Lecture 2: Knowledge Graph Embedding Models

Relational Learning

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Advanced Topics in Machine Learning, University of Oxford

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Overview

- A glimpse at embedding models
  - Translational models: TransE and RotatE
  - Bilinear models: RESCAL, DistMult, and ComplEx
  - Box embedding models
- Overview of the embedding models
- Temporal knowledge graph completion
- Outlook and discussions
- Summary

A Glimpse at Embedding Models

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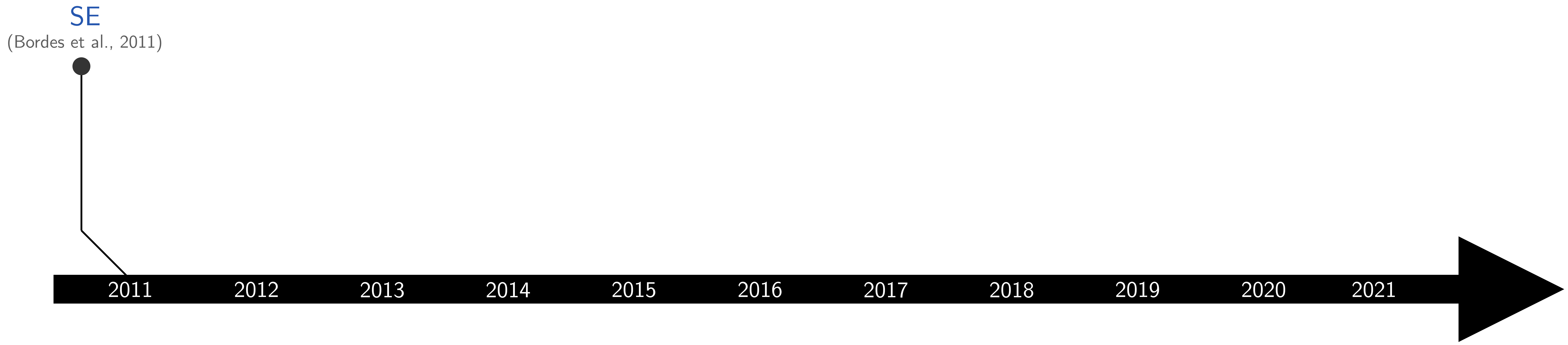

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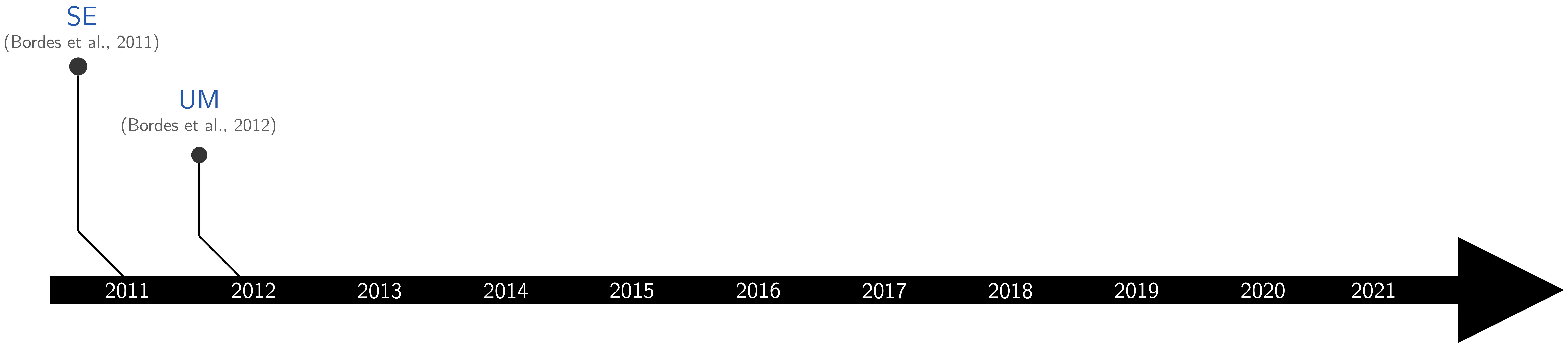

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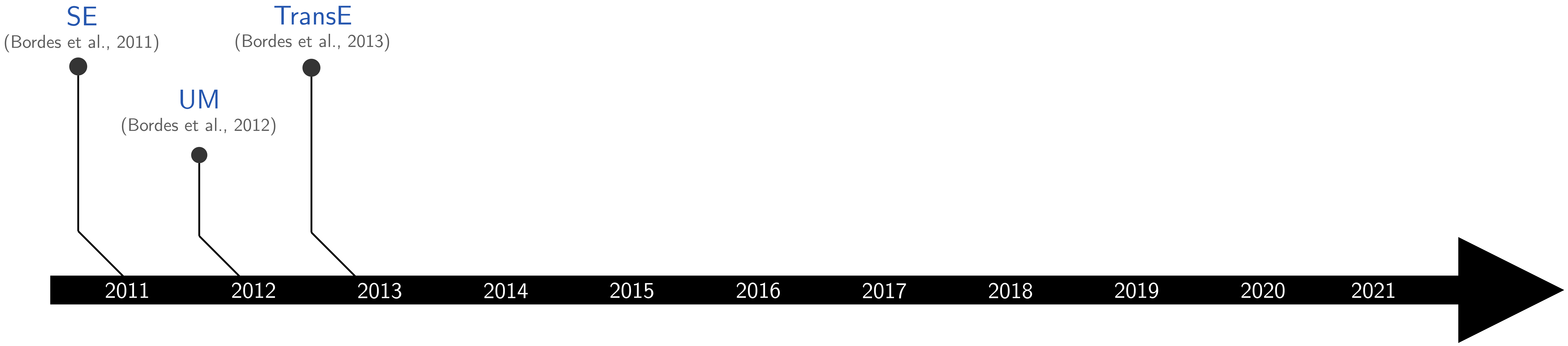

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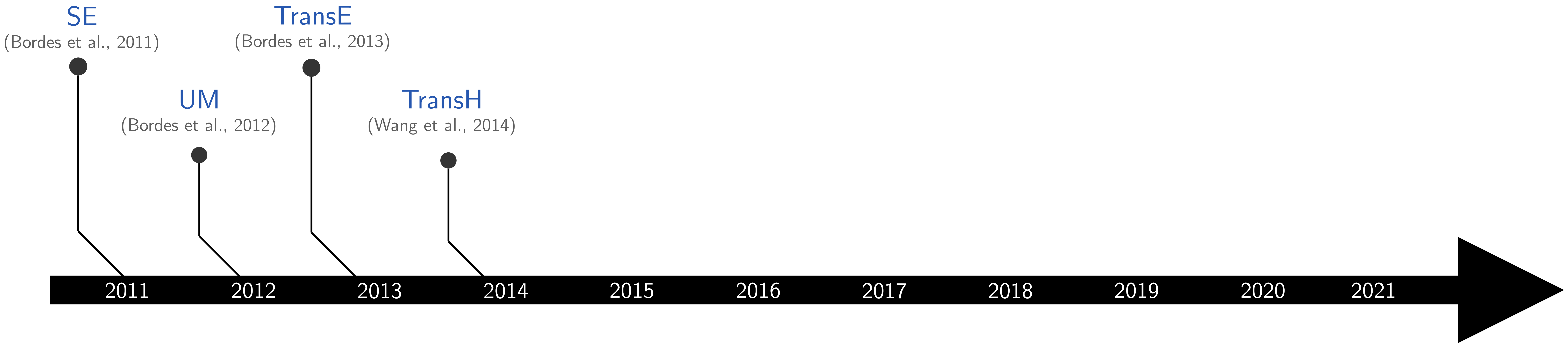

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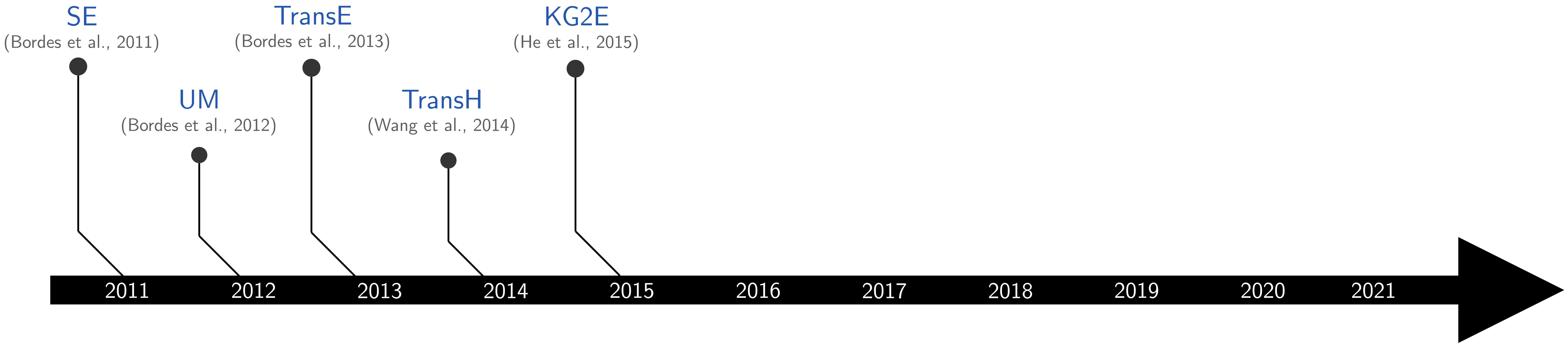

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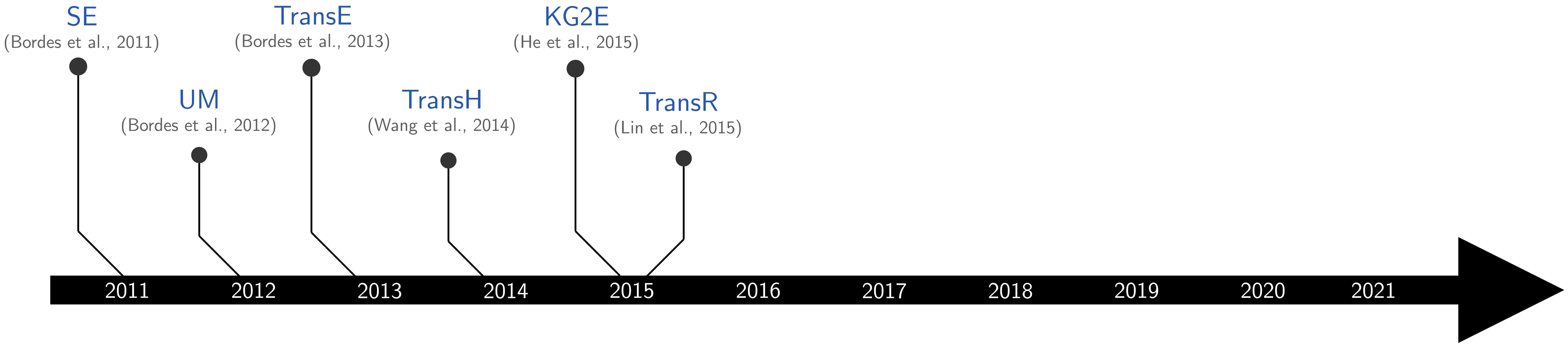

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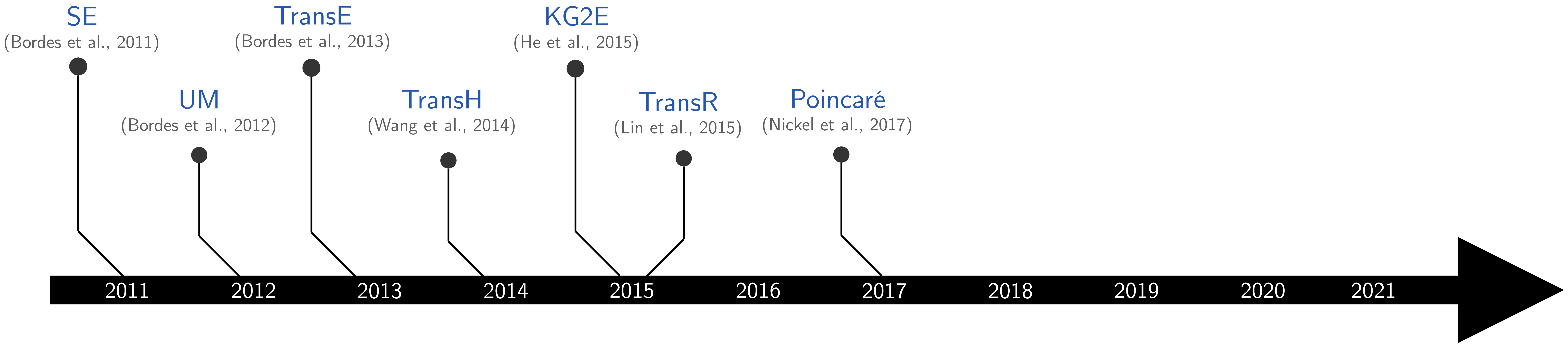

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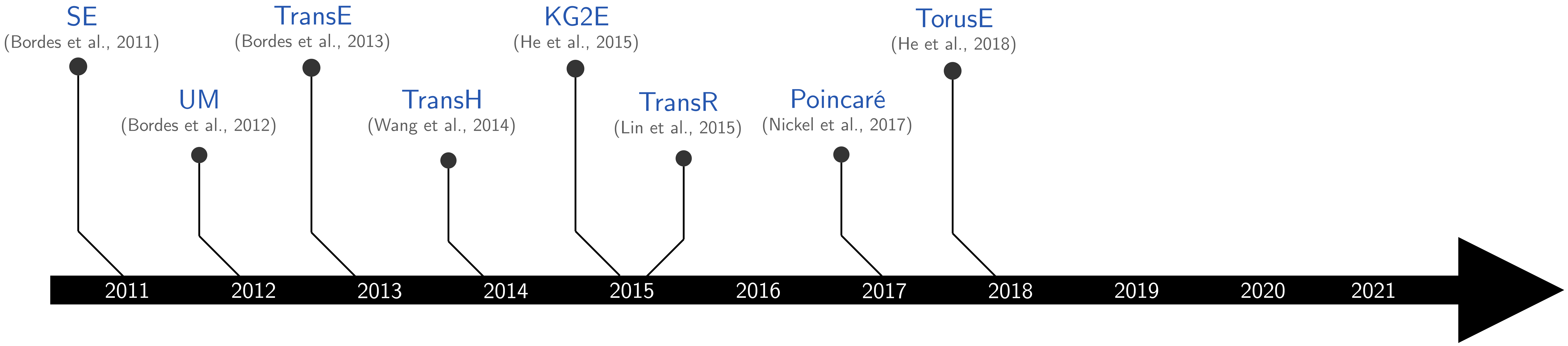

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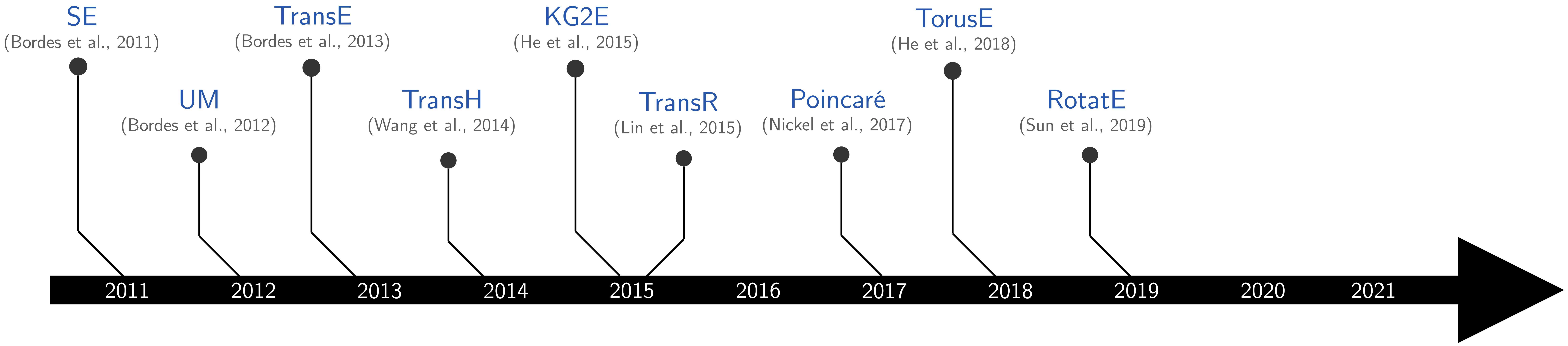

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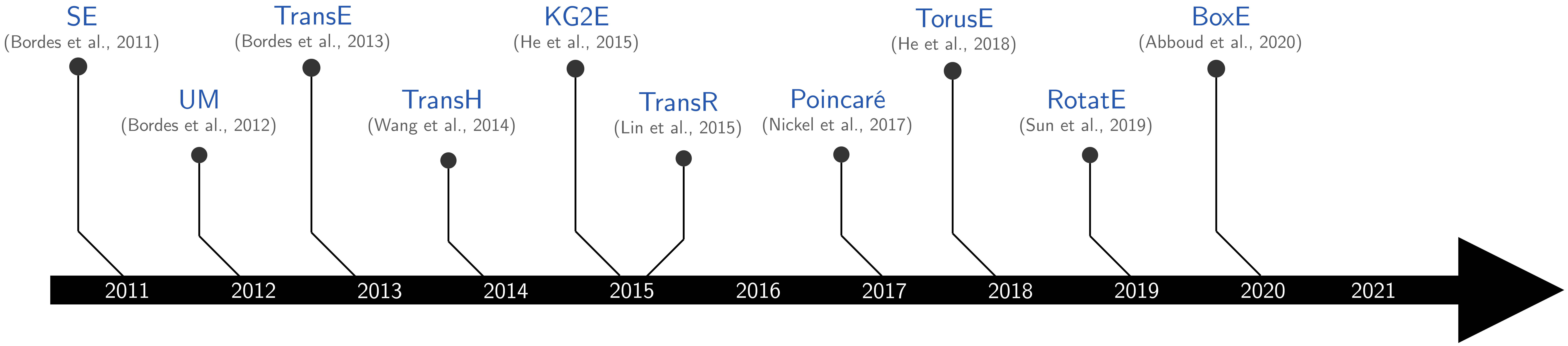

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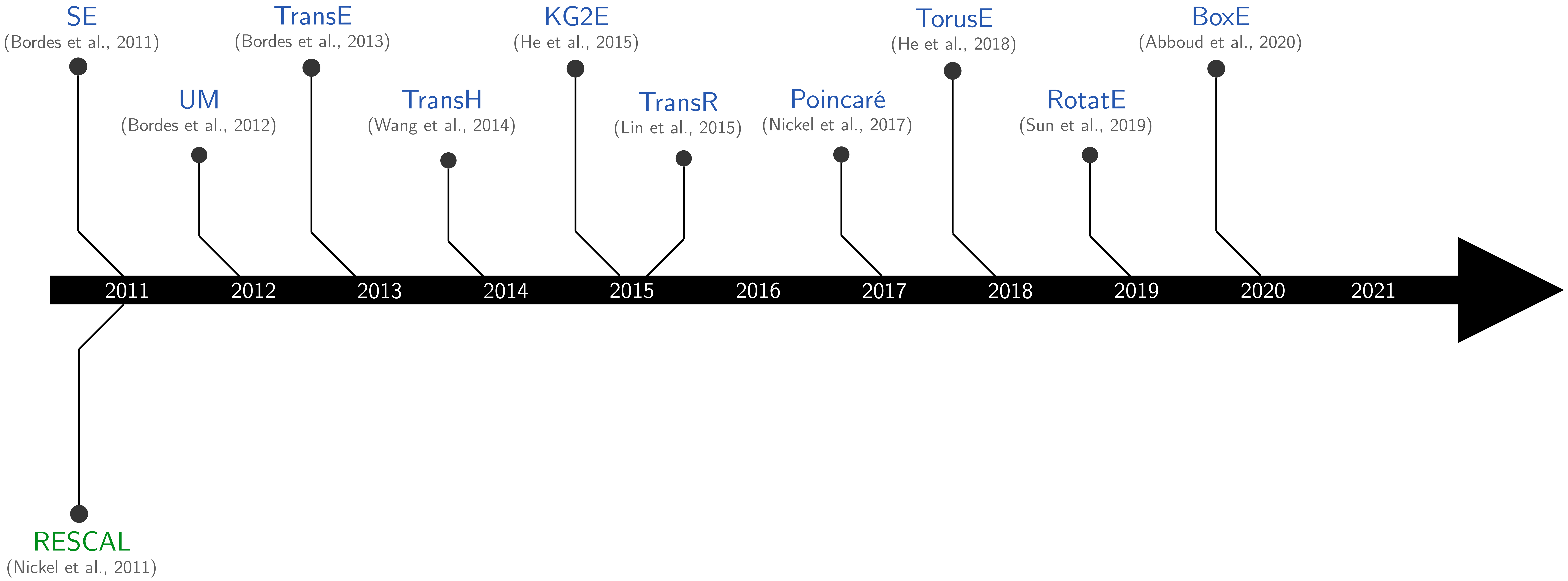

