Knowledge Graph Lab

TU WIEN

ExpressivE: A Spatio-Functional Embedding For Knowledge Graph Completion

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TU Wien

ICLR 2023 Spotlight Presentation

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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- Knowledge graph completion (KGC)
  - Automatically infer missing triples

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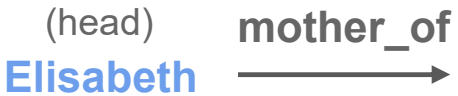
- Knowledge graphs are highly incomplete
  - 75% of the triples of Freebase lack a nationality (West et al., 2014)
- Knowledge graph completion (KGC)
  - Automatically infer missing triples
- Knowledge graph embedding models (KGEs)
  - Embed knowledge graphs into vector spaces

Knowledge Graphs

Knowledge Graphs

(head)
Elisabeth

Knowledge Graphs



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Knowledge Graph Embedding Models

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

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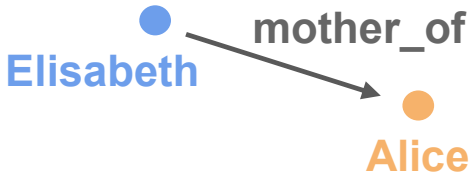

(head) **mother_of** (tail)

Elisabeth → **Alice**

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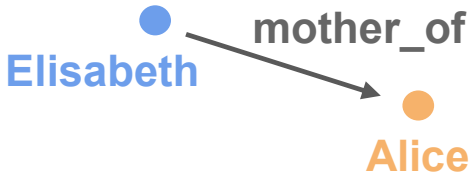

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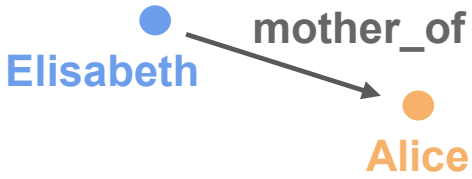

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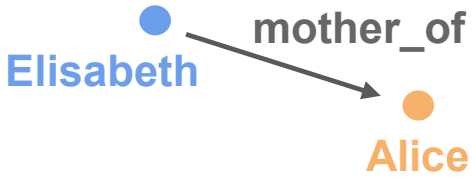

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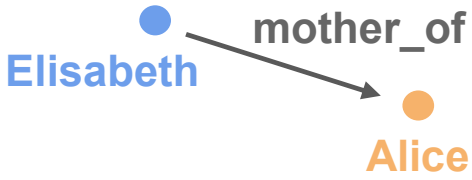

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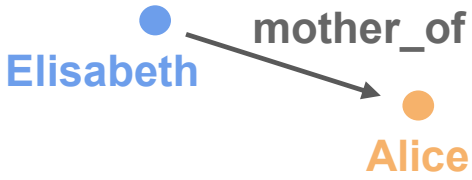

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- Bilinear Models
  - ComplEx (Trouillon et al., 2016), TuckER (Balazevic et al., 2019)

Knowledge Graph Embedding Models

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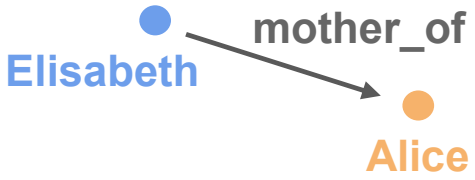

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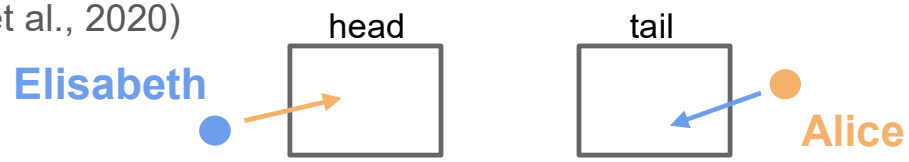

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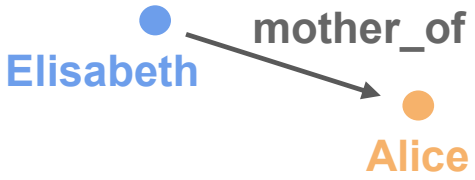

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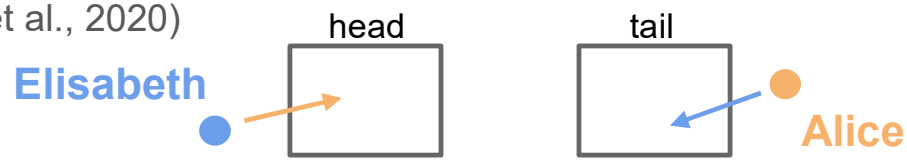

- Bilinear Models
  - ComplEx (Trouillon et al., 2016), TuckER (Balazevic et al., 2019)

- 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: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow \perp$	✓	✓	✓

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X mother_of Y ⇒ X parent_of 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.: $r_1(X,Y) \wedge r_2(Y,Z) \Leftrightarrow r_3(X,Z)$	✗	✗	✗
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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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  - **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.: $r_1(X,Y) \wedge r_2(Y,Z) \Leftrightarrow r_3(X,Z)$	✗	✗	✗
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Intersection: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow r_3(X,Y)$	✓	✗	✗
Mutual exclusion: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow \perp$	✓	✓	✓

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)

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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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X father_of Y ∧ Y parent_of Z ⇒ X grand_parent_of Z

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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.: $r_1(X,Y) \wedge r_2(Y,Z) \Rightarrow r_3(X,Z)$	✗	✗
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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)

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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.: $r_1(X,Y) \wedge r_2(Y,Z) \Rightarrow r_3(X,Z)$	✗	✗
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Mutual exclusion: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow \perp$	✓	✓

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.: $r_1(X,Y) \wedge r_2(Y,Z) \Leftrightarrow r_3(X,Z)$	✓	✓	✗	✗	✗
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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: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow \perp$	✓	✓	✓	✓	✓

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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: $r_1(X,Y) \wedge r_2(X,Y) \Rightarrow \perp$	✓	✓	✓	✓	✓	✓

Challenge: Expressiveness

- Spatial and Bilinear Models
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- 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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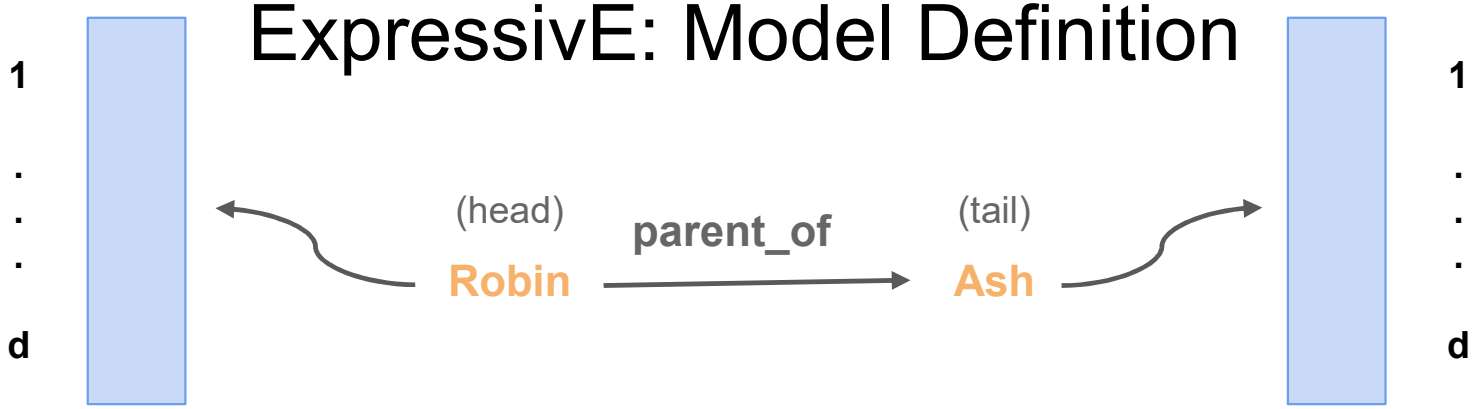

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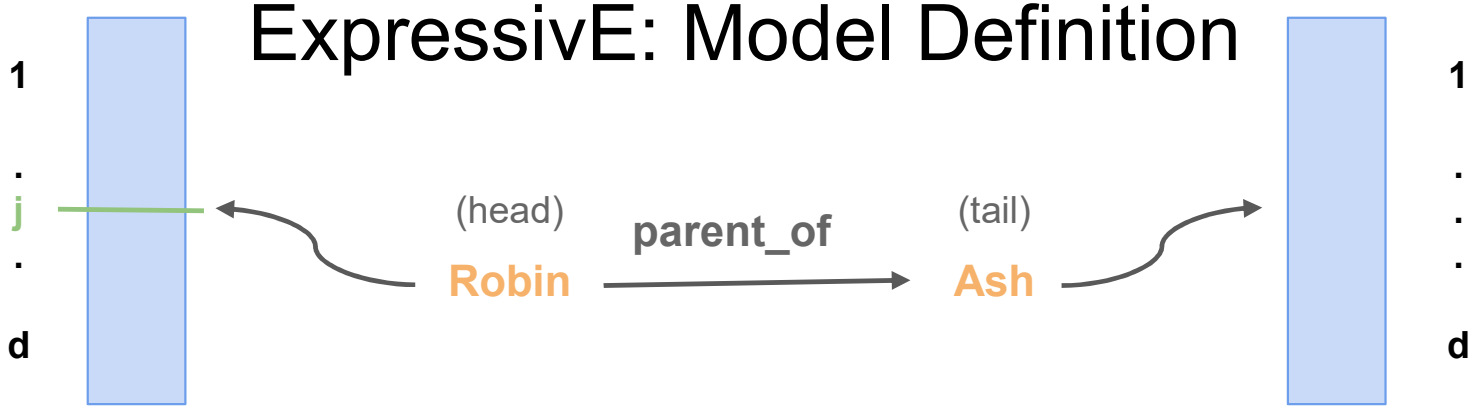

