Expressive and Geometrically Interpretable Knowledge Graph Embeddings

Aleksandar Pavlović and Emanuel Sallinger

TU Wien

AIROV 2024

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ExpressivE, ICLR 2023

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ExpressivE, ICLR 2023

SpeedE, NAACL 2024

AIROV 2024

Knowledge Graph Completion

- Knowledge graphs are highly incomplete
  - 75% of the triples of Freebase lack a nationality (West et al., 2014)

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  - 75% of the triples of Freebase lack a nationality (West et al., 2014)
- Knowledge graph completion (KGC)
  - Automatically infer missing triples
- Knowledge graph embedding models (KGEs)
  - Embed knowledge graphs into vector spaces

Knowledge Graphs

Knowledge Graphs

(head)

Elisabeth

Knowledge Graphs

(head)
Elisabeth

mother_of →

Knowledge Graphs

Knowledge Graph Embedding Models

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- Functional Models
  - TransE (Bordes et al., 2013), RotatE (Sun et al., 2019)

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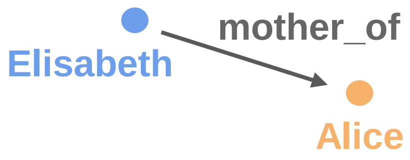

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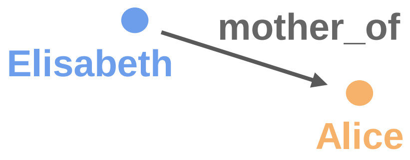

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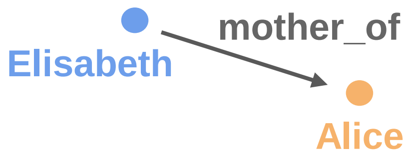

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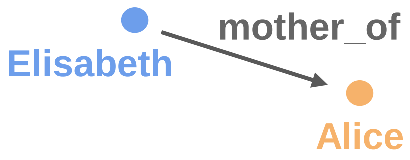

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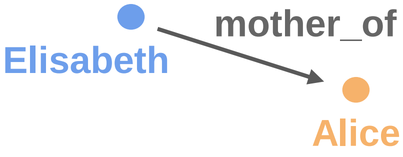

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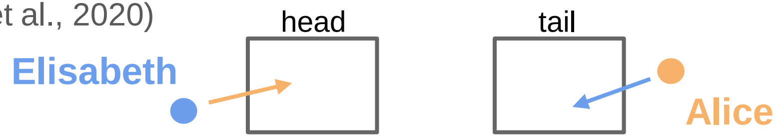

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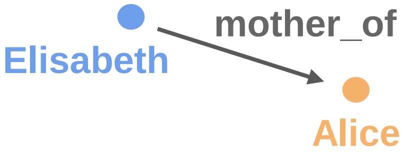

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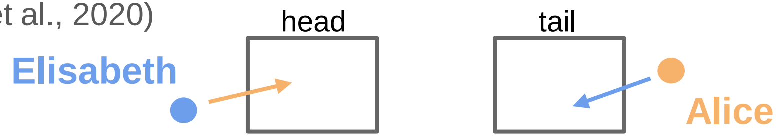

- Bilinear Models
  - ComplEx (Trouillon et al., 2016), TuckER (Balazevic et al., 2019)

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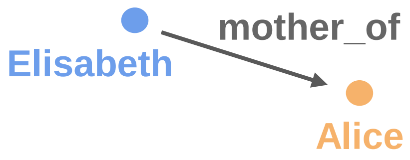

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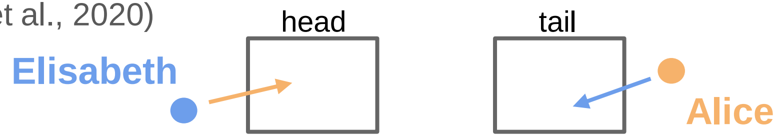

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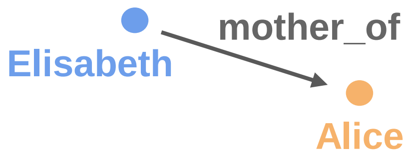

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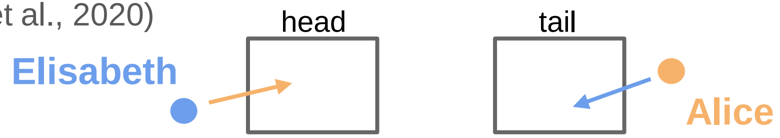

- Bilinear Models
  - ComplEx (Trouillon et al., 2016), TuckER (Balazevic et al., 2019)

- Neural Models

Inference Patterns

- Generalization capabilities

Inference Pattern
Symmetry: $r_1(X,Y) \Rightarrow r_1(Y,X)$
Anti-symmetry: $r_1(X,Y) \Rightarrow \neg r_1(Y,X)$
Inversion: $r_1(X,Y) \Leftrightarrow r_2(Y,X)$
Comp. def.: $r_1(X,Y) \wedge r_2(Y,Z) \Leftrightarrow r_3(X,Z)$
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Inference Patterns

- Generalization capabilities
  - Analyzing inference patterns that can be captured by a model

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Inference Patterns

- Generalization capabilities
  - Analyzing inference patterns that can be captured by a model
  - Hierarchy and composition are fundamental patterns that have been extensively studied:
    - (Bordes et al., 2013; Sun et al., 2019; Zhang et al., 2019; Lu & Hu, 2020, Yang et al., 2015a; Trouillon et al., 2016; Kazemi & Poole, 2018; Abboud et al., 2020)

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Inference Patterns

- Bilinear and Spatial Models
  - **Can** represent **hierarchy patterns** (Trouillon et al., 2016; Abboud et al., 2020)

Inference Pattern	BoxE	ComplEx	DistMult
Symmetry: $r_1(X, Y) \Rightarrow r_1(Y, X)$	✓	✓	✓
Anti-symmetry: $r_1(X, Y) \Rightarrow \neg r_1(Y, X)$	✓	✓	✗
Inversion: $r_1(X, Y) \Leftrightarrow r_2(Y, X)$	✓	✓	✗
Comp. def.: $r_1(X, Y) \wedge r_2(Y, Z) \Leftrightarrow r_3(X, Z)$	✗	✗	✗
Gen. comp.: $r_1(X, Y) \wedge r_2(Y, Z) \Rightarrow r_3(X, Z)$	✗	✗	✗
Hierarchy: $r_1(X, Y) \Rightarrow r_2(X, Y)$	✓	✓	✓
Intersection: $r_1(X, Y) \wedge r_2(X, Y) \Rightarrow r_3(X, Y)$	✓	✗	✗
Mutual exclusion: $r_1(X, Y) \wedge r_2(X, Y) \Rightarrow \bot$	✓	✓	✓

Inference Patterns

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X mother_of Y ⇒ X parent_of Y

Inference Pattern	BoxE	ComplEx	DistMult
Symmetry: $r_1(X, Y) \Rightarrow r_1(Y, X)$	✓	✓	✓
Anti-symmetry: $r_1(X, Y) \Rightarrow \neg r_1(Y, X)$	✓	✓	✗
Inversion: $r_1(X, Y) \Leftrightarrow r_2(Y, X)$	✓	✓	✗
Comp. def.: $r_1(X, Y) \wedge r_2(Y, Z) \Leftrightarrow r_3(X, Z)$	✗	✗	✗
Gen. comp.: $r_1(X, Y) \wedge r_2(Y, Z) \Rightarrow r_3(X, Z)$	✗	✗	✗
Hierarchy: $r_1(X, Y) \Rightarrow r_2(X, Y)$	✓	✓	✓
Intersection: $r_1(X, Y) \wedge r_2(X, Y) \Rightarrow r_3(X, Y)$	✓	✗	✗
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Inference Patterns

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  - **Can** represent **hierarchy patterns** (Trouillon et al., 2016; Abboud et al., 2020)
  - **Cannot** represent any notion of **composition** (Sun et al., 2019; Abboud et al., 2020)

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Anti-symmetry: $r_1(X,Y) \Rightarrow \neg r_1(Y,X)$	✓	✓	✗
Inversion: $r_1(X,Y) \Leftrightarrow r_2(Y,X)$	✓	✓	✗
Comp. def.: $r_1(X,Y) \wedge r_2(Y,Z) \Leftrightarrow r_3(X,Z)$	✗	✗	✗
Gen. comp.: $r_1(X,Y) \wedge r_2(Y,Z) \Rightarrow r_3(X,Z)$	✗	✗	✗
Hierarchy: $r_1(X,Y) \Rightarrow r_2(X,Y)$	✓	✓	✓
Intersection: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow r_3(X,Y)$	✓	✗	✗
Mutual exclusion: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow \bot$	✓	✓	✓

Inference Patterns

- Functional Models
  - Can represent a limited notion of composition (Zhang et al., 2019; Abboud et al., 2020; Lu & Hu, 2020; Gao et al., 2020)

X mother_of Y ∧ Y parent_of Z ⇔ X grand_mother_of Z

Inference Pattern	RotatE	TransE
Symmetry: $r_1(X,Y) \Rightarrow r_1(Y,X)$	✓	✗
Anti-symmetry: $r_1(X,Y) \Rightarrow \neg r_1(Y,X)$	✓	✓
Inversion: $r_1(X,Y) \Leftrightarrow r_2(Y,X)$	✓	✓
Comp. def.: $r_1(X,Y) \wedge r_2(Y,Z) \Leftrightarrow r_3(X,Z)$	✓	✓
Gen. comp.: $r_1(X,Y) \wedge r_2(Y,Z) \Rightarrow r_3(X,Z)$	✗	✗
Hierarchy: $r_1(X,Y) \Rightarrow r_2(X,Y)$	✗	✗
Intersection: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow r_3(X,Y)$	✓	✓
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Symmetry: $r_1(X,Y) \Rightarrow r_1(Y,X)$	✓	✗
Anti-symmetry: $r_1(X,Y) \Rightarrow \neg r_1(Y,X)$	✓	✓
Inversion: $r_1(X,Y) \Leftrightarrow r_2(Y,X)$	✓	✓
Comp. def.: $r_1(X,Y) \wedge r_2(Y,Z) \Leftrightarrow r_3(X,Z)$	✓	✓
Gen. comp.: $r_1(X,Y) \wedge r_2(Y,Z) \Rightarrow r_3(X,Z)$	✗	✗
Hierarchy: $r_1(X,Y) \Rightarrow r_2(X,Y)$	✗	✗
Intersection: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow r_3(X,Y)$	✓	✓
Mutual exclusion: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow \perp$	✓	✓

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X mother_of Y ∧ Y parent_of Z ⇒ X grand_parent_of Z
X father_of Y ∧ Y parent_of Z ⇒ X grand_parent_of Z

mother_of = father_of

(Abboud et al., 2020)