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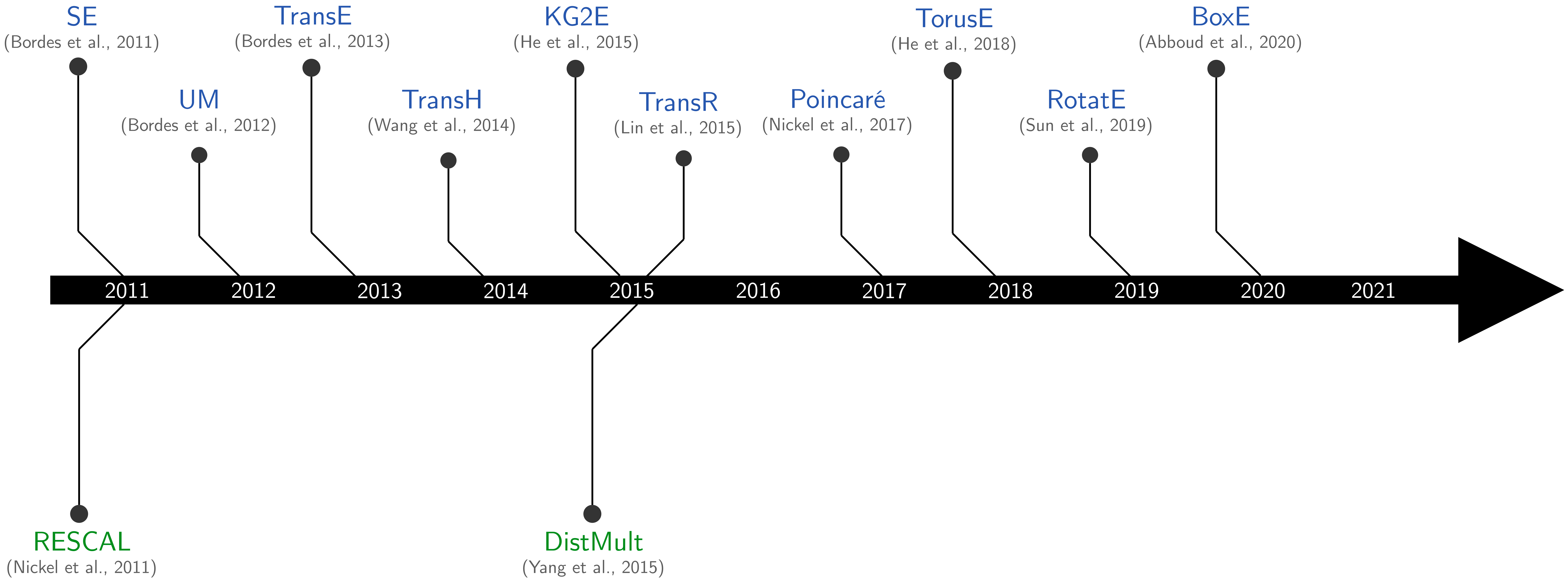

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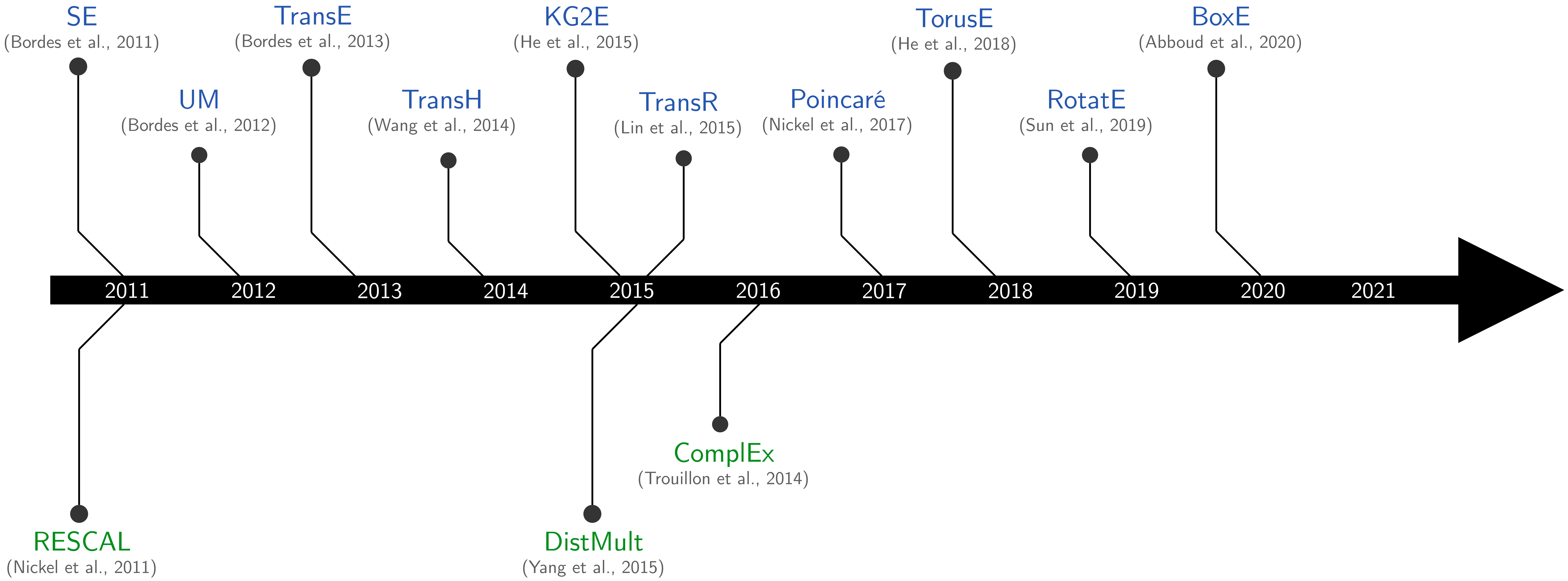

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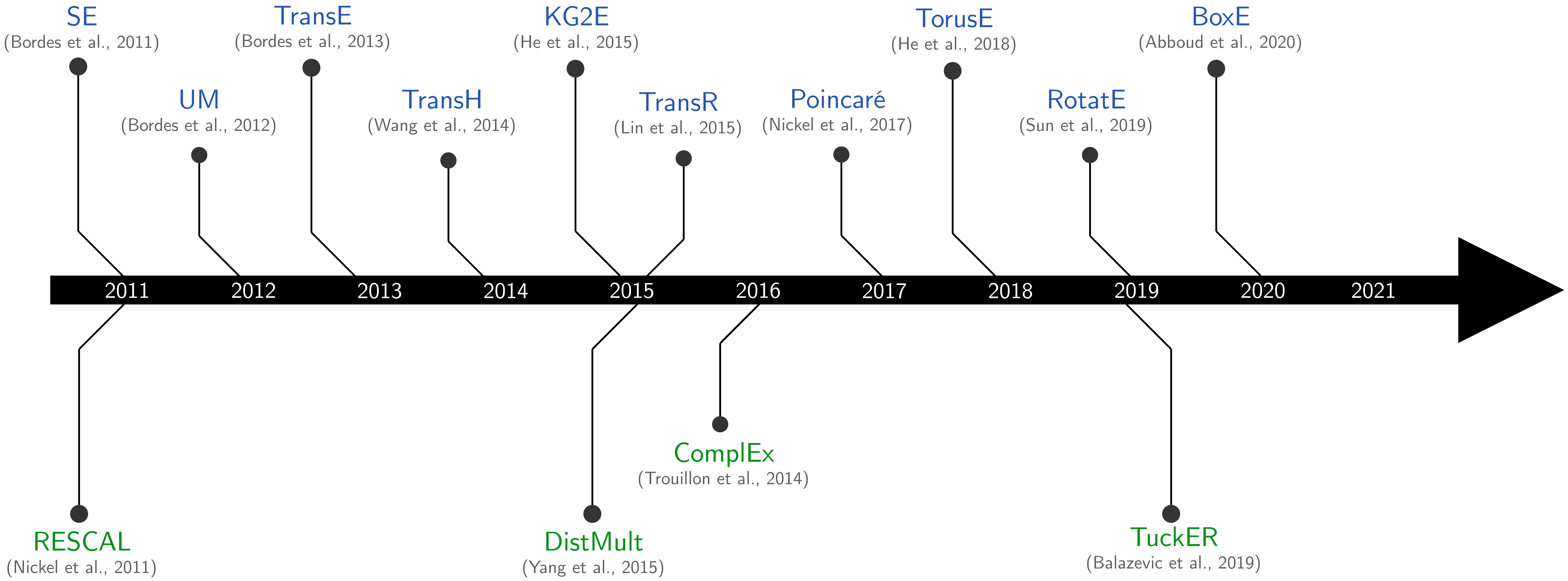

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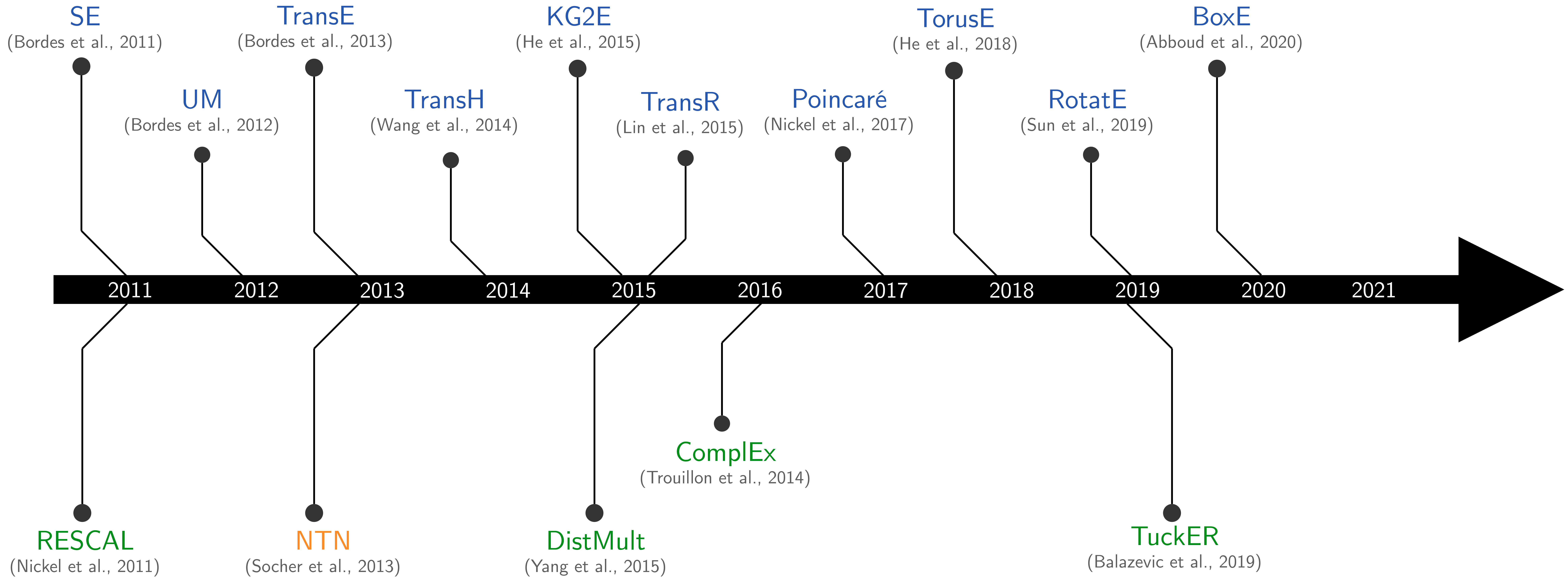

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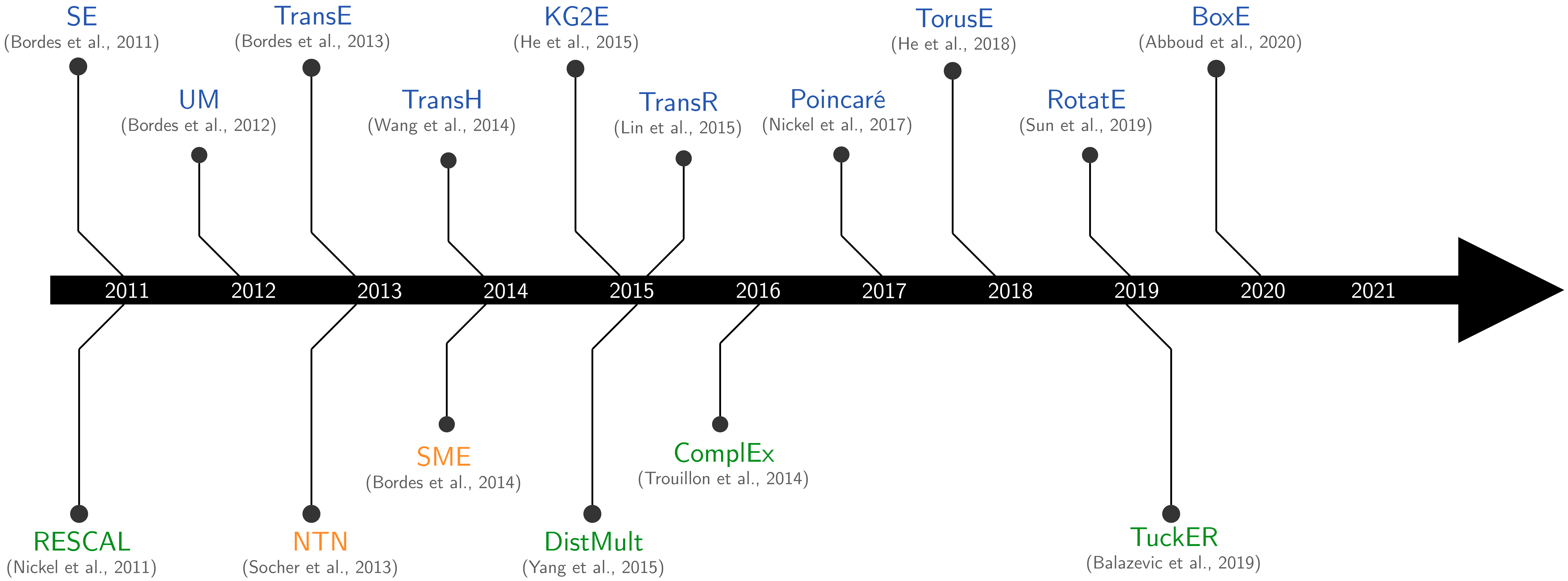

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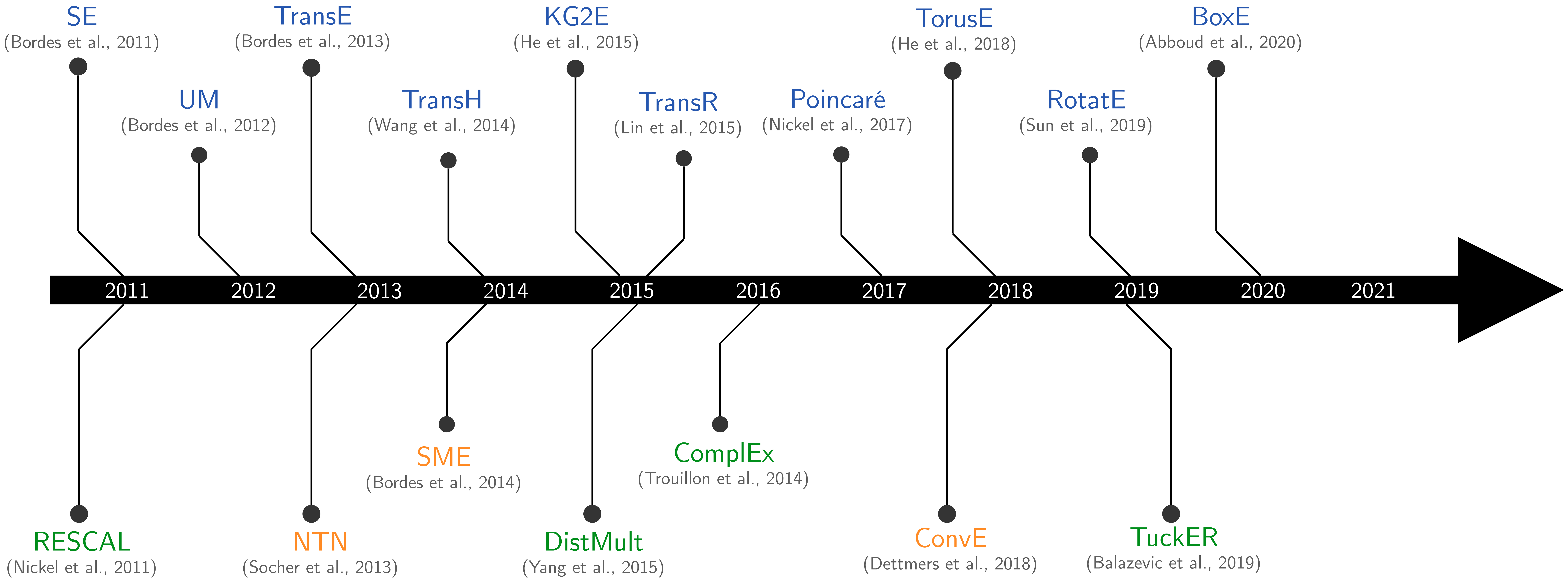

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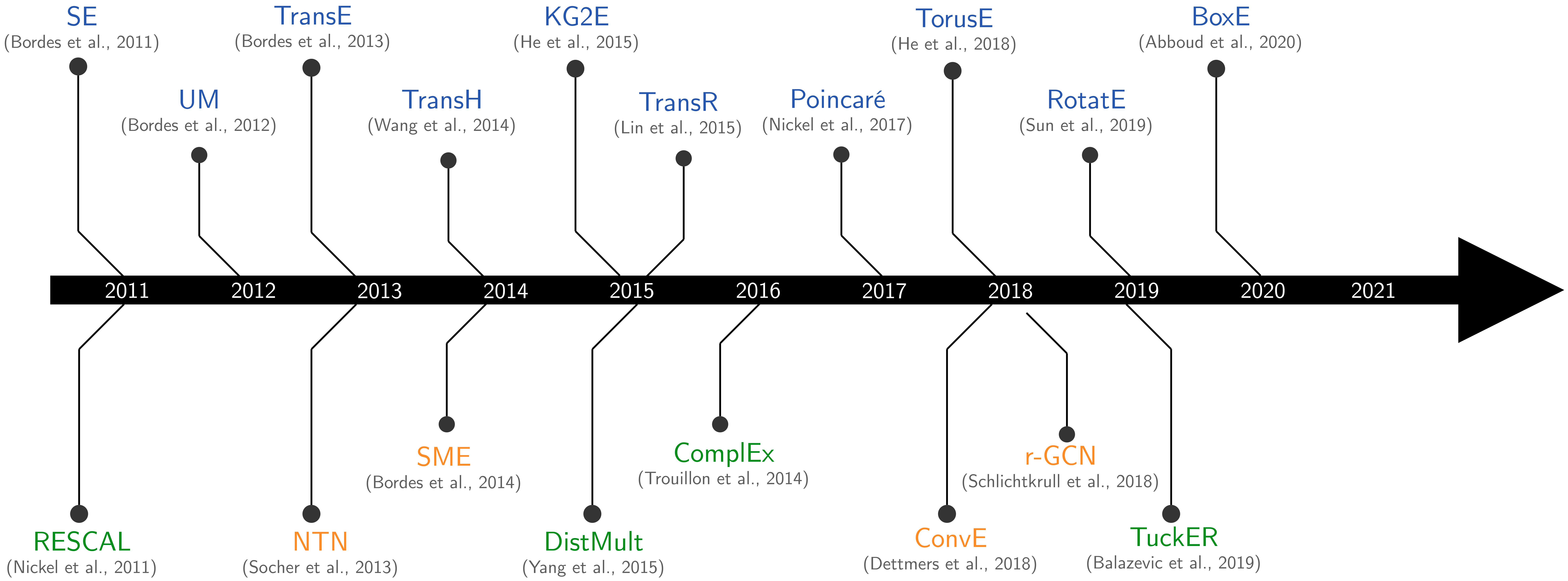