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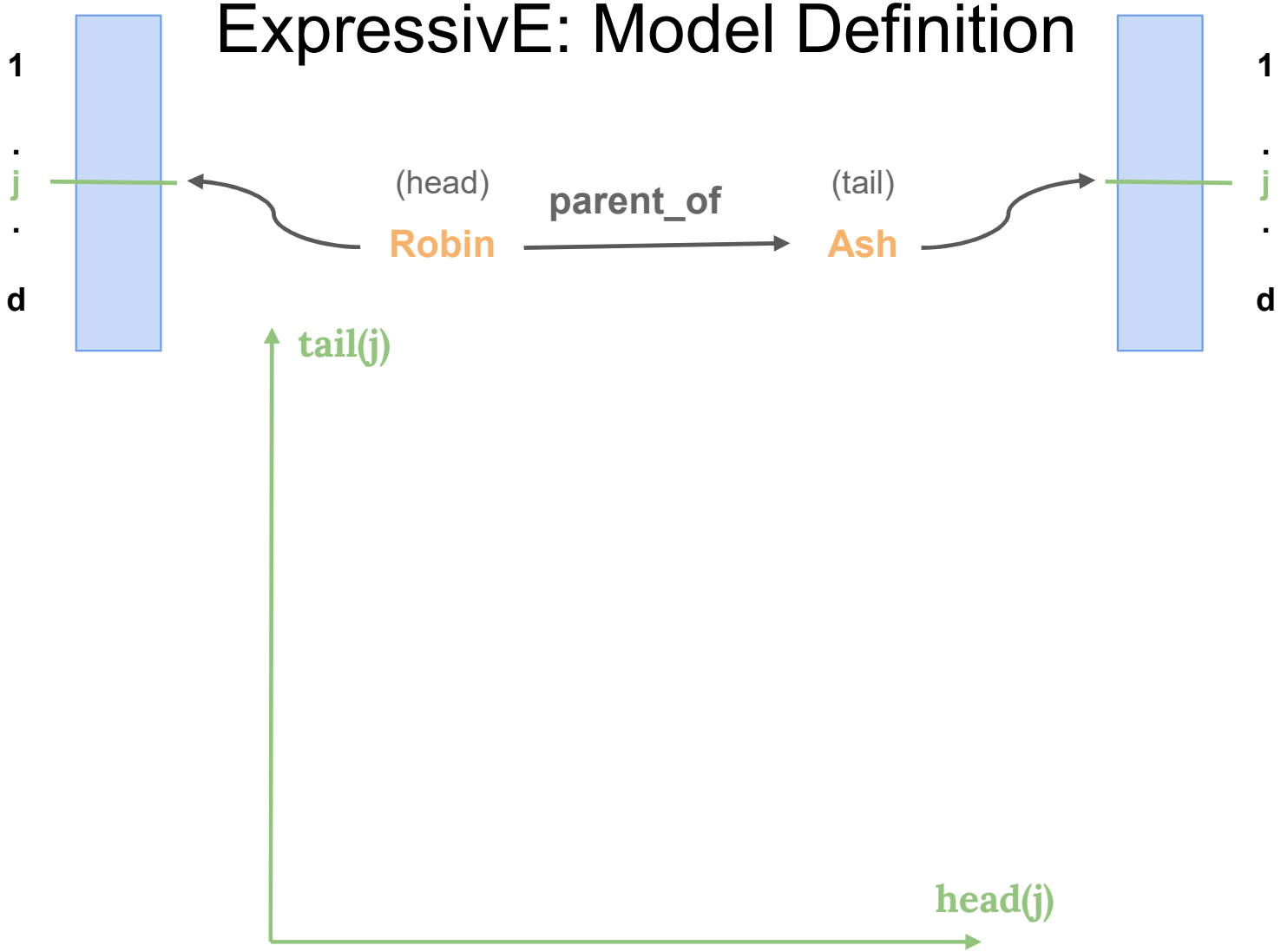

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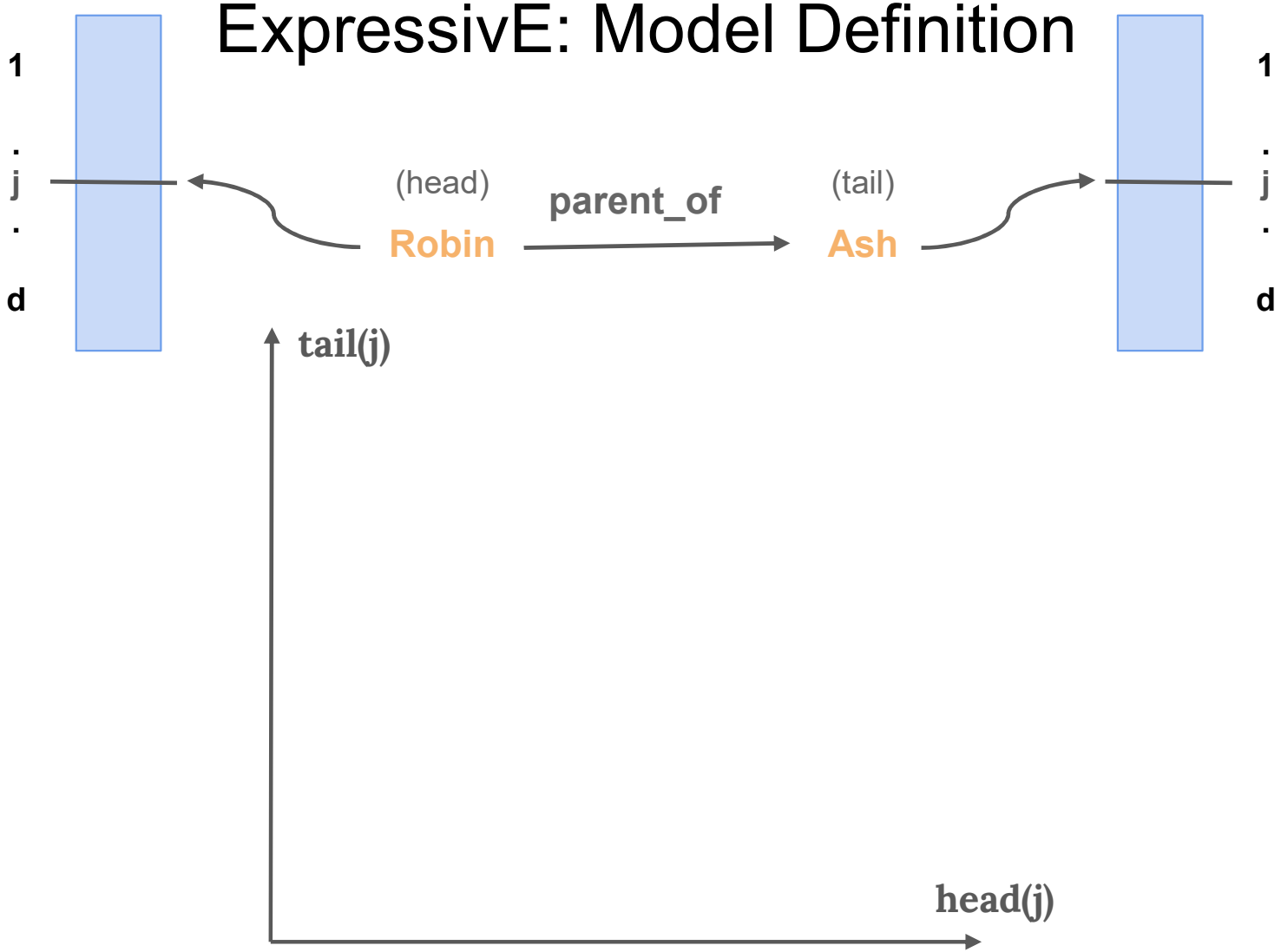

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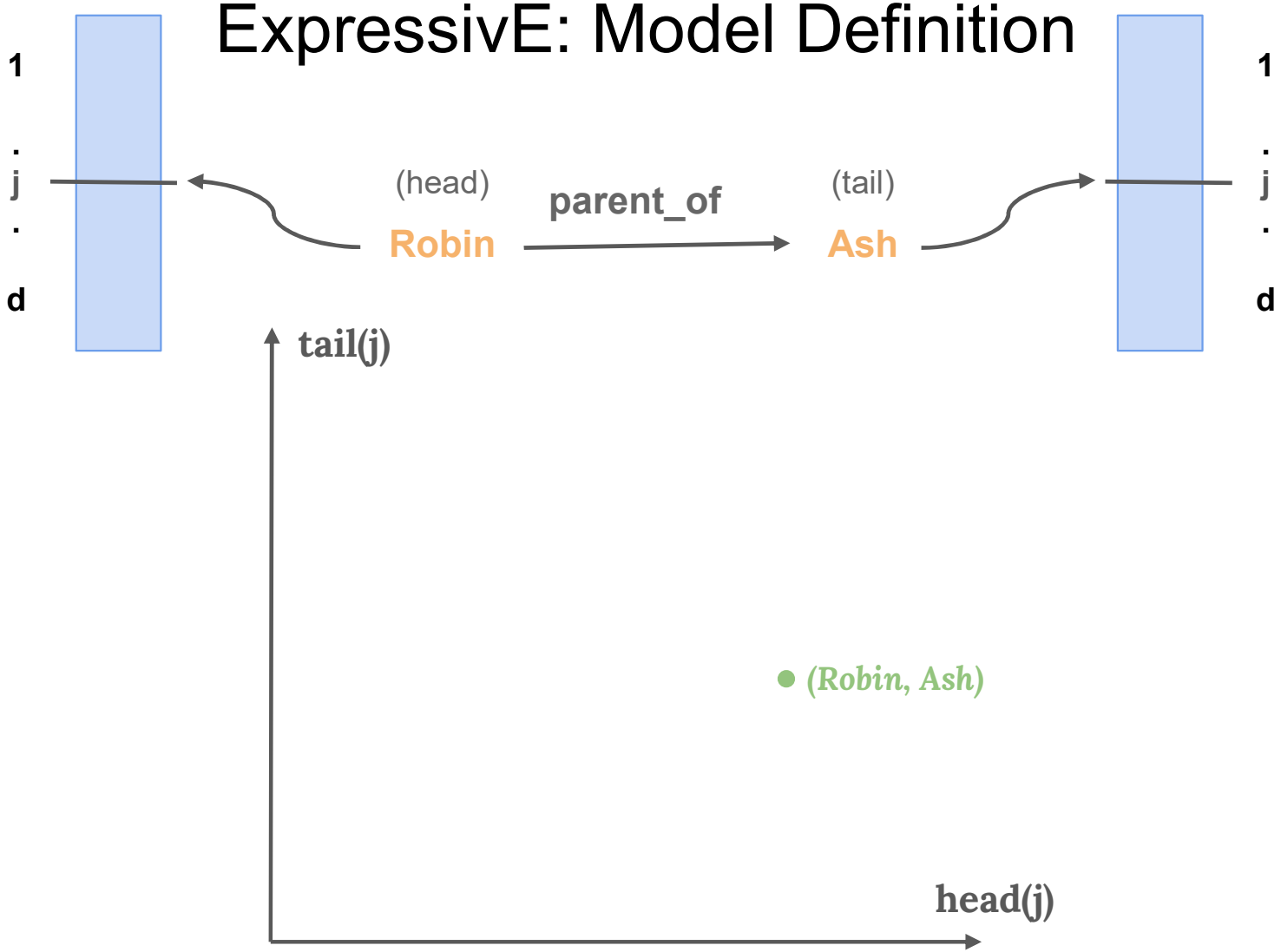

