o v\|$$

DistMult (Yang et al. 14)

- $s_R(u, v) = -\sum_{i=1}^{n} u_i r_i v_i$

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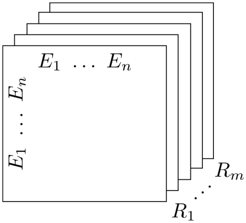
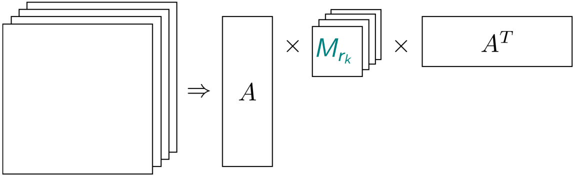
- Generalizations
  - Distinguish whether entities in subject or object position
  - ComplEx (Trouillon et al. 16)
    relate those entity types by complex conjugation
  - SimplE (Kazemi/Poole 18)
    for each $R(u, v)$ consider $R^{-}(v, u)$

RESCAL





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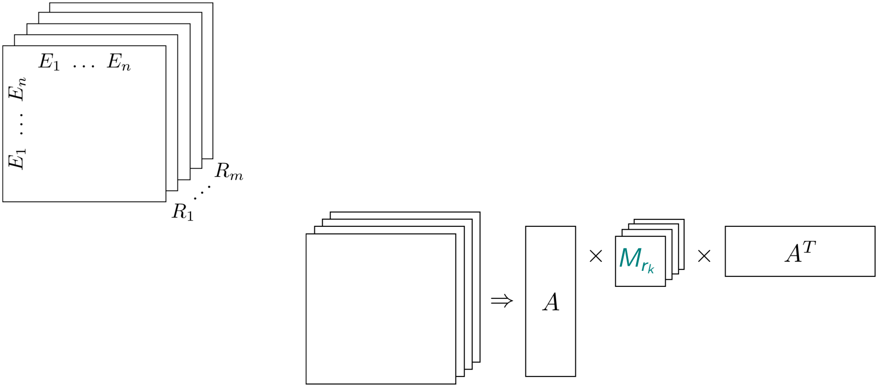

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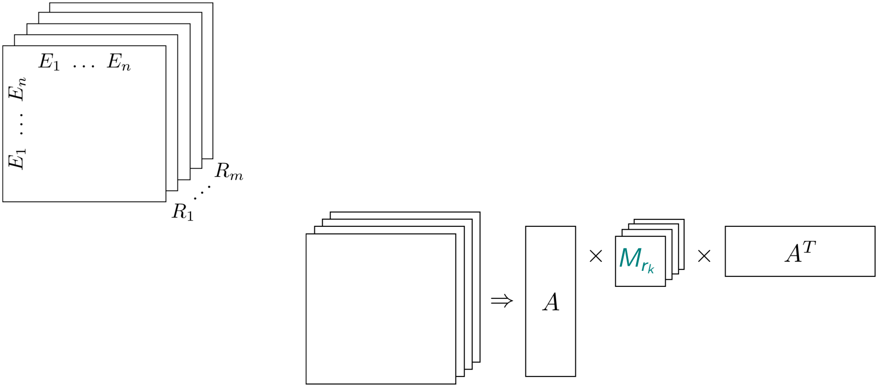

- $s_{R_k}(u, v) = -u^T M_{r_k} v$
- Limitation: suffers from overfitting

Expressivity Criterion

- Usually one considers low-dimensional spaces
- But nonetheless must be sufficiently high to embed knowledge expressed in KGs
  - P: set of valid triples in KG
  - N: set of non-valid triples in KG $(N \cap P = \emptyset)$

Expressivity Criterion

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Definition (Kazemi/Poole 18)

An embedding model is fully expressive iff there are a dimension n, an embedding e, and a threshold λ_R such that:

- for all $R(u, v) \in P$: $s_R(e(u), e(v)) \leq \lambda_R$
- for all $R(u, v) \in N$: $s_R(e(u), e(v)) > \lambda_R$

Results on Expressiveness (Kazemi/Poole 18)

Model	Fully expressive?
TransE (and all extensions)	-
DistMult	-
SimplE	+
ComplEx	+
RESCAL	+

- TransE not sufficiently general, RESCAL tends to overfitting
- And now?