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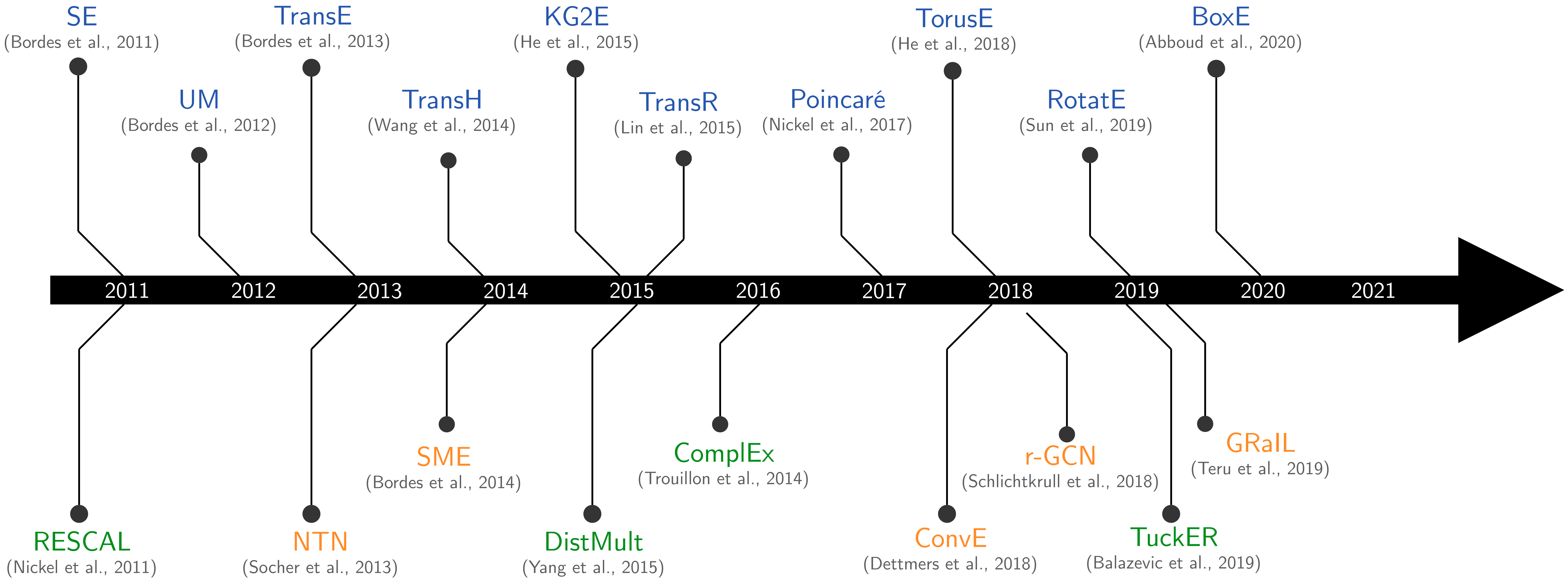

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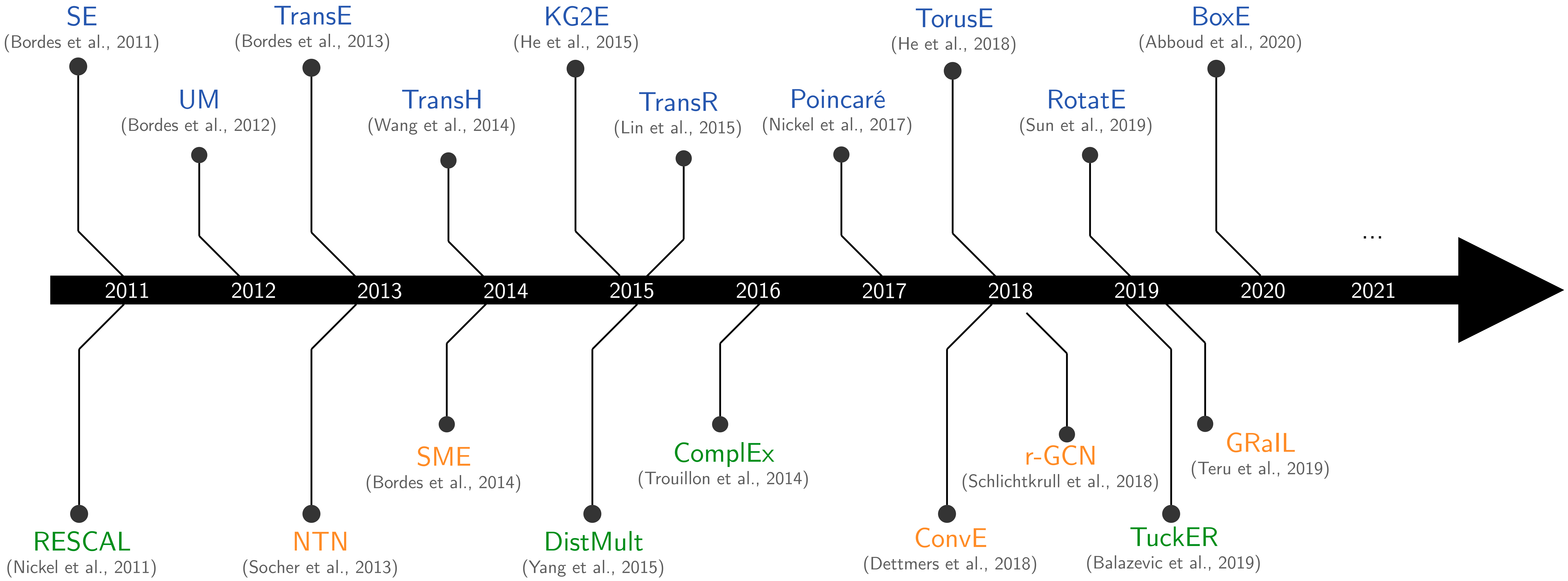

Translational Models

TransE

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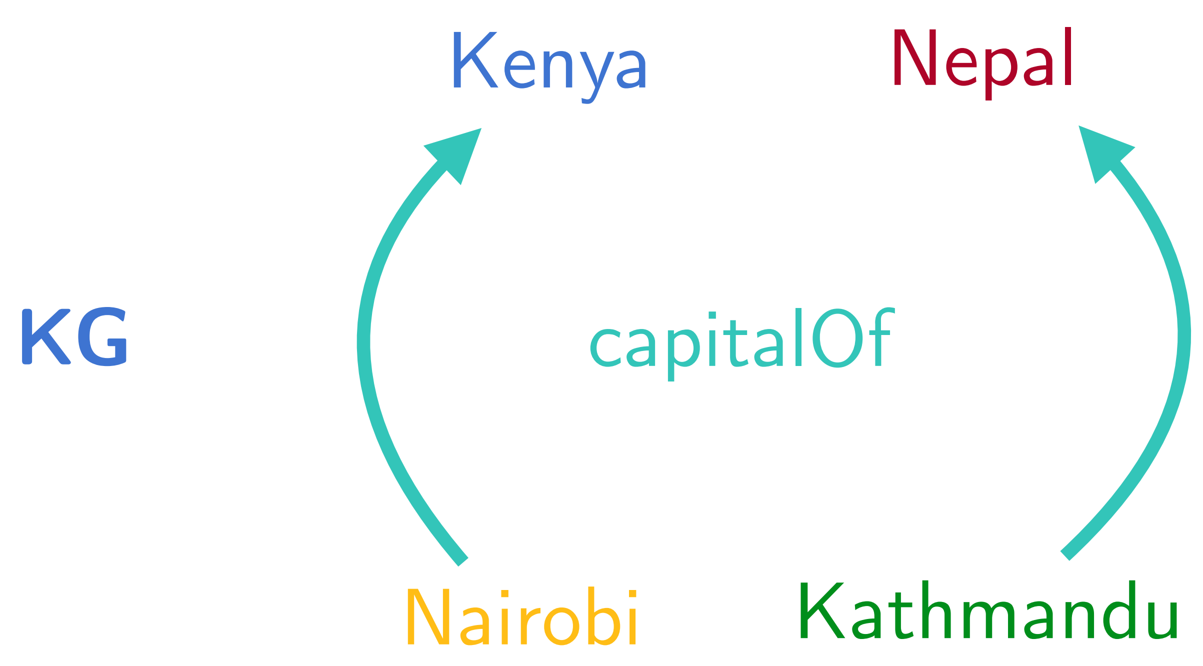

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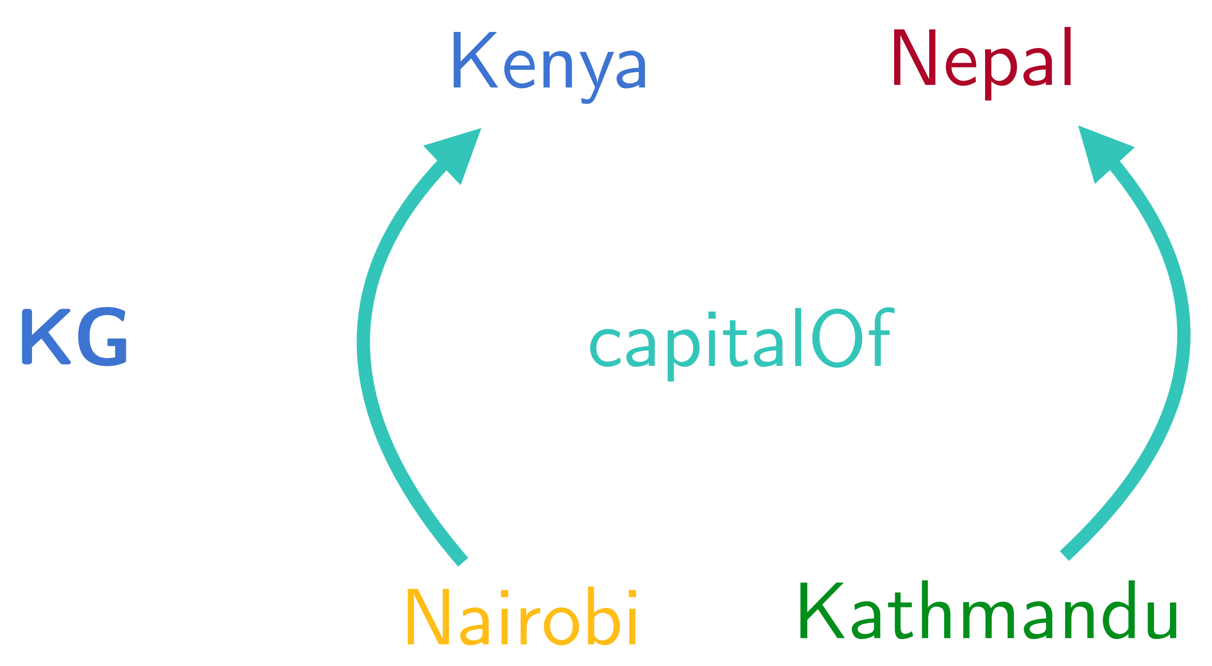

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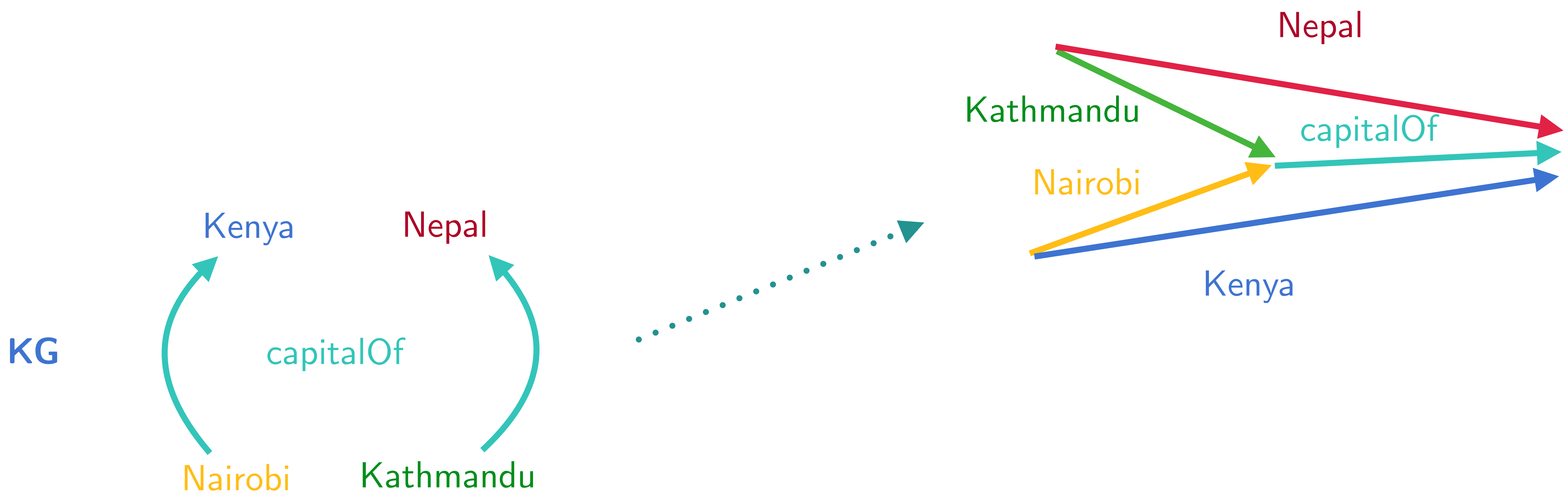

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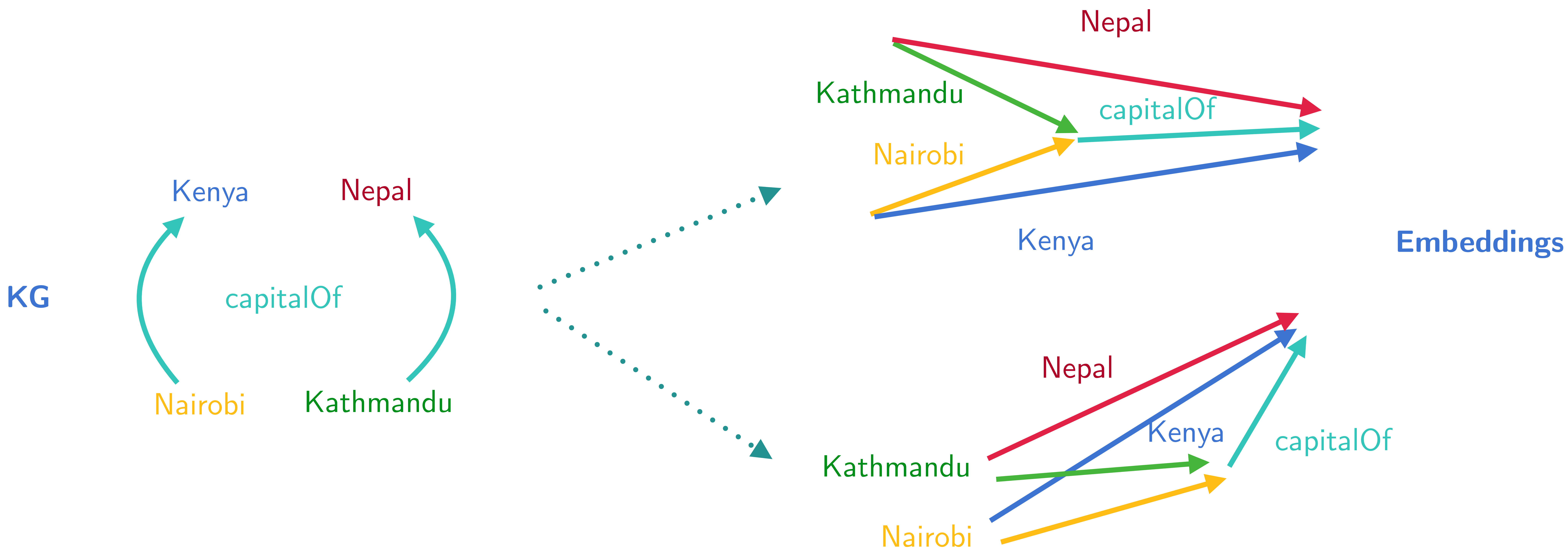

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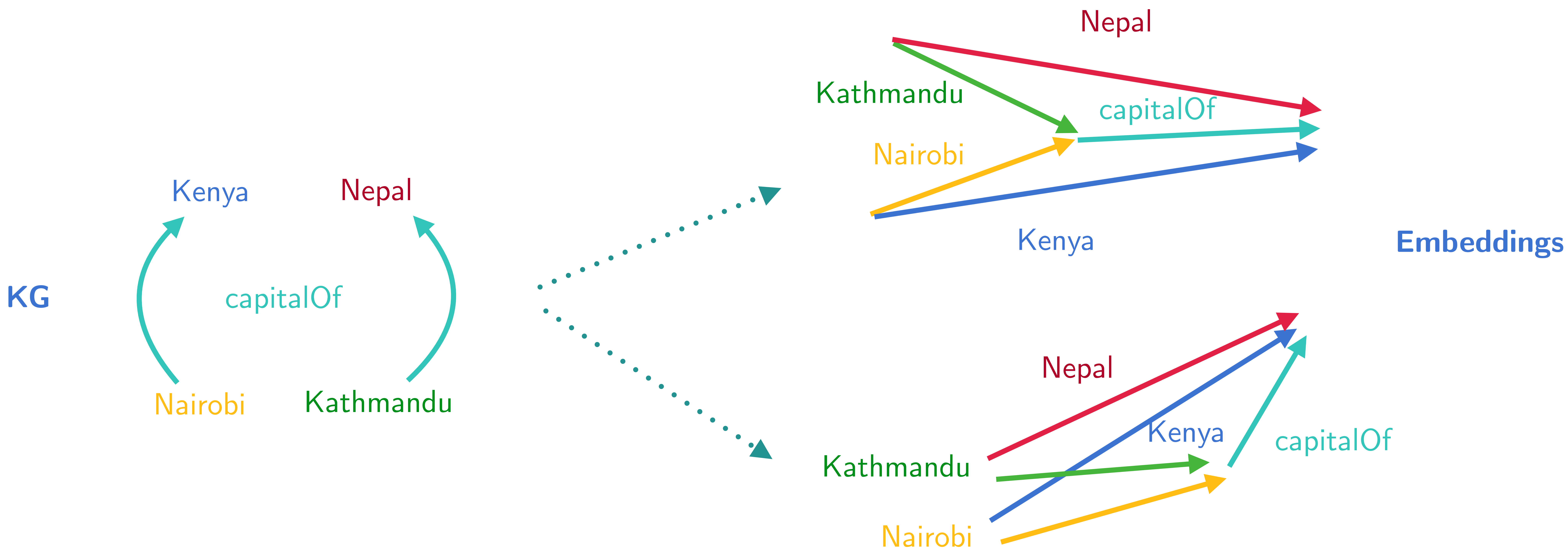

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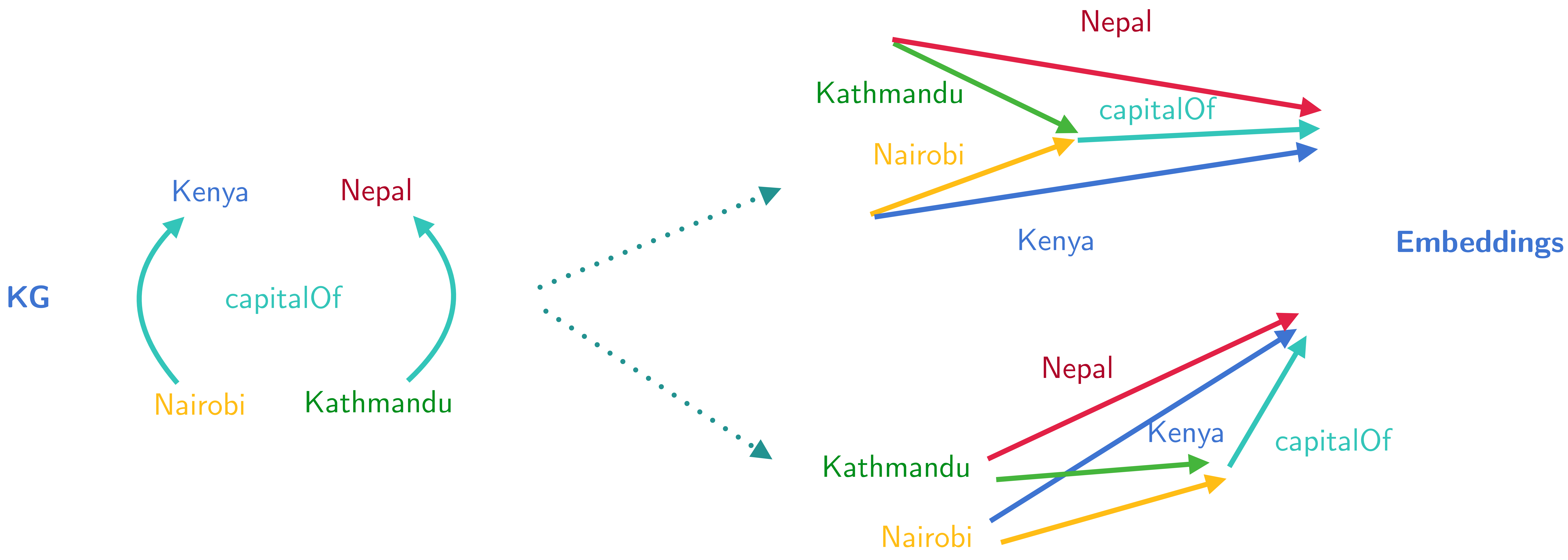
TransE



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- Optimized to minimize (resp., maximize) the dissimilarity of true facts (resp., negative facts).

TransE: Optimization, Loss, Training

Decoder: Consider a distance measure d, e.g., L_1 or L_2 norm, where $d(\mathbf{h} + \mathbf{r}, \mathbf{t}) = \|\mathbf{h} + \mathbf{r} - \mathbf{t}\|$ represents how dissimilar $\mathbf{h} + \mathbf{r}$, and $\mathbf{t}$ are. Hence, $-\|\mathbf{h} + \mathbf{r} - \mathbf{t}\|$ defines a similarity measure.

Loss: TransE defines the loss function:

$$\mathscr{L} = \sum_{r(h,t) \in G} \sum_{r(h',t') \in N^{r(h,t)}} \left[d(\mathbf{h} + \mathbf{r}, \mathbf{t}) - d(\mathbf{h}' + \mathbf{r}, \mathbf{t}') + \gamma \right]_+ ,$$

where γ is a margin hyper-parameter, $N^{r(h,t)}$ is a set of negative samples for $r(h,t)$, and $[x]_+$ denotes the positive part of x.