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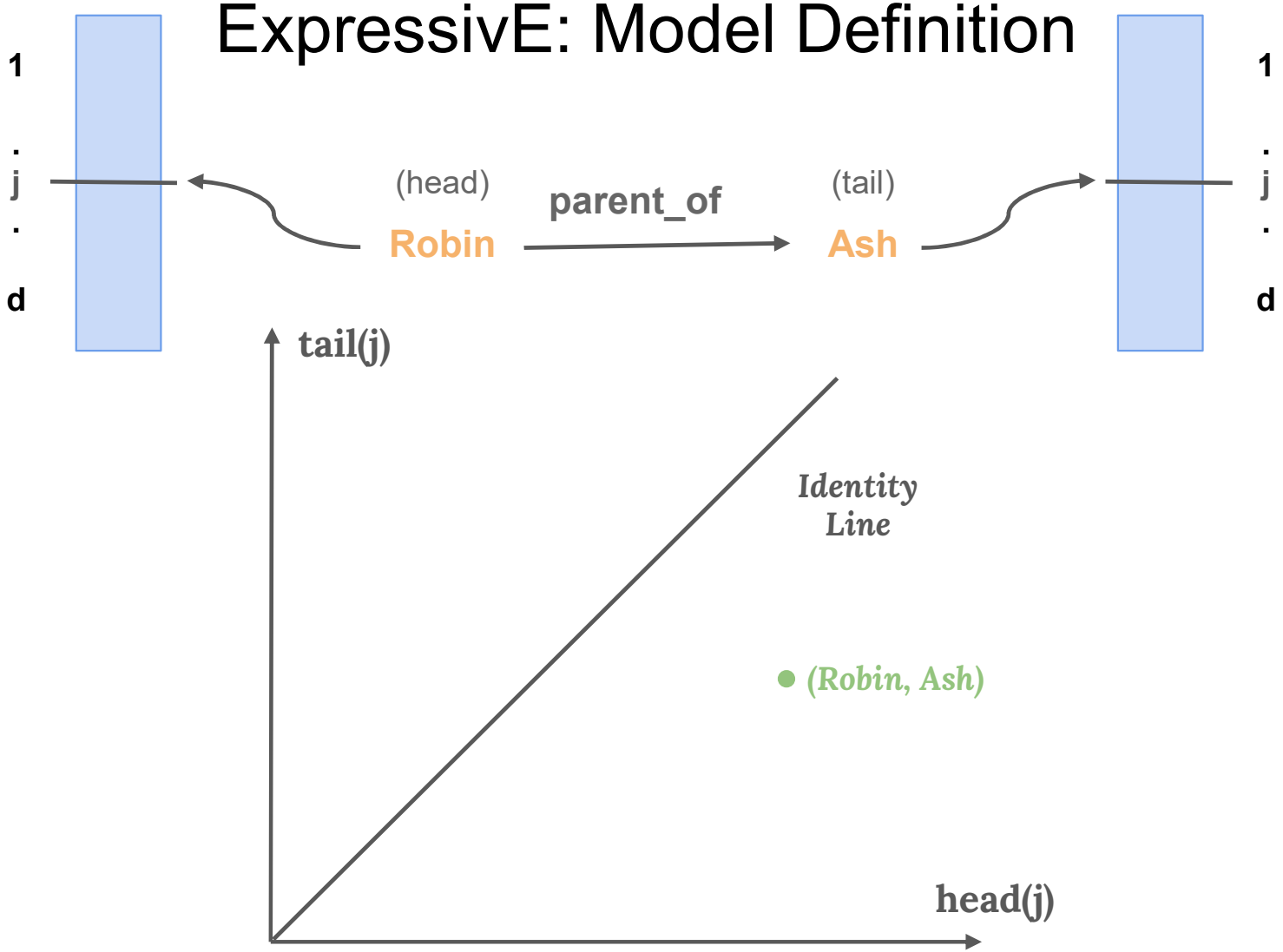

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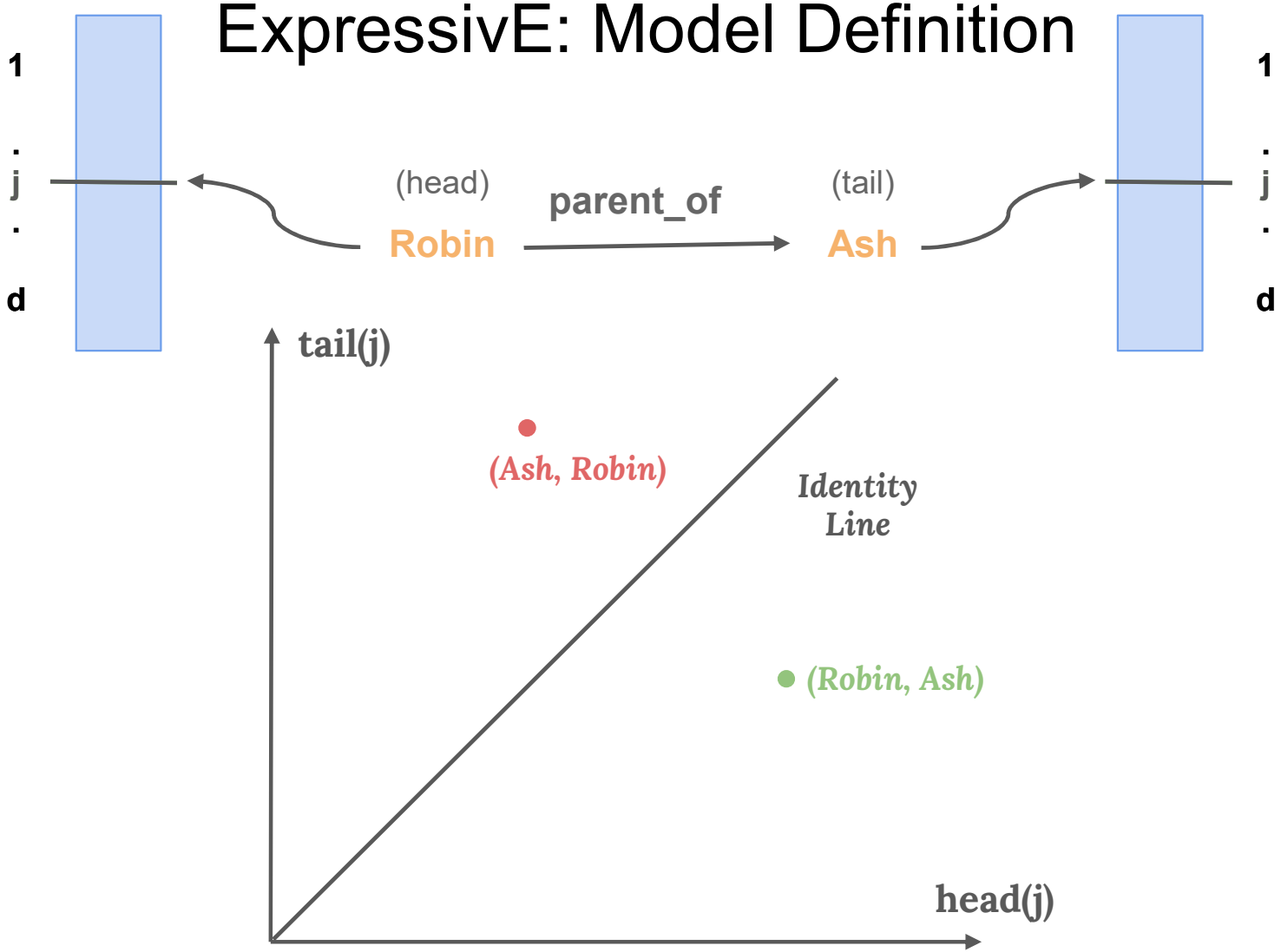