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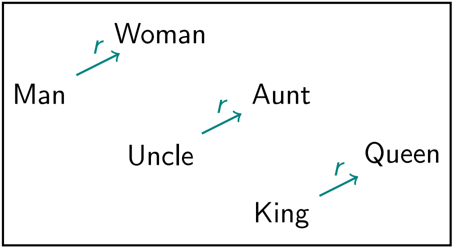
- TransE not sufficiently general, RESCAL tends to overfitting
- And now?
- Here comes logic
  - "Logic focussed" semantics for concepts and relations
  - Add logically specified background knowledge

Logico-geometrical Semantics

- Represent concepts as sets (set of vectors, not single vector)
- Represent binary relations as sets of pairs of objects



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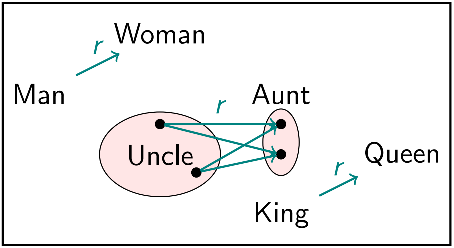

Adding Background Knowledge

Some completions due to background knowledge/ontology

Example

Ontology :

$$\{\forall X, Y, Z. subfield(X, Y) \wedge worksIn(Z, X) \rightarrow worksIn(Z, Y)\}$$

$$\begin{aligned} KG_2 \quad = \quad & \{worksIn(alice,AI), subfield(AI,CS), manyPubls(alice,bob), \\ & worksIn(bob,AI), \qquad \text{(by induction)} \\ & worksIn(alice,CS) \qquad \text{(by deduction)}\} \end{aligned}$$

Ontologies in Description Logics

Definition (Description logics (DLs))

Logics for use in knowledge representation with special attention on a good balance of expressibility and feasibility of reasoning services

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Logics for use in knowledge representation with special attention on a good balance of expressibility and feasibility of reasoning services

- Can be mapped to fragments of FOL
- Usage
  - Ontology representation language
  - Foundation for standard web ontology language (OWL)
- Have been investigated for ca. 30 years now
  - Many theoretical insights on various different purpose DLs
  - Various reasoners

Family of DLs

- Variable-free logics centered around concepts
- concepts = one-ary predicates in FOL = classes in OWL

Example (Concepts)

- $Students$ ("students")
- $Students \sqcap Male$ (" Male students")
- $\exists attends.MathCourse$ ("Those attending a math course")
- $\forall hasFriends.Freaks$ ("Those having only freaks as friends")
- $Person \sqcap \forall attends.(Course \sqcap \neg Easy)$ ("Persons attending only non-easy courses")

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- Concepts: semantics

- Interpretation
  $\mathcal{I} = (\Delta^\mathcal{I}, \cdot^\mathcal{I})$
- $A^\mathcal{I} \subseteq \Delta^\mathcal{I}$ for all $A \in N_C$
- $c^\mathcal{I} \in \Delta^\mathcal{I}$ for all $c \in N_i$
- $r^\mathcal{I} \subseteq \Delta^\mathcal{I} \times \Delta^\mathcal{I}$
  for all $r \in N_{Ro}$

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- $(C \sqcap D)^{\mathcal{I}} = C^{\mathcal{I}} \cap D^{\mathcal{I}}$
- $(C \sqcup D)^{\mathcal{I}} = C^{\mathcal{I}} \cup D^{\mathcal{I}}$
- $\neg C = \Delta^{\mathcal{I}} \setminus C^{\mathcal{I}}$
- $(\forall r.C)^{\mathcal{I}} = \{d \in \Delta^{\mathcal{I}} \mid$ for all $e \in \Delta^{\mathcal{I}}$: If $(d, e) \in r^{\mathcal{I}}$ then $e \in C^{\mathcal{I}}\}$
- $(\exists r.C)^{\mathcal{I}} = \{d \in \Delta^{\mathcal{I}} \mid$ there is $e \in \Delta^{\mathcal{I}}$ s.t. $(d, e) \in r^{\mathcal{I}}$ and $e \in C^{\mathcal{I}}\}$

Tbox and Abox

- Terminological box (tbox) $\mathcal{T}$
  - Finite set of general concept inclusions (GCIs)

$$C \sqsubseteq D$$

  - Semantics: $\mathcal{I} \models C \sqsubseteq D$ iff $C^{\mathcal{I}} \subseteq D^{\mathcal{I}}$.