Favors higher values of similarity for true facts than for negative ones: implementation of the intended criterion.

Optimization: By stochastic gradient descent, where all embeddings are initialized randomly; at each iteration, the parameters are updated by taking a gradient step with constant learning rate. The algorithm is stopped based on its performance on a validation set.

How Expressive is TransE?

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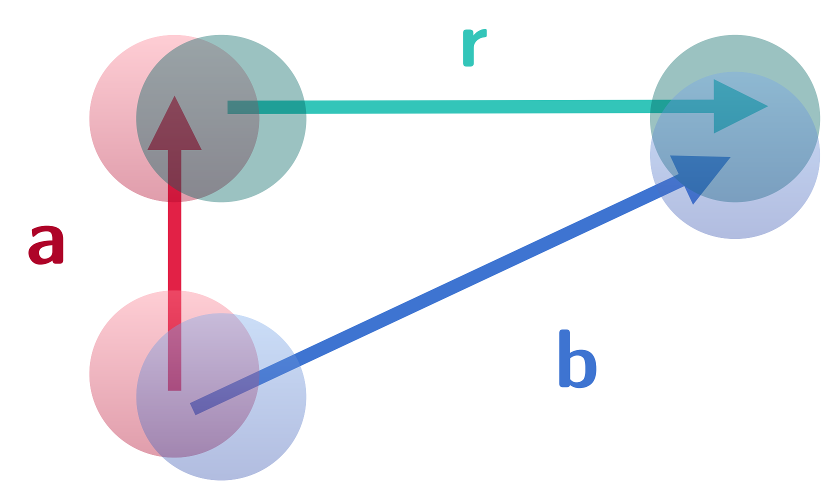

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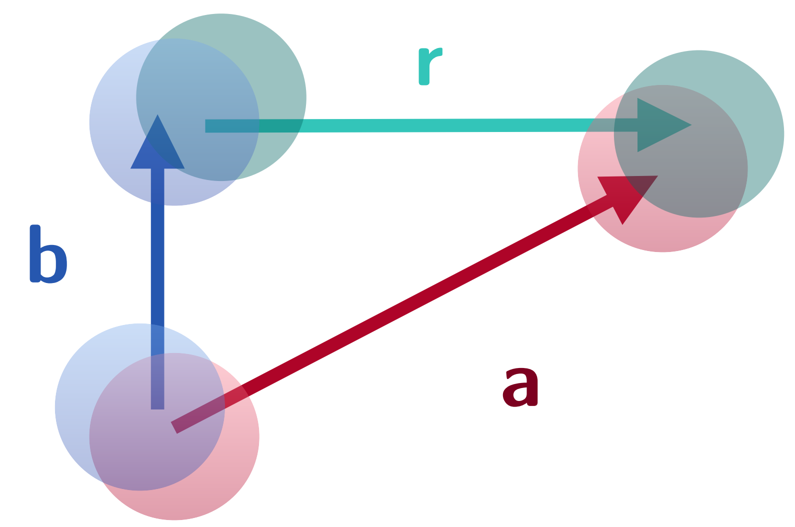

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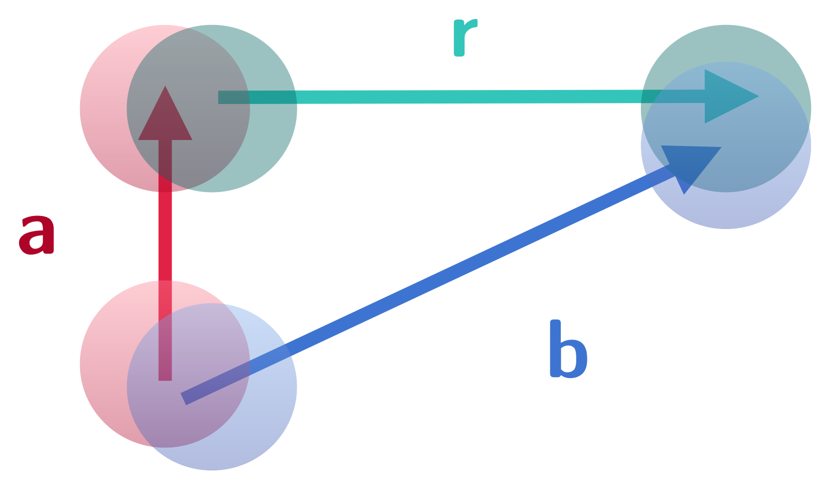

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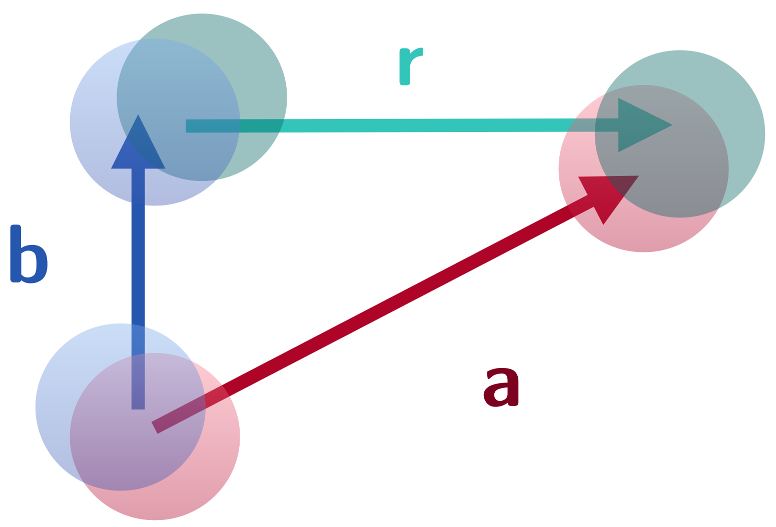
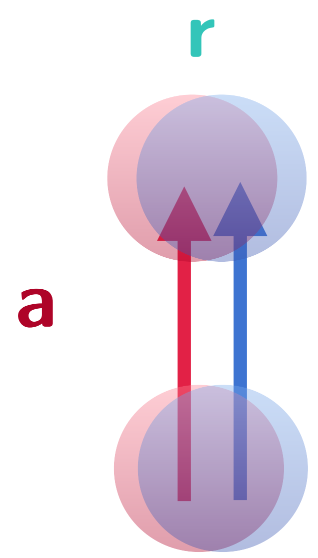


(iii) $r(a,b)$ & $r(b,a)$



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The relation r can be made symmetric only by additionally forcing r to be reflexive, hence leading to loss of generality.

TransE is not fully expressive: it cannot encode the set of true facts $\{r(a,b), r(b,a)\}$ and the set of false facts $\{r(a,a), r(b,b)\}$.

Consider a relation such as cousinOf with entities alice, bob to see a problematic example.

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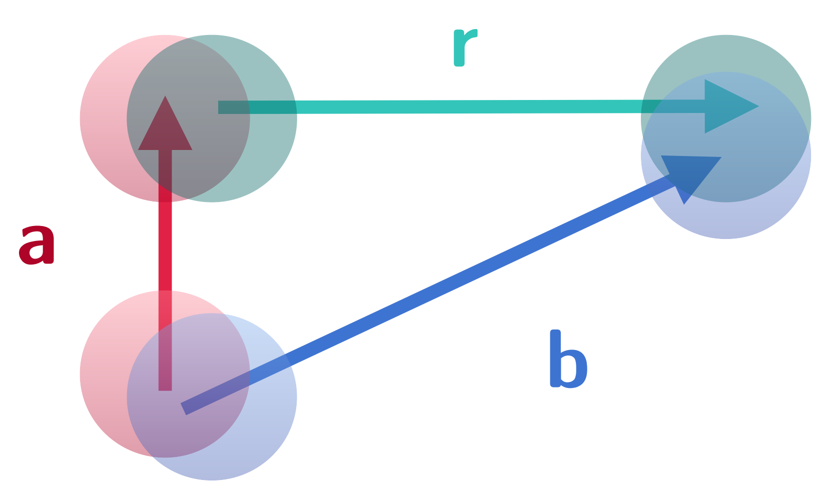

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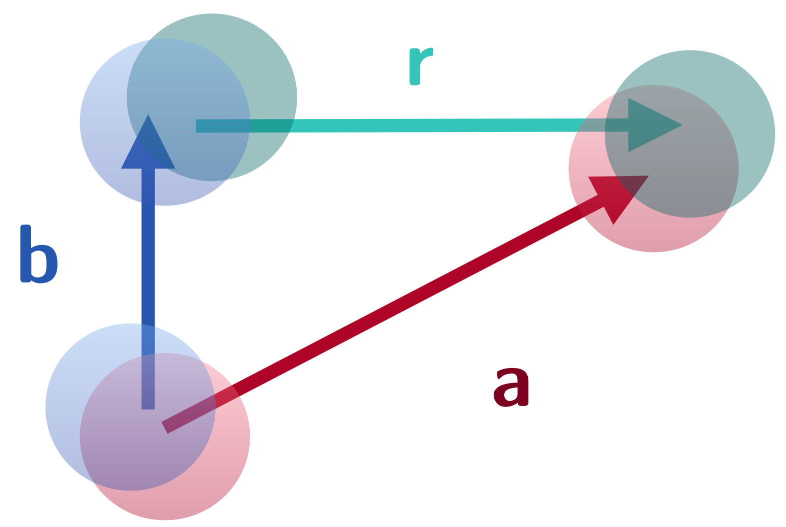

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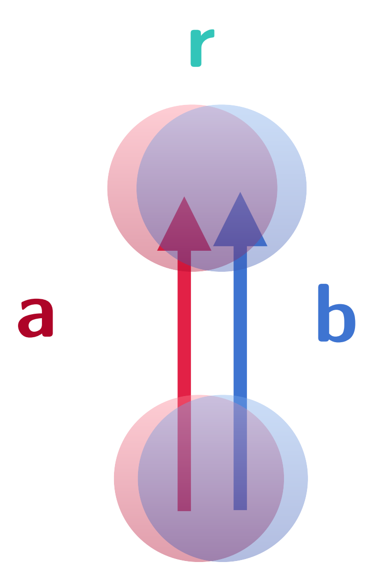

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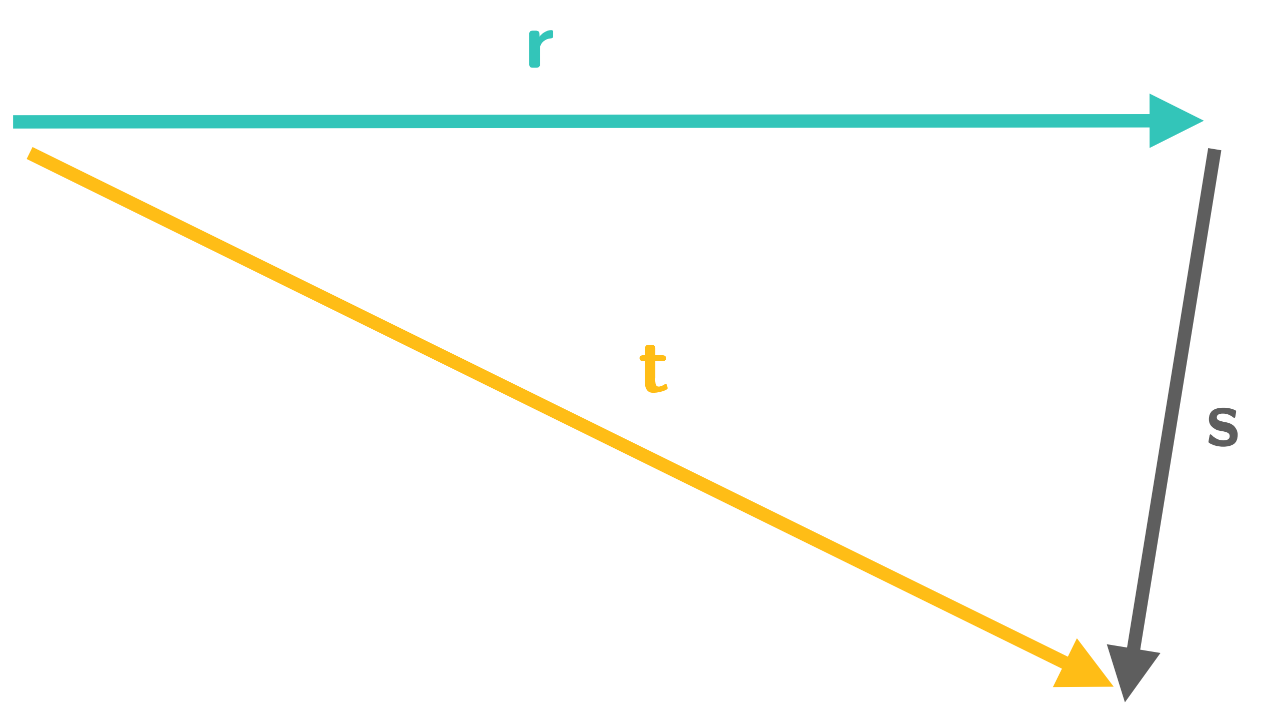

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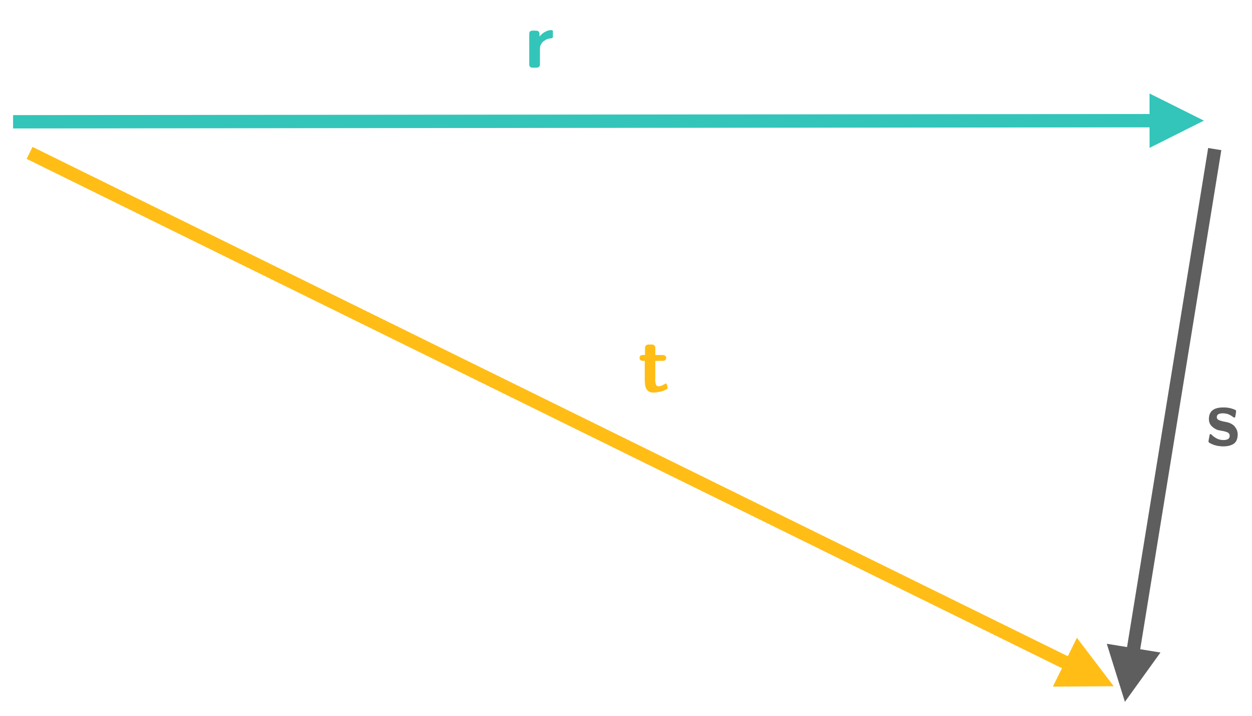

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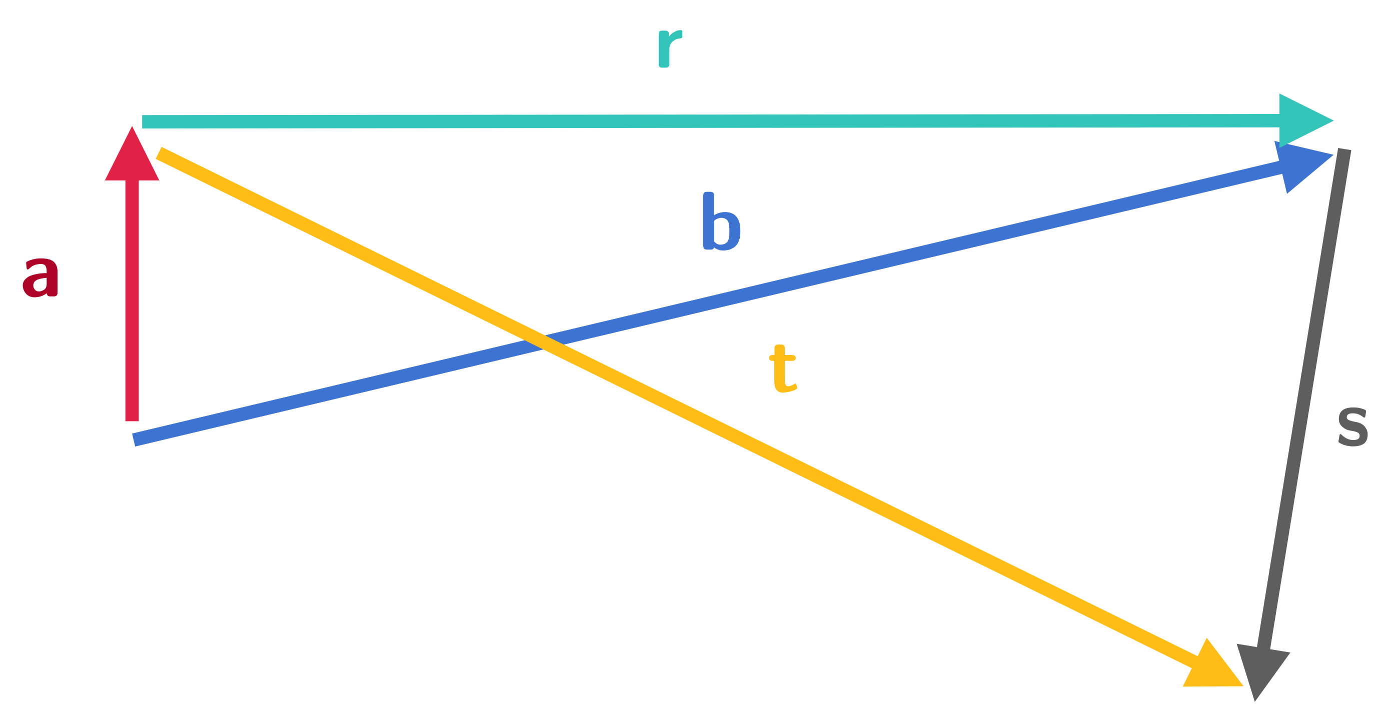

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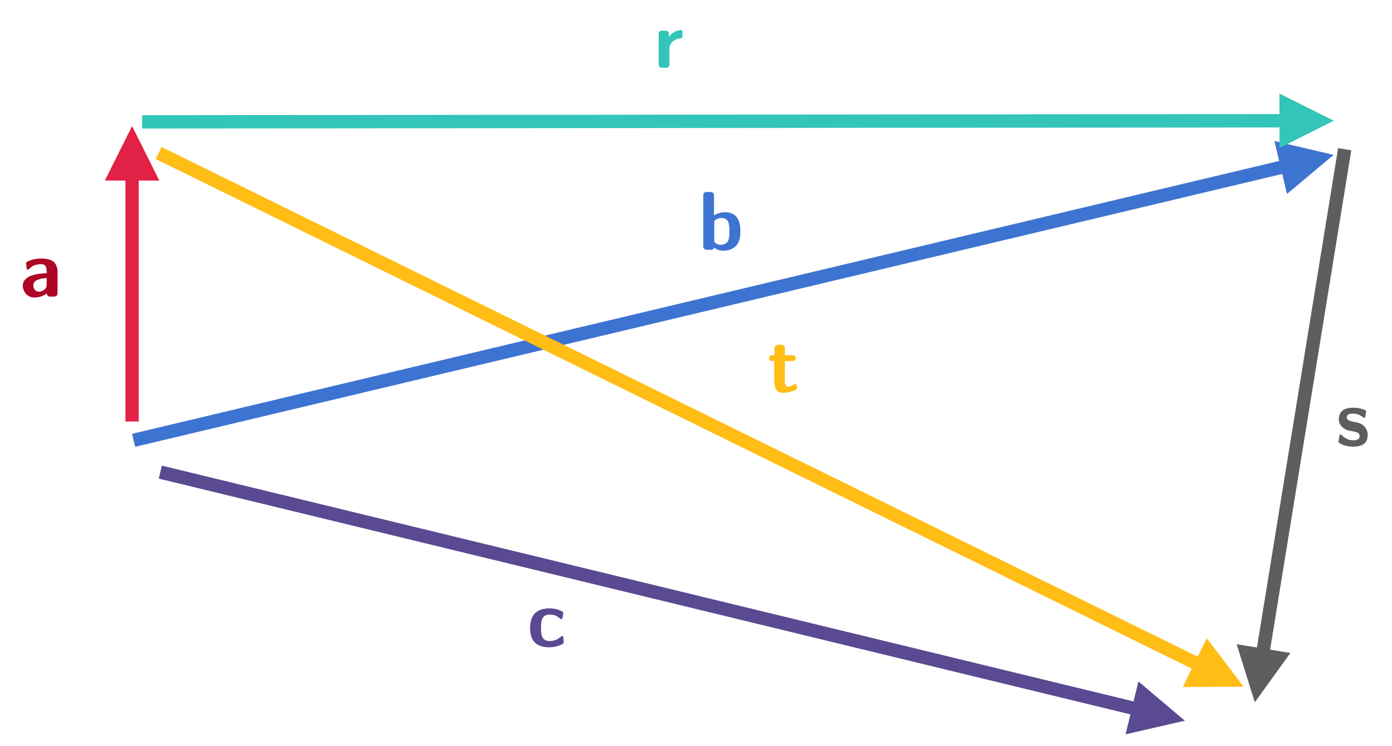