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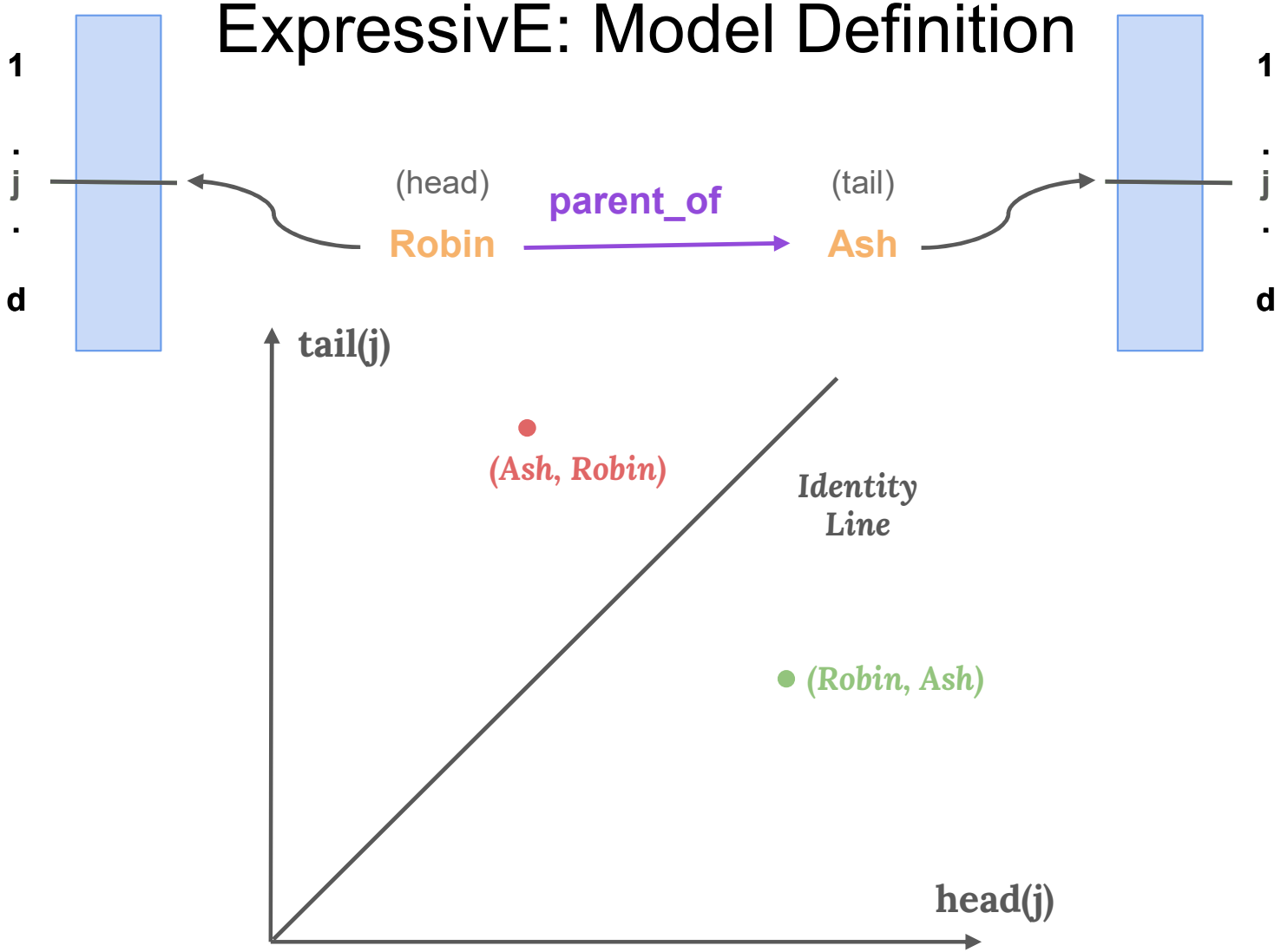

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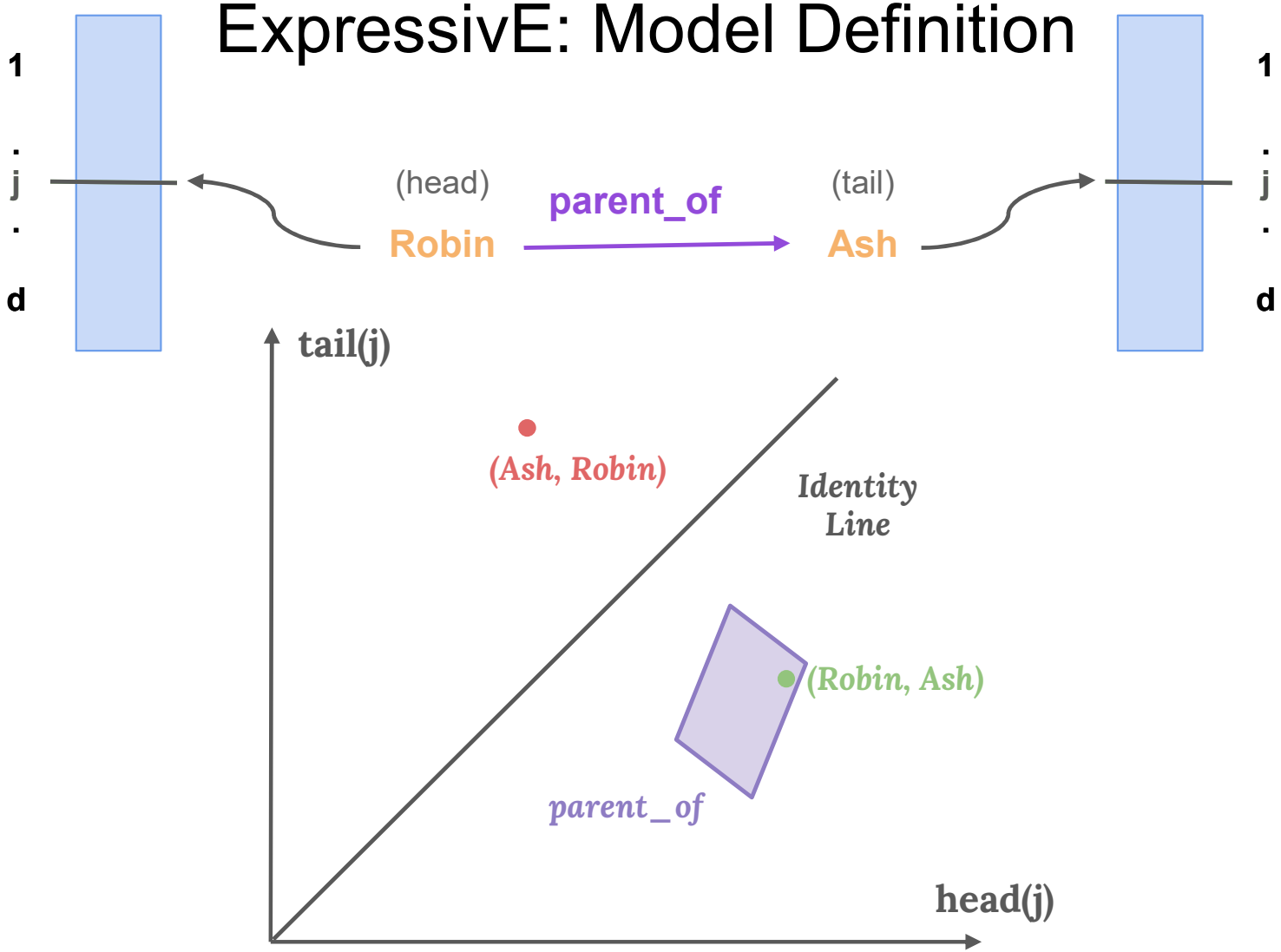

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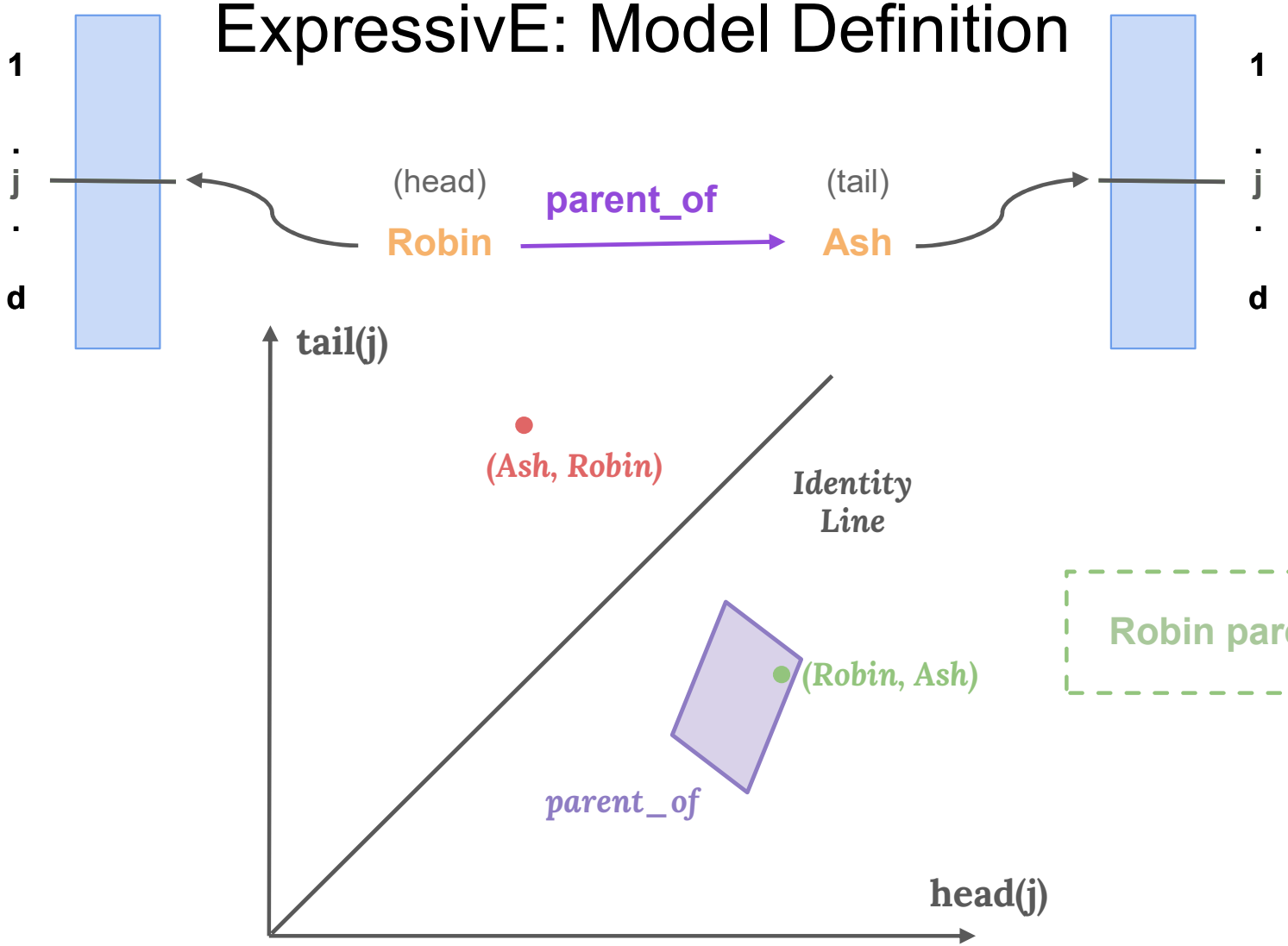