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- Assertional box (abox) $\mathcal{A}$
  - Finite set of assertions
  - Assertion: $C(a)$, $r(a, b)$
  - Semantics:
    $\mathcal{I} \models C(a)$ iff $a^{\mathcal{I}} \in C^{\mathcal{I}}$
    $\mathcal{I} \models r(a, b)$ iff $(a^{\mathcal{I}}, b^{\mathcal{I}}) \in r^{\mathcal{I}}$.

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- Ontology: $(\sigma, \mathcal{T}, \mathcal{A})$

Definition (Basic Reasoning services)

- Model: $\mathcal{I} \models \mathcal{O}$ iff $\mathcal{I} \models \mathcal{T} \cup \mathcal{A}$ iff $\mathcal{I} \models ax$ for all $ax \in \mathcal{T} \cup \mathcal{A}$.
- Satisfiability/Consistency: $\mathcal{O}$ is satisfiable iff $\mathcal{T} \cup \mathcal{A}$ is satisfiable iff it has a model
- Entailment: $\mathcal{O} \vDash ax$ iff: For all $\mathcal{I}$: If $\mathcal{I} \models \mathcal{O}$ then $\mathcal{I} \models ax$.
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Definition (Extended Reasoning services)

- Query answering: Certain answers $cert(Q(x), \mathcal{O}) = \{\vec{a} \in N_i \mid \mathcal{O} \vDash Q[\vec{x}/\vec{a}]\}$
- ...

Example (Certain Answers for Conjunctive Queries)

$$\mathcal{T} = \{ \top \sqsubseteq \mathit{Male} \sqcup \mathit{Female}, \mathit{Male} \sqcap \mathit{Female} \sqsubseteq \bot \}$$

$$\mathcal{A} = \{ \mathit{friend}(\mathit{john}, \mathit{susan}), \mathit{friend}(\mathit{john}, \mathit{andrea}), \mathit{female}(\mathit{susan}), \mathit{likes}(\mathit{susan}, \mathit{andrea}), \mathit{likes}(\mathit{andrea}, \mathit{bill}), \mathit{Male}(\mathit{bill}) \}$$

$$Q(x) = \exists y, z(\mathit{friend}(x, y) \wedge \mathit{Female}(y) \wedge \mathit{likes}(y, z) \wedge \mathit{Male}(z))$$

- $\mathit{cert}(Q(x), \mathcal{O}) = ?$

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- We have to consider all possible models of the ontology
- But here there are actually two classes:
  Andrea is male vs. Andrea is not male.

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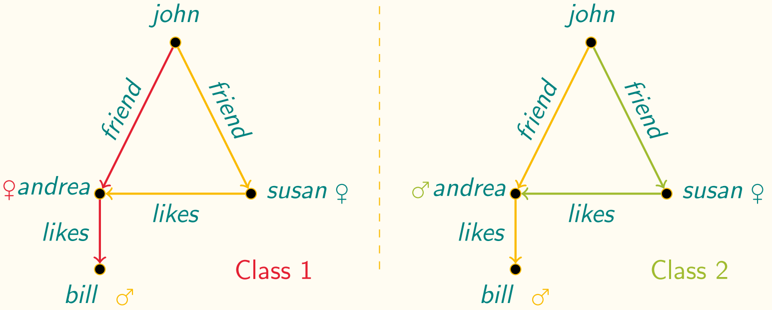


$$\mathit{cert}(Q(x), \mathcal{O}) = \{\mathit{john}\}$$

Cone-Embedding for $\mathcal{ALC}$ Ontologies

Aim

Find ML-feasible geometric models such that $\mathcal{ALC}$ ontology is classically satisfiable iff it is satisfiable by such a geometric model.