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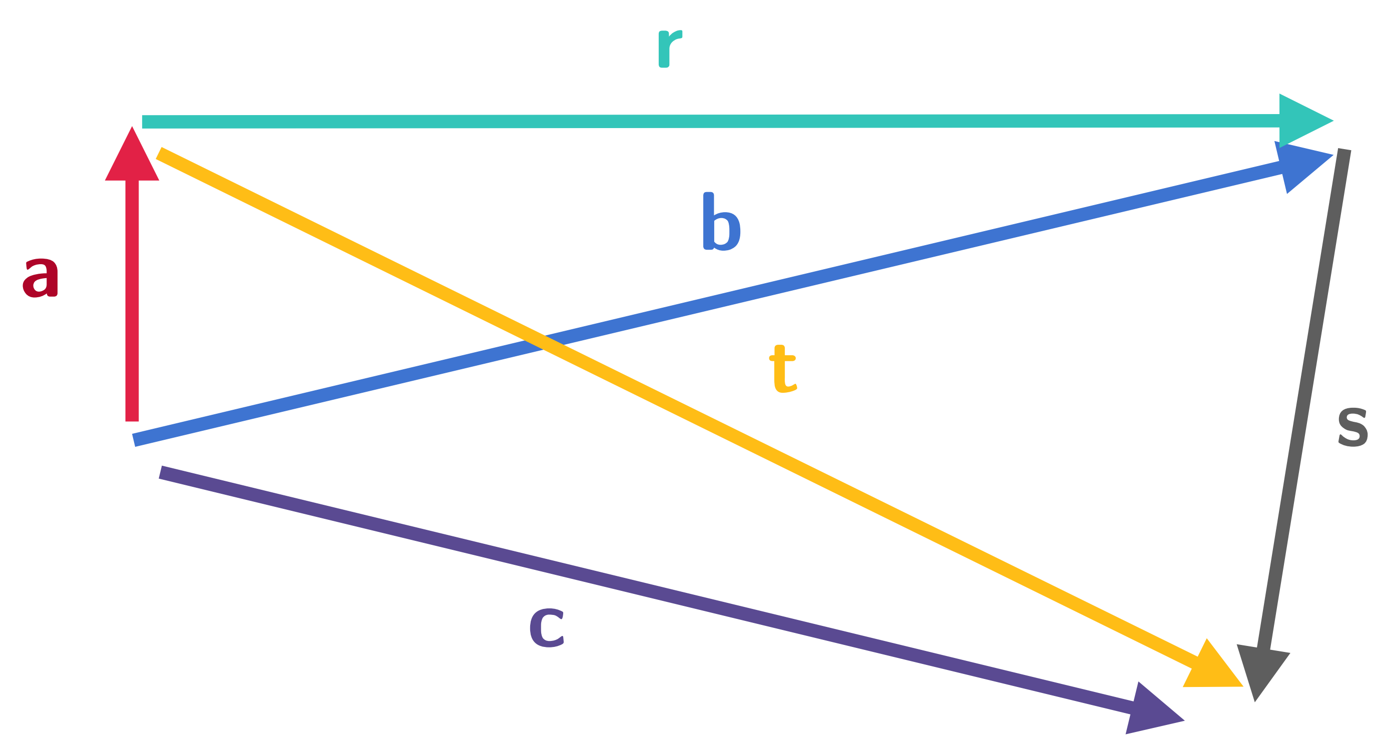

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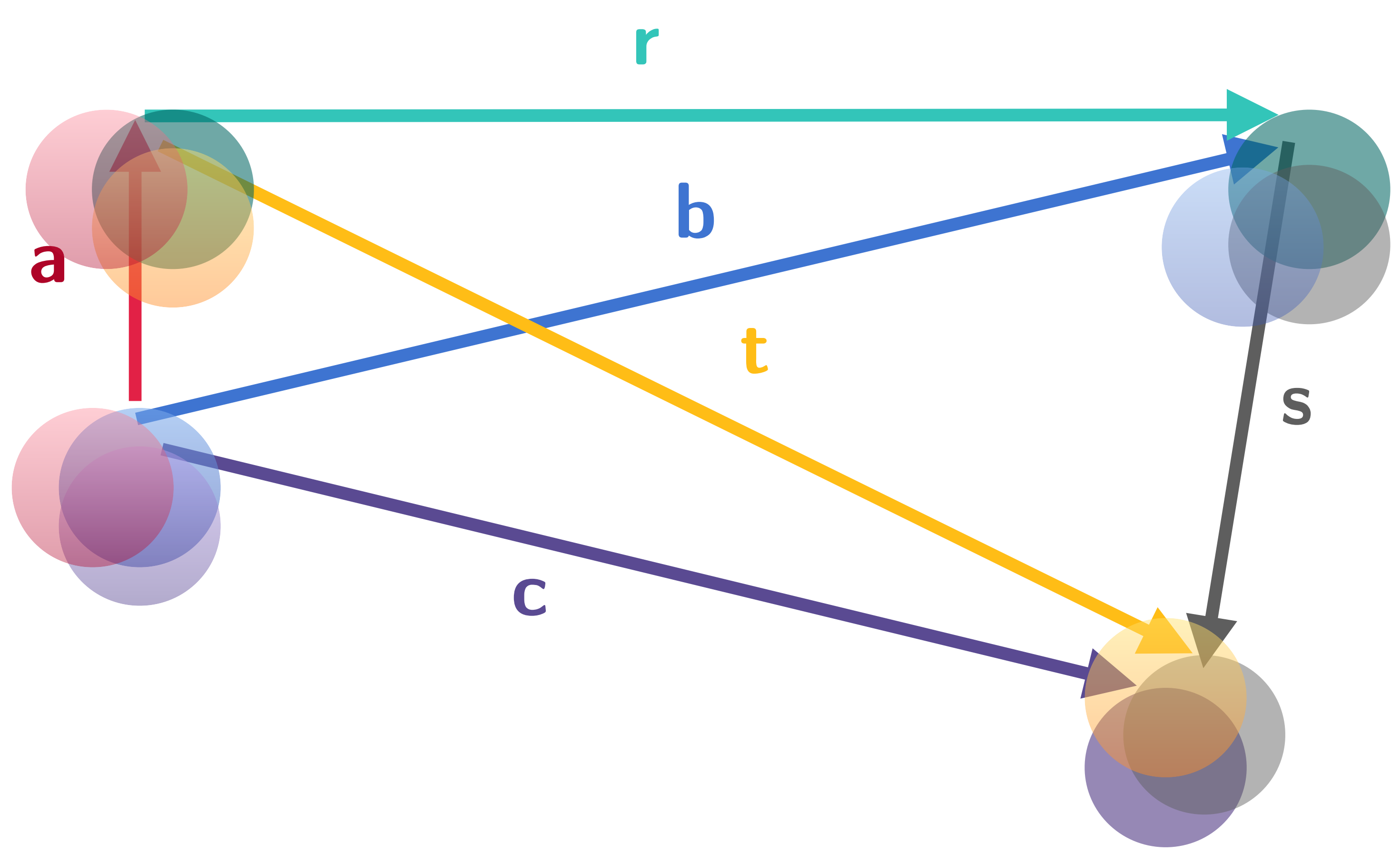

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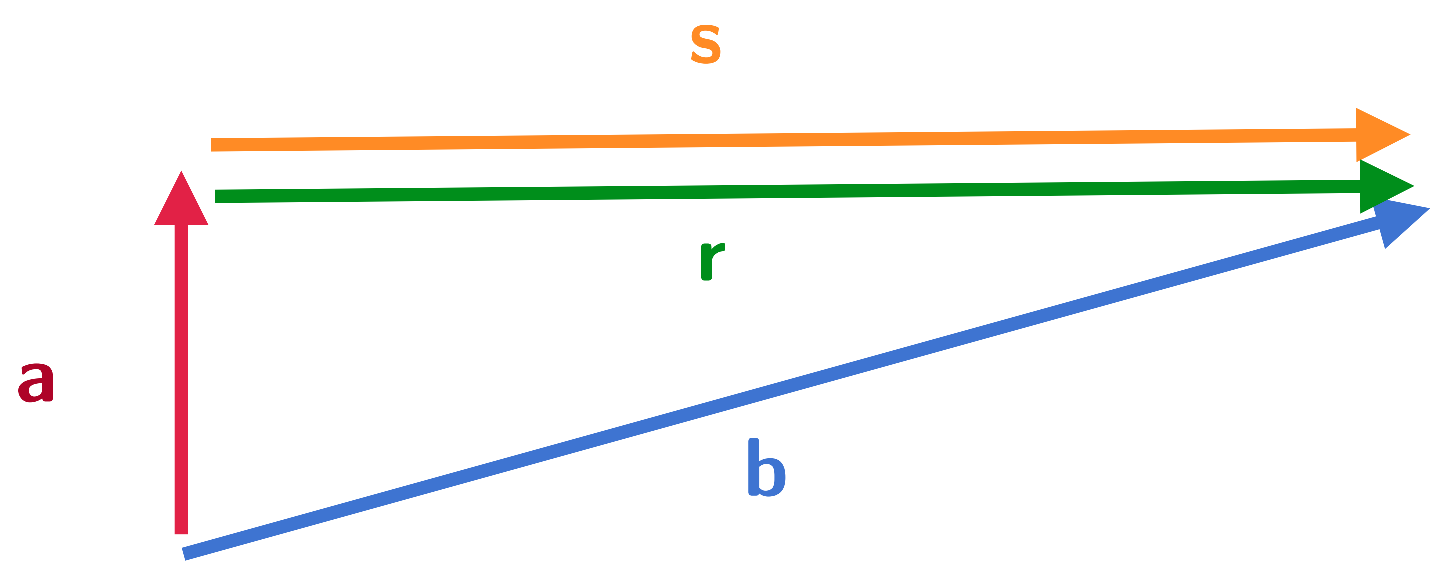
Which Inference Patterns Can TransE Not Capture?

TransE cannot capture symmetry: a relation can be symmetric only by forcing it to be reflexive.

What about the hierarchy pattern: $\forall x, y\ r(x, y) \Rightarrow s(x, y)$?



Only by setting $\mathbf{r} \approx \mathbf{s}$, and, this would imply relation equivalence: TransE cannot capture hierarchy either.

The lack of ability to capture the hierarchy pattern is also a serious limitation, as it is also prevalent in datasets (e.g., the relation capitalOf implies the relation cityIn).

Other Limitations of TransE

1-to-n, n-to-1, n-to-n, relations refer to the cardinality of the relation in terms of the head and tail entities.

TransE does not efficiently learn the representations for n-to-n relations in a KG:

locatedIn(Oxford, Oxfordshire)

locatedIn(Oxford, UK)

We need Oxfordshire $\approx$ UK to realize these, since the elements locatedIn, Oxford are shared in the scoring.

Similarly for 1-to-n relations, i.e., Bob $\approx$ Chris in:

motherOf(Anne, Bob)

motherOf(Anne, Chris)

Other translational models are proposed to reduce the effect of this problem; see, e.g., TransH and TransR.

RotatE

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RotatE defines each relation r as a rotation from an entity h to an entity t in the complex vector space.

Euler's formula: $e^{i\theta} = cos\theta + i\ sin\theta$, i.e., a unitary complex number tracing the unit circle in the complex plane as θ ranges through reals.

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Encoder: Entities $h, t \in E$ and relations $r \in R$, through d-dimensional complex vectors $\mathbf{h}, \mathbf{t}, \mathbf{r} \in \mathbb{C}^d$, where each element r_i of $\mathbf{r}$ is of the form $e^{i\theta_{r,i}}$ (with modulus $| r_i | = 1$).

Decoder: Consider a dissimilarity measure $d(\mathbf{h} \odot \mathbf{r}, \mathbf{t}) = \|\mathbf{h} \odot \mathbf{r} - \mathbf{t}\|$, where $\odot$ denotes element-wise product, corresponding to a counterclockwise rotation in every dimension i by $\theta_{r,i}$ radians about the origin of the complex plane. Hence, $-\|\mathbf{h} \odot \mathbf{r} - \mathbf{t}\|$ defines a similarity measure.

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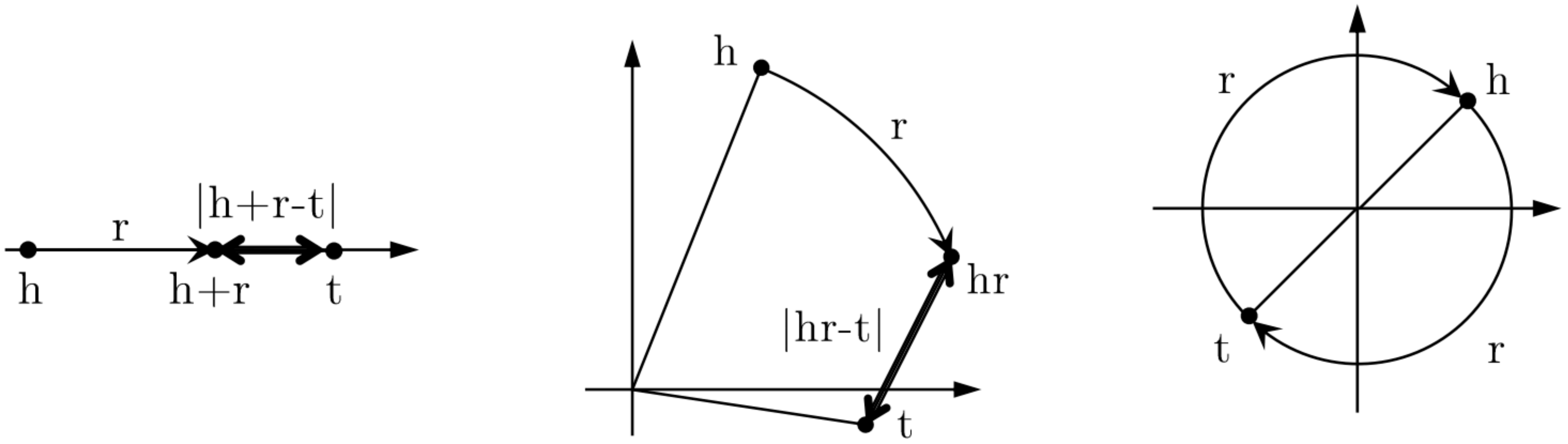
Loss: For every fact $r(h, t)$, RotatE minimizes the following loss function:

$$\mathscr{L} = -\log \sigma(\gamma - d(\mathbf{h} \odot \mathbf{r}, \mathbf{t})) - \sum_{r(h',t') \in N^{r(h,t)}} \frac{1}{k} \log \sigma(d(\mathbf{h}' \odot \mathbf{r}, \mathbf{t}') - \gamma),$$

where γ is a fixed margin, σ is the sigmoid function, and $N^{r(h,t)}$ is a set of k negative samples for $r(h, t)$.

RotatE vs TransE



(a) TransE models $\mathbf{r}$ as translation in real line.

(b) RotatE models $\mathbf{r}$ as rotation in complex plane.

(c) RotatE: an example of modeling symmetric relations $\mathbf{r}$ with $r_i = -1$

Figure (Sun et al): Comparing 1-dimensional embeddings of the models TransE and RotatE. Rotations in each individual dimension enable RotatE to capture symmetry.

RotatE can emulate TransE as a special case, see Theorem 4 of (Sun et al).

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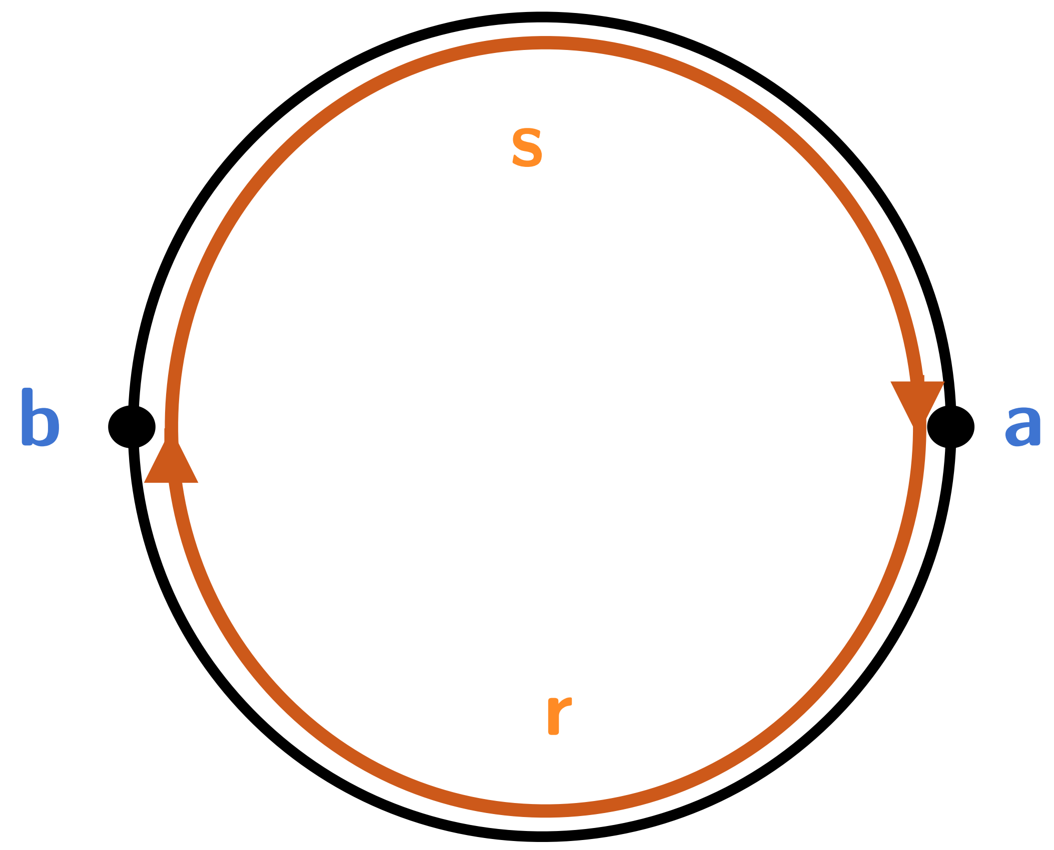

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RotatE cannot fit the sets facts:

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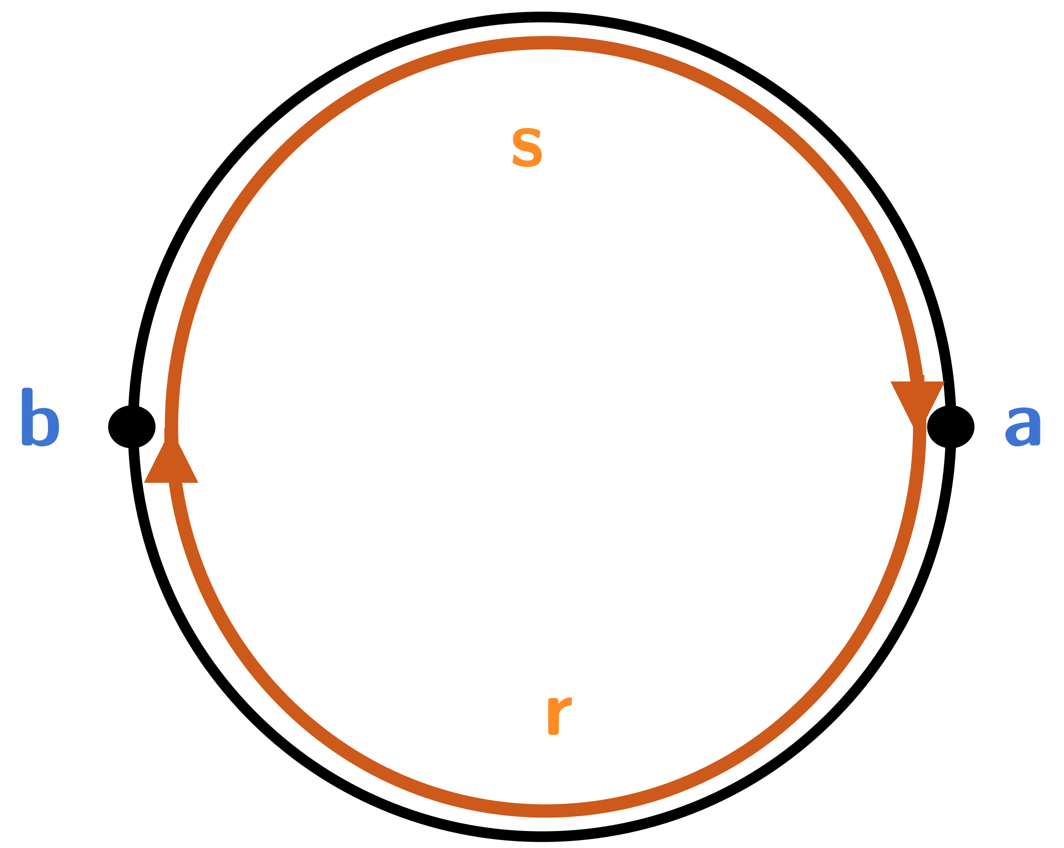