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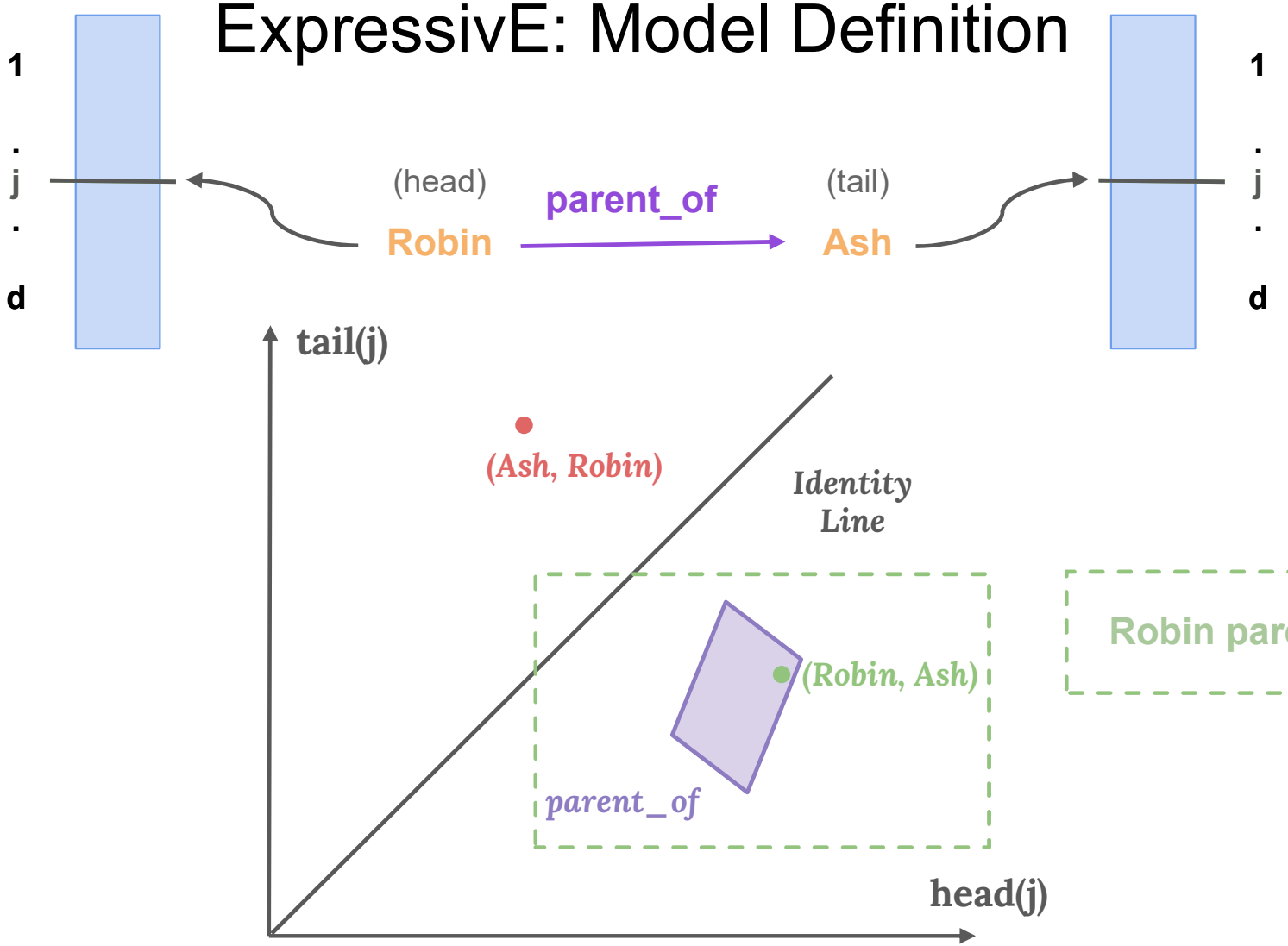

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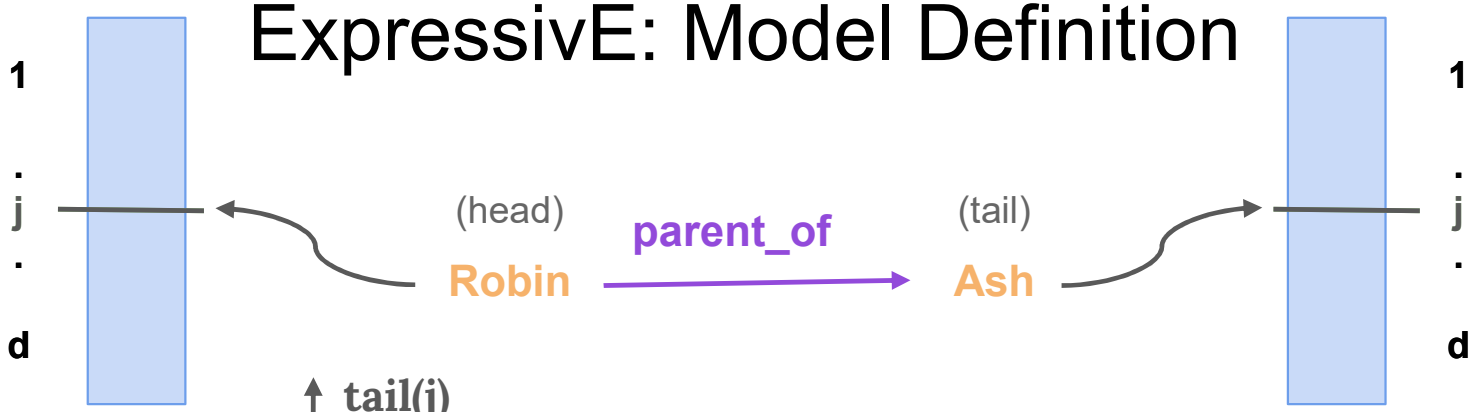

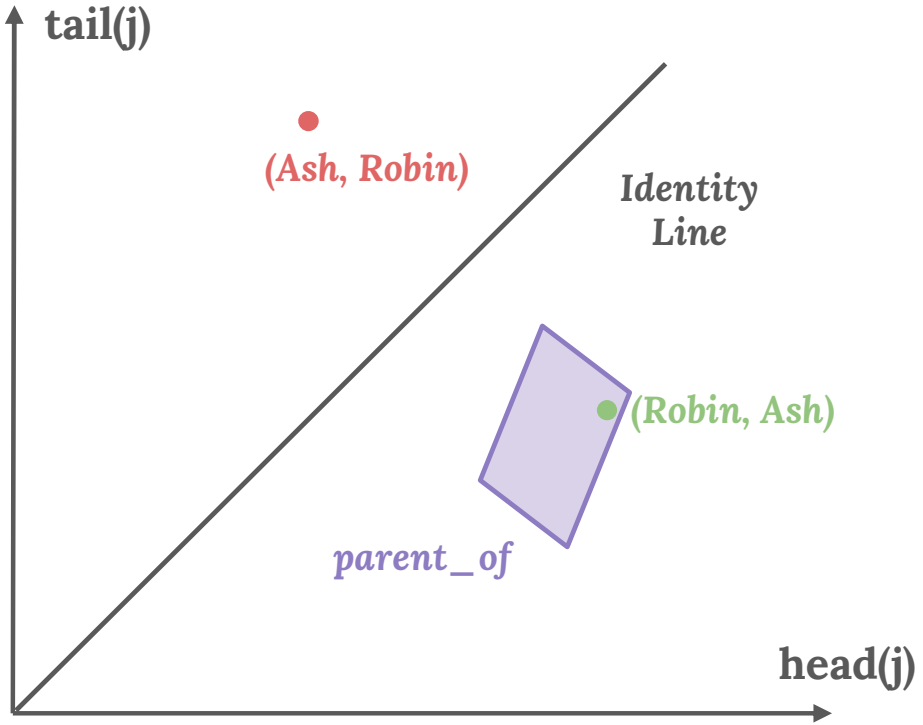

Ash parent_of Robin

Robin parent_of Ash

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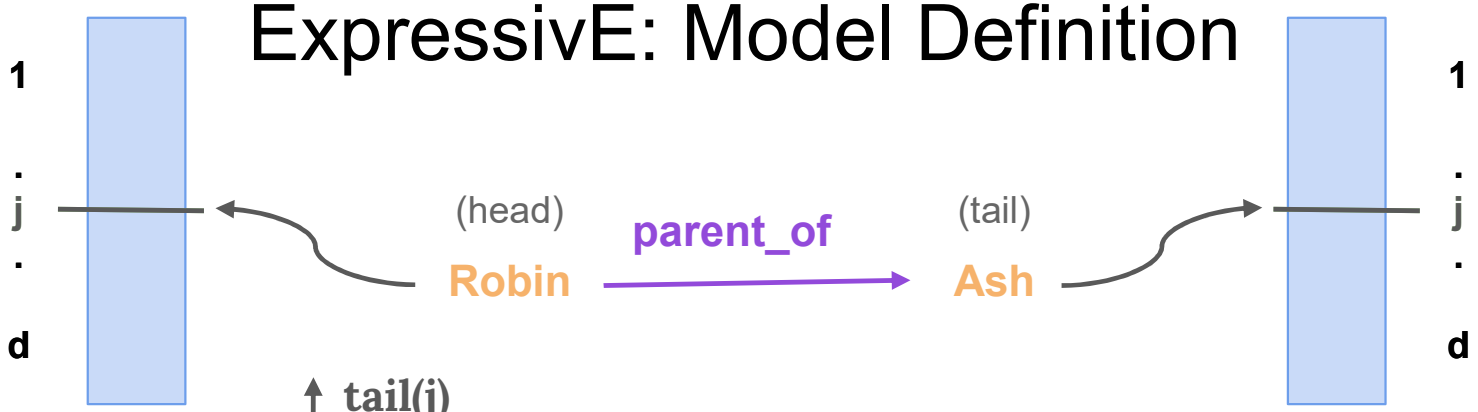