Inference Pattern	RotatE	TransE
Symmetry: $r_1(X,Y) \Rightarrow r_1(Y,X)$	✓	✗
Anti-symmetry: $r_1(X,Y) \Rightarrow \neg r_1(Y,X)$	✓	✓
Inversion: $r_1(X,Y) \Leftrightarrow r_2(Y,X)$	✓	✓
Comp. def.: $r_1(X,Y) \wedge r_2(Y,Z) \Leftrightarrow r_3(X,Z)$	✓	✓
Gen. comp.: $r_1(X,Y) \wedge r_2(Y,Z) \Rightarrow r_3(X,Z)$	✗	✗
Hierarchy: $r_1(X,Y) \Rightarrow r_2(X,Y)$	✗	✗
Intersection: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow r_3(X,Y)$	✓	✓
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Gen. comp.: $r_1(X,Y) \wedge r_2(Y,Z) \Rightarrow r_3(X,Z)$	✗	✗
Hierarchy: $r_1(X,Y) \Rightarrow r_2(X,Y)$	✗	✗
Intersection: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow r_3(X,Y)$	✓	✓
Mutual exclusion: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow \bot$	✓	✓

Challenge: Inference Patterns

Inference Pattern	RotatE	TransE	BoxE	ComplEx	DistMult
Symmetry: $r_1(X,Y) \Rightarrow r_1(Y,X)$	✓	✗	✓	✓	✓
Anti-symmetry: $r_1(X,Y) \Rightarrow \neg r_1(Y,X)$	✓	✓	✓	✓	✗
Inversion: $r_1(X,Y) \Leftrightarrow r_2(Y,X)$	✓	✓	✓	✓	✗
Comp. def.: $r_1(X,Y) \wedge r_2(Y,Z) \Leftrightarrow r_3(X,Z)$	✓	✓	✗	✗	✗
Gen. comp.: $r_1(X,Y) \wedge r_2(Y,Z) \Rightarrow r_3(X,Z)$	✗	✗	✗	✗	✗
Hierarchy: $r_1(X,Y) \Rightarrow r_2(X,Y)$	✗	✗	✓	✓	✓
Intersection: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow r_3(X,Y)$	✓	✓	✓	✗	✗
Mutual exclusion: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow \bot$	✓	✓	✓	✓	✓

Challenge: Inference Patterns

- Challenge 1:
  - Contemporary KGEs cannot capture **general** composition

Inference Pattern	RotatE	TransE	BoxE	ComplEx	DistMult
Symmetry: $r_1(X,Y) \Rightarrow r_1(Y,X)$	✓	✗	✓	✓	✓
Anti-symmetry: $r_1(X,Y) \Rightarrow \neg r_1(Y,X)$	✓	✓	✓	✓	✗
Inversion: $r_1(X,Y) \Leftrightarrow r_2(Y,X)$	✓	✓	✓	✓	✗
Comp. def.: $r_1(X,Y) \wedge r_2(Y,Z) \Leftrightarrow r_3(X,Z)$	✓	✓	✗	✗	✗
Gen. comp.: $r_1(X,Y) \wedge r_2(Y,Z) \Rightarrow r_3(X,Z)$	✗	✗	✗	✗	✗
Hierarchy: $r_1(X,Y) \Rightarrow r_2(X,Y)$	✗	✗	✓	✓	✓
Intersection: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow r_3(X,Y)$	✓	✓	✓	✗	✗
Mutual exclusion: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow \perp$	✓	✓	✓	✓	✓

Challenge: Inference Patterns

- Challenge 1:
  - Contemporary KGEs cannot capture **general** composition

- Challenge 2:
  - Capturing composition **and** hierarchy jointly is an open problem

Inference Pattern	RotatE	TransE	BoxE	ComplEx	DistMult
Symmetry: $r_1(X, Y) \Rightarrow r_1(Y, X)$	✓	✗	✓	✓	✓
Anti-symmetry: $r_1(X, Y) \Rightarrow \neg r_1(Y, X)$	✓	✓	✓	✓	✗
Inversion: $r_1(X, Y) \Leftrightarrow r_2(Y, X)$	✓	✓	✓	✓	✗
Comp. def.: $r_1(X, Y) \wedge r_2(Y, Z) \Leftrightarrow r_3(X, Z)$	✓	✓	✗	✗	✗
Gen. comp.: $r_1(X, Y) \wedge r_2(Y, Z) \Rightarrow r_3(X, Z)$	✗	✗	✗	✗	✗
Hierarchy: $r_1(X, Y) \Rightarrow r_2(X, Y)$	✗	✗	✓	✓	✓
Intersection: $r_1(X, Y) \wedge r_2(X, Y) \Rightarrow r_3(X, Y)$	✓	✓	✓	✗	✗
Mutual exclusion: $r_1(X, Y) \wedge r_2(X, Y) \Rightarrow \perp$	✓	✓	✓	✓	✓

Challenge: Inference Patterns

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- Challenge 2:
  - Capturing composition **and** hierarchy jointly is an open problem

Inference Pattern	ExpressivE	RotatE	TransE	BoxE	ComplEx	DistMult
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Anti-symmetry: $r_1(X,Y) \Rightarrow \neg r_1(Y,X)$	✓	✓	✓	✓	✓	✗
Inversion: $r_1(X,Y) \Leftrightarrow r_2(Y,X)$	✓	✓	✓	✓	✓	✗
Comp. def.: $r_1(X,Y) \wedge r_2(Y,Z) \Leftrightarrow r_3(X,Z)$	✓	✓	✓	✗	✗	✗
Gen. comp.: $r_1(X,Y) \wedge r_2(Y,Z) \Rightarrow r_3(X,Z)$	✓	✗	✗	✗	✗	✗
Hierarchy: $r_1(X,Y) \Rightarrow r_2(X,Y)$	✓	✗	✗	✓	✓	✓
Intersection: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow r_3(X,Y)$	✓	✓	✓	✓	✗	✗
Mutual exclusion: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow \bot$	✓	✓	✓	✓	✓	✓

Challenge: Expressiveness

- Spatial and Bilinear Models
  - **Are** fully expressive (except DistMult (Yang et al., 2015a))

Challenge: Expressiveness

- Spatial and Bilinear Models
    - **Are** fully expressive (except DistMult (Yang et al., 2015a))

- Functional Models
    - Not fully expressive, i.e., **cannot** represent any arbitrary knowledge graph
    - **Struggle** with one-to-many, many-to-one, and many-to-many relations

Challenge: Expressiveness

- Spatial and Bilinear Models
  - **Are** fully expressive (except DistMult (Yang et al., 2015a))

- Functional Models
  - Not fully expressive, i.e., **cannot** represent any arbitrary knowledge graph
  - **Struggle** with one-to-many, many-to-one, and many-to-many relations

- Challenge 3:
  - Model that **is** fully expressive
  - **Can** handle one-to-many, many-to-one, and many-to-many relations
  - While **keeping** the ability of functional models to capture composition

ExpressivE: Model Definition

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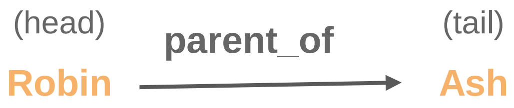

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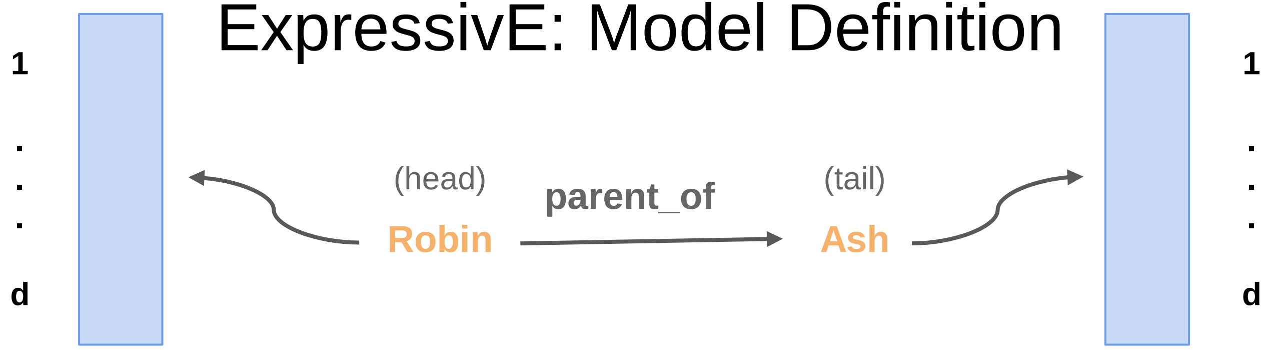

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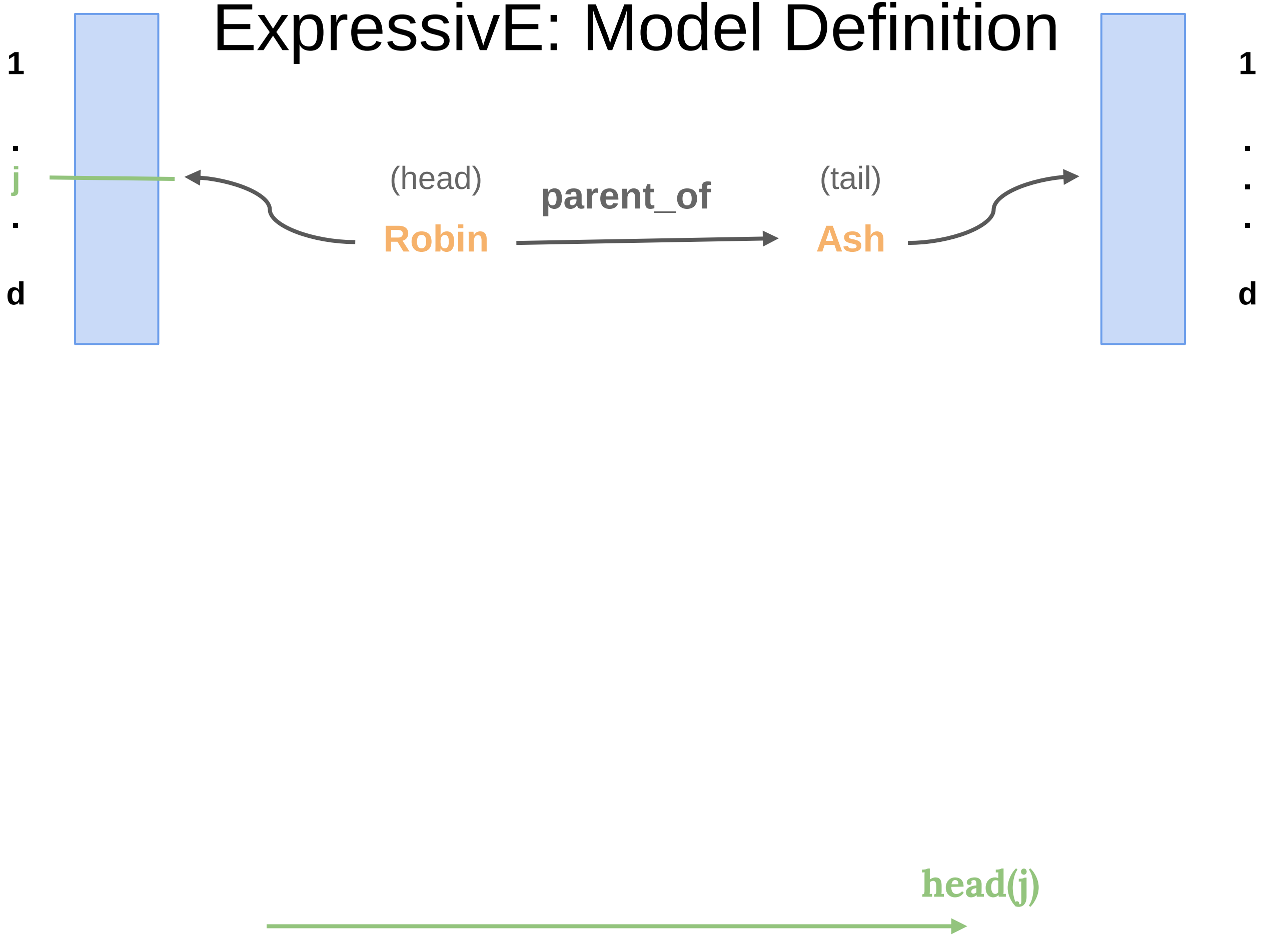