Simple Case: Propositional $\mathcal{ALC}$

- Boolean concepts

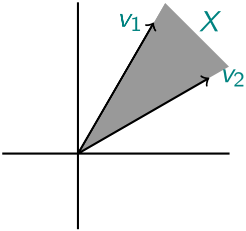
$$C \longrightarrow A \mid \bot \mid \top \mid \neg C \mid C \sqcap C \mid C \sqcup C$$

- Tbox restricted to Boolean concepts
- Geometric model for Boolean concepts based on closed convex cones
- Embedding space
  - $E = \mathbb{R}^n$ for some $n \in \mathbb{N}$
  - Scalar product for $v, w \in E$

$$\langle v, w \rangle = \sum_{1 \leq i \leq n} v_i w_i$$

Cones

- $X \subseteq E$ is a convex cone iff for all $v, w \in X, \lambda, \mu \in \mathbb{R}_{\geq 0}$: $\lambda v + \mu w \in X$



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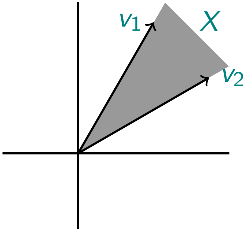

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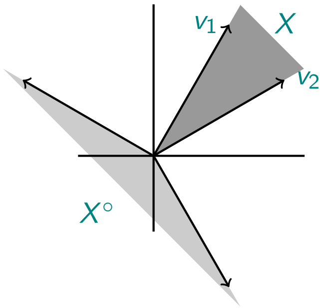
$$X^\circ = \{v \in E \mid \forall w \in X : \langle v, w \rangle \leq 0\}$$



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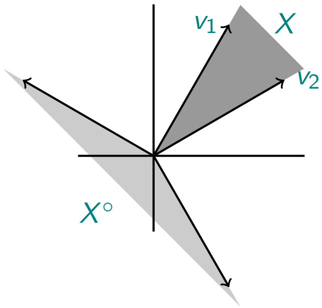


Proposition

For closed convex cones X, Y:

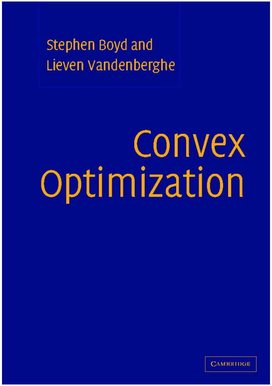
- X° *is a closed convex cone*
- $(X^\circ)^\circ = X$
- $conicHull(X \cup Y) = (X^\circ \cap Y^\circ)^\circ$

Definition (Cone-Semantics of $\mathcal{ALC}$ concepts (First Try))

- A geometric interpretation $\mathcal{I}$ interprets all atomic concepts by closed convex cones in E
- Semantics for arbitrary concepts under $\mathcal{I}$
  - $(\top)^{\mathcal{I}} = \Delta$
  - $(\bot)^{\mathcal{I}} = \{\vec{0}\}$
  - $(C \sqcap D)^{\mathcal{I}} = C^{\mathcal{I}} \cap D^{\mathcal{I}}$
  - $(\neg C)^{\mathcal{I}} = C^{\circ}$
  - $(C \sqcup D)^{\mathcal{I}} = (\neg(\neg C \sqcap \neg D))^{\mathcal{I}}$

Why Convex Cones?

1. ML-feasibility:
   convex (even conic) optimization



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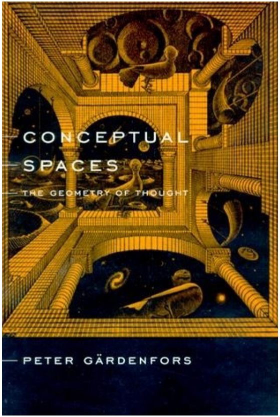

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3. Logic: polarity as negation

Lemma (Farkas' Lemma)

Let X be the convex cone generated by vectors $v_1, \ldots, v_n \in \mathbb{R}^n$ and consider $w \in \mathbb{R}^n$. Then either $w \in X$ or there is $z \in \mathbb{R}^n$ such that $\langle z, v_i \rangle \leq 0$ for all i, and $\langle z, w \rangle \geq 0$.