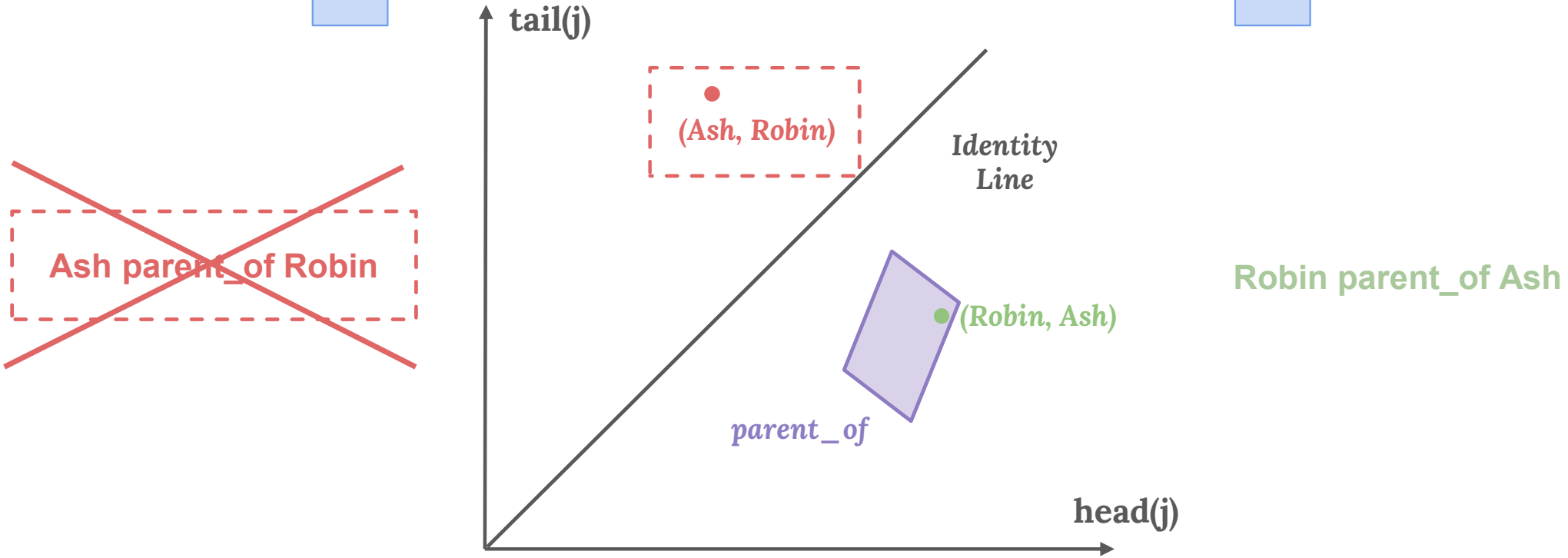

Fully Expressiveness

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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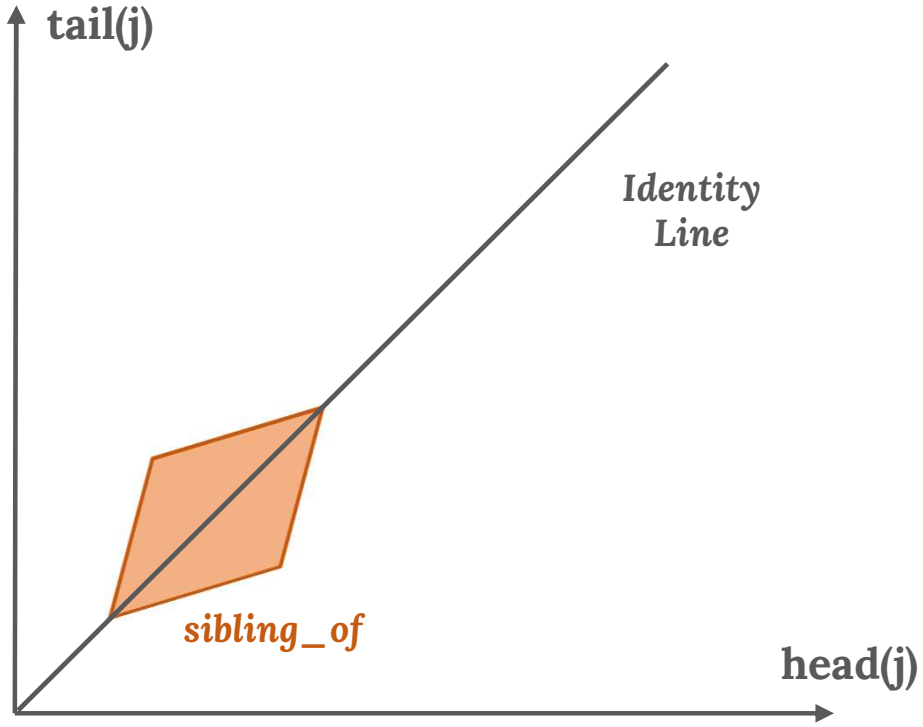

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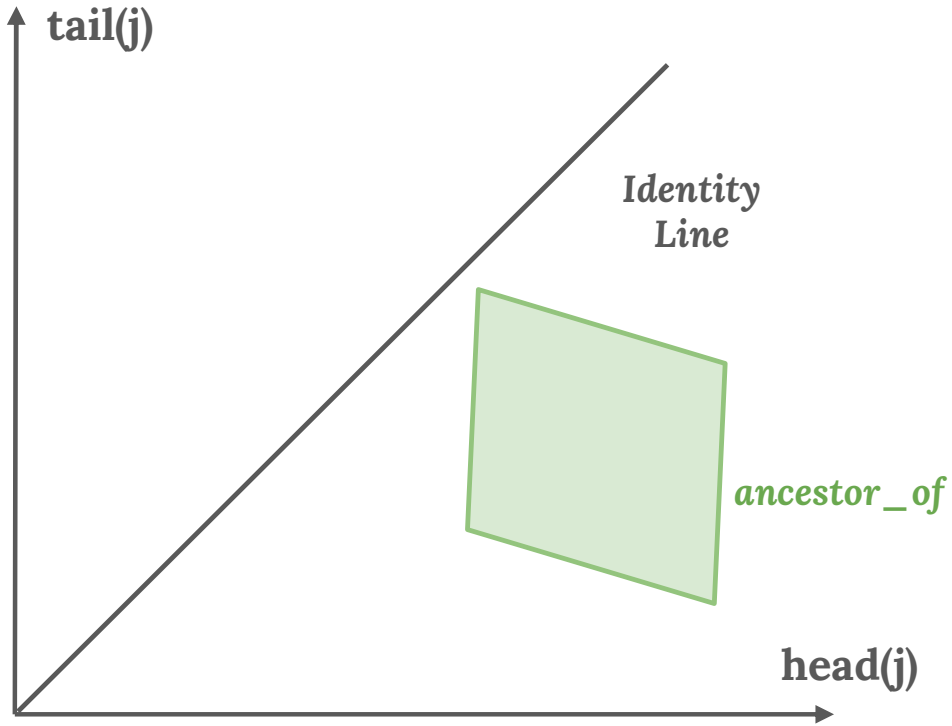

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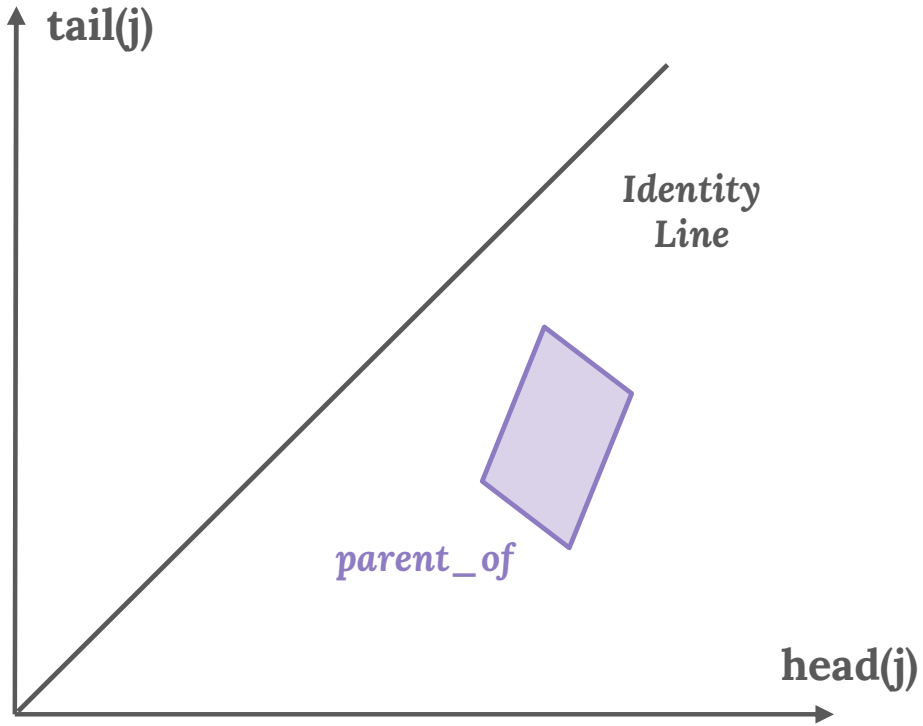