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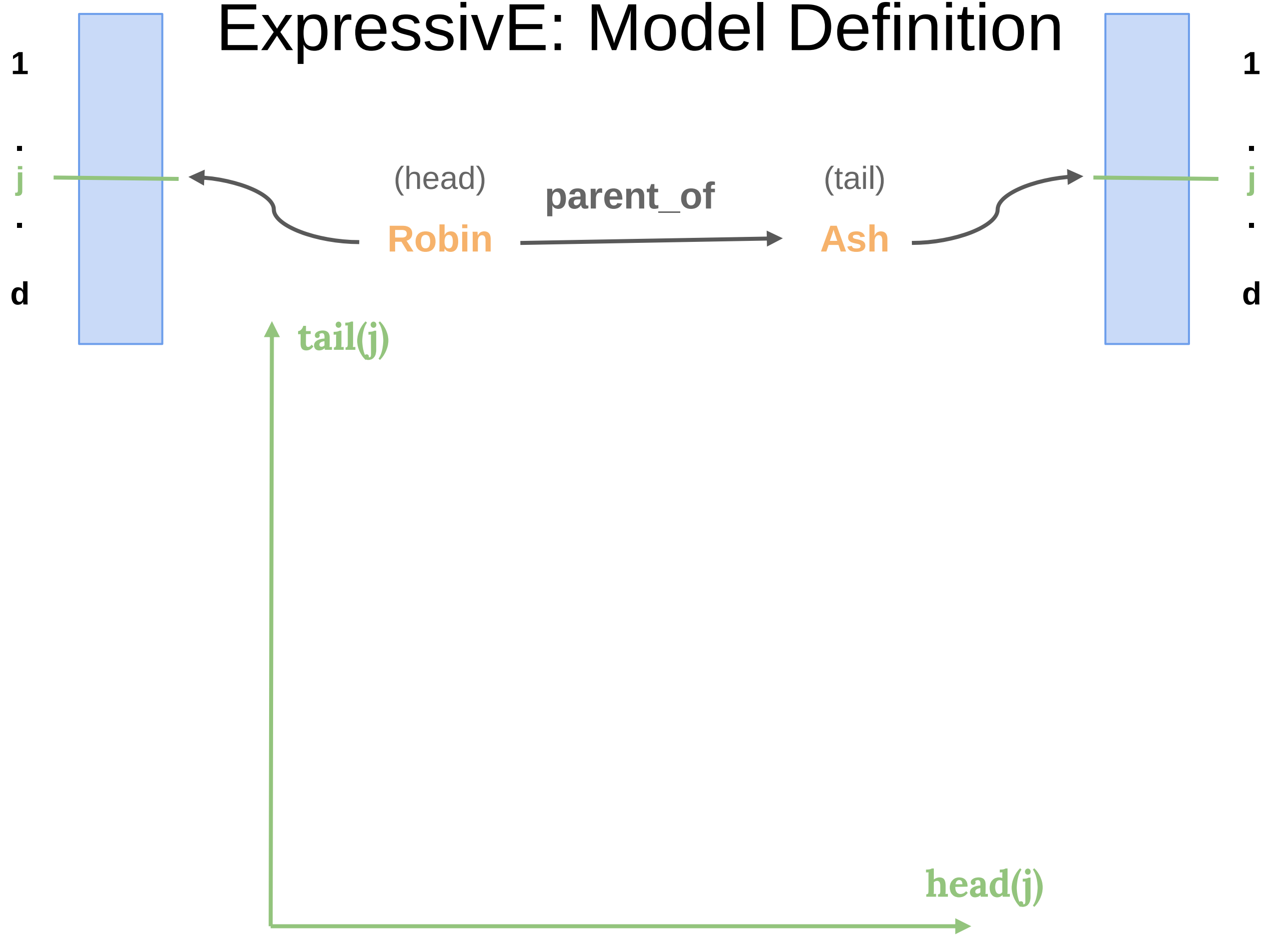

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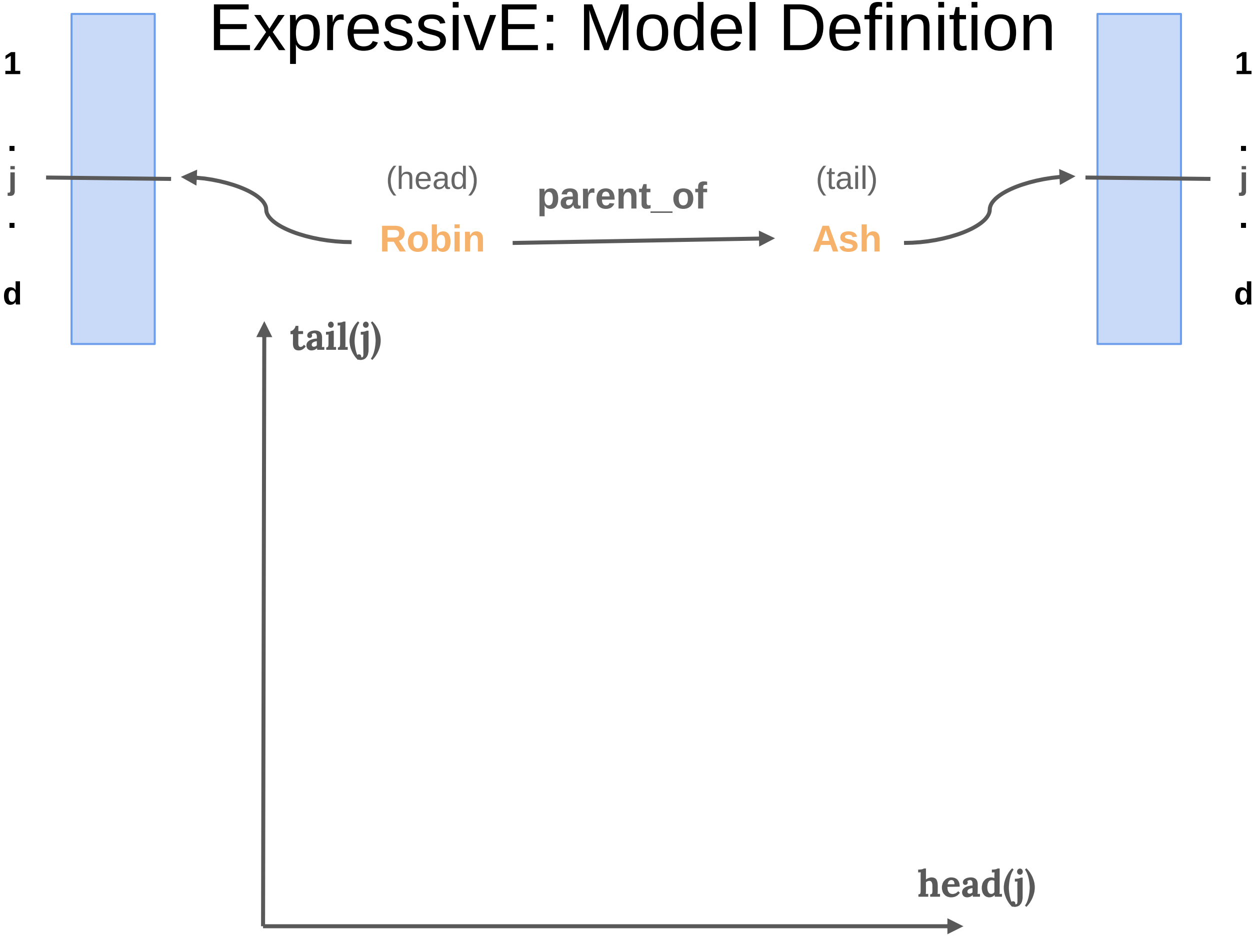

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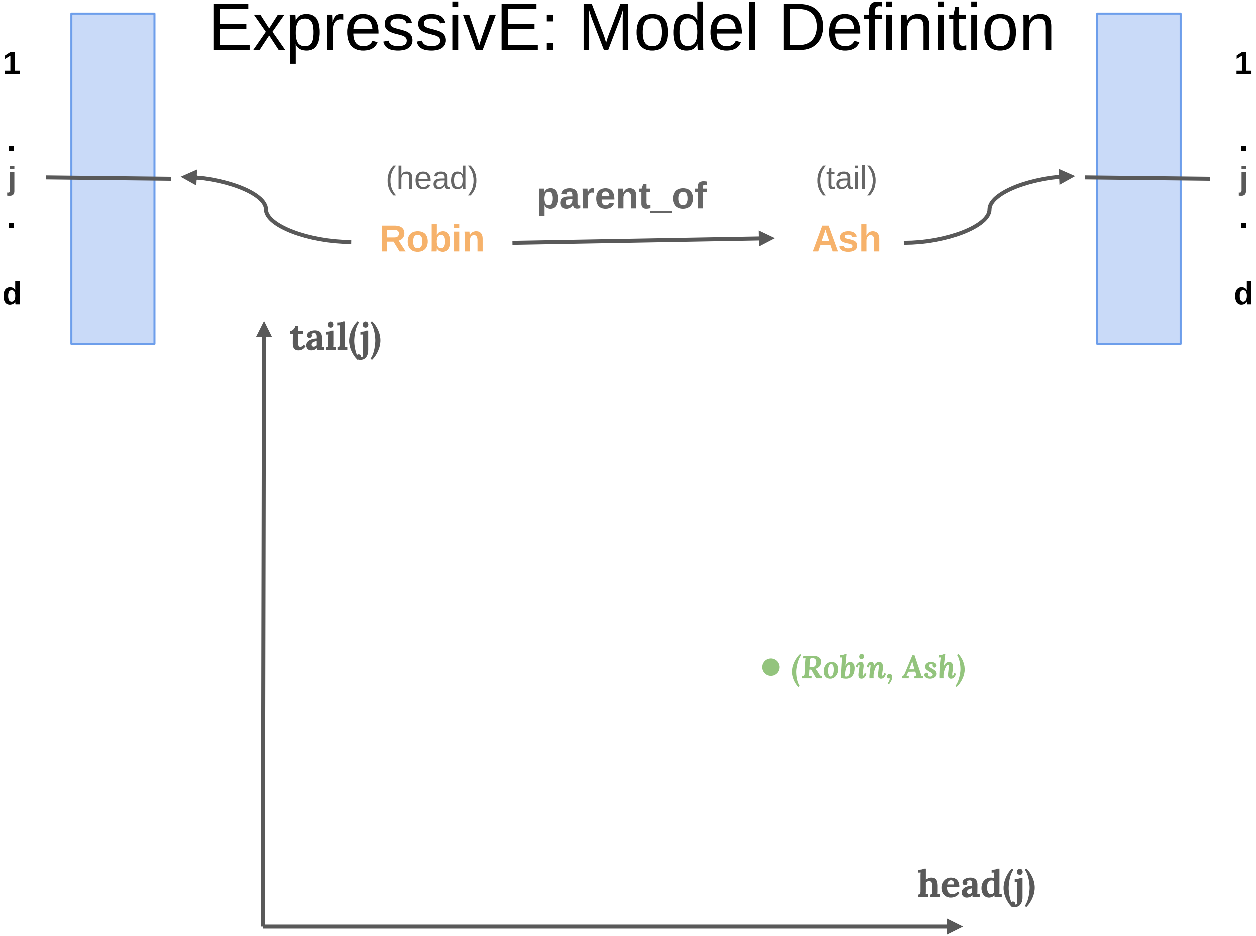