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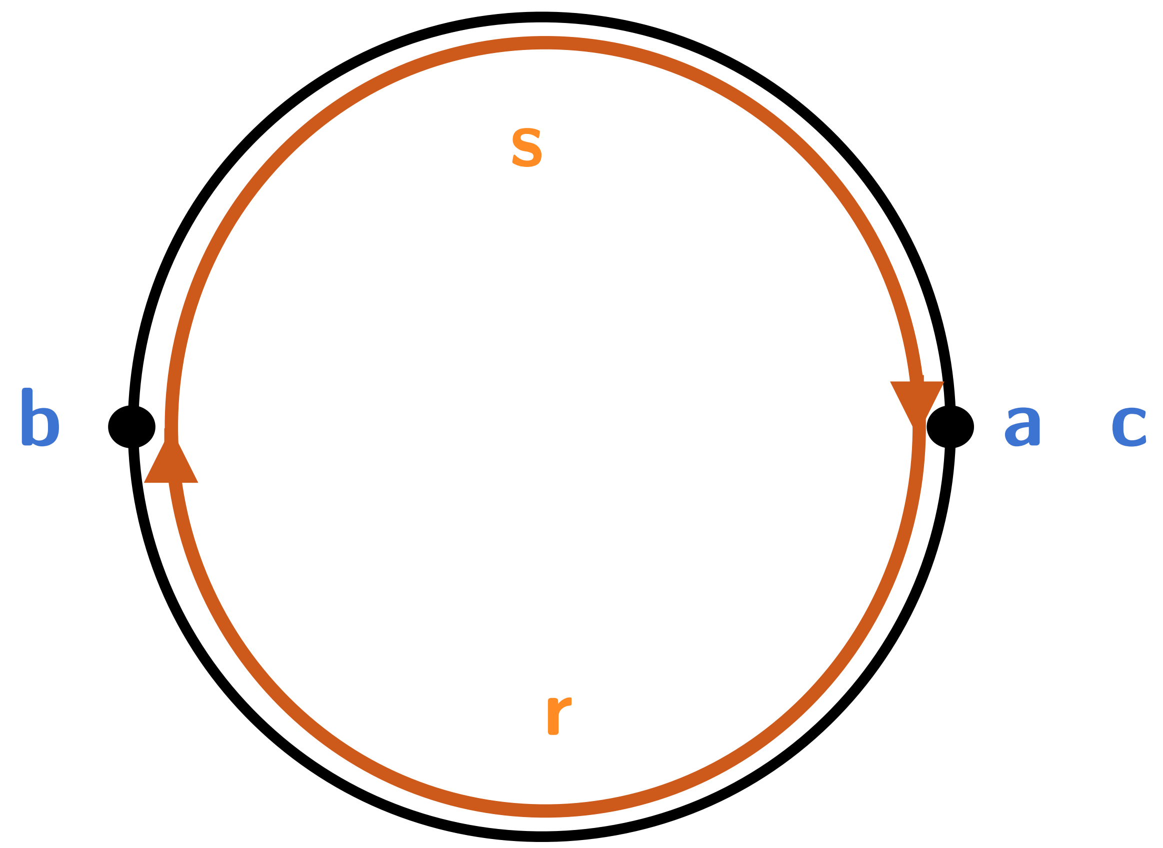

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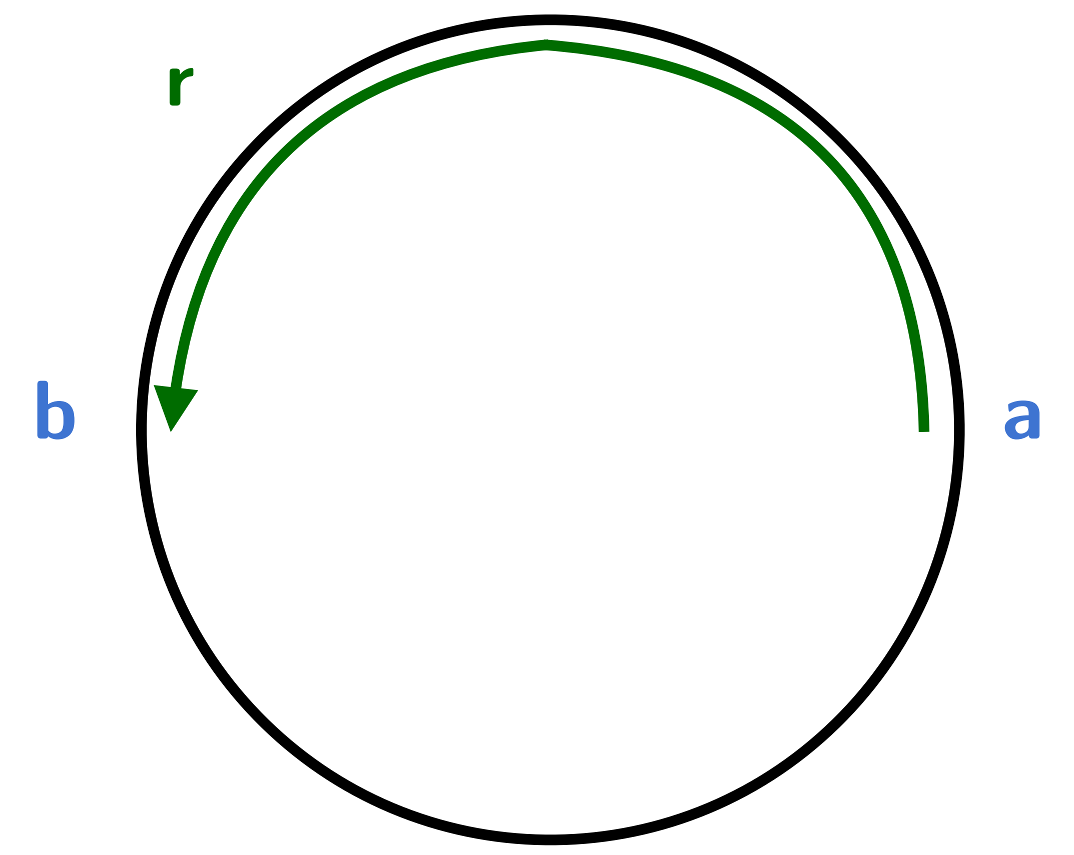

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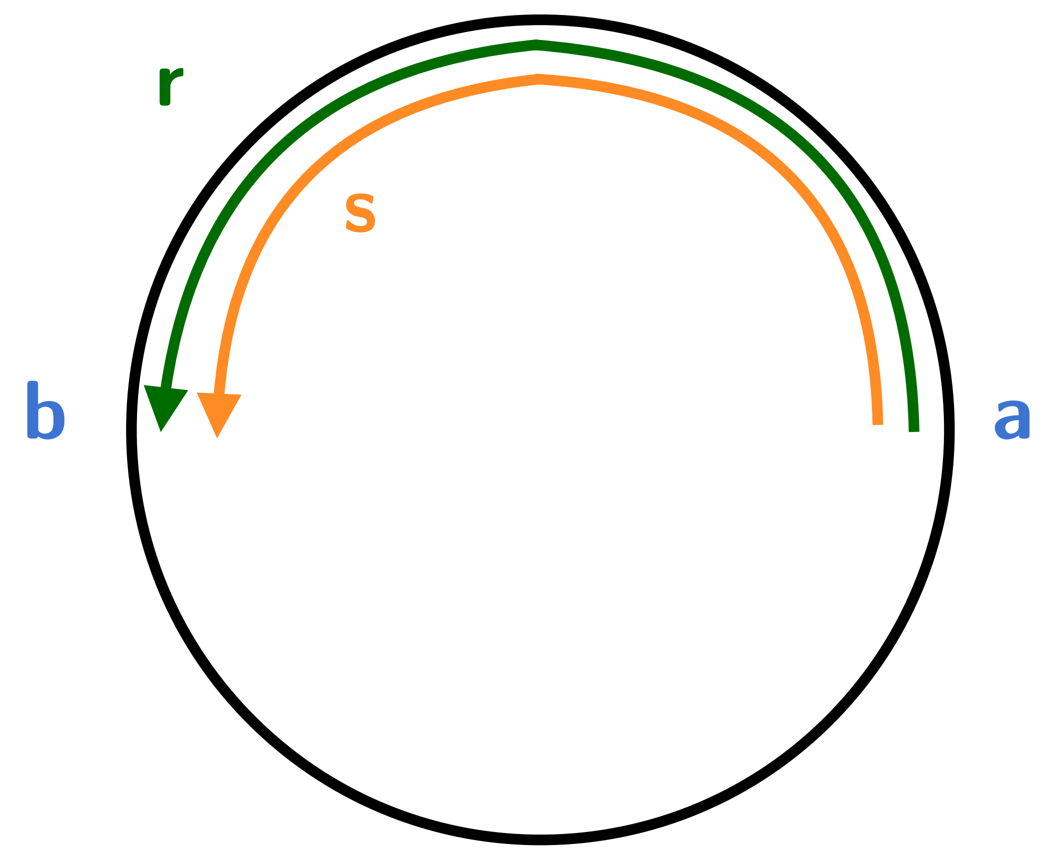

Bilinear Models

Tensor Representation of a KG

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A KG G can be represented by defining, for every relation $r \in R$, an adjacency matrix $\mathbf{M}_r \in \mathbb{R}^{|E| \times |E|}$:

$$\mathbf{M}_{r[i,j]} = \begin{cases} 1 & \text{if } r(e_i, e_j) \in G, \\ 0 & \text{otherwise.} \end{cases}$$

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Similarly, we can represent G in terms of a tensor $\mathbf{T} \in \mathbb{R}^{|E| \times |E| \times |R|}$:

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Bilinear models use a bilinear product, to represent the relationships, hence the name "bilinear".

Bilinear models use tensor/matrix representation for relations and fall under tensor factorization methods.

RESCAL

$$\mathbf{h}^\top \begin{bmatrix} 0.5 & 1 & 0.2 \\ 1 & 0.2 & 0 \\ 0.3 & 0.5 & 0.8 \end{bmatrix}_r \mathbf{t}$$

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RESCAL is the first bilinear model and has inspired a line of research.

Encoder: Entities $h, t \in E$ through vectors $\mathbf{h}, \mathbf{t} \in \mathbb{R}^d$, and relations $r \in R$, as a matrix $\mathbf{M}_r \in \mathbb{R}^d \times \mathbb{R}^d$.

Decoder: Scores a fact $r(h, t)$ as $\mathbf{h}^\top \mathbf{M}_r \mathbf{t}$, which captures all interactions between the components of $\mathbf{h}$ and $\mathbf{t}$ and defines a similarity measure.

Loss: Exact formulation can vary, depending on regularization terms etc.

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Expressiveness: RESCAL is fully expressive, as it is possible to fit arbitrary set of true and false facts using the power of full rank matrix. This requires $O(d^2)$ parameters per relation, and is impractical for large-scale KGs.

Problem: Using a full rank matrix is prone to overfitting, and this has motivated a line of research, where several restrictions are imposed on the representation.

DistMult

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DistMult is a bilinear model that restricts RESCAL to a diagonal matrix.

Encoder: DistMult does not allow an arbitrary matrix $\mathbf{M}_r \in \mathbb{R}^d \times \mathbb{R}^d$ for a relation $r \in R$ and restricts this to be the diagonal matrix $\mathbf{D}_r$.

Decoder: DistMult scores a fact $r(h, t)$ similar to RESCAL, with the restriction to the diagonal matrix: $\mathbf{h}^\top \mathbf{D}_r \mathbf{t}$.

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Expressiveness: DistMult is not fully expressive since $\mathbf{h}^\top \mathbf{D}_r \mathbf{t} = \mathbf{t}^\top \mathbf{D}_r \mathbf{h}$.

DistMult cannot differentiate between head entity and tail entity: all relations are modeled as symmetric regardless, i.e., even anti-symmetric relations.

Scalability: While very inexpressive, DistMult is scalable, i.e., linear in d.

ComplEx

$$\mathbf{h}^\top \begin{bmatrix} 1+i & 0 & 0 \\ 0 & 2+i & 0 \\ 0 & 0 & 3+2i \end{bmatrix}_r \bar{\mathbf{t}}$$

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ComplEx is another bilinear model which extends DistMult to the complex domain.

Encoder: Entities $h, t \in E$ through d-dimensional vectors $\mathbf{h}, \mathbf{t} \in \mathbb{C}^d$ in complex space, and relations $r \in R$, as a diagonal matrix $\mathbf{D}_r \in \mathbb{C}^d \times \mathbb{C}^d$ in this space.

Decoder: Scores a fact $r(h, t)$ as $\text{Re}(\mathbf{h}^\top \mathbf{D}_r \bar{\mathbf{t}})$, where $\bar{\mathbf{t}}$ defines the complex conjugate of $\mathbf{t}$, and Re denotes the real part of a complex vector.

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Expressiveness: By the use of complex conjugates, ComplEx introduces asymmetry and thus can also model asymmetric relations. ComplEx is fully expressive for KGs.

ComplEx is an interesting trade-off, as it generalizes DistMult to a fully expressive model, while still using diagonal matrices, which are less prone to overfitting.

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Both ComplEx and DistMult can capture the hierarchy pattern: For DistMult, set $s = \lambda r$, for a scalar $\lambda > 1$: Then $\mathbf{h}^\top \mathbf{D_r} \mathbf{t} < \mathbf{h}^\top \mathbf{D_s} \mathbf{t}$, and and hence $\forall x, y \; r(x, y) \Rightarrow s(x, y)$. The argument for ComplEx is analogous.

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Models such as RESCAL and TuckER are same as ComplEx in terms of inference patterns.

Box Embedding Models

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A probabilistic embedding model is proposed based on Box Lattice Measures (Vilnis et al.): every class (i.e., unary relation) and entity in a KG are represented by a box. Entity-class membership, as well as relation similarity, is captured by means of box intersection in the lattice representation space.

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Neither of these approaches facilitate means for using box embeddings for KG completion.

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Encoder: Each entity $h, t \in E$ in terms of two d-dimensional vectors $\mathbf{h}, \mathbf{b_h} \in \mathbb{R}^d$ and $\mathbf{t}, \mathbf{b_t} \in \mathbb{R}^d$; each (binary) relation $r \in R$, in terms of two d-dimensional hyper-rectangles, or boxes, $\mathbf{r^h}, \mathbf{r^t} \in \mathbb{R}^d$, corresponding to a head box and a tail box, respectively.

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Idea: The embedding $\mathbf{h}$ (resp., $\mathbf{t}$) defines the base position of an entity h (resp., t), and the embedding $\mathbf{b_h}$ (resp., $\mathbf{b_t}$) defines its translational bump, which translates other entities from their base positions to their final embeddings by "bumping" them.

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Decoder: Consider a distance measure $\text{dist}(\mathbf{e}, \mathbf{B})$ which defines how close an entity embedding $\mathbf{e}$ is to the center of a box $\mathbf{B}$. BoxE scores a fact $r(h, t)$ as the sum of the L-x norms of such function:

$$\left\| \text{dist}(\mathbf{h}^{\mathbf{r}(\mathbf{h},\mathbf{t})}, \mathbf{r}^{\mathbf{h}}) \right\|_x + \left\| \text{dist}(\mathbf{t}^{\mathbf{r}(\mathbf{h},\mathbf{t})}, \mathbf{r}^{\mathbf{t}}) \right\|_x$$

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Box sizes are dynamic and their position matters: Every relation may be represented with boxes of different size and their relative position in relation to entities are part of scoring.

The final entity representation is dynamic: Every entity can have a potentially different final embedding relative to a different fact, since the bump vector depends on the other entity occurring in the fact.

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A fact citizenOf(Hitchcock, UK) holds when the final embedding of the entity Hitchcock appears in the box $\text{citizenOf}^{(h)}$ and the the final embedding of the entity UK appears in the box $\text{citizenOf}^{(t)}$.

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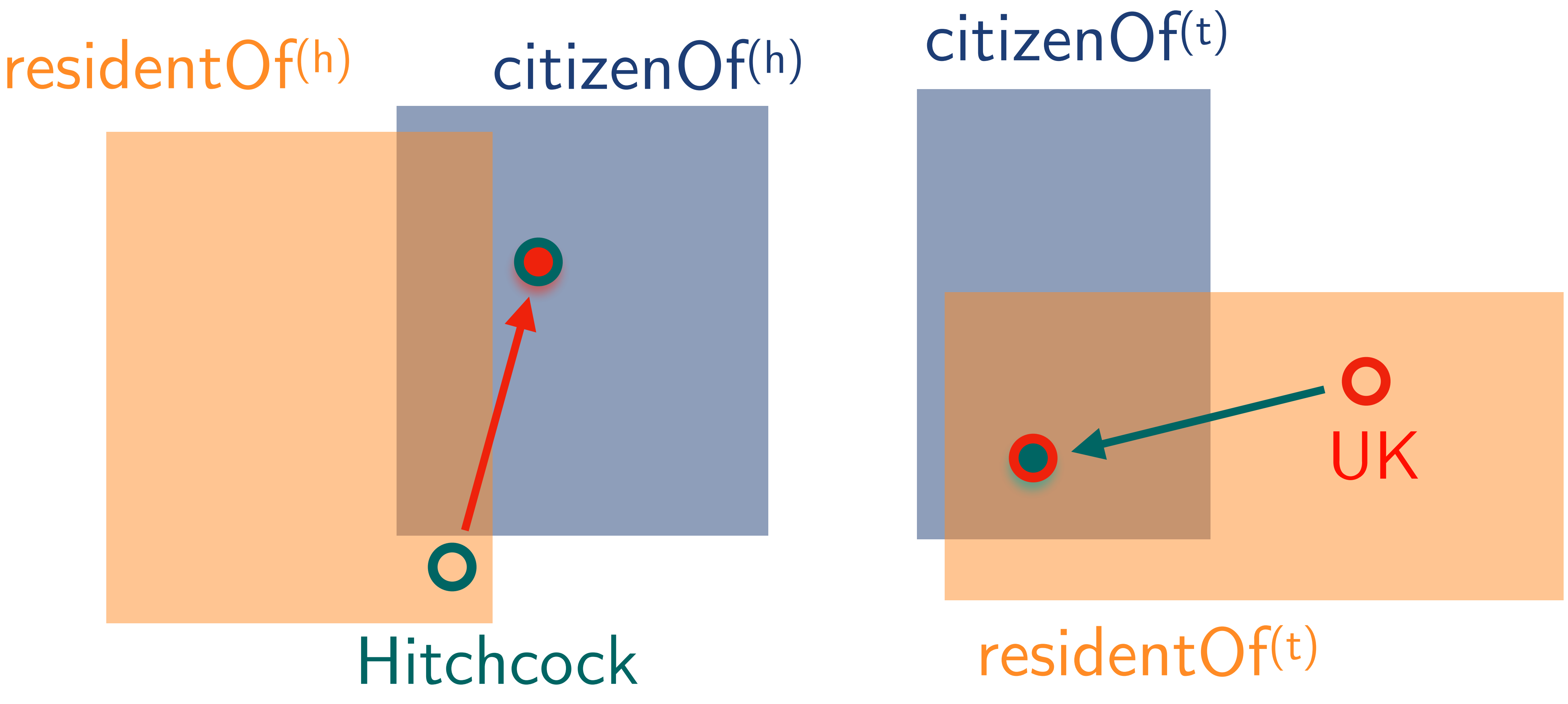