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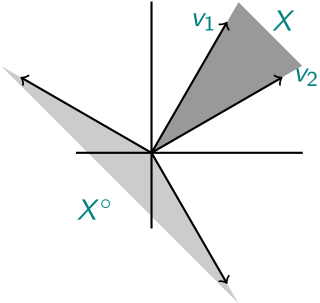

Lemma (Farkas' Lemma)

Let X be the convex cone generated by vectors $v_1, \ldots, v_n \in \mathbb{R}^n$ and consider $w \in \mathbb{R}^n$. Then either $w \in X$ or there is $z \in \mathbb{R}^n$ such that $\langle z, v_i \rangle \leq 0$ for all i, and $\langle z, w \rangle \geq 0$.

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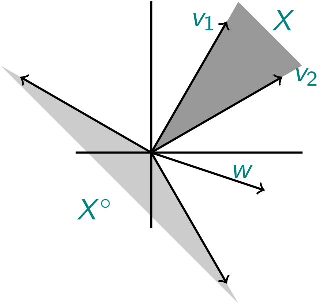

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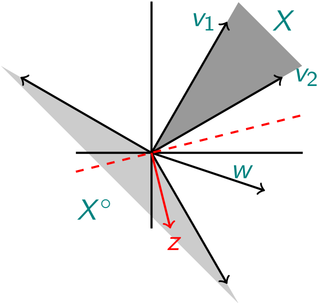

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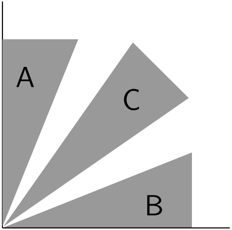

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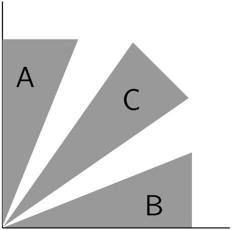

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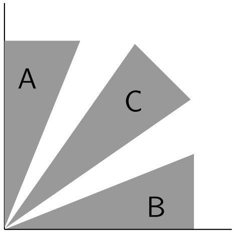

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- Distributivity law not fulfilled
- What should we do?
  1. Restrict cones (today)
  2. Search for a (the) logic of cones (not today)

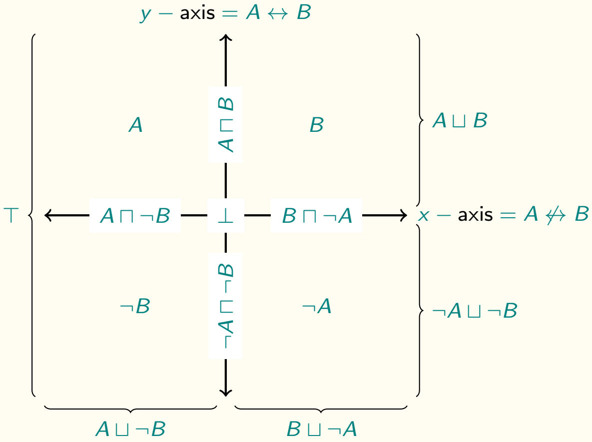
Searching for $\mathcal{ALC}$-cones (Nomen est Omen)

Definition

X is an al-cone in $\mathbb{R}^n$ iff $X = X_1 \times \cdots \times X_n$

where each $X_i \in \{\mathbb{R}, \mathbb{R}_+, \mathbb{R}_-, \{0\}\}$

Example (Boolean Algebra over Two Atomic Concepts)



Al-Cones Do the Job

Proposition

Boolean $\mathcal{ALC}$-ontologies are classically satisfiable iff they are by a geometric model over $\mathbb{R}^n$ based on al-cones of the form $X_1 \times \cdots \times X_n$ with $X_i \in \{\{0\}, \mathbb{R}^+, \mathbb{R}^-, \mathbb{R}\}$ for $i \in \{1, \ldots, n\}$.