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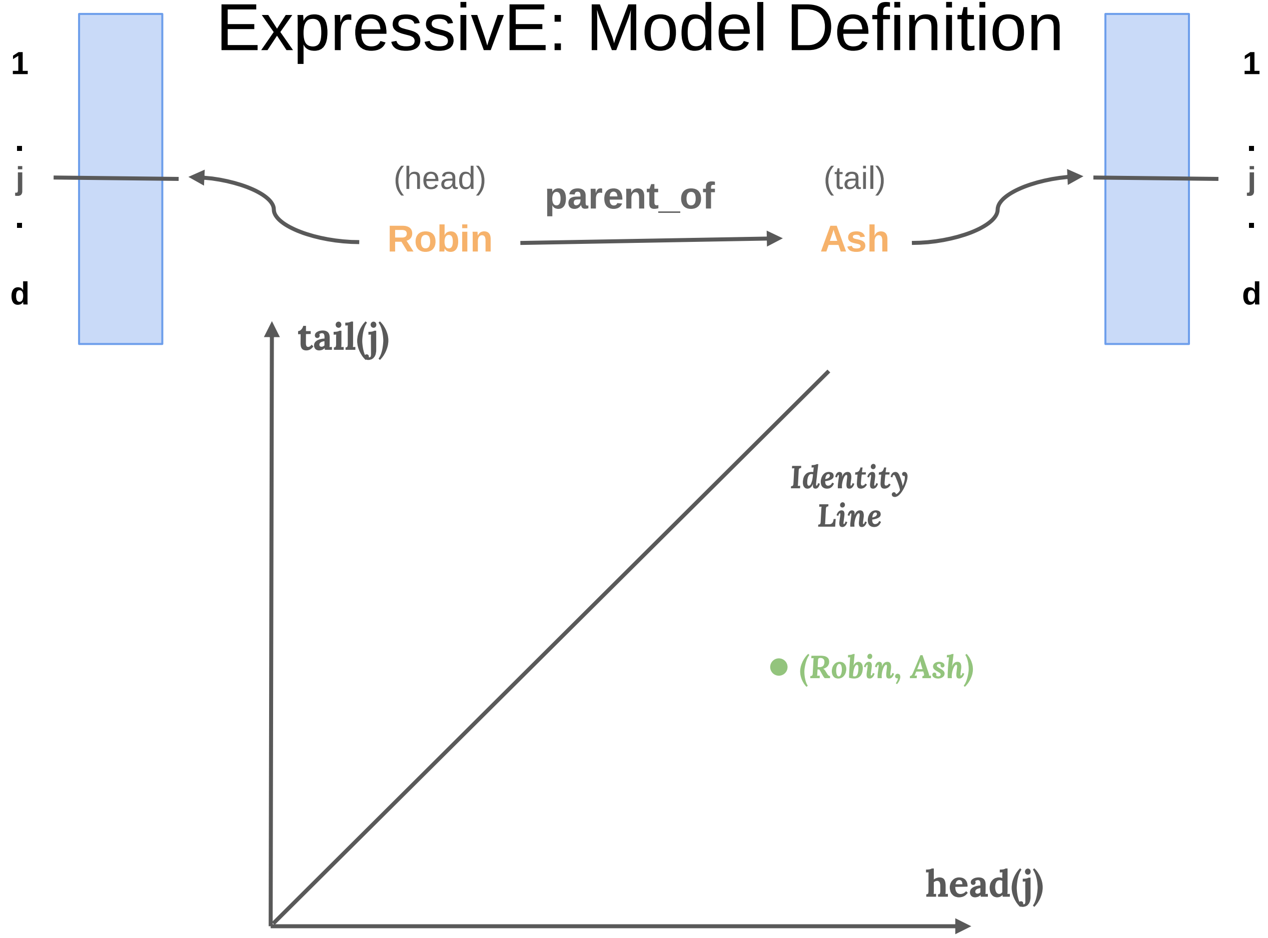

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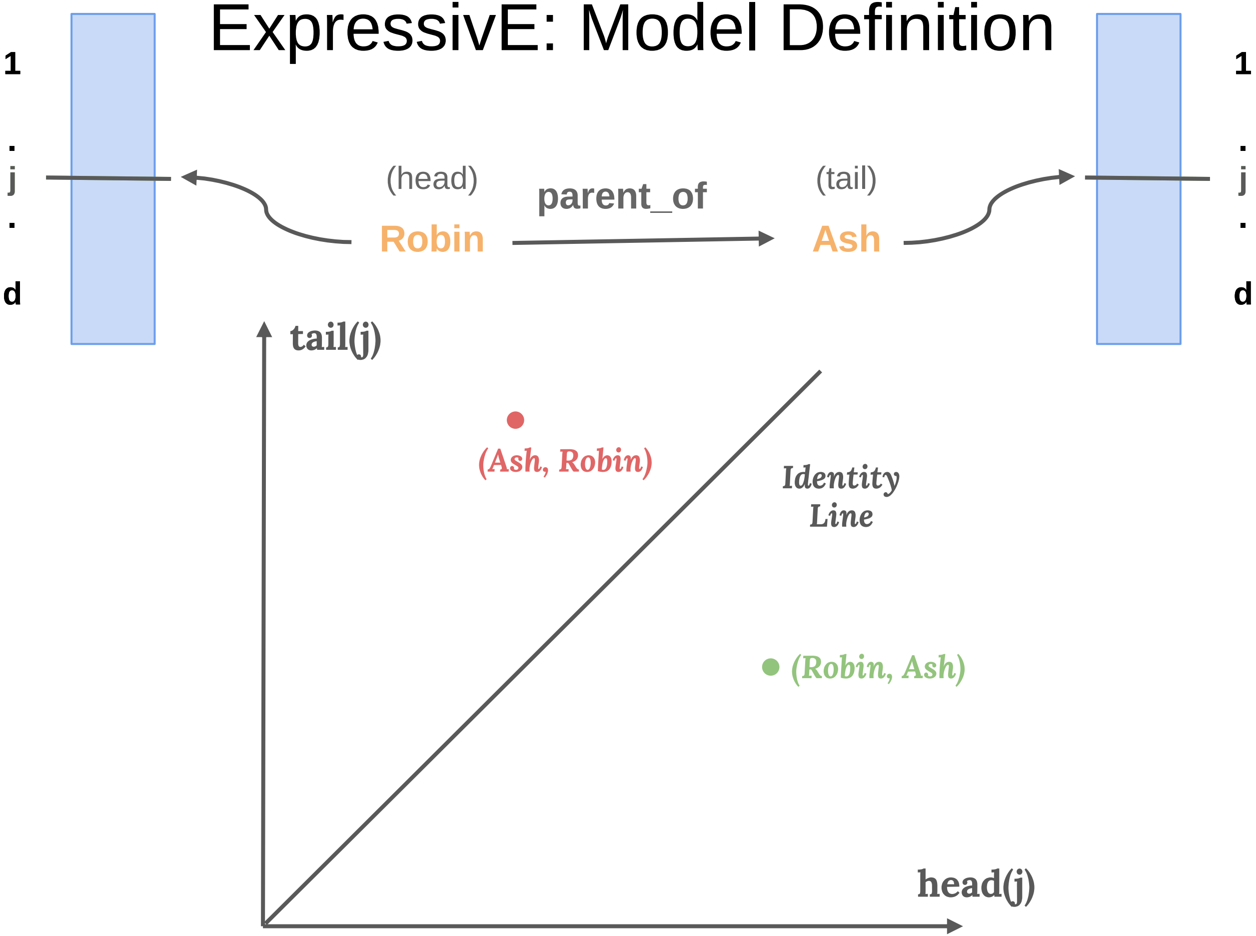