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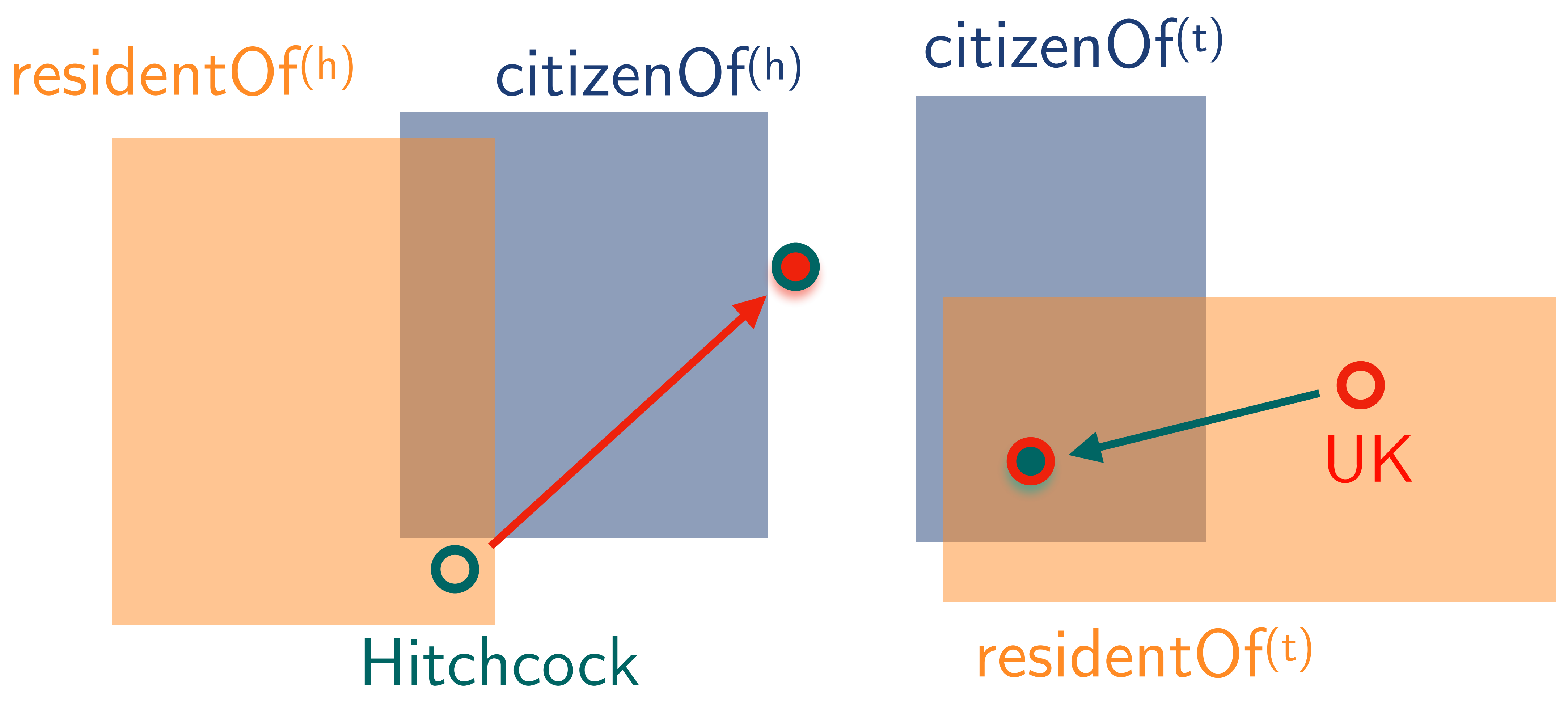

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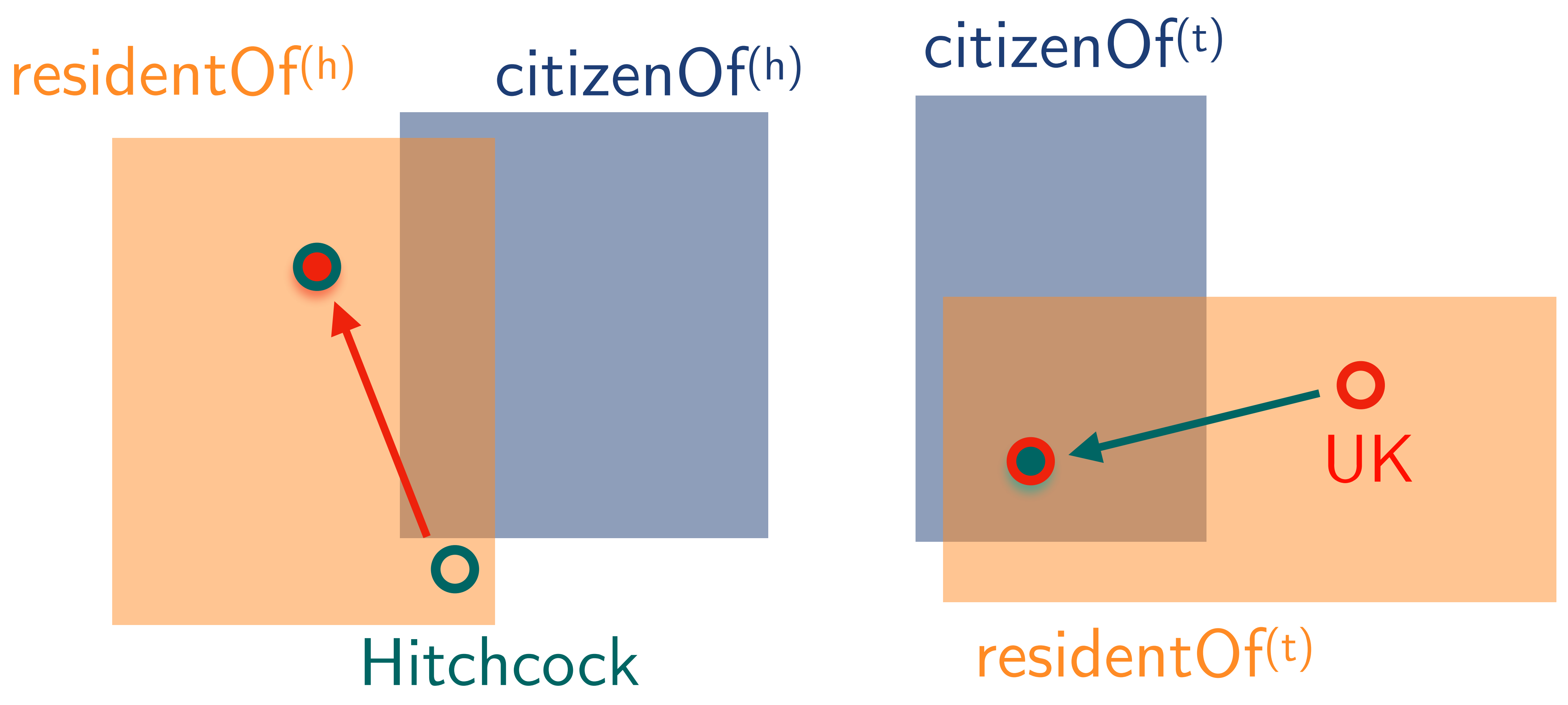

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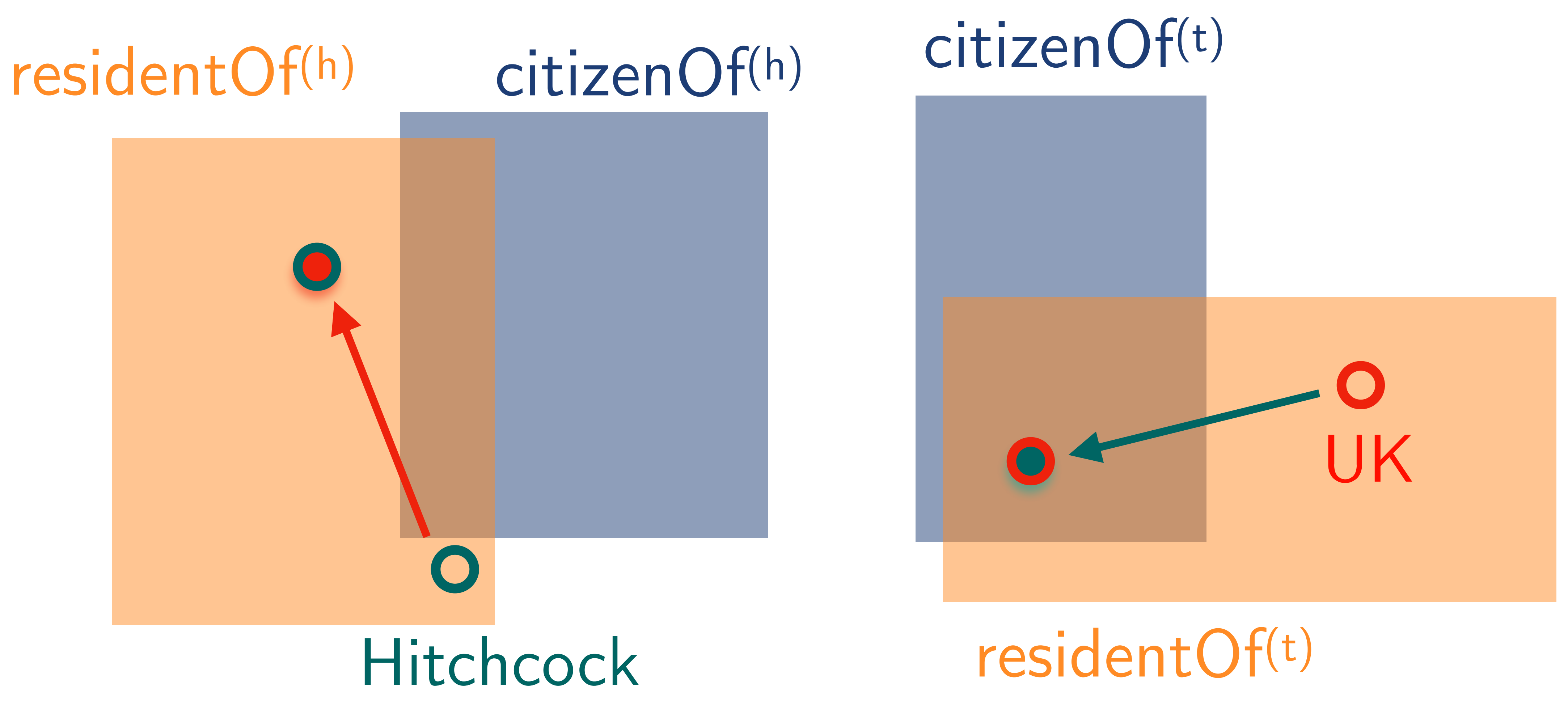

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Expressiveness: BoxE is fully expressive. Any fact $r(h,t)$ can be made false in the model, by defining a bump vector for, e.g., the head entity h such that the tail entity t is pushed outside of the tail box of r in a single dimension. This operation can be done for all false facts without "harming" true facts, using $E \times R$ dimensions.

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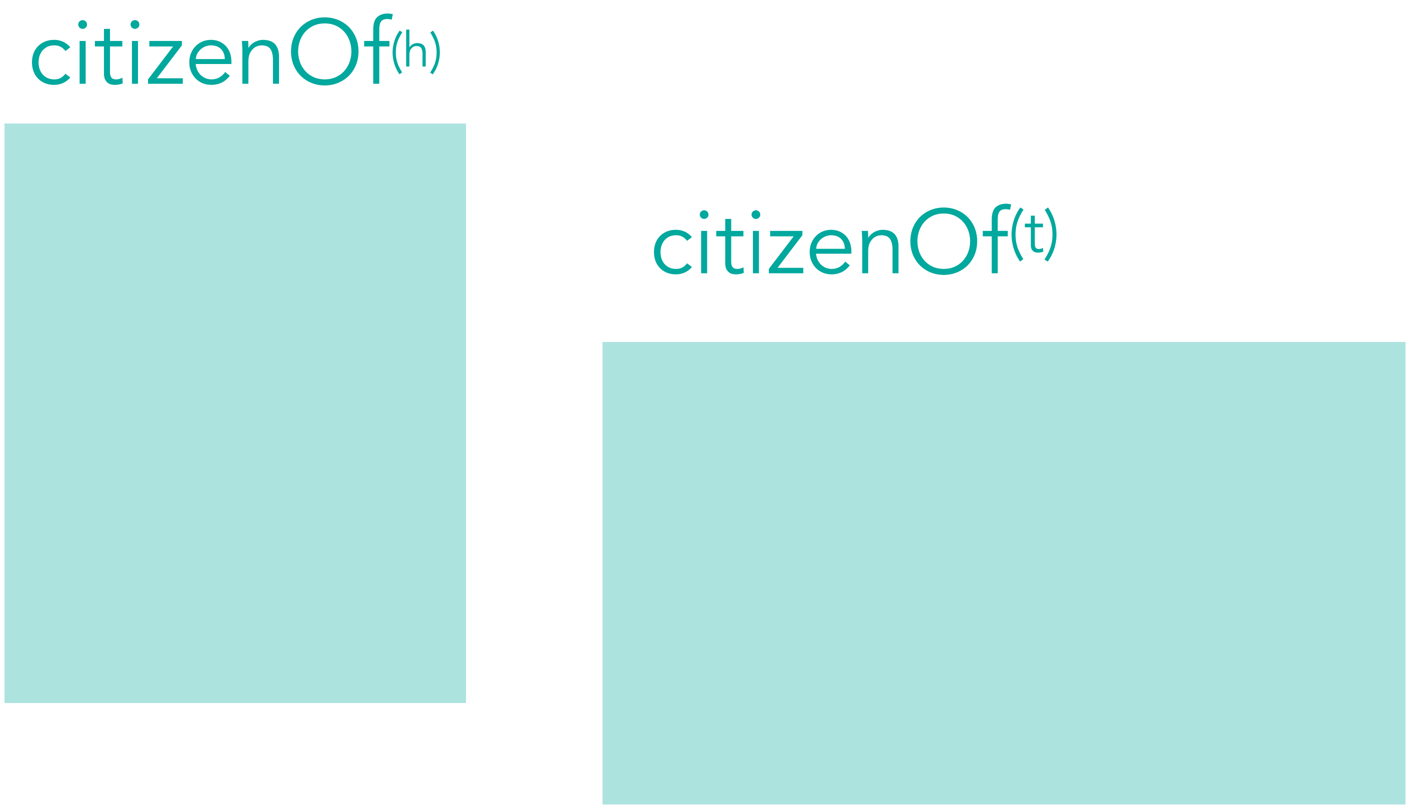

Anti-symmetry

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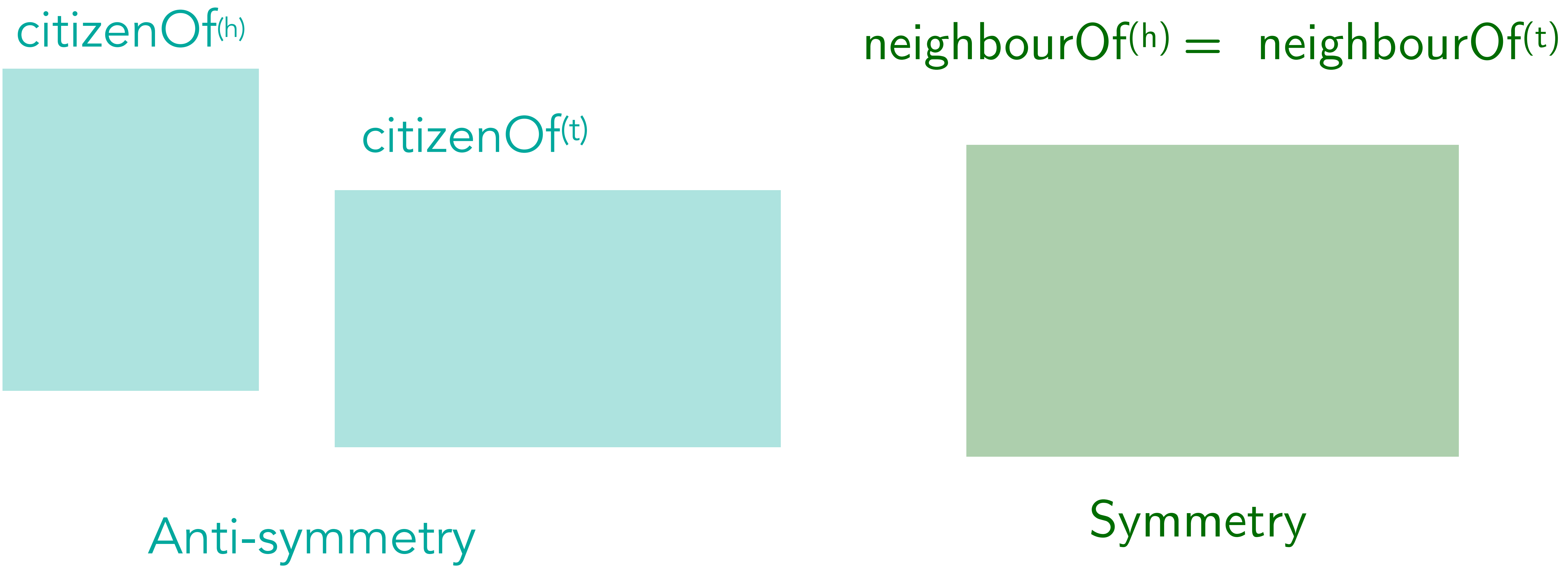

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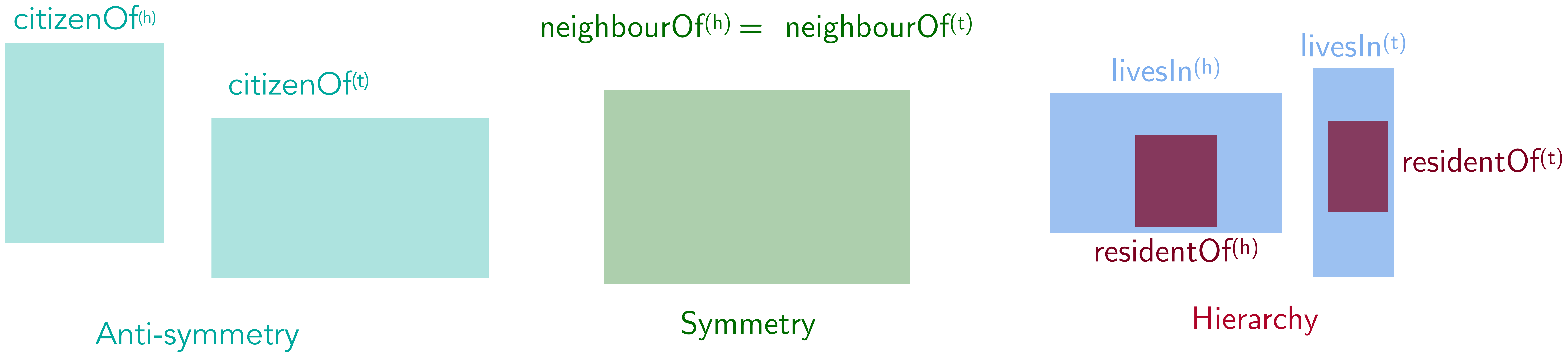

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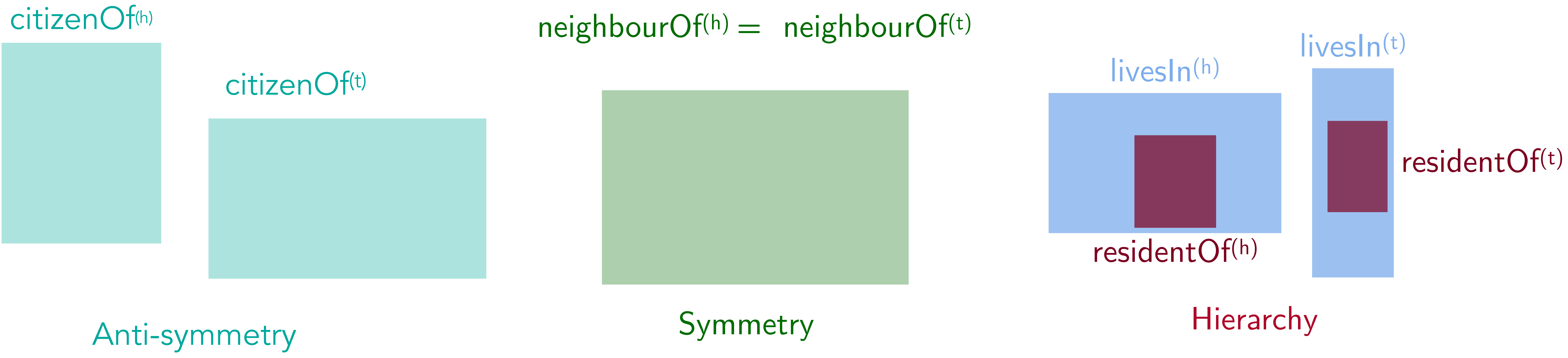

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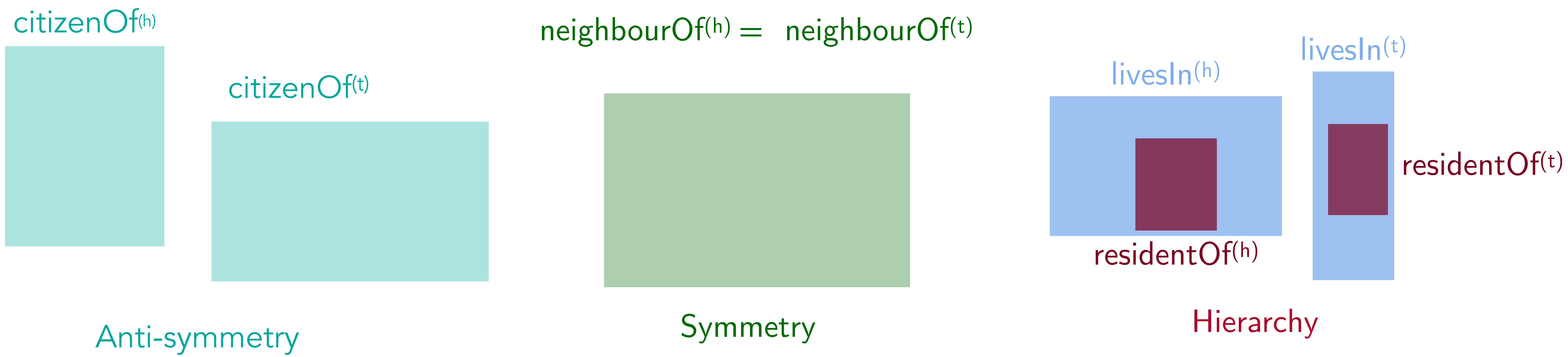

Other inference patterns, e.g., inverse, mutual exclusion, intersection can be captured by configuring boxes.