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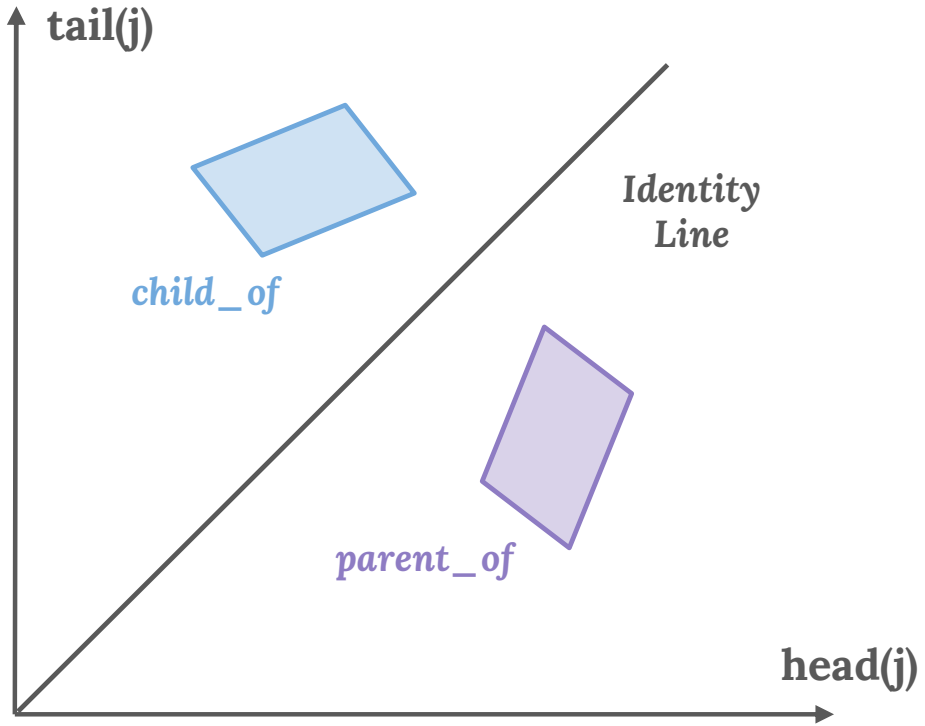

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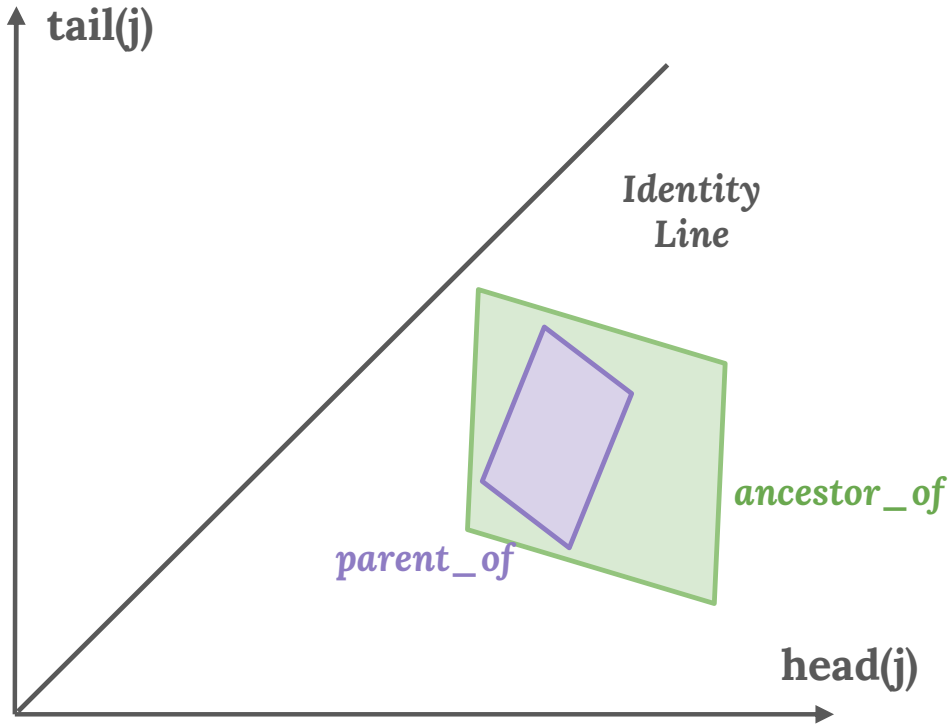

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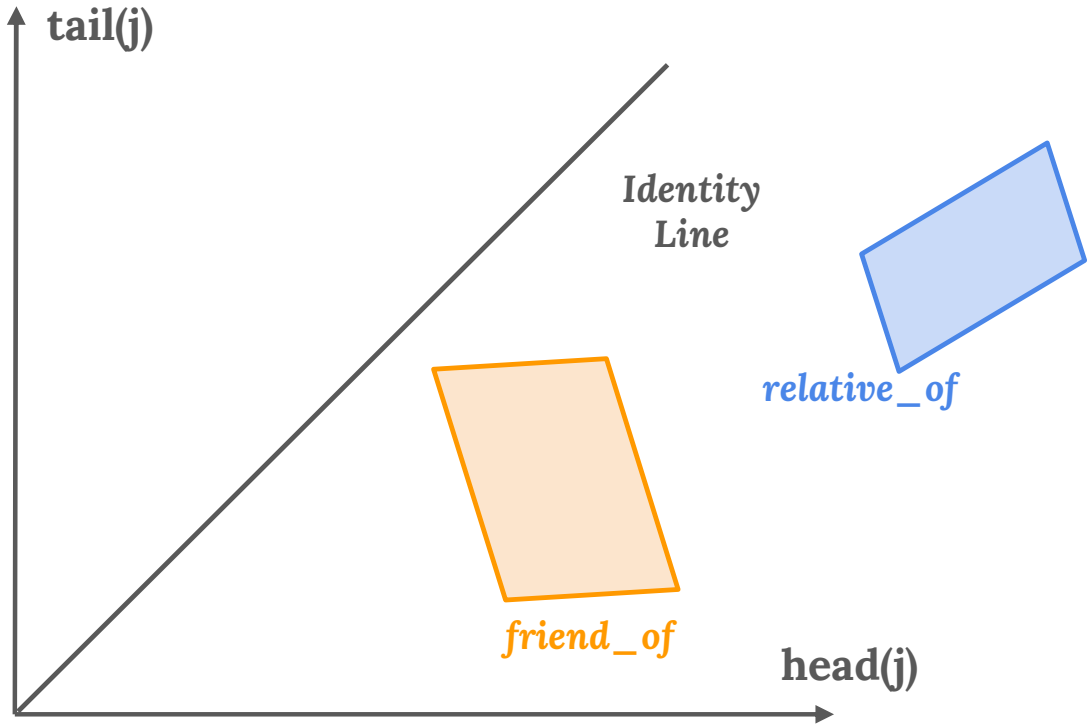

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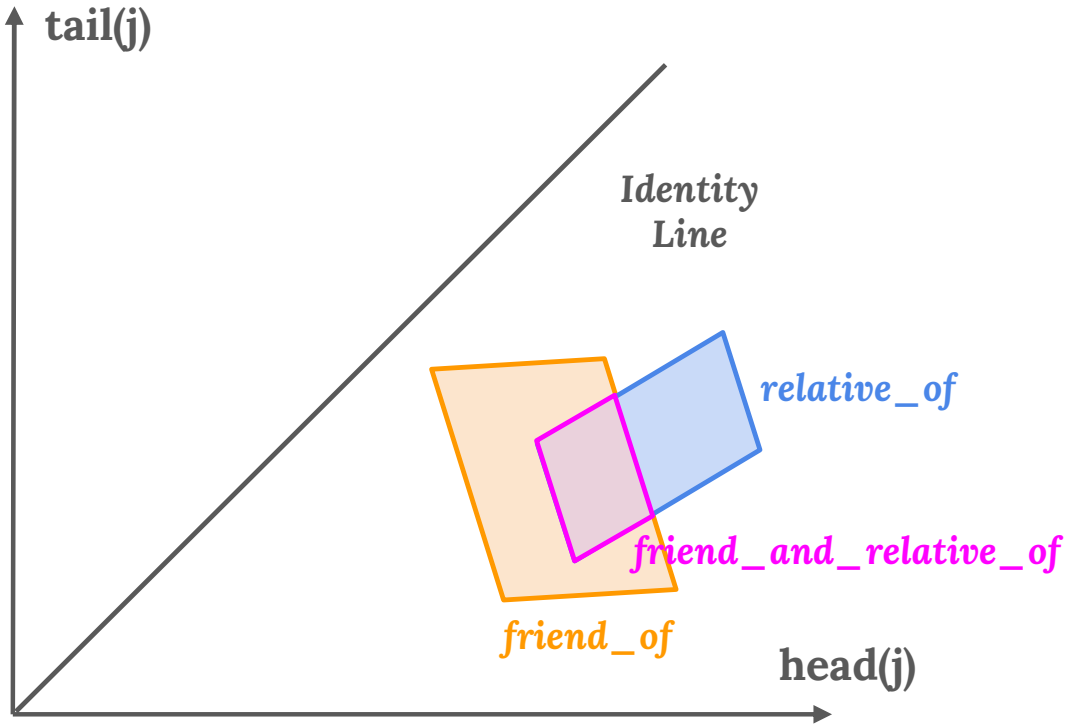

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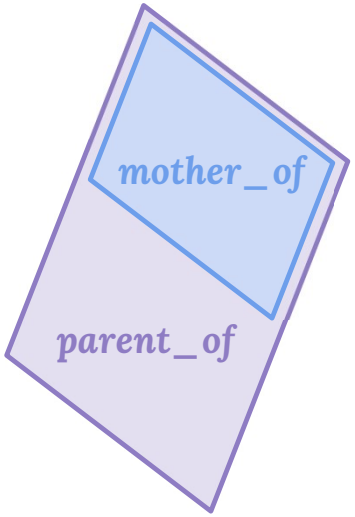