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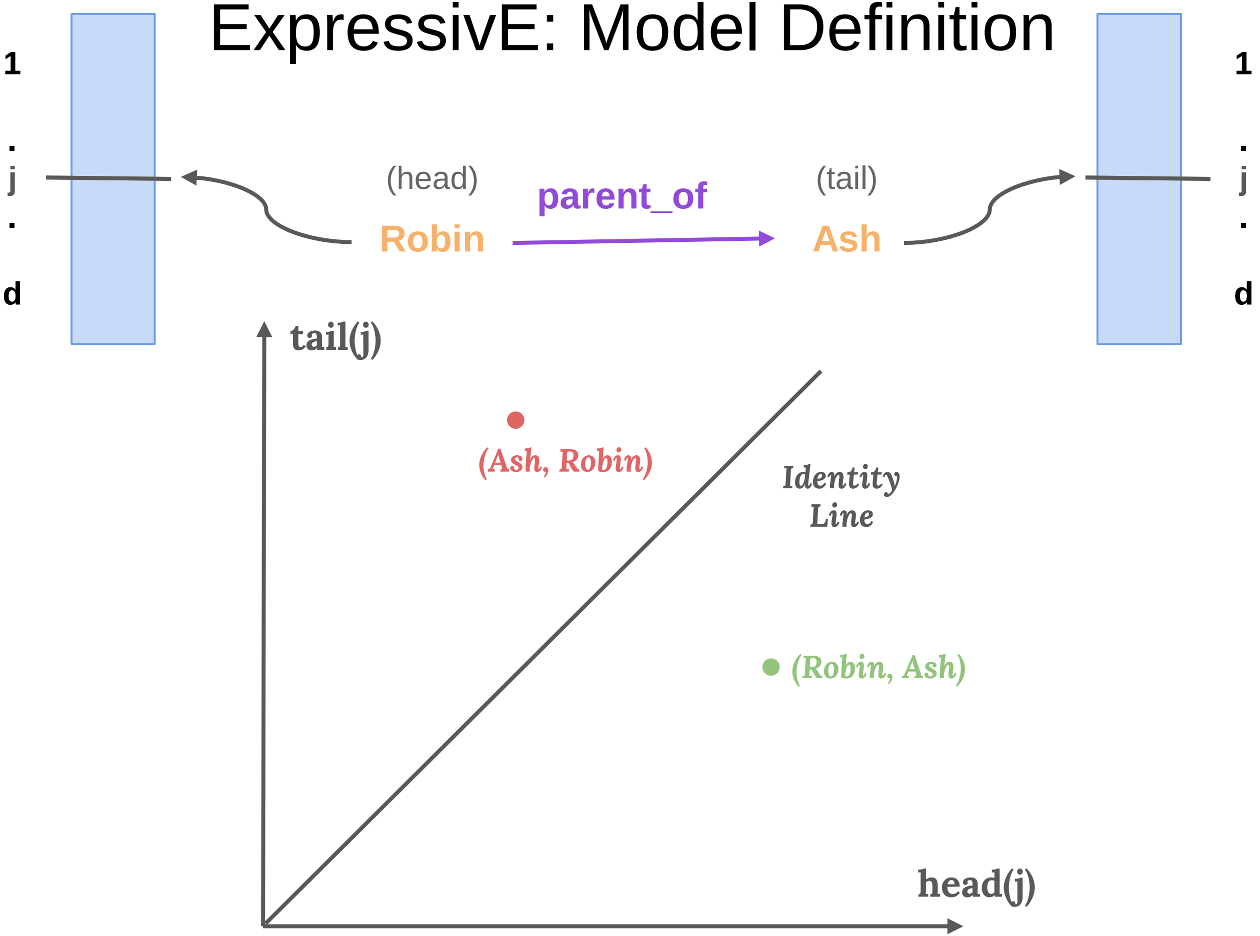

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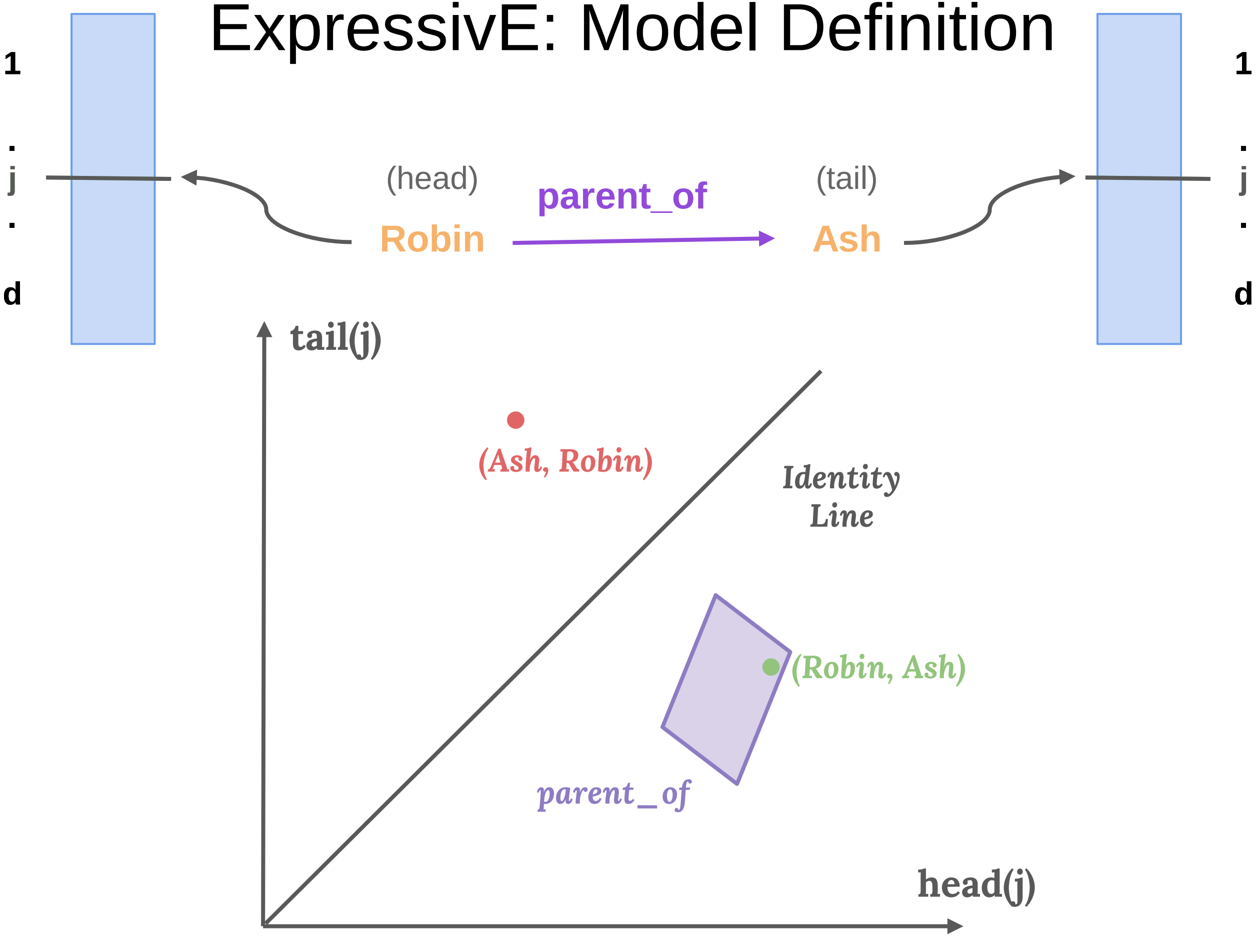

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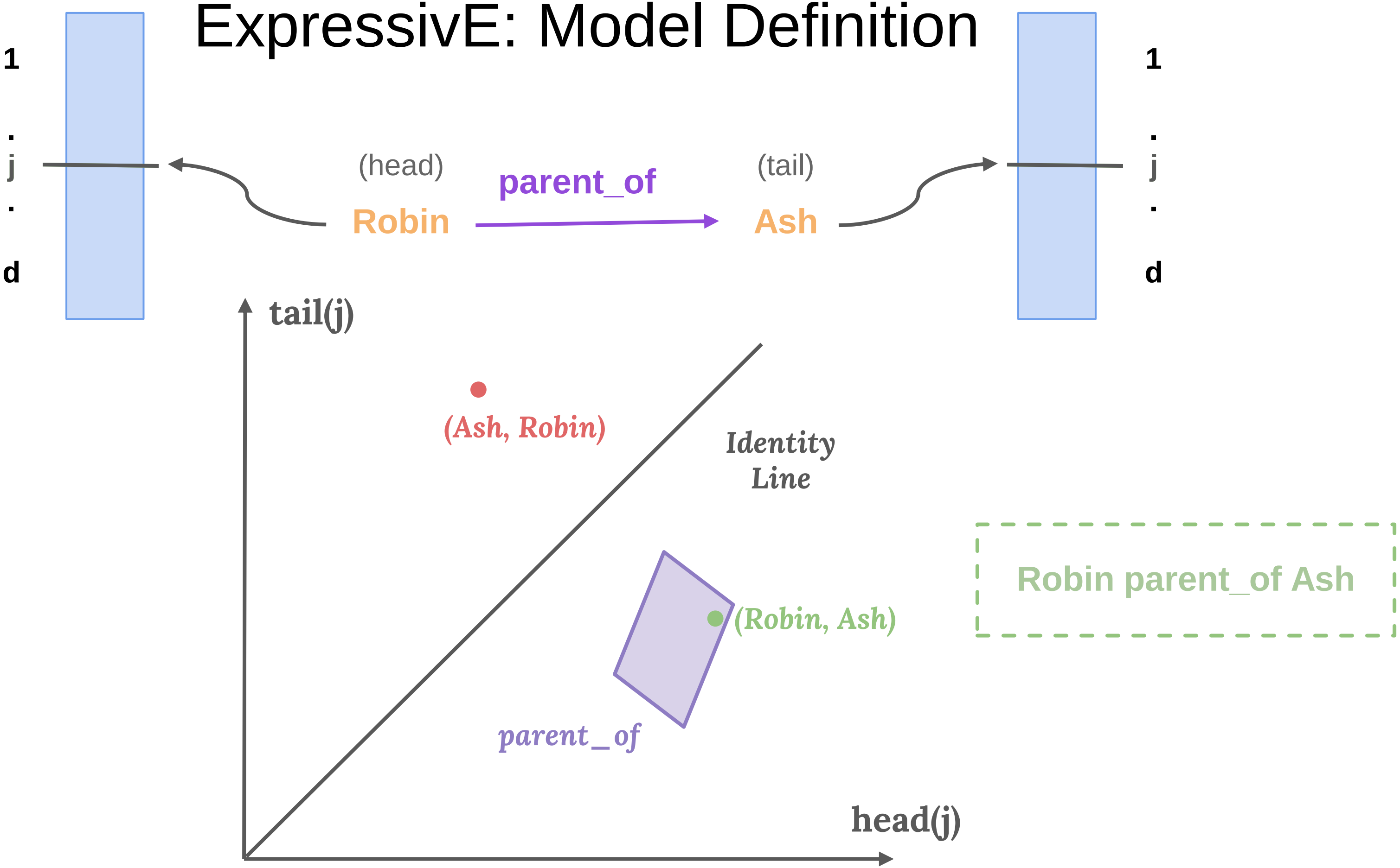