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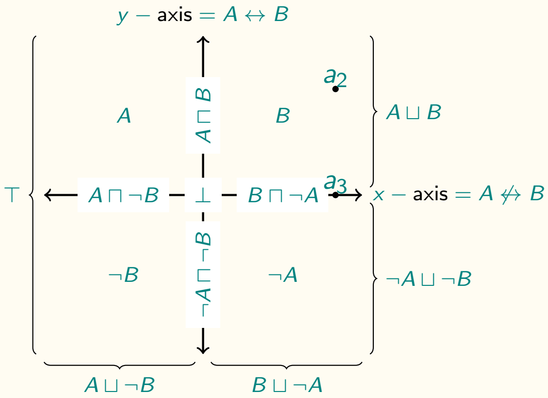
- Hypothesis space $\mathcal{H} = \{$ rotation(α) of al-cone system $\}$

Example



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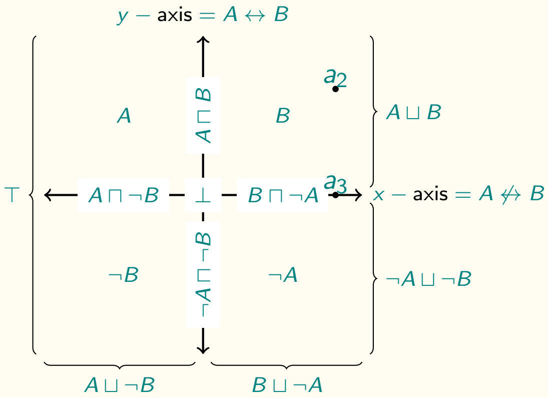

- Our geometric models are partial models
- Construction before not faithful: any $c \in A \sqcup B$ must be A or B, though ontology does not say so.

Faithful Models

Proposition

For classically satisfiable Boolean $\mathcal{ALC}$-ontologies there is a concept-faithful and tbox-faithful geometric model on some $\mathbb{R}^{2n}$ based on al-cones of the form $X_1 \times \cdots \times X_{2n}$ with $X_{2i} \in \{\{0\}, \mathbb{R}^+, \mathbb{R}^-, \mathbb{R}\}$ and $X_{2i+1} = X_{2i}$.

Al-Cone Models for Full $\mathcal{ALC}$

- Previous construction does not work because tbox-induced Boolean algebra not atomic
- Approximative solution: consider rank bound
- Roles are interpreted "classically"

Proposition

$\mathcal{ALC}$-ontologies are classically satisfiable iff they are satisfiable by a (abox faithful, m-rank-concepts faithful) geometric model on some finite $\mathbb{R}^n$ using sets of the form $X_1 \times \cdots \times X_n$ with $X_i \in \{\{0\}, \mathbb{R}^+, \mathbb{R}^-, \mathbb{R}\}$.

Embeddings for Ontologies in Other Logics

Embedding for Datalog$^{\pm}$

- Existential rules (with atoms B_i, H_j)

$$B_1 \wedge \cdots \wedge B_n \rightarrow \exists X_1, \ldots, X_j . H_1 \wedge \cdots \wedge H_k$$

Example

$$\mathit{short\text{-}talk}(X) \wedge \mathit{well\text{-}planed}(X) \rightarrow \exists t . \mathit{lasts}(X, t) \wedge t < 1h$$

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- Integrity constraints capture only one aspect of negation (disjointness), but not covering (no negation on lhs)

Geometric Models Based on Convex Sets

Theorem (Basulto/Schockaert 18)

For all Datalog$^{\pm}$ KBs $\mathcal{O}$ with quasi-chained rules only:
$\mathcal{O}$ is classically satisfiable iff it is satisfiable by a geometric model that interprets all relations by convex sets.

$B_1 \wedge \dots \wedge B_n \rightarrow \exists X_1, \dots, X_j . H_1 \wedge \dots \wedge H_k$ is quasi-chained iff:

$$\mid (var(B_1) \cup \dots \cup var(B_{i-1})) \cap var(B_i) \mid \leq 1$$

Summary

- KG embedding as means to resolve trade-off

  ML-feasible geometric structures vs. logical semantics

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Thanks for your attention!

References

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  http://www.inf.unibz.it/~calvanese/teaching/2010-08-ESSLLI-DL-QA/
- Reasoning Web Summer School 2014 course by Kontchakov on Description Logics
  http://rw2014.di.uoa.gr/sites/default/files/slides/An_Introduction_to_Description_Logics.pdf
- Lecture notes by Calvanese in 2013/2014 course on Ontology and Database Systems
  https://www.inf.unibz.it/~calvanese/teaching/14-15-odbs/lecture-notes/
- Course notes by Franz Baader on Description Logics
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