This approach does not work for the composition pattern: $\forall x, y, z \ r(x, y) \wedge s(y, z) \Rightarrow t(x, z)$! BoxE cannot capture composition as an inference pattern.

Generalized Inference Patterns

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Example: Bilinear models can separately capture the hierarchy rules:

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Jointly capturing these imposes either $\forall x, y \ r_1(x, y) \Rightarrow r_2(x, y)$ or $\forall x, y \ r_2(x, y) \Rightarrow r_1(x, y)$ (Gutiérrez-Basulto et al.).

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A simple relational hierarchy cannot be captured by any of these systems. BoxE can capture these inference patterns also in this general sense, and can capture, e.g., relational hierarchies.

Rule Languages

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To better assess the inductive capacity of a model, show the rule language it can capture.

Overview of Embedding Models

Embedding Models: Representation and Scoring

Model	Entity representation	Relation representation	Scoring function
TransE	$\mathbf{h}, \mathbf{t} \in \mathbb{R}^d$	$\mathbf{r} \in \mathbb{R}^d$	$-\|\mathbf{h} + \mathbf{r} - \mathbf{t}\|$
RotatE	$\mathbf{h}, \mathbf{t} \in \mathbb{C}^d$	$\mathbf{r} \in \mathbb{C}^d$	$-\|\mathbf{h} \odot \mathbf{r} - \mathbf{t}\|$
RESCAL	$\mathbf{h}, \mathbf{t} \in \mathbb{R}^d$	$\mathbf{M}_r \in \mathbb{R}^d \times \mathbb{R}^d$	$\mathbf{h}^\top \mathbf{M}_r \mathbf{t}$
DistMult	$\mathbf{h}, \mathbf{t} \in \mathbb{R}^d$	$\mathbf{D}_r \in \mathbb{R}^d \times \mathbb{R}^d$	$\mathbf{h}^\top \mathbf{D}_r \mathbf{t}$
ComplEx	$\mathbf{h}, \mathbf{t} \in \mathbb{C}^d$	$\mathbf{D}_r \in \mathbb{C}^d \times \mathbb{C}^d$	$\mathrm{Re}(\mathbf{h}^\top \mathbf{D}_r \bar{\mathbf{t}})$
BoxE	$\mathbf{h}, \mathbf{t}, \mathbf{b_h}, \mathbf{b_t} \in \mathbb{R}^d$	Hyper-rect's $\mathbf{r^h}, \mathbf{r^t} \in \mathbb{R}^d$	$-\left(\left\| \mathrm{dist}(\mathbf{h}^{\mathbf{r}(\mathbf{h},\mathbf{t})}, \mathbf{r^h}) \right\|_x + \left\| \mathrm{dist}(\mathbf{t}^{\mathbf{r}(\mathbf{h},\mathbf{t})}, \mathbf{r^t}) \right\|_x \right)$

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Summary of the models covered in the lecture: Entity representations $h, t \in E$ and relation representations $r \in R$ are given, along with the scoring function for an arbitrary fact $r(h, t)$. Please refer to the original works for the details.

Embedding Models: Expressiveness and Inferences

Inference pattern	**TransE**	**RotatE**	**BoxE**	**DistMult**	**ComplEx**
Symmetry	N/N	Y/Y	Y/Y	Y/Y	Y/Y
Anti-symmetry	Y/Y	Y/Y	Y/Y	N/N	Y/Y
Inversion	Y/N	Y/Y	Y/Y	N/N	Y/Y
Composition	Y/N	Y/N	N/N	N/N	N/N
Hierarchy	N/N	N/N	Y/Y	Y/N	Y/N
Intersection	Y/N	Y/N	Y/Y	N/N	N/N
Mutual exclusion	Y/Y	Y/Y	Y/Y	Y/N	Y/N

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A summary of the inference patterns / generalized inference patterns that can be captured by selected models.

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Another bilinear model TuckER, coincides with ComplEX in terms of the listed inference patterns.

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We will revisit knowledge graph completion in the context of graph neural networks.

Temporal Knowledge Graph Completion

Temporal Knowledge Graphs

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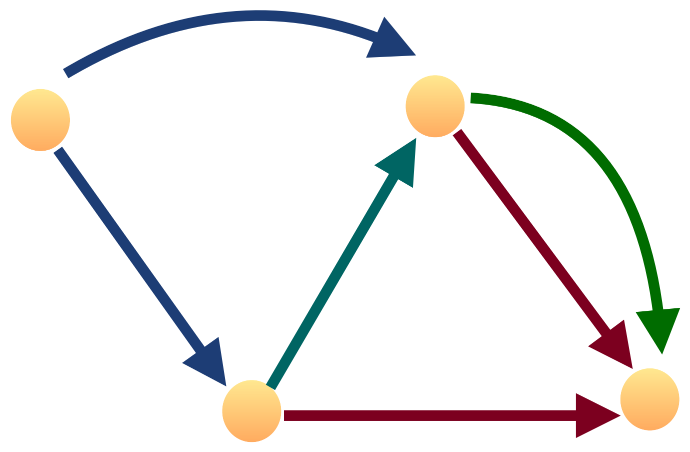
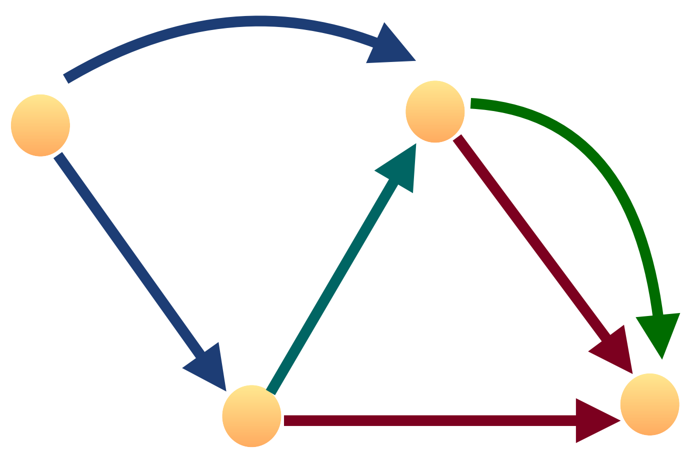
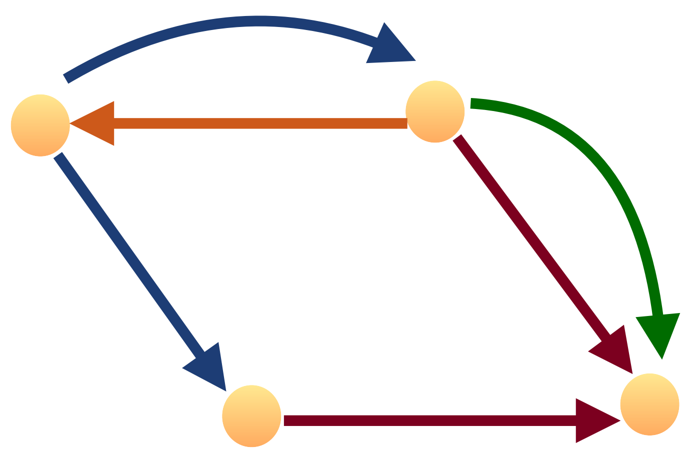


t_1

Temporal Knowledge Graphs

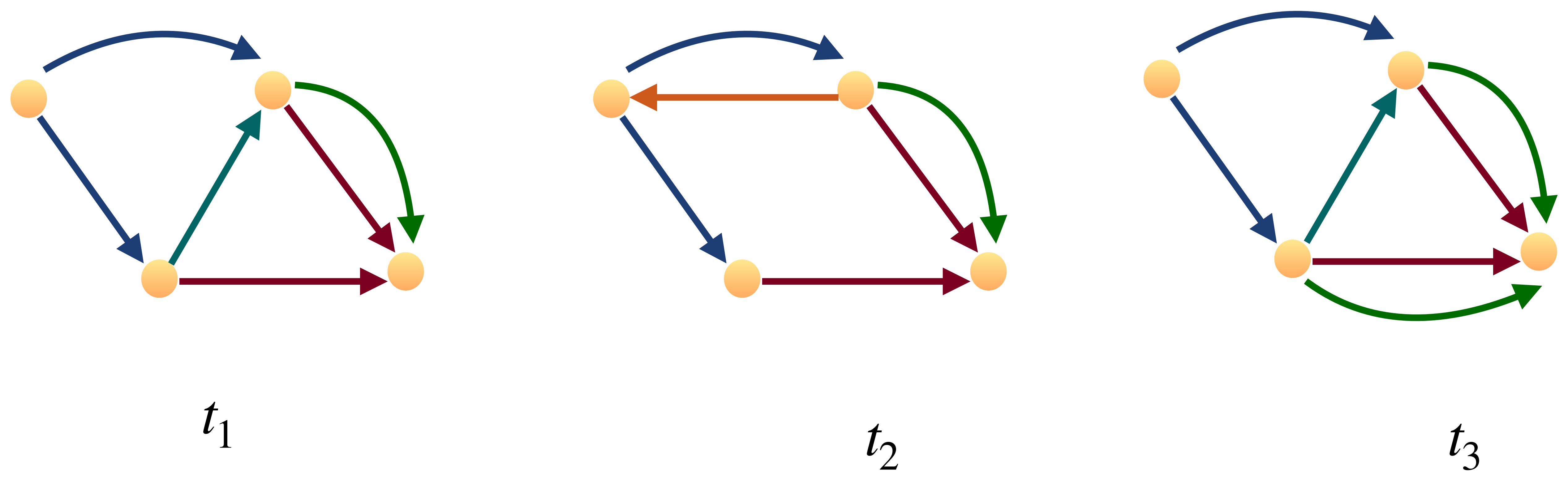


t_1



t_2

Temporal Knowledge Graphs



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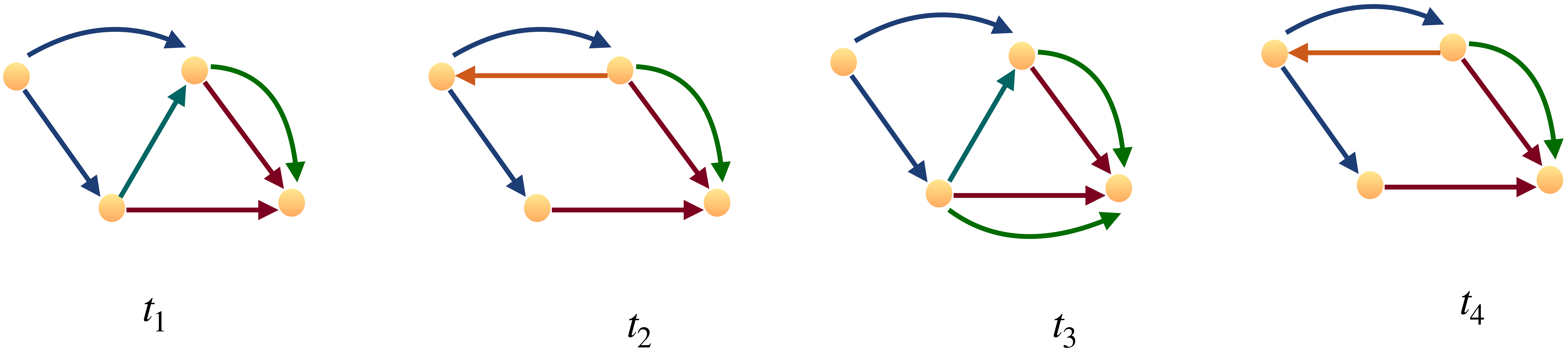

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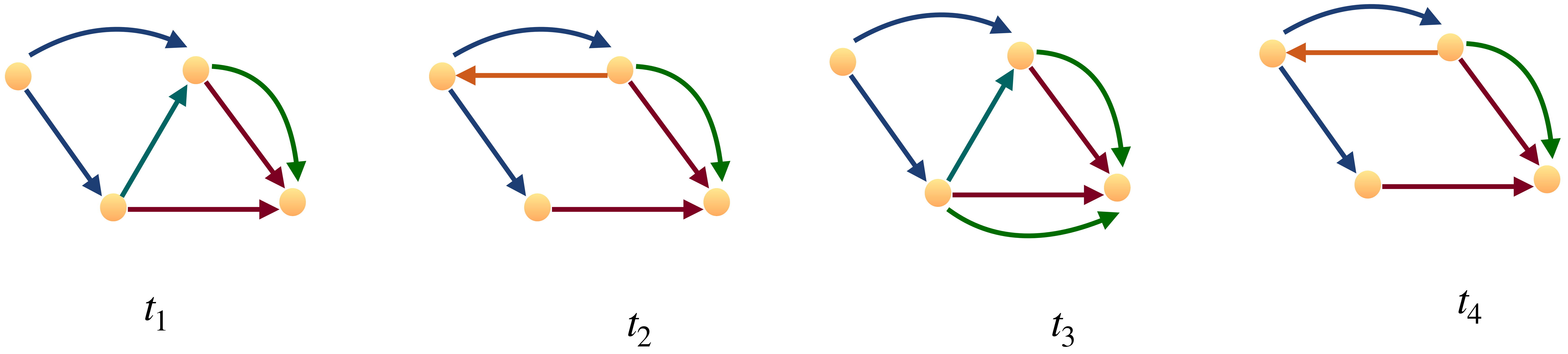
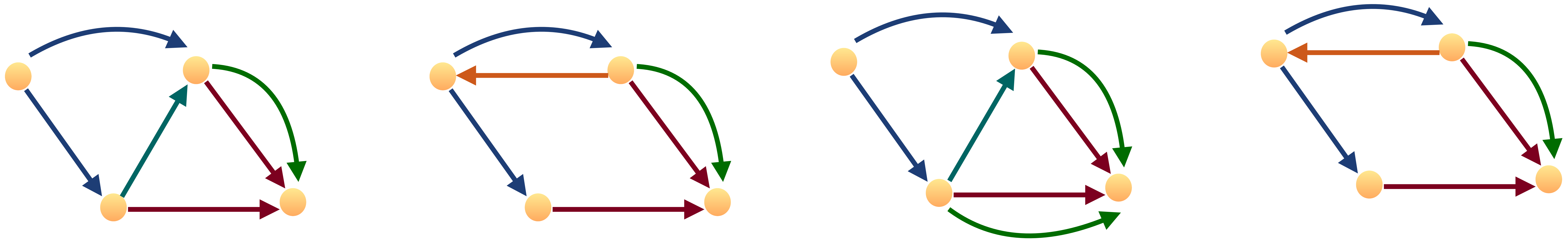


Temporal knowledge: Knowledge changes over time and we can capture this with timestamps T.

Temporal facts: A temporal fact is of the form $r(h, t \mid \tau)$, where $r \in R$, and $h, t \in E$, and $\tau \in T$, indicating the timestamp where the fact holds.

Temporal KGs: A temporal KG is a finite set of temporal facts, or equivalently a sequence of KGs.

Temporal Knowledge Graph Completion



t_1 t_2 t_3 t_4

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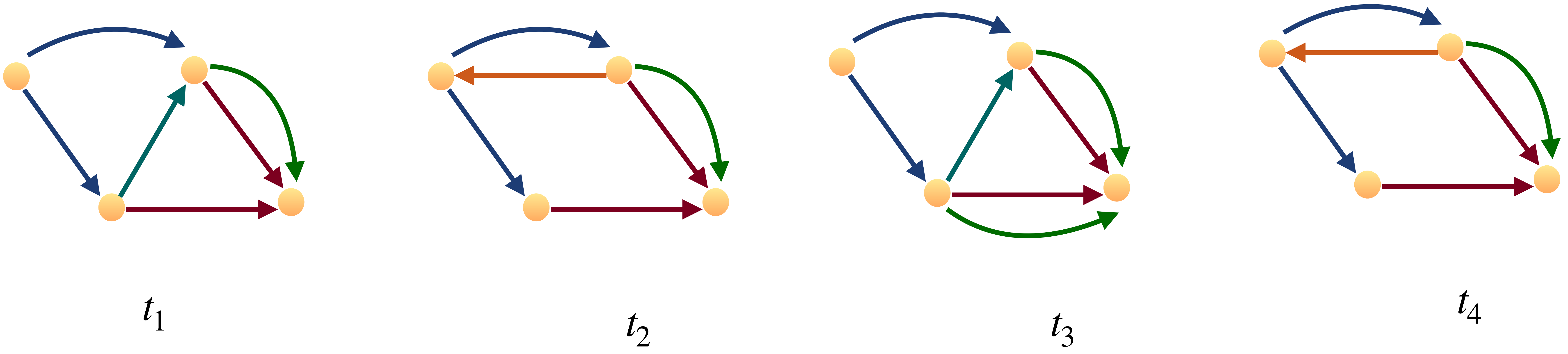

Temporal KG completion: Given a temporal KG G, temporal KG completion is to predict (temporal) facts that are missing from G. There are two regimes:

Interpolation: Observations over timestamps $\tau_1 \ldots \tau_n$ and predictions/completion over timestamps $\tau_1 \ldots \tau_n$.

Extrapolation: Observations over timestamps $\tau_1 \ldots \tau_n$ and predictions/completions over unseen timestamps.

Extrapolation is very hard, but already interpolation is hard: facts must be predicted in the right timestamps.

Temporal Knowledge Graph Completion

Dataset	|E|	|R|	|T|	Training	Validation	Test	Timespan	Granularity
ICEWS14	7,128	230	365	72,826	8,963	8,941	1 year	Daily
ICEWS05-15	10,488	251	4017	386,962	46,092	46,275	11 years	Daily
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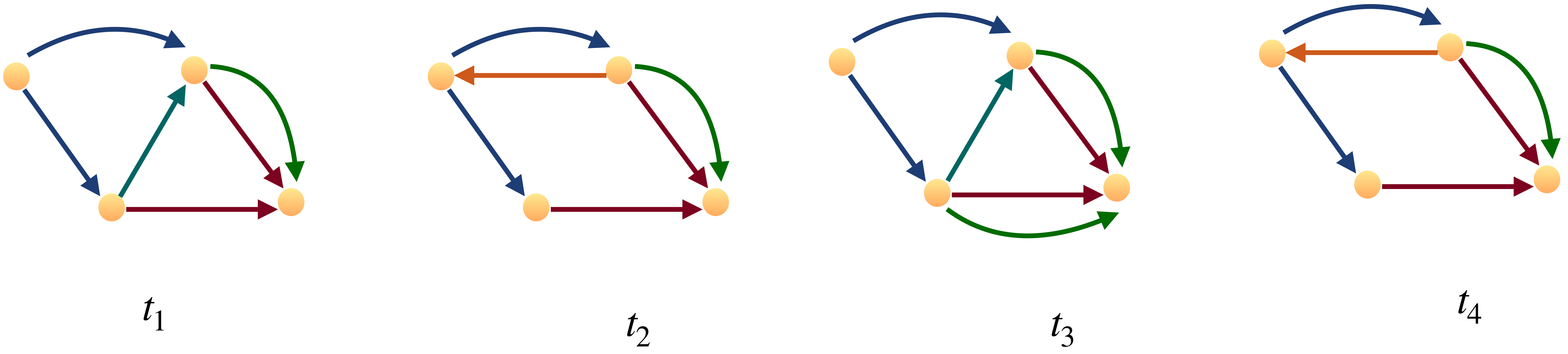
Datasets: ICEWS14 and ICEWS5-15 (Garcia-Duran et al, 2018): subsets of the Integrated Crisis Early Warning System (ICEWS) dataset, which stores temporal socio-political facts starting from the year 1995. GDELT: a subset of Global Database of Events, Language, and Tone temporal KG (Leetaru and Schrodt 2013).

A Brief Look at TTransE



Encoder: TTransE (Leblay and Chekol, 2018) extends TransE by additionally encoding each timestamp $\tau \in \mathbf{T}$ into the space $\boldsymbol{\tau} \in \mathbb{R}^d$.

Decoder: Score a temporal fact $r(h, t \mid \tau)$ based on how similar $\mathbf{h} + \mathbf{r} + \boldsymbol{\tau}$ and $\mathbf{t}$ are: $-\|\mathbf{h} + \mathbf{r} + \boldsymbol{\tau} - \mathbf{t}\|$

Remark: Any translational model can be extended in this simple way and more sophisticated proposals exist.

Outlook and Discussions

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- **Rule injection**: KGs usually have an accompanying schema, or an ontology, encoding the general domain knowledge in the form of first-order rules. Ideally, all predictions in the KG completion task should comply with such knowledge. Is it possible to inject such knowledge into the embedding models and to what extent?

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- **Other tasks**: Tasks beyond KG completion, e.g., entity classification, query answering with embedding models.

Summary

- KG completion with shallow embedding models:
  - Translational models, e.g., TransE, RotatE.
  - Bilinear models, e.g., RESCAL, DistMULT, ComplEx.
  - Box embeddings, e.g., BoxE.
- Many other embedding models build on similar, or analogous ideas.
- Temporal KG completion
- We evaluated the respective models in terms of:
  - Model expressiveness
  - Model inductive capacity and inference patterns

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