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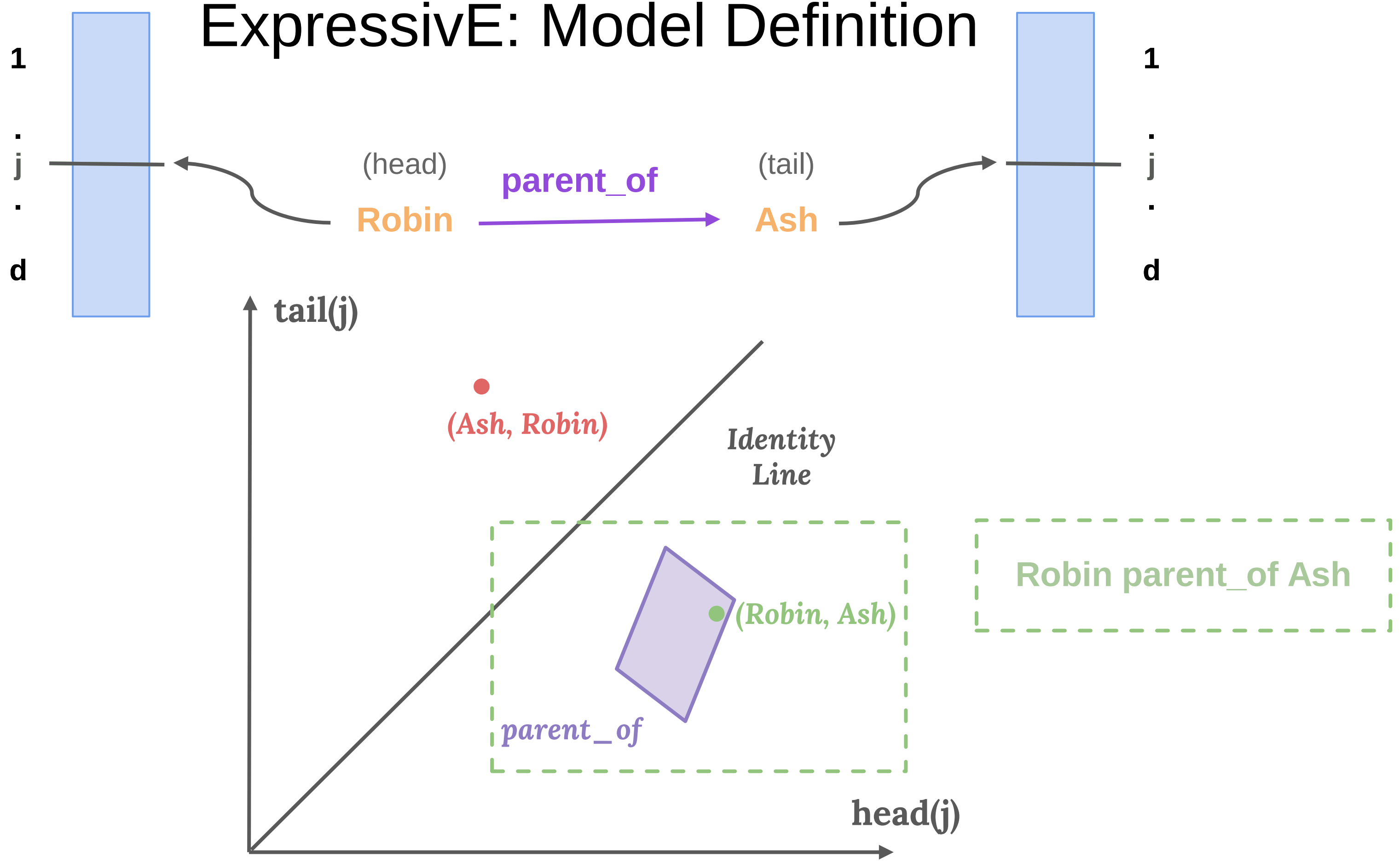

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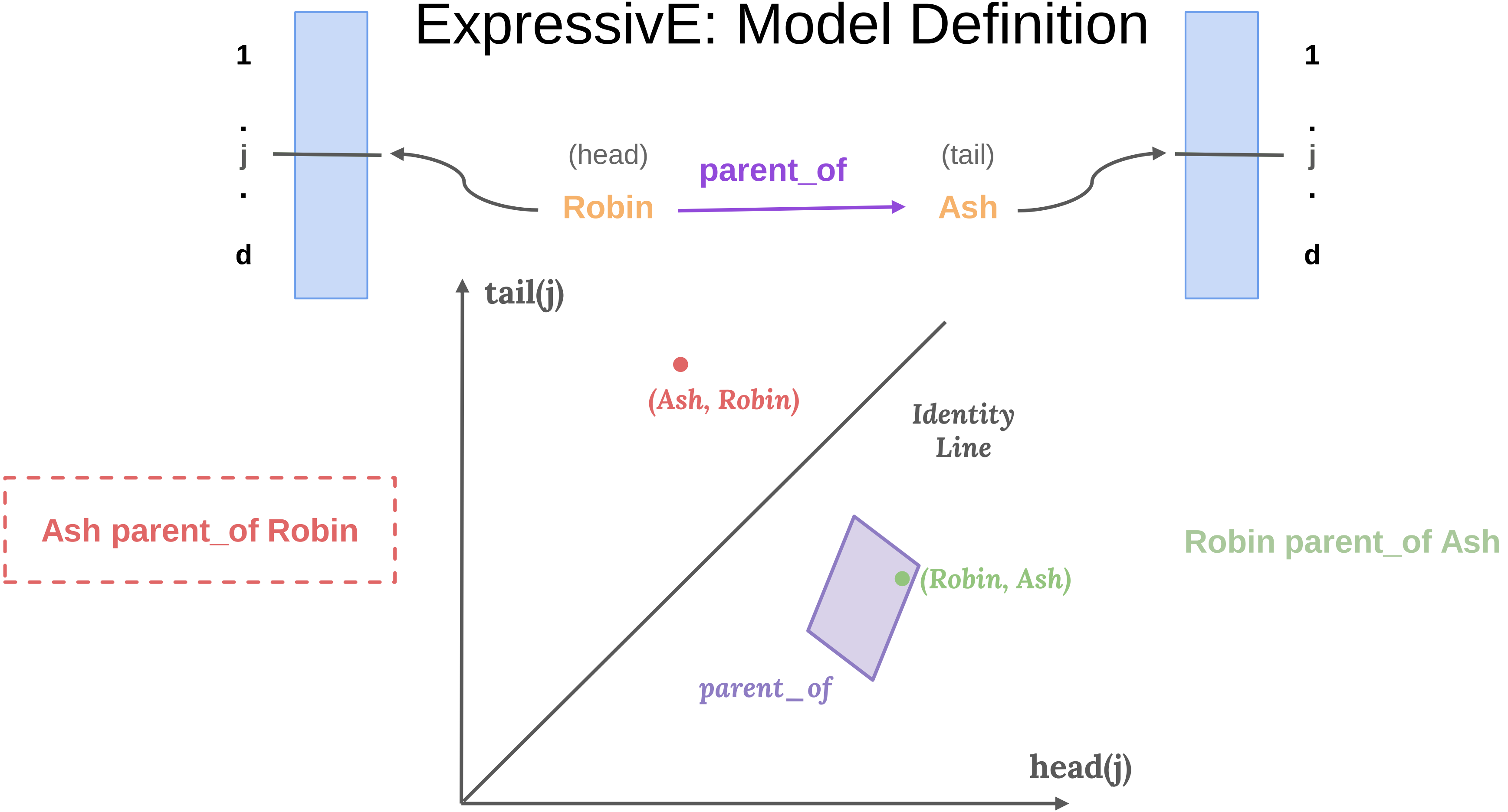

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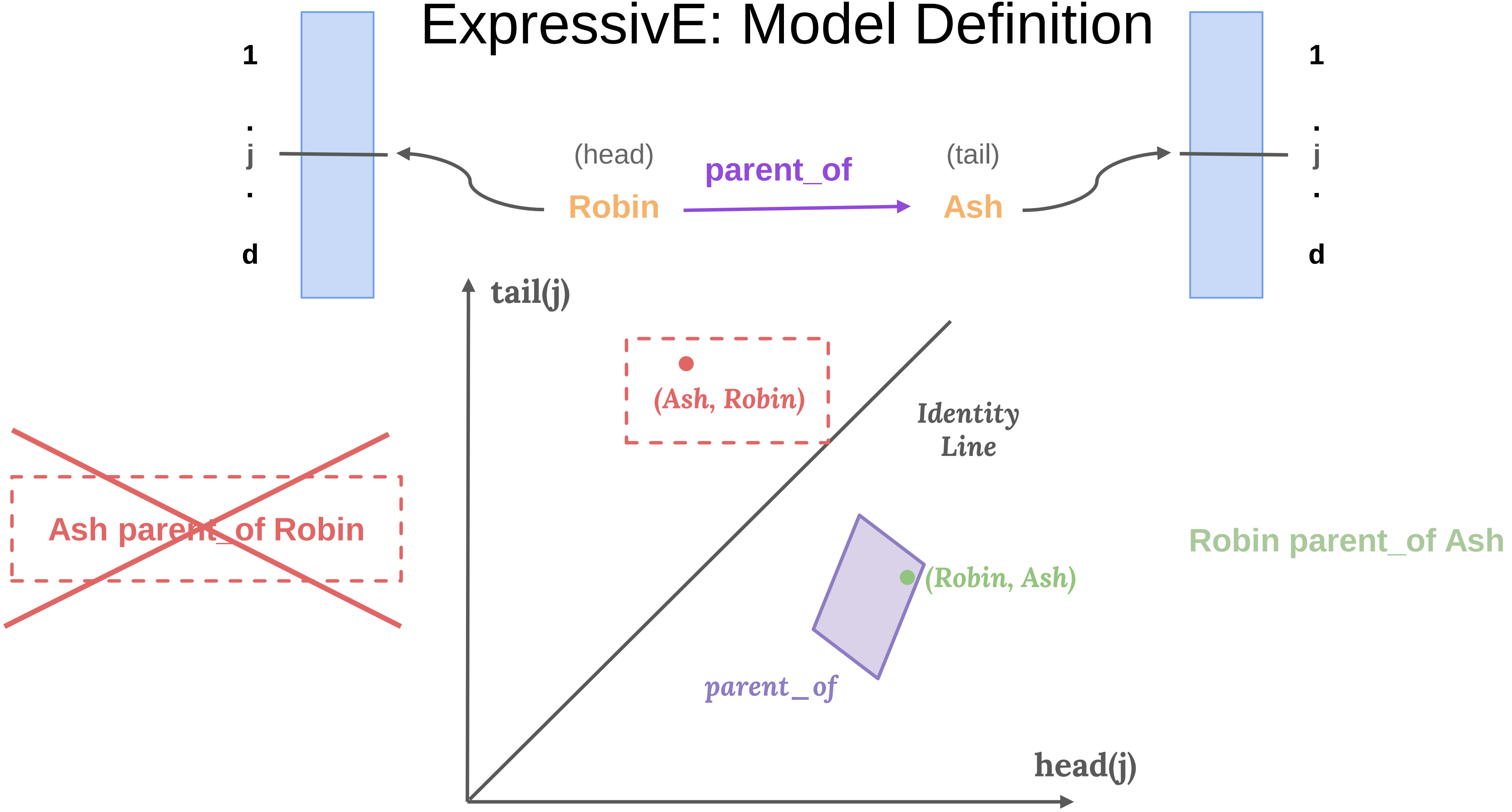

Fully Expressiveness

Theorem 5.1 (Expressive Power) *ExpressivE can capture any arbitrary graph* G *over* $\boldsymbol{R}$ *and* $\boldsymbol{E}$ *if the embedding dimensionality* d *is at least in* $O(|\boldsymbol{E}| * |\boldsymbol{R}|)$.