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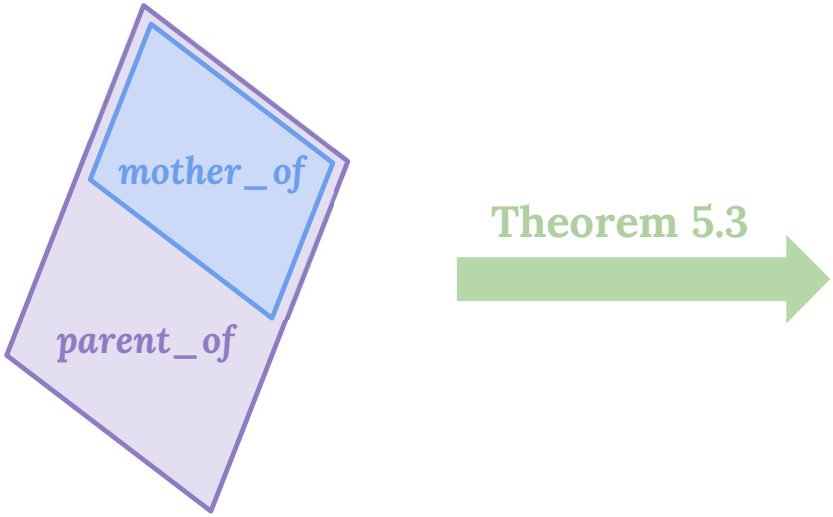

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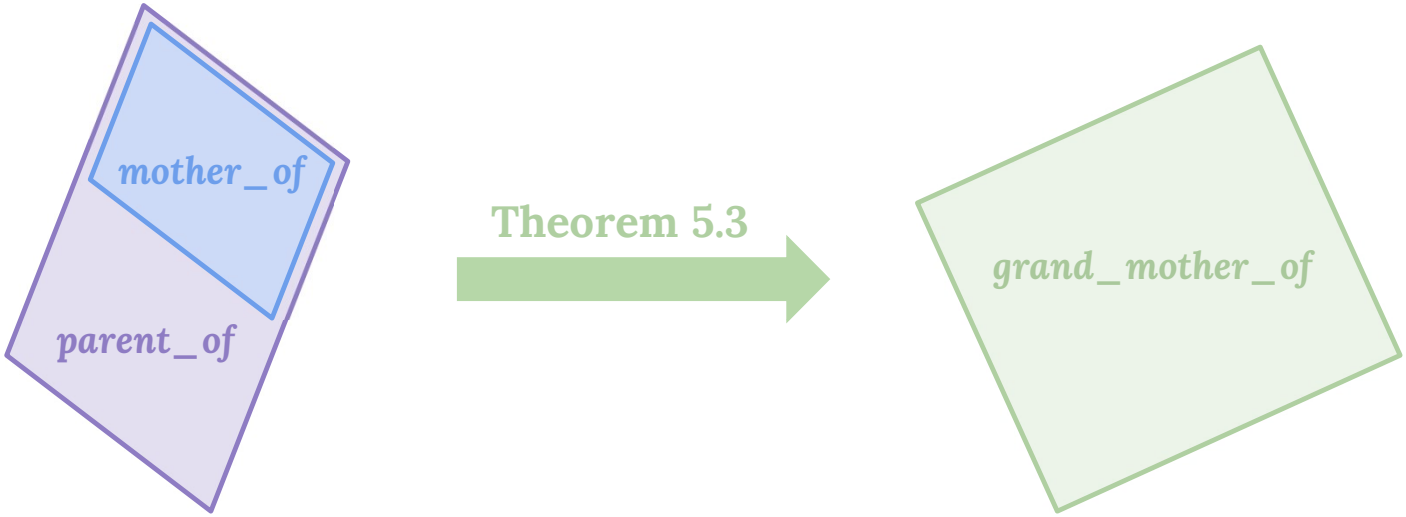

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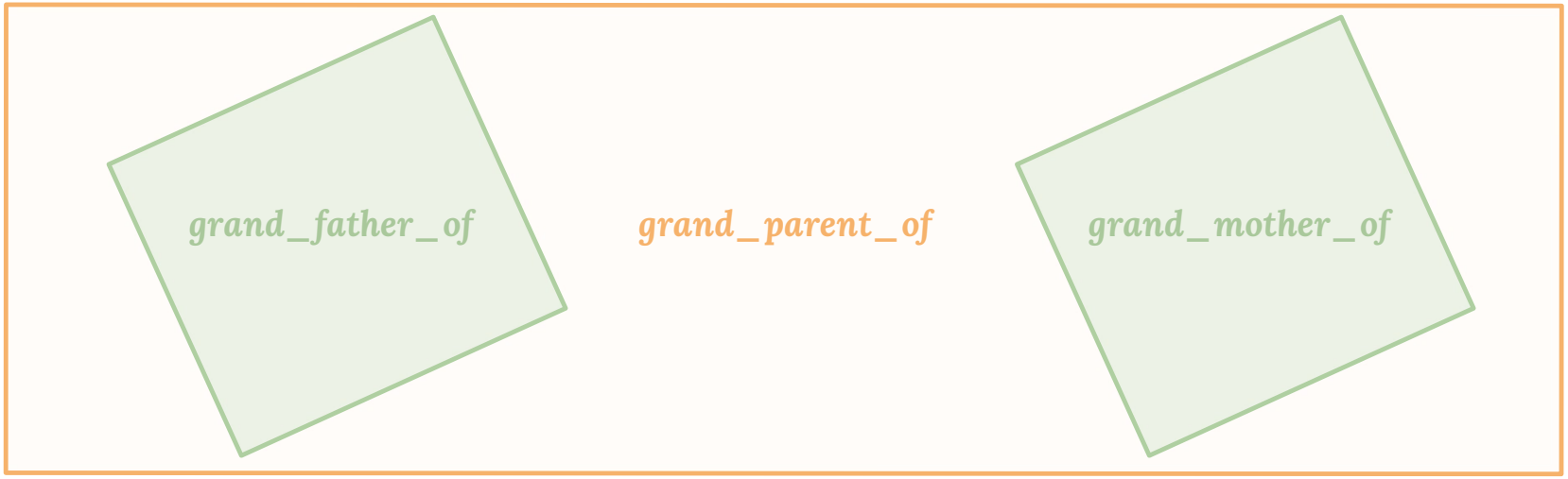

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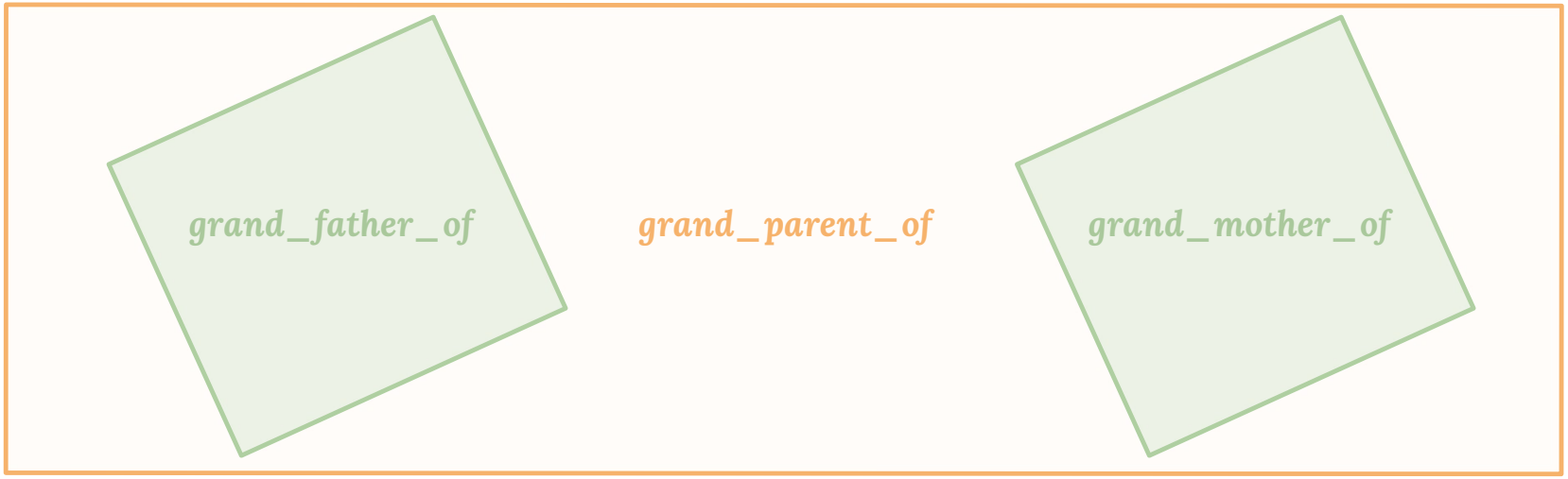

Representing relations as regions naturally allows for one-to-many, many-to-one, and many-to-many relations

Evaluation on KGC

Family	Model	WN18RR				FB15k-237			
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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:
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Additional Results

Relation Name	ExpressivE	RotatE	BoxE
member_meronym	**0.233**	0.199	0.226
hypernym	**0.189**	0.162	0.159
has_part	**0.198**	0.187	0.168
instance_hypernym	0.352	0.326	**0.425**
synset_domain_topic_of	0.363	**0.384**	0.323
member_of_domain_usage	0.288	0.333	**0.360**
member_of_domain_region	0.123	0.188	**0.189**
also_see	**0.649**	0.631	0.517
derivationally_related_from	**0.956**	0.943	0.902
similar_to	**1.000**	**1.000**	**1.000**
verb_group	**0.972**	0.843	0.876

Task	**Predicting Head**				**Predicting Tail**			
Cardinality	1-1	1-N	N-1	N-N	1-1	1-N	N-1	N-N
ExpressivE	**0.976**	0.290	0.105	**0.941**	**0.976**	0.141	**0.327**	**0.938**
RotatE	0.833	**0.294**	0.103	0.930	0.875	0.107	0.288	0.925
BoxE	0.877	0.272	**0.146**	0.883	0.893	**0.147**	0.246	0.884

Head Rel.	**_verb_group**				**_also_see**			**_syn_dto**
Model	S_1	C_2	C_3	C_4	C_5	C_6	S_7	C_8
Base Exp.	**1.000**	**1.000**	**1.000**	**1.000**	**0.818**	**0.907**	**0.985**	**0.621**
RotatE	0.865	0.760	0.760	0.760	0.771	0.893	0.975	0.599
BoxE	0.906	0.801	0.806	0.806	0.632	0.645	0.727	0.547

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  - can handle **one-to-many, many-to-one, and many-to-many** relations
  - achieves very **strong** performance on KGC, while solely using **half** the number of parameters of its closest relatives

Thank you