Generalization Capabilities

Theorem 5.2 *ExpressivE captures (a) symmetry, (b) anti-symmetry, (c) inversion, (d) hierarchy, (e) intersection, and (f) mutual exclusion.*

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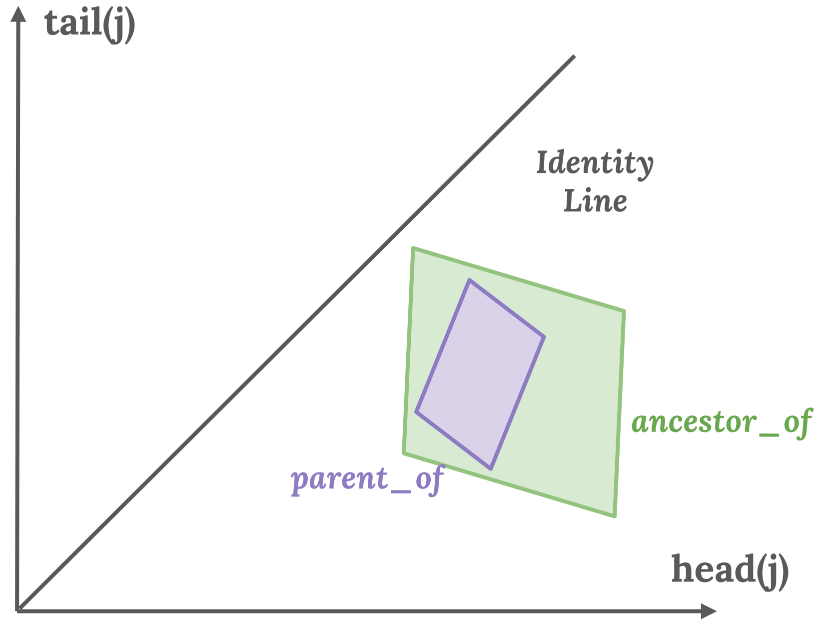

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Theorem 5.4 *ExpressivE captures compositional definition and general composition.*

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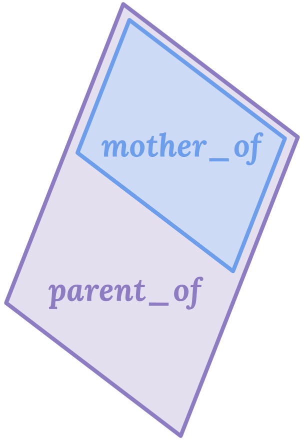
X mother_of Y ∧ Y parent_of Z ⇔ X grand_mother_of Z



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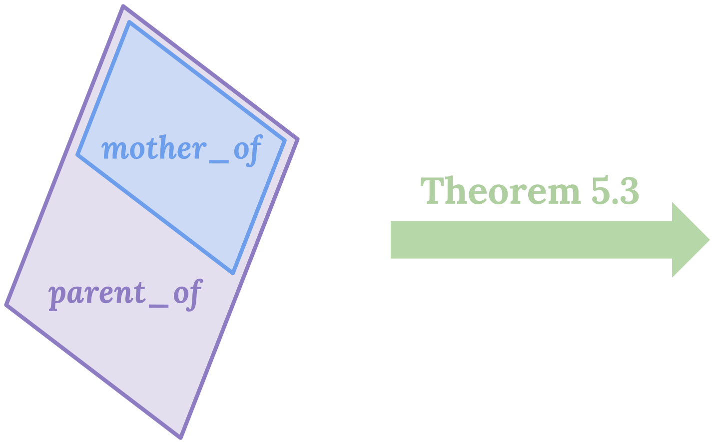

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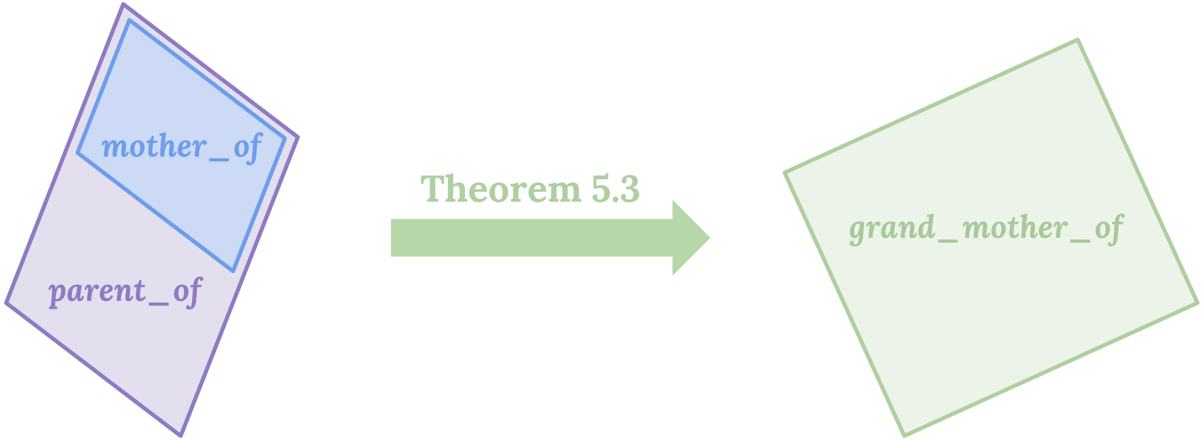

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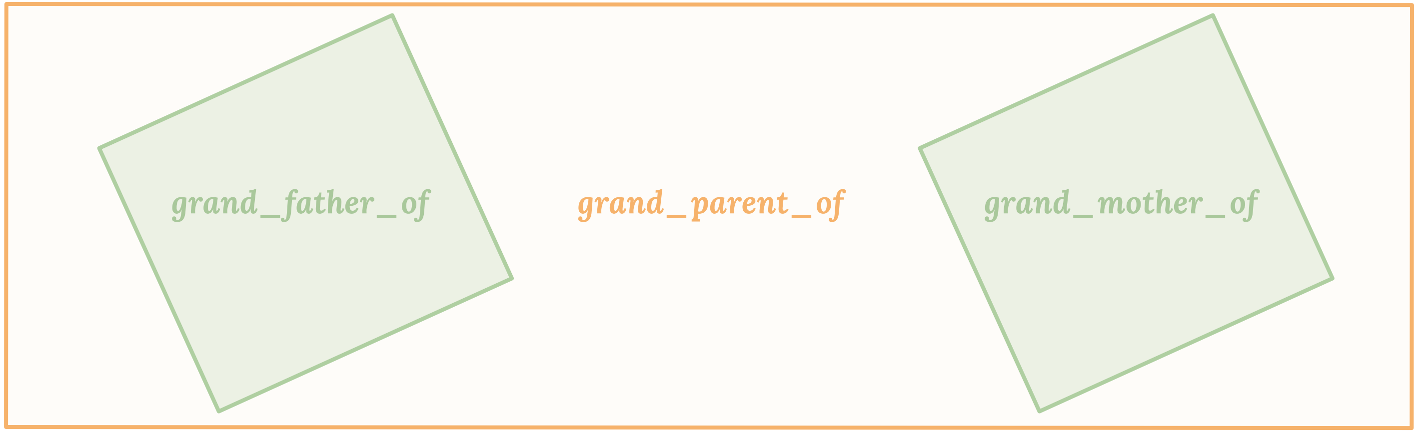

Evaluation on KGC

Family	Model	WN18RR				FB15k-237			
		H@1	H@3	H@10	MRR	H@1	H@3	H@10	MRR
Func. & Spatial	Base ExpressivE	**.464**	**.522**	.597	**.508**	.243	.366	.512	.333
	Func. ExpressivE	.407	.519	**.619**	.482	**.256**	**.387**	.535	**.350**
	BoxE	.400	.472	.541	.451	.238	.374	**.538**	.337
	RotatE	.428	.492	.571	.476	.241	.375	.533	.338
	TransE	.013	.401	.529	.223	.233	.372	.531	.332
Bilinear	DistMult	-	-	.531	.452	-	-	.531	.343
	ComplEx	-	-	**.547**	**.475**	-	-	.536	.348
	TuckER	**.443**	**.482**	.526	.470	**.266**	**.394**	**.544**	**.358**

Best-published MRR and Hit@K:
BoxE: (Abboud et al., 2020)
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Benchmark	Dimensionality	ExpressivE	BoxE	RotatE
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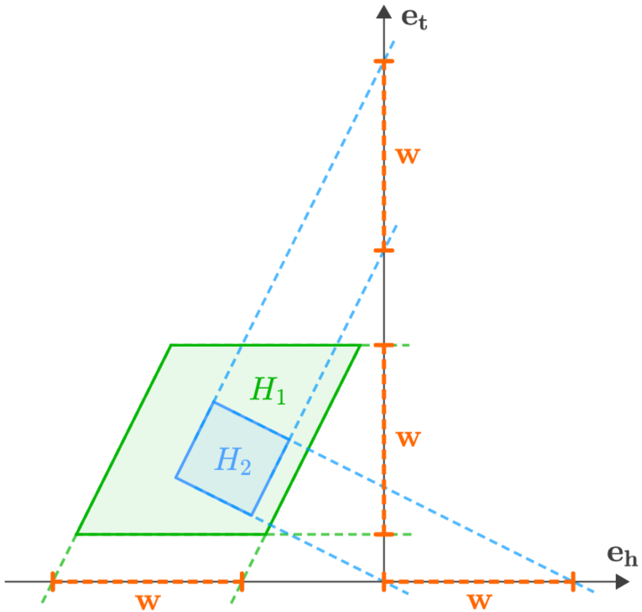

Extension of ExpressivE: SpeedE

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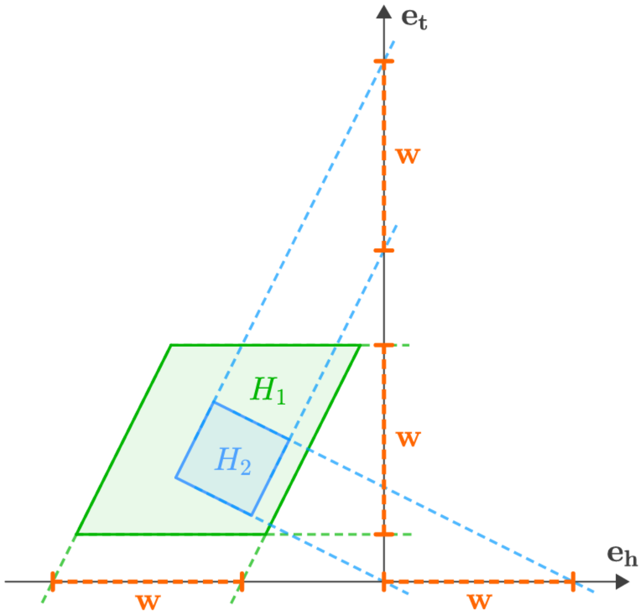

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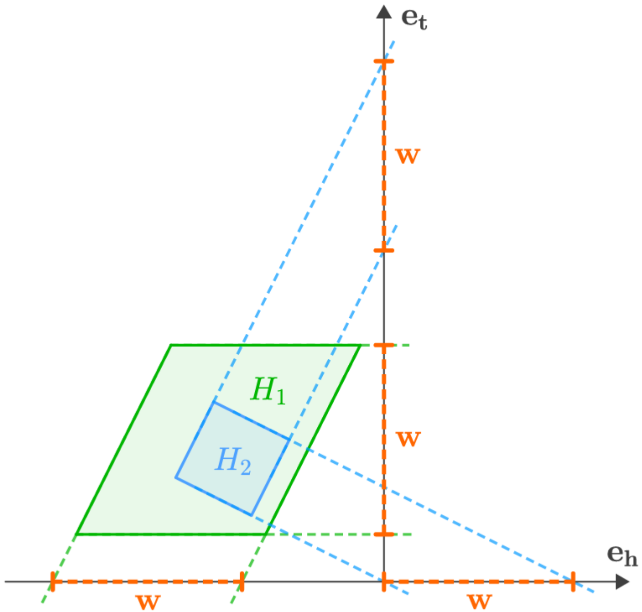

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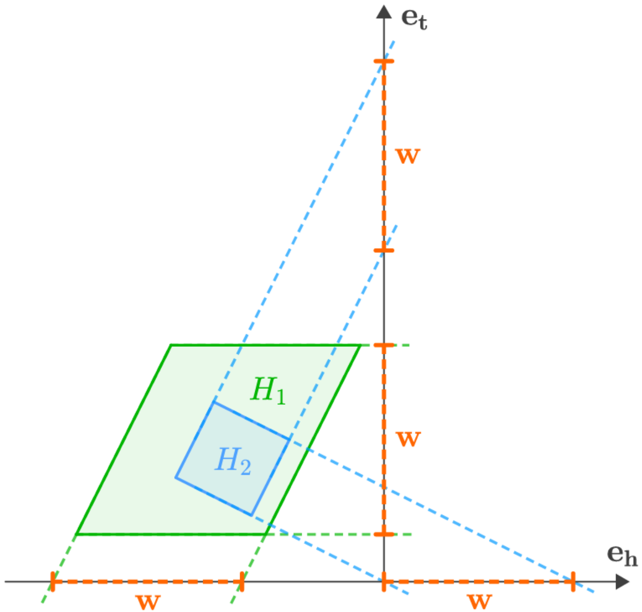

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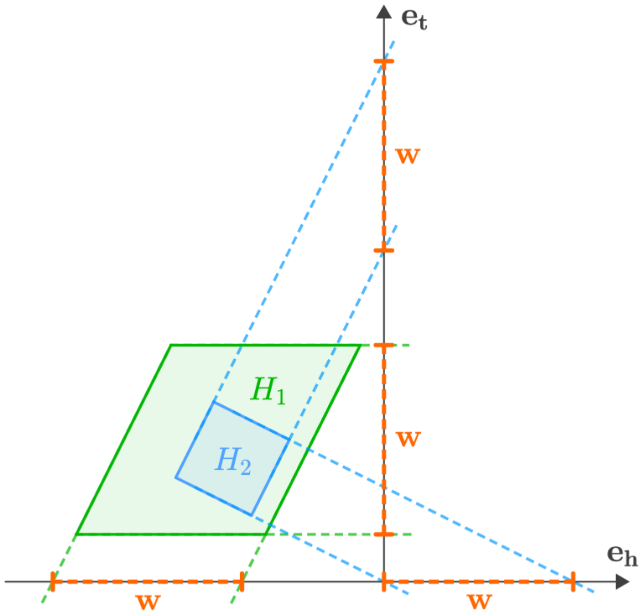

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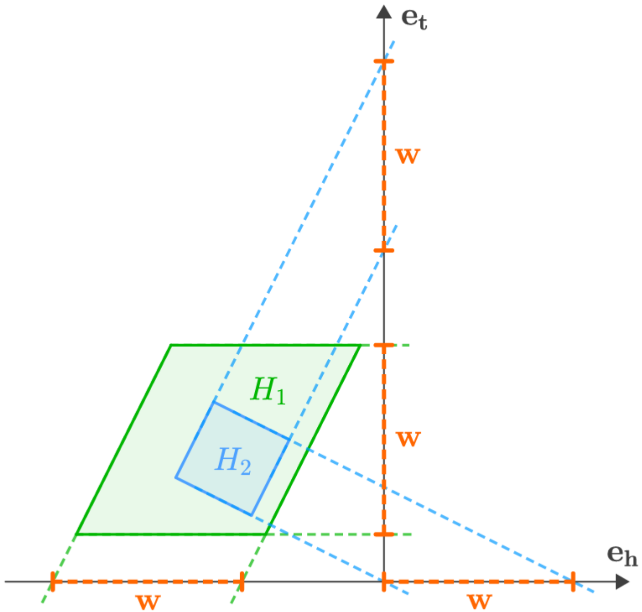
  - Increased space and time efficiency
    - Allows application in **low-resource** settings



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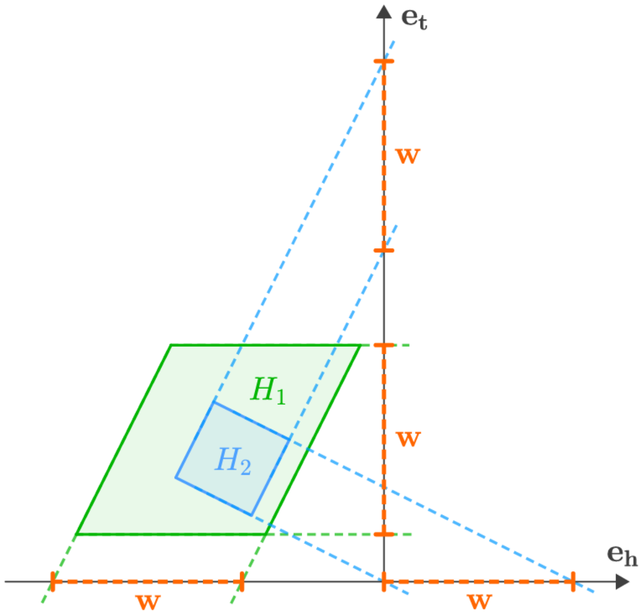
- SpeedE's advancements
  - **Higher scalability**
  - Increased space and time efficiency
    - Allows application in **low-resource** settings
  - Increased KGC prediction performance
    - Especially for **low-dimensional** embeddings



SpeedE: Low-Dimensional KGC

Space	Model	WN18RR				FB15k-237				YAGO3-10			
		MRR	H@1	H@3	H@10	MRR	H@1	H@3	H@10	MRR	H@1	H@3	H@10

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	MuRE	.458	.421	.471	.525	.313	.226	.340	.489	.283	.187	.317	.478
	RefE	.455	.419	.470	.521	.302	.216	.330	.474	.370	.289	.403	.527
	RotE	.463	.426	.477	.529	.307	.220	.337	.482	.381	.295	.417	.548
	AttE	.456	.419	.471	.526	.311	.223	.339	.488	.374	.290	.410	.537
	HAKE	.416	.389	.427	.467	.296	.212	.323	.463	.253	.164	.286	.430
Non-Euclidean	RotatE	.387	.330	.417	.491	.290	.208	.316	.458	.235	.153	.260	.410
	ComplEx-N3	.420	.390	.420	.460	.294	.211	.322	.463	.336	.259	.367	.484
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	RefH	.447	.408	.464	.518	.312	.224	.342	.489	.381	.302	.415	.530
	RotH	**.472**	.428	**.490**	**.553**	.314	.223	.346	.497	.393	.307	.435	.559
	AttH	.466	.419	.484	.551	**.324**	**.236**	**.354**	**.501**	**.397**	**.310**	**.437**	**.566**
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	AttE	.456	.419	.471	.526	.311	.223	.339	.488	.374	.290	.410	.537
	HAKE	.416	.389	.427	.467	.296	.212	.323	.463	.253	.164	.286	.430
Non-Euclidean	RotatE	.387	.330	.417	.491	.290	.208	.316	.458	.235	.153	.260	.410
	ComplEx-N3	.420	.390	.420	.460	.294	.211	.322	.463	.336	.259	.367	.484
	MuRP	.465	.420	.484	.544	.323	.235	.353	**.501**	.230	.150	.247	.392
	RefH	.447	.408	.464	.518	.312	.224	.342	.489	.381	.302	.415	.530
	RotH	**.472**	.428	**.490**	**.553**	.314	.223	.346	.497	.393	.307	.435	.559
	AttH	.466	.419	.484	.551	**.324**	**.236**	**.354**	**.501**	**.397**	**.310**	**.437**	**.566**
	ConE	.471	**.436**	.486	.537	-	-	-	-	-	-	-	-

Best-published MRR and H@K are from:
SpeedE, Min_SpeedE, ExpressivE: Benchmarked by us
ConE: (Baietal.,2021)
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The rest: (Chamietal.,2020)

SpeedE: Low-Dimensional KGC

Space	Model	WN18RR				FB15k-237				YAGO3-10			
		MRR	H@1	H@3	H@10	MRR	H@1	H@3	H@10	MRR	H@1	H@3	H@10
Euclidean	ExpressivE	.485	.442	.499	.571	.298	.208	.331	.476	.333	.257	.367	.476
	TuckER	.428	.401	-	.474	.306	.223	-	.475	-	-	-	-
	MuRE	.458	.421	.471	.525	.313	.226	.340	.489	.283	.187	.317	.478
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		MRR	H@1	H@3	H@10	MRR	H@1	H@3	H@10	MRR	H@1	H@3	H@10
Euclidean	SpeedE	**.493**	**.446**	**.512**	**.584**	**.320**	**.227**	**.356**	**.504**	**.413**	**.332**	**.453**	**.564**
	Min_SpeedE	.485	.442	.499	.573	.319	.226	**.356**	.502	.410	.328	.449	.563
	ExpressivE	.485	.442	.499	.571	.298	.208	.331	.476	.333	.257	.367	.476
	TuckER	.428	.401	-	.474	.306	.223	-	.475	-	-	-	-
	MuRE	.458	.421	.471	.525	.313	.226	.340	.489	.283	.187	.317	.478
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SpeedE: Space and Time Efficency

Model	Dim.	MRR	Conv. Time	#Parameters
SpeedE	**50**	**.500**	**6min**	**2M**
ExpressivE	200	**.500**	31min	8M
HAKE	500	.497	50min	41M
ConE	500	.496	1.5h	20M
RotH	500	.496	2h	21M

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Model	**Time per Epoch**		
	WN18RR	FB15k-237	YAGO3-10
SpeedE	7s	22s	88s
ExpressivE	15s	46s	185s
RotH	42s	112s	520s
AttH	43s	113s	533s

Summary

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  - the **same** KGC performance on WN18RR
  - reaching SotA performance with **low-dimensional** embeddings

ExpressivE, ICLR 2023

SpeedE, NAACL 2024

Thank